ABSTRACT

Internal combustion engines are widely used in transportation and power generation. Since their invention, internal combustion engines were designed with the intention of using petroleum byproducts, which have been abundant while environmental issues were the least of concerns. In today’s world, diminishing and unreliable petroleum reserves, the issue of global warming due to accumulation of greenhouse gases in the atmosphere and the harmful effects of exhaust fumes on humans raise concerns. These issues emphasize on the need for alternative fuels and clean combustion technologies. Stationary engines, used in powerplants and large scale ships in particular, are affected by the aforementioned issues. The motivation behind this work is to answer to the needs of this particular application by investigating use of gaseous fuel in a dual fuel gas engines under lean premixed conditions and discovering advanced combustion strategies.

In this study, a single cylinder micro-pilot fuel injected dual fuel gas engine is operated using various gases in two separate experimental sessions; engine performance, exhaust gas emissions and visual characteristics of combustion are measured in order to discuss combustion characteristics in a gas engine with usable end-gas autoignition, which is named as PREmixed Mixture Ignition in the End-gas Region combustion. Engine performance, exhaust emissions and visual characteristics of combustion activity are measured by performance tests and visualization study.

In the first part of this study, premixed natural gas mixture with equivalence ratio 0.6 is ignited using split pilot fuel injection strategy. Performance tests and visualization study has shown that Split pilot fuel injection can be used to suppress knocking to obtain PREMIER combustion by delaying the growth of flame kernels and reducing their size and suppress knocking, by which the maxima of feasible engine output and thermal efficiency were extended to the promixity of knocking condition. Additionally, this strategy promoted normal combustion to PREMIER combustion by widening flame kernels and accelerating their rate of growth, which advanced overall combustion activity and increased the probability of the occurrence of end-gas autoignition. The range of operating conditions that can be converted to PREMIER combustion by split fuel injection was limited. Heavy knocking or normal combustion with low engine output cannot be converted to PREMIER combustion. When the end of delivery of the second injection coincided with the appearance of flame kernels, spray penetration supported flame kernel development by increasing both the sizes and growth speeds. When second injection started before full development of flame kernels, the sprays and
kernel initiation zones interacted and produced larger flame kernels than was achievable with single injection. When the flame kernels were partially grown during injection, the final size and growth rate of the flame kernels are affected adversely. When the second injection occurred after full growth of the flame kernels formed by the first injection, a fraction of the second spray was consumed in the vicinity of the injector and the kernels grew towards the injector, restricting the final size and growth rate of flame; this condition yielded poor result because the fraction of fuel consumed around the injector did not provide any input to propagating flames.

On the second part of the study, combustion characteristics of methane-hydrogen mixtures are investigated based on their suitability for operation in pilot fuel ignited dual fuel gas engine operation under PREMIER combustion. First, the optimum equivalence ratio for use of pure methane is found as 0.56, which is used for evaluating characteristics of methane-hydrogen mixtures comparatively. Results showed that increasing hydrogen content of gaseous fuel mixtures improved thermal efficiency while maintaining engine output, which was possible due to increased flame propagation speed, shortened end-gas autoignition delay and higher rates of reaction completeness. These occurrences also improved operation stability at normal combustion conditions; however engine operation of PREMIER combustion cases were equally stable throughout the fueling range. In-cylinder pressure levels were lower for mixtures with higher hydrogen fraction due to reduced knock resistance. Addition of H₂ improved carbon monoxide and unburned hydrocarbon emissions systematically due to both reduced amount of hydrocarbon based fuel in the cylinder mixture and a higher level of combustion completeness. NOₓ emissions do not change significantly, which also shows that there is no trade-off of NOₓ versus carbon dioxide and unburned hydrocarbon emissions. Knocking resistance of hydrogen mixtures were strongly influenced by flame propagation speed and associated heat release; however no significant drawbacks regarding engine operation were observed. Mixtures with higher hydrogen concentrations required more retarded pilot fuel injection but the duration required for occurrence of end-gas heat release is observed to happen faster when H₂ concentration is increased. A distinct hydrogen concentration limit of 60% by volume was observed, above which PREMIER combustion is not achievable due to abrupt occurrence of super knocking. At this condition, in-cylinder mixture was susceptible to premature ignition due to possible presence of hot spots in combustion chamber.

On the third part of this work, the results of the second part were used for identifying the phenomenon as end-gas autoignition and discussing the differences between the end-gas autoignition characteristics of knocking and PREMIER combustion. Livengood-Wu integral method was applied using an
ignition delay time correlation obtained from the literature and a constant temperature ignition delay table obtained from CHEMKIN. The reasonable agreement between Livengood-Wu integral with both approaches support the proposition that end-the distinct second stage heat release peak appears due to autoignition. Absence of rapid pressure rise and pressure oscillations during PREMIER combustion operation indicated that it is a knock-free autoignition phenomenon. Heat releases of cycles with end-gas autoignition were faster and an operating condition with higher number of cycles with such characteristics yielded higher thermal efficiency. The earliest end-gas autoignition timing without knocking is not influenced by fuel type in a significant level. Fuel mixtures with higher reactivity reach at end-gas autoignition condition faster, requiring a more retarded injection timing for delaying start of combustion. Lower heating value of hydrogen reduced volumetric energy density of the unburned mixture, due to which autoignition of a larger volume was completed over a longer period for the same amount of energy. This also allowed a larger fraction of the in-cylinder mixture to be consumed by autoignition without knocking. While fuel mixtures with higher hydrogen fractions had inferior knock resistance in terms of maximum in-cylinder pressure and its derivative, the operation range with usable end-gas autoignition was wider, the end-gas volume was larger and the amount of end-gas heat release was higher. Due to these advantages, thermal efficiency can be improved while maintaining the engine output. It was concluded that the amount of heat release during end-gas autoignition, its duration and the expansion rate of the cylinder during this occurrence decide whether or not knocking occurred.
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Cagdas AKSU
2.7. Properties of the fuels used in this work ......................................................................... 30

3. Experimental setup ................................................................................................................ 32

3.1. The test engine .................................................................................................................. 32

3.1.1. Specifications of the test engine .................................................................................. 32

3.1.2. Piston types, configurations and adjustment of compression ratio ............................... 33

3.1.3. Visualization parts ....................................................................................................... 34

3.2. Air induction and the supercharging systems .................................................................. 37

3.3. Natural gas injection system ............................................................................................ 38

3.4. Gaseous fuel supply system ............................................................................................ 40

3.5. Pilot fuel injection system ............................................................................................... 41

3.6. The main control panel .................................................................................................... 44

3.7. Data measuring, processing and recording devices .......................................................... 46

3.7.1. In-cylinder pressure measurement .............................................................................. 46

3.7.2. Crank angle, cam angle and top dead center sensors ................................................. 47

3.7.3. Data logger ................................................................................................................. 48

3.8. The timer circuit and auxiliary devices .......................................................................... 48

3.9. Exhaust gas analyzers ..................................................................................................... 52

3.10. Imaging equipment and setup ...................................................................................... 53

4. Calibration of measurement devices, data acquisition and processing ......................... 56

4.1. Calibration of pressure data ............................................................................................ 56

4.2. Calibration of natural gas flowrate ................................................................................ 56

4.1.3. Calibration of amount of pilot fuel injection ............................................................... 57
4.2. Continuous to cyclic data transformation ................................................................. 58
  4.2.1. Recorded data file format .................................................................................. 58
  4.2.2. Processing method of crank angle and top dead center signals ....................... 58
  4.2.3. Determination of start of cycles and preparation of crank angle position data .... 59
  4.2.4. Cutting the time series pressure data into separate cycles .............................. 59
4.3. Filtering ..................................................................................................................... 60
  4.3.1. Median filter ..................................................................................................... 60
  4.3.2. Moving average filter ..................................................................................... 61
  4.3.3. Finite impulse response (FIR) filters .............................................................. 61
  4.3.4. FIR filter windowing and Dolph-Chebyshev window ...................................... 63
  4.3.5. Savitzky-Golay filter ..................................................................................... 63
4.4. Specifics of the procedures for determination of performance characteristics ...... 64
  4.4.1. Numerical differentiation and integration ....................................................... 64
  4.4.2. Rate of heat release and mass fraction burned (MFB) ..................................... 64
  4.4.3. Unburned mixture temperature ...................................................................... 65
  4.4.4. Determination of end-gas autoignition timing by Livengood-Wu integral method 66
4.5. Image processing ..................................................................................................... 66
  4.5.1. Image recording and conversion ...................................................................... 66
  4.5.2. Background subtraction .................................................................................. 67
  4.5.3. Noise removal by median filter ...................................................................... 67
  4.5.4. Image derivation ............................................................................................ 67
5. Extension of PREMIER Combustion Operation Range Using Split Micro Pilot Fuel Injection 69
5.1. Motivation ....................................................................................................................... 69
5.2. Specifics of the experimental setup, test procedure and data analysis ......................... 70
5.3. Engine performance in single injection mode................................................................. 74
   5.3.1. Pressure history and rate of heat release................................................................. 74
   5.3.2. Engine performance and operation stability ........................................................... 76
5.4. Effect of split injection on engine performance and operation range of PREMIER combustion................................................................. 78
   5.4.1. Pressure history, rate of heat release, and fraction of PREMIER combustion cycles 78
   5.4.2. Engine performance and operation stability ........................................................... 83
   5.4.3. Effects of split injection on combustion characteristics ........................................... 85
   5.4.4. Suppression of knocking to PREMIER combustion by split fuel injection............ 90
   5.4.5. Promotion of normal combustion to PREMIER combustion with split injection.... 93
5.5. Summary of observations................................................................................................. 97
5.6. Raw in-cylinder images of all recorded conditions ......................................................... 98
   6.1. Motivation ................................................................................................................ 102
   6.2. Specifics of the experimental setup, test procedure and data analysis ....................... 102
   6.3. Preliminary experiments using methane ..................................................................... 106
      6.3.1. Pressure histories and rate of heat release characteristics of methane ............... 106
      6.3.2. Engine performance of methane ....................................................................... 113
      6.3.3. Exhaust emissions of methane.......................................................................... 115
6.3.4. Determination of the optimum equivalence ratio ......................................................... 117

6.4. Methane-hydrogen mixtures .............................................................................................................. 118

6.4.1. Pressure histories and rate of heat release characteristics of methane-hydrogen mixtures .................................................................................................................................................. 118

6.4.2. Engine performance of methane-hydrogen mixtures ......................................................... 123

6.4.3. Exhaust emissions of methane-hydrogen mixtures ............................................................. 125

6.4.4. An overview of combustion characteristics of methane-hydrogen mixtures under PREMIEIR combustion operation ........................................................................................................................................... 127

6.4.5. Determination of change of combustion and knocking characteristics with addition of hydrogen .................................................................................................................................................. 130

6.5. Summary of observations ............................................................................................................. 131

7. Investigation of end-gas autoignition characteristics of PREMIEIR combustion using methane-hydrogen mixtures .................................................................................................................................................. 133

7.1. Motivation ........................................................................................................................................ 133

7.2. Summary of pressure history, rate of heat release, performance and general combustion characteristics .................................................................................................................................................. 133

7.3. Distinction between knocking and non-knocking cycles and a quantitative approach to definition of PREMIEIR combustion operation range ........................................................................................................................................... 139

7.4. Difference between maximum pressures and maxima of rate of pressure rise rates of knocking and non-knocking cycles .................................................................................................................................................. 144

7.5. Confirmation of end-gas combustion behavior using Livengood-Wu integrals ................. 146

7.6. End-gas autoignition characteristics of methane-hydrogen mixtures in PREMIEIR combustion .................................................................................................................................................. 149

7.7. Summary of observations ............................................................................................................. 157
8. Conclusions.................................................................158

References.................................................................................161
List of figures

Figure 2.1: Typical P-v diagrams of ideal (a) naturally aspirated Otto, (b) naturally aspirated Diesel, (c) supercharged Otto and (d) supercharged Diesel cycles ................................................................. 15
Figure 2.2: Typical P-v diagram of a four stroke cycle in a real engine .............................................................................. 17
Figure 2.3: The dimensions required for obtaining instantaneous cylinder volume .......................................................... 18
Figure 2.4: Graphical representation of a one dimensional flame propagation mechanism ........................................... 22
Figure 2.5: Schematic representation of droplet combustion model .................................................................................. 23
Figure 2.6: Graphical explanation of spark ignition, compression ignition and dual fuel compression ignition combustion mechanisms ............................................................................................................. 27
Figure 2.8: Pressure histories and rates of heat release of normal combustion, PREMIER combustion and knocking cycles using natural gas as the primary fuel .......................................................... 30
Figure 3.1: The test engine in (a) metal engine and (b) visualization settings ......................................................................... 33
Figure 3.2: Simplified sketches of combustion chamber geometries of all experimental conditions .................................. 34
Figure 3.3: Imaging parts ....................................................................................................................................................... 36
Figure 3.4: Visible area of the sapphire window .......................................................................................................................... 36
Figure 3.5: Outline of the supercharger and intake air heater systems .............................................................................. 37
Figure 3.6: Outline of natural gas supply and calibration system .............................................................................................. 39
Figure 3.7: Gaseous fuel supply system ......................................................................................................................................... 41
Figure 3.8: Pilot fuel injection system ........................................................................................................................................... 42
Figure 3.9: Orientation of pilot fuel sprays ................................................................................................................................. 44
Figure 3.10: The functions of the main control panel ................................................................................................................. 46
Figure 3.11: The generalized circuit diagram of photointerrupters .............................................................................................. 48
Figure 3.12: Circuit diagram of TIME98 sequencer input signal conditioning ............................................................................ 50
Figure 3.13: Circuit diagram of TIME98 sequencer output signals and connection to auxiliary devices ....................... 51
Figure 3.14: Outline of the visualization setup .............................................................................................................................. 54
Figure 3.15: The visualization setup ........................................................................................................................................... 55
Figure 5.1: Experimental setup of (a) performance experiments and (b) visualization ........................................................................ 71
Figure 5.2: Examples of background images, in-cylinder images and the first derivatives derived after background subtraction ...................................................................................................................... 74
Figure 5.3: Typical pressure histories and rates of heat release of normal combustion, PREMIER combustion and knocking operation ...................................................................................................... 75
Figure 5.4: Engine performance and operation stability with single injection: (a) indicated mean effective pressure, (b) thermal efficiency and (c) coefficient of variation of indicated mean effective pressure. 77
Figure 5.5: Pressure histories and rate of heat release characteristics of all experimental conditions with first injection timings of (a) $\theta_{inj}=6^\circ$BTDC, (b) $\theta_{inj}=5^\circ$BTDC, (c) $\theta_{inj}=4^\circ$BTDC, (d) $\theta_{inj}=3^\circ$BTDC. 79
Figure 5.6: Number of cycles with occurrence of end-gas autoignition. 81
Figure 5.7: Distinction of PREMIER combustion from knocking: (a) Knocking intensities and (b) maxima of in-cylinder pressures. 82
Figure 5.8: Comparison of engine performance and operation stability of all experimental conditions: (a) indicated mean effective pressure, (b) thermal efficiency and (c) coefficient of variation of indicated mean effective pressure. 84
Figure 5.9: PREMIER combustion operation range with split pilot fuel injection. 85
Figure 5.10: A typical rate of heat release in PREMIER combustion and its second derivative. 86
Figure 5.11. Flame kernel development at 5°ATDC: (a) $\theta_{inj}=5^\circ$BTDC single injection, (b) $\theta_{inj}=5^\circ$BTDC/1°BTDC, and (c) $\theta_{inj}=5^\circ$BTDC/5°ATDC. 88
Figure 5.12: Closeup view of inward kernel growth with second injection at $\theta_2=5^\circ$ATDC. (a) $\theta_{inj}=6^\circ$BTDC/5°ATDC, (b) $\theta_{inj}=5^\circ$BTDC/5°ATDC, (c) $\theta_{inj}=4^\circ$BTDC/5°ATDC and (d) $\theta_{inj}=3^\circ$BTDC/5°ATDC. 89
Figure 5.13: Pressure histories and rates of heat release of $\theta_{inj}=6^\circ$BTDC single injection and $\theta_{inj}=6^\circ$BTDC/TDC split injection. 90
Figure 5.14: Visual investigation of suppression of knocking: (a) $\theta_{inj}=6^\circ$BTDC single injection with $m_{inj}=0.6$mg/cycle and (b) $\theta_{inj}=6^\circ$BTDC/TDC split injection. Additional reference graph on suppression of flame kernel growth at (c) $\theta_{inj}=6^\circ$BTDC/5°ATDC. 92
Figure 5.15: Comparison of pressure histories and ROHR of single- and split-injection strategies at $\theta_{inj}=4^\circ$BTDC and $\theta_{inj}=4^\circ$BTDC/TDC. 93
Figure 5.16: Visual investigation of promotion of normal combustion to PREMIER combustion: (a) $\theta_{inj}=4^\circ$BTDC single injection, (b) $\theta_{inj}=4^\circ$BTDC/0.5°BTDC. Additional reference graph on suppression of flame kernel growth at (c) $\theta_{inj}=4^\circ$BTDC/5°ATDC. 95
Figure 5.17: Visual investigation improvement of heat release characteristics: (a) $\theta_{inj}=3^\circ$BTDC single injection, (b) $\theta_{inj}=3^\circ$BTDC/0.5°ATDC. Additional reference graph on suppression of flame kernel growth at (c) $\theta_{inj}=3^\circ$BTDC/5°ATDC. 96
Figure 5.18: Unprocessed in-cylinder images of (a) $\theta_{inj}=6^\circ$BTDC single injection, (b) $\theta_{inj}=6^\circ$BTDC/TDC and (c) $\theta_{inj}=6^\circ$BTDC/5°ATDC. 98
Figure 5.19: Unprocessed in-cylinder images of (a) $\theta_{inj}=5^\circ$BTDC single injection, (b) $\theta_{inj}=5^\circ$BTDC/1$^\circ$BTDC and (c) $\theta_{inj}=5^\circ$BTDC/5$^\circ$ATDC ................................................................. 99

Figure 5.20: Unprocessed in-cylinder images of (a) $\theta_{inj}=4^\circ$BTDC single injection, (b) $\theta_{inj}=4^\circ$BTDC/0.5$^\circ$BTDC and (c) $\theta_{inj}=4^\circ$BTDC/5$^\circ$ATDC ..................................................................................................................................... 100

Figure 5.21: Unprocessed in-cylinder images of (a) $\theta_{inj}=3^\circ$BTDC single injection, (b) $\theta_{inj}=3^\circ$BTDC/0.5$^\circ$ATDC and (c) $\theta_{inj}=3^\circ$BTDC/5$^\circ$ATDC ..................................................................................................................................... 101

Figure 6.1: Outline of the experimental setup ........................................................................................................................................ 103

Figure 6.2: Pressure histories and rate of heat release characteristics at most beneficial injection timings... 107

Figure 6.3: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.60................................................................................................................................... 108

Figure 6.4: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.58................................................................................................................................... 109

Figure 6.5: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.56................................................................................................................................... 110

Figure 6.6: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.54................................................................................................................................... 111

Figure 6.7: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.52................................................................................................................................... 112

Figure 6.8: Performance characteristics of pure methane at tested equivalence ratios: (a) Indicated mean effective pressure, (b) thermal efficiency and (c) coefficient of variation of indicated mean effective pressure. ................................................................................................................................... 114

Figure 6.9: Exhaust emission characteristics in pure methane operation: (a) Nitrogen oxide, (b) unburned hydrocarbon and (c) carbon monoxide emissions. ........................................................................................................................................ 116

Figure 6.10: Comparison of all engine performance and exhaust emission characteristics at most beneficial injection timing: (a) $P_{mi}$, (b) thermal efficiency, (c) COV($P_{mi}$); (d) NOx, (e) CO and (f) HCemissions. ................................................................. 117

Figure 6.11: (a) Pressure histories of and (b) rate of heat release characteristics at the most beneficial injection timings of all fueling cases. ........................................................................................................................................ 120

Figure 6.12: Pressure histories of methane-hydrogen mixtures: (a) 100% CH$_4$, (b) 90% CH$_4$/10% H$_2$, (c)80% CH$_4$/20% H$_2$, (d)70% CH$_4$/30% H$_2$, (e)60% CH$_4$/40% H$_2$, (f)50% CH$_4$/50% H$_2$, and (g) 40% CH$_4$/60% H$_2$. ........... 121

Figure 6.13: Rate of heat release of methane-hydrogen mixtures: (a) 100% CH$_4$, (b) 90% CH$_4$/10% H$_2$, (c)80% CH$_4$/20% H$_2$, (d)70% CH$_4$/30% H$_2$, (e)60% CH$_4$/40% H$_2$, (f)50% CH$_4$/50% H$_2$, and (g) 40% CH$_4$/60% H$_2$. ........... 122
Figure 6.14: Super knocking observed during 40% CH₄/60% fueling condition.......................................................... 123

Figure 6.15: Performance characteristics of methane-hydrogen mixtures at tested equivalence ratios: (a) Indicated mean effective pressure, (b) thermal efficiency and (c) coefficient of variation of indicated mean effective pressure............................................................................................................................................. 124

Figure 6.16: Exhaust emission characteristics of methane-hydrogen mixtures: (a) Nitrogen oxide, (b) unburned hydrocarbon and (c) carbon monoxide emissions................................................................. 126

Figure 6.17: Mass fraction burned characteristics of methane-hydrogen mixtures at the most beneficial injection timing ................................................................................................................................................. 128

Figure 6.18: Flame propagation heat release duration of methane-hydrogen mixtures at the most beneficial injection timing. ............................................................................................................................... 129

Figure 6.19: End-gas autoignition delay duration of methane-hydrogen mixtures at the most beneficial injection timing. ................................................................................................................................................ 130

Figure 6.20: Maxima of rate of change of heat release rates in all fueling and injection timing conditions.... 131

Figure 7.1: 80 cycle averages of (a) In-cylinder pressure and (b) rate of heat release at the most beneficial injection timing conditions............................................................................................................................... 135

Figure 7.2: (a) Indicated mean effective pressure and (b) thermal efficiency of methane-hydrogen mixtures including low engine output and knocking operating conditions................................................................. 136

Figure 7.3: Mass fraction burned durations of (a) 0%-10%, (b) 10%-30% and (c) 30%-75% ............................ 138

Figure 7.4: Comparisons of (a) pressure histories and rate of heat release characteristics, (b) power spectral densities and (c) knocking intensities of knocking, PREMIER combustion and normal combustion cycles. .... 140

Figure 7.5: Distinction between combustion modes: (a) the number of cycles with end-gas autoignition, (b) the maxima of knocking intensities and (c) number of knocking cycles................................................................. 142

Figure 7.6: PREMIER combustion operation and normal-to-PREMIER combustion transition ranges......... 143

Figure 7.7: Maxima of in-cylinder pressures vs. maxima of rate pressure rise rates............................................ 145

Figure 7.8: Maximum rate of pressure rise without knocking by hydrogen concentration ............................ 146

Figure 7.8: Average End-gas autoignition timings, their estimations and the deviation between actual and estimated errors................................................................................................................................. 148

Figure 7.10: Graphical representation of the parameters that describe PREMIER combustion. ...................... 150

Figure 7.10: Mass fraction burned before occurrence of end-gas autoignition.................................................. 151

Figure 7.12: End-gas autoignition timings and delays......................................................................................... 153
Figure 7.13: End-gas autoignition characteristics: (a) end-gas autoignition heat release durations, (b) end-gas autoignition heat release and (c) PREMIER combustion indices.
List of Tables

Table 2.1: Van der Waals constants of gases found in the composition of working fluid. ......................... 10
Table 2.2: Benedict-Webb-Rubin equation of state parameters of gases used in this work [100]. ............... 11
Table 2.3: Properties of test fuels .............................................................................................................. 31
Table 3.1: Engine specifications ................................................................................................................ 32
Table 5.1: Configuration of the test engine and operating conditions .............................................................. 70
Table 5.2: List of fuel delivery strategies ..................................................................................................... 72
Table 6.1: Engine and test bench specifications ............................................................................................. 104
Table 6.2: List of injection timings at tested fueling conditions ....................................................................... 104
Table 6.3: Fueling and intake air conditions of methane-hydrogen mixtures .................................................. 105
Table 7.1: Maximum rate of pressure rise without knocking by hydrogen concentration ............................... 146
Table 7.2: Constant pressure ignition delay correlation parameters from the literature .............................. 149
Table 7.3: Coefficients of Methane-hydrogen mixture ignition delays suggested by Gersen et.al. [1] ............ 149
1. **Introduction**

1.1. **Research Background**

1.1.1. **Use of Gaseous Fuels in Dual Fuel Engines**

Considering use of large scale dual fuel internal combustion engines, Biogas, biomass gas and natural gas are considered as suitable energy resources due to their local availability and clean combustion characteristics. An extensive literature survey is carried out on these three types of gaseous fuels.

Biomass is defined as biological matter obtained from animals or plants wastes. Apart from directly burning, such materials can be processed into of biofuels, such as bioethanol, biodiesel, biogas, through thermal, chemical or biochemical methods. The gaseous biofuels can be classified into two sub-categories: digester gas and producer gas.

Digester gas is generated through methane fermentation, i.e. anaerobic fermentation of waste materials, such as food scraps, sewage and agricultural wastes like animal dungs or crops; this type consists of CH$_4$ as the fuel component, CO$_2$ and traces of H$_2$, H$_2$S, N$_2$ and others as non-reactive components. Composition of digester gas depends on the sort of source waste material, fermentation time, humidity, temperature, pressure and many other parameters [1]. Feasibility of biogas as a fuel has been under investigation started in 1980’s and the possibility of conversion of existing engines is researched commonly in spark ignition (SI) engines [2-6]. Use of biogas in SI engines has been investigated extensively and the operation is often commented as unstable due to high diluent concentration of the gas [7-21]. In contrast, Dual fuel compression ignition (CI) engines are well-known to suit combustion of lean mixtures [22-30]. Karim stated that presence of CO$_2$ may alter the nature of combustion, such as extending ignition delay period, causing incomplete combustion under light loads and promoting emission of UHC and CO while satisfying a wider operation range until knock occurs [22]. Effects of CO$_2$ concentration on engine performance was experimentally investigated and compared to that of natural gas [23-25]. It was observed that CO$_2$ concentrations up to 30% have positive effects on engine performance, while higher than 40% will deteriorate operation stability [23]. Comparing exhaust emissions, it was observed that NOx emissions were significantly lower for biogas, while the rest of emission characteristics were comparable between these two gaseous fuels [24]. Chen et. al. studied effects of preheating inlet charge, and observed that this approach is especially beneficial in terms of power output and thermal efficiency at leaner conditions [26]. Apart from biogas-diesel
dual fuel approach, use of biodiesel and vegetable oils for pilot injection was tested, and properties of biogas combustion were compared to that of other gaseous fuels [27-30]. In these studies, apart from an expectable increase in pilot fuel supply rate due to different heating values of biofuels, no apparent drawbacks were observed. Common observations in these studies were improved NOx emissions and knock resistance versus deteriorated CO and UHC in comparison to natural gas. In addition, it can be concluded that, while improved knock resistance extends dual fuel operation range, knocking prevails.

Producer gas is obtained via gasification of materials like wood chips and sawdust. Hydrogen is the main fuel of biomass gas, also known as producer gas, alongside with CO and a small fraction of CH₄, which is commonly produced by processing biological wastes like wood chips. Producer gas is widely studied for use in SI engines [31-36]. Most of the studies reported several problems about compatibility of producer gas with spark ignition operation. N₂ and CO₂ are common diluents in the composition, total fraction of which may exceed 60% depending on the biomass source and the processing method. Spark ignition engines exhibited poor performance in excessive presence of diluents where misfiring or instability were common problems in addition, compositional instability of producer gas at significant levels, which also had a negative impact on operation stability as well. In contrast, dual fuel CI operation is known to be less sensitive to such parameters due to a consistently large initial flame kernel created by the pilot fuel. In contrast, dual fuel CI approach is not well understood yet. So far, most of the producer gas dual fuel combustion efforts are made mostly on practical use, such as in-site use for electricity generation [37-41].

Natural gas is a mixture of mainly methane as the primary combustible gas, with traces of other hydrocarbon gases and diluents, the fractions of which depend on the region of extraction and purification processes. Due to its methane-rich composition, natural gas is a clean-burning fuel and it is drawing more attention as the demand for petroleum alternatives continue to increase. Compared to biogas and biomass gas, it has found use in practical large scale dual fuel gas engines, such as those used in large vessels or local powerplants. Natural gas constituted 14% of total final consumption of world energy sources in 1973, which increased to 15.1% in 2013; the fraction used for transportation increased from 2.7% to 6.9% over this 40-year interval [43]. Use of natural gas in spark ignition (SI) engines and CI engines has been researched extensively. Especially, its use in dual-fuel CI has attracted much attention due to the high level of attainable thermal efficiency. Dual-fuel CI engines in general are suitable platforms for using gaseous fuels with high autoignition temperatures, one of which is natural gas. In this combustion mode, an air-gaseous fuel mixture is ignited by the pilot fuel. By its nature, autoignition of the pilot fuel creates a large zone of flames, the flame.
kernel. A profound improvement over SI, the CI configuration eliminates smoke emission and enables lean operation by reducing the risk of misfiring; however, increased unburned hydrocarbon (HC) and carbon monoxide (CO) emissions remain an issue \[22,44\]. In addition, dual fuel operation range is limited by knocking at the higher load end and by misfiring at the lower load end \[22, 44-46\]. Moreover, exhaust emissions are a trade-off of CI versus SI processes, where soot and NOx emissions are lower but CO and unburned hydrocarbon emissions are higher than those of direct-injection CI engines. Various researchers have addressed these problems by explaining the effects of use of alternative fuels as pilot fuel, pilot fuel quantity, fuel properties, injection timing, equivalence ratio, intake pressure, temperature and use of EGR \[47–60\]. Basic natural gas-diesel pilot injection dual fuel technology is currently used in public transportation buses, stationary engines used for power generation, and large-scale ships.

1.1.2 Advancement in Dual Fuel Engines and Advanced Combustion Technologies

A common interest in dual-fuel gas engine research is to minimise the pilot fuel injection quantity to reduce diesel fuel dependency while the gaseous fuel is functioning as the major energy source. In these systems, gaseous fuel is fed into the intake air and pilot fuel serves as the source of ignition. Several researchers have focused on this particular application \[61–68\]. These studies report reduction of exhaust emissions and improvement of thermal efficiency over direct injection CI engines. Maximization of thermal efficiency is a common goal; however this goal can be achieved by increasing in-cylinder pressure. This high pressure is also the main reason for the increased temperature, which causes knocking under borderline operating conditions \[22, 44-46, 50\]. This approach is especially beneficial because the fraction of unburned methane rejected in the exhaust gases, a phenomenon known as “methane slip,” is reduced \[65-67\]. Additionally, use of split pilot fuel injection is also reported to improve operation stability \[62, 68\].

Conventional approaches to the use of gaseous fuels in CI engines have strict limitations; thus, more advanced combustion strategies are being investigated, such as Homogeneous Charge Compression Ignition (HCCI) and Reactivity Controlled Compression Ignition (RCCI). HCCI relies of autoignition of in-cylinder mixture \[69-80\]. At the time of discovery of HCCI combustion, it was envisioned that homogeneous air-fuel mixture would undergo autoignition, making complex combustion controls obsolete \[69\]. In contrast, autoignition phenomenon often yields knocking unless a proper combustion controlling strategy is applied, which limits engine operation under this combustion mode to low load operation \[70-72\]. The initial approach to this problem was to control in-cylinder mixture properties by clever manipulation of temperature, air/fuel...
ratio or introduction of different matters, such as ozone [73-78]. Despite the fact that practical operation range of HCCI combustion is extended, it is still very narrow for utilization in practical engines; therefore the efforts to combine HCCI combustion with either SI or CI engines is a trending research topic [79-82]. This approach also introduces a new combustion control strategy, where either the spark discharge or autoignition of fuel injection can assist the start of combustion. The particular case of control of combustion by pilot fuel injection provides the foundation of RCCI combustion in terms of mixture preparation and presence of autoignition to a certain extent [83-86]. RCCI combustion concept was first suggested as control of combustion by in-cylinder fuel blending; this approach intends to control the reactivity of in-cylinder mixture, which manipulates autoignition and heat release characteristics [83]. This concept is suggested to provide thermal efficiency levels up to 60% [84]. Introduced at the end of the first decade of 2000’s, the characteristics and control strategies are still under investigation [85-86]. While the improvement of the combustion efficiency is the common attractive trait of both HCCI and RCCI combustion, neither is suitable for high load operation. In order to improve the thermal efficiency of internal combustion engines at high loads, a different approach is required.

1.1.3. PREMIER Combustion

Dual-fuel operation at high loads has been researched in the laboratory using dual-fuel gas engines with various fuels, where ignition source was micro pilot fuel injection. Under heavy load conditions, two-stage combustion has been observed as a precursor to knocking with no sign of fluctuations or rapid increase in pressure [87–95]. The thermal efficiency of the engine shows noticeable improvements, with zero smoke emissions. From more recent studies, it is now understood that the end-gas region can exhibit autoignition simultaneous with flame propagation; this phenomenon has been named “PREMIER” (PREmixed Mixture Ignition in the End Gas Region) combustion [91]. This name has been in use for this type of combustion since its introduction. A visualization study has also proven that it is possible to obtain knock-free end-gas autoignition [96]. In PREMIER combustion mode, the end-gas region reaches autoignition conditions due to pressure and temperature build-up; simultaneous heat release from two different combustion modes causes more rapid heat release when the engine enters the expansion cycle. While attainable thermal efficiency in this combustion mode is superior to normal operation, the operation range is narrow, limited to the prior-to-knocking operating region. Currently PREMIER combustion is at an early stage of research, and new strategies that can extend its operation range are required in order to provide the tools and methodology required for future practical applications.
1.2. Objectives of this study

The aim of this work is to investigate the characteristics of end-gas autoignition and discover its relation to in-cylinder mixture conditions. The research was carried out in three separate sub-topics in order to investigate both the operational characteristics regarding practical engine use and verification of the hypotheses that were formed in during previous works by detailed explanation of development and occurrence of knock-free end-gas autoignition phenomenon [89-94]. In the first part of the work, we investigated possibility of use of split fuel injection strategy as a means for extending the operation range of PREMIER combustion by means of both performance tests and in-cylinder visualization of flame kernel development. Homogeneous mixture of natural gas and air is used as the primary fuel and ignited with both single and split micro pilot diesel fuel injection. In the second part of this work, performance and exhaust emission characteristics of methane and hydrogen mixtures are compared to those of pure methane, and end-gas autoignition characteristics of methane-hydrogen mixtures are evaluated in a methane number range from 100 to 50.

Both performance tests and visualization were performed in a pilot fuel injected dual fuel gas engine at various fuel supply and intake conditions. Intake air temperature and pressure were stabilized in all cases. Engine performance was evaluated based on the pressure history and its derivatives, which was collected by a pressure transducer connected to the cylinder head. Exhaust emissions were recorded by using a combined exhaust gas analyser for NOx and CO, and dedicated hydrocarbon emission analyser connected to the exhaust line. During visualization experiments, an extended block and piston were installed between the cylinder head and the engine block, which provided optical access by installing a sapphire window to the extended piston crevice and a mirror to the extended body that reflects the image to the camera. A high speed camera was used for capturing in-cylinder images, and a metal halide lamp was used as the light source for exposing the spray patterns.

Many important clues were found on the characteristics of PREMIER combustion phenomenon and the operating conditions required for achieving this type of combustion. First of all, it is possible to control the end-gas region autoignition behaviour by optimizing initial flame kernel characteristics. Secondly, operating range of PREMIER combustion depends on both reactivity of the gaseous fuel; however the width of the operating range is not dependant on the fuel properties as long as premature ignition does not occur. Finally,
it is confirmed by both Livengood-Wu integral method and visualization that the end-gas region activity is actually autoignition.

1.3. Outline of the thesis

This thesis consists of 8 chapters

Chapter 1 briefly summarizes the proceedings of the research field and identifies the importance of the current work. The discussion involves the need for alternative fuels, their characteristics and the need for advanced combustion mechanisms that can answer the needs for more efficient use of these fuels. The discussion on advanced combustion mechanisms inform on the progress made until date and identify their shortcomings. Finally, the importance of PREMIER combustion and its difference compared to HCCI and RCCI combustion concepts is explained. Next, the aim of this work is described as investigation of both fundamental characteristics of PREMIER combustion and the parameters that affect its operating range.

Chapter 2 introduces the theoretical and conceptual background of combustion in an internal combustion engine. In the beginning, a brief introduction to physics, thermodynamics and chemistry of combustion is presented. On the next stage, exhaust emissions formation mechanism are explained and their impact on the environment is briefly mentioned. Following, combustion mechanisms in spark ignition engines, compression ignition engines, and dual fuel compression ignition gas engines are explained. Based on that information, the mechanism of PREMIER combustion and its characteristics are defined. Finally, properties of test fuels are listed.

Chapter 3 explains the experimental setup in details and introduces measurement devices. The test engine and its specifications, configurations and basics of engine operation are discussed. Engine speed governing system, supercharging system, pilot fuel and natural gas injection and calibration systems, gaseous fuel supply system, the main control unit, injection control unit and exhaust gas analysers are introduced in details with their intended uses.

Chapter 4 informs on data acquisition and processing methods. In this section, the procedure of data recording, its conversion to pressure versus crank angle arrays and evaluation of rate of heat release, mass fraction burned, unburned mixture temperature and end-gas autoignition timing is explained in details. In visualization part, image capturing and recording process, noise elimination and image derivation processes are explained.
**Chapter 5** discusses the effect of split pilot fuel injection on engine performance and combustion, which was evaluated from the results of both performance tests and visualization of pilot fuel sprays and flame kernels. Results showed that it is possible to extend operation range of PREMIER combustion by both suppressing knocking and promoting normal combustion to PREMIER combustion. In-cylinder images showed that it is possible to control the flame kernel size using the split pilot fuel injection. Growth rate can be increased or retarded and flame kernel size can be increased or decreased depending on the relation between timings of the first and second injections. This has shown that progress of combustion can be controlled by manipulating flame kernel characteristics.

**Chapter 6** explains combustion characteristics of methane-hydrogen mixtures in a pilot fuel injected dual fuel engine by comparing to those of pure methane. In the first stage of this work, preliminary tests were performed using only methane in order to identify the optimum equivalence ratio condition based on pressure history, heat release characteristics, engine performance, operation stability and exhaust emissions, and the equivalence ratio of 0.56 was found to be the most suitable condition. On the second stage of the study, methane-hydrogen mixtures are tested at the equivalence ratio of 0.56 and total energy supply rate of 2.6 kJ per cycle; hydrogen fraction of the fuel mixture was increased from 0 to 60% by volume in 10% increments, where 60% was found to be unsuitable due to premature ignition of the premixed mixture and consequent super knocking. It was possible to maintain the engine output and achieve higher thermal efficiency, lower carbon monoxide and hydrocarbon emissions and improved operation stability at lower maximum in-cylinder pressure levels without sacrificing NOx emissions. Replacing methane by hydrogen allowed for reduced emissions while higher reactivity and faster heat release due to addition of hydrogen was the cause of these improvements.

**Chapter 7** discusses end-gas autoignition characteristics in PREMIER combustion operation using the data set of methane-hydrogen mixtures with added knocking and low engine output conditions. Livengood-Wu integral method was applied and the cause of second stage rapid heat release was confirmed as autoignition. It was also found out that higher reactivity of hydrogen shortens the duration from start of combustion to the end-gas autoignition, preserves a larger fraction of the mixture for end-gas autoignition. It was also observed that end-gas autoignition did not occur instantaneously, taking a certain amount of time until completion. It is also found out that the timing and duration end-gas heat release, the amount of autoignition heat release, reactivity of the fuel and volumetric heat content of the unburned mixture were all decisive factors on whether or not the end-gas heat release activity is PREMIER combustion or knocking. Lower volumetric heat
content of fuel mixtures with higher fractions tended to allow a higher amount of end-gas heat release without knocking.

Chapter 8 summarizes the conclusions of the study.
2. Theoretical Background

2.1. Equation of state correlations

An equation of state is a correlation between the physical state of a gaseous matter and its surroundings. These equations interpret the dependence between the quantitative properties of a gaseous matter, pressure, volume and temperature of the matter. They are commonly utilized in thermodynamics. In this work, three types of equations of state are used, which will be explained in this section.

2.1.1. Ideal gas equation

Ideal gas law is the most commonly used equation of state. This model assumes that the gas has a monatomic structure, is at a high temperature and low pressure. The equation is given as:

\[ PV = nR_u T \]  

Where \( P \) is pressure in Pascal (Pa), \( V \) is volume in cubic meters (m\(^3\)), \( n \) is the molar quantity of the gas in moles (1 mole of matter consist of 6.022\( \times 10^{23} \) atoms or molecules), \( R_u \) is the universal gas constant as 8.314 joules per kelvin per mole (J/K*mol) and \( T \) is the temperature in Kelvin. It should be noted that the alternative units can be used, as long as the magnitudes of order are matched.

2.1.2. Van der Waals Equation of State

The behavior of a real gas typically deviates from the Ideal gas approximation. Van der Waals equation incorporates the effect of intermolecular attractions into the ideal gas equation. The governing equations are as follows:

\[ \left( p + \frac{n^2a}{V^2} \right)(V + b) = nR_u T \]  

In this equation, \( a \) is a measure of average attraction between molecules and \( b \) is the volume that is occupied by the molecules. Both parameters are functions of molecular characteristics that can be derived using characteristics, but are commonly tabulated in the literature. In this work, the values of \( a \) and \( b \) are obtained from the literature for the gases that are relevant to this work and are tabulated in table 2.1 [99]. A particular
The benefit of Van der Waals equation of state regarding this work is, it improves the precision of approximations while it does not have high computational demands.

<table>
<thead>
<tr>
<th>name</th>
<th>Molecular structure</th>
<th>a</th>
<th>B</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>H₂</td>
<td>0.2453</td>
<td>0.02651</td>
</tr>
<tr>
<td>methane</td>
<td>CH₄</td>
<td>2.300</td>
<td>0.04301</td>
</tr>
<tr>
<td>Ethane</td>
<td>C₂H₆</td>
<td>5.570</td>
<td>0.06499</td>
</tr>
<tr>
<td>Propane</td>
<td>C₃H₈</td>
<td>9.385</td>
<td>0.09044</td>
</tr>
<tr>
<td>i-Butane</td>
<td>C₄H₁₀</td>
<td>13.36</td>
<td>0.1168</td>
</tr>
<tr>
<td>n-butane</td>
<td>C₄H₁₀</td>
<td>13.93</td>
<td>0.1168</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>N₂</td>
<td>1.370</td>
<td>0.0387</td>
</tr>
<tr>
<td>Oxygen</td>
<td>O₂</td>
<td>1.382</td>
<td>0.03186</td>
</tr>
<tr>
<td>CO₂</td>
<td>CO₂</td>
<td>3.658</td>
<td>0.04286</td>
</tr>
<tr>
<td>Water vapor</td>
<td>H₂O</td>
<td>5.537</td>
<td>0.03049</td>
</tr>
</tbody>
</table>

2.1.3. Benedict-Webb-Rubin Equation of State

Benedict-Webb-Rubin (BWR) equation of state is an empirical approximation of behavior of gases. It consists of eight coefficients that are determined experimentally. This equation is especially popular, because it is possible to obtain both vapor and liquid qualities. Benedict-Webb-Rubin equation is as following [100]:

\[
P = RT\rho + (B_0RT - A_0 - C_0/T^2)\rho^2 + (bRT - a)\rho^3 + a\alpha\rho^6 + (C_0\rho^3/T^2)(1 + \gamma\rho^2)\exp(-\gamma\rho^2)\]

In this equation, \(\rho\) is density, \(P\) is pressure, \(R\) is the universal gas constant and \(T\) is temperature in Kelvin. \(A_0\), \(B_0\), \(C_0\), \(a\), \(b\), \(c\), \(\alpha\) and \(\gamma\) are matter specific constants. \(C_0\) is constant for temperatures above the boiling range of a matter, and its it defined as function of temperatures below that threshold; however the
gases used in this study never encounter temperatures below their boiling points, so it is safe to use $C_0$ as constant. Table 2.2 lists Benedict-Webb-Rubin equation of state constants for the gases used in this work.

Table 2.2: Benedict-Webb-Rubin equation of state parameters of gases used in this work [100].

<table>
<thead>
<tr>
<th></th>
<th>A0</th>
<th>B0</th>
<th>C0</th>
<th>a</th>
<th>b</th>
<th>c</th>
<th>alfa</th>
<th>gamma</th>
</tr>
</thead>
<tbody>
<tr>
<td>(r)</td>
<td>2</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td>3</td>
<td>2</td>
<td></td>
</tr>
<tr>
<td>Hydrogen</td>
<td>1.57E+05</td>
<td>2.08E-02</td>
<td>3.66E+07</td>
<td>1.65E+02</td>
<td>3.38E-04</td>
<td>7.37E+05</td>
<td>1.17E-04</td>
<td>3.23E-03</td>
</tr>
<tr>
<td>methane</td>
<td>1.82E+05</td>
<td>4.55E-02</td>
<td>3.23E+09</td>
<td>4.41E+03</td>
<td>2.52E-03</td>
<td>3.64E+08</td>
<td>3.30E-04</td>
<td>1.05E-02</td>
</tr>
<tr>
<td>Ethane</td>
<td>4.22E+05</td>
<td>6.28E-02</td>
<td>1.82E+10</td>
<td>3.50E+04</td>
<td>1.11E-02</td>
<td>3.32E+09</td>
<td>2.43E-04</td>
<td>1.18E-02</td>
</tr>
<tr>
<td>Propane</td>
<td>6.96E+05</td>
<td>9.73E-02</td>
<td>5.15E+10</td>
<td>9.60E+04</td>
<td>2.25E-02</td>
<td>1.31E+10</td>
<td>6.07E-04</td>
<td>2.20E-02</td>
</tr>
<tr>
<td>i-Butane</td>
<td>1.04E+06</td>
<td>1.38E-01</td>
<td>8.61E+10</td>
<td>1.96E+05</td>
<td>4.24E-02</td>
<td>2.90E+10</td>
<td>1.07E-03</td>
<td>3.40E-02</td>
</tr>
<tr>
<td>n-Butane</td>
<td>1.02E+06</td>
<td>1.24E-01</td>
<td>1.01E+11</td>
<td>1.91E+05</td>
<td>4.00E-02</td>
<td>3.21E+10</td>
<td>1.10E-03</td>
<td>3.40E-02</td>
</tr>
<tr>
<td>Nitrogen</td>
<td>1.07E+05</td>
<td>4.07E-02</td>
<td>8.17E+08</td>
<td>1.51E+03</td>
<td>1.98E-03</td>
<td>5.55E+07</td>
<td>2.92E-04</td>
<td>7.50E-03</td>
</tr>
<tr>
<td>Oxygen</td>
<td>9.63E+04</td>
<td>3.53E-08</td>
<td>3.31E+09</td>
<td>1.65E+04</td>
<td>3.58E-03</td>
<td>1.30E+09</td>
<td>3.93E+00</td>
<td>3.01E-02</td>
</tr>
<tr>
<td>Carbon dioxide</td>
<td>2.77E+05</td>
<td>4.99E-02</td>
<td>1.40E+10</td>
<td>1.39E+04</td>
<td>4.12E-03</td>
<td>1.51E+09</td>
<td>8.47E-05</td>
<td>5.39E-03</td>
</tr>
</tbody>
</table>

(Pressure in Pa, volume in m$^3$, temperature in K)

The eight constants of a mixture are obtained from the properties of the components of the mixture by using the following correlation [100]:

$$X_{\text{mix}} = \left( \sum_{i=1}^{n} Y_i X_i^{1/r} \right)^r$$

where $n$ is the number of components in a mixture, $X_{\text{mix}}$ is the parameter of the mixture, $Y_i$ is the mole fraction of component 1, and $X_i$ is the mole fraction of the component I, and $r$ is the specific constant for the parameter i. The values of $r$ are tabulated in table 2.2.

2.2. Thermodynamic processes in heat engines.

Internal combustion engines are heat engines that convert heat to work; the process of conversion of heat to work is explained by the second law of thermodynamics. The fundamental statement of second law of
thermodynamics is, “although all work can be concerted completely to heat, heat cannot be completely and continuously converted into work” [104].

Based on this statement, the definition of a heat engine is conceptualized as a cyclic device that operates between two reservoirs; the system draws heat from a high temperature reservoir, converts a fraction of the heat to work, and rejects the remaining heat to a low temperature reservoir. In a reversible system, the heat exchange and work output can be correlated to the state of the working fluid as:

\[ \int \delta Q - \int \delta W = \Delta U = 0 \quad 2.5 \]

Where \( \delta Q \) and \( \delta W \) refer to instantaneous portion of the heat exchange and work output, and \( \Delta U \) is the total change of internal energy of the fluid system. The internal energy of a fluid in a system is typically a function of temperature; the state of the fluid changes with addition or extraction of heat. Assuming that the behavior of the working fluids can be defined as ideal gases, the relationship between the change of internal energy and temperature can be assumed constant. Based on this assumption, the definition of constant volume specific heat becomes:

\[ c_v = \left( \frac{du}{dT} \right)_v \quad 2.6 \]

The lower-case annotation of internal energy indicates the internal energy per unit mass. In a different approach, the combination of the compression or expansion work done by the working fluid can be combined with internal energy, which is referred to as enthalpy. Enthalpy is a function of temperature as well, and its relation to temperature is given as:

\[ c_p = \left( \frac{dh}{dT} \right)_p \quad 2.6 \]

Entropy (s) of a system describes availability of energy for conversion to work. In an ideal gas system, the relation between temperature and entropy is described as:

\[ dS = \left( \frac{dQ}{dT} \right)_{rev} \quad 2.7 \]
The subscript, rev, refers to a reversible process. By definition, entropy of the system can be constant, only if there is no heat exchange is involved; therefore constant entropy processes are compression and expansion work of a well-isolated reversible system. In presence of heat exchange, the change of entropy per unit mass is defined as

\[ Tds = dh - v_dP \]  

2.7

Additionally, entropy change of a system between states 1 and 2 are given as

\[ s_2 - s_1 = \int_1^2 c_p \frac{dT}{T} - R \ln \frac{P_2}{P_1} \]  

2.8a

\[ s_2 - s_1 = \int_1^2 c_v \frac{dT}{T} - R \ln \frac{v_2}{v_1} \]  

2.8b

The relationships between temperature, pressure and specific volume in an isentropic process are:

\[ \frac{P_2}{P_1} = \left( \frac{T_2}{T_1} \right)^{\frac{k}{k-1}} \]  

2.8a

\[ \frac{v_2}{v_1} = \left( \frac{T_2}{T_1} \right)^{\frac{1}{k-1}} \]  

2.8b

\[ \frac{P_2}{P_1} = \left( \frac{v_2}{v_1} \right)^{-k} \]  

2.8c

Based on the aforementioned correlations, the working principles of spark ignition and compression ignition cycles are defined as Otto and Diesel cycles, named after the inventors of the corresponding engines. These ideal models correlate the four stroke operation in terms of a closed system, which involve four processes: isentropic compression, heat addition, isentropic expansion, constant volume heat rejection. The difference between these two models is the approach to the heat addition stage. It is assumed that constant volume heat addition occurs in Otto cycle and constant pressure heat addition occurs in Diesel cycle. Theoretically, constant volume heat addition is inherently superior to constant pressure heat addition process at equal
compression ratios in terms of thermal efficiency; however the maximum compression ratio applicable to spark ignition engines is limited in practice.

When discussing the four cycle process in an internal combustion engine, the simplest versions of Otto and Diesel cycles fail to explain the phenomenon as a whole; therefore the fluid exchange process needs to be included to the process. Fluid exchange process may occur under atmospheric conditions for both intake and exhaust, or the intake pressure can be increased by an application called “supercharging. The P-V diagrams of both naturally aspirated and supercharged Otto and Diesel cycles are given in figure 2.1. The equivalence of the processes occurring in a real engine and in the thermodynamic cycle can be explained as following [97]:

Process 1-2: Compression. It is assumed that compression process is adiabatic and there is not heat exchange between the control volume and the boundaries. A process occurring under these conditions is also called as isentropic, because lack of heat exchange preserves entropy at its initial state.

Process 2-3: Combustion. This process is assumed to occur under adiabatic conditions. In spark ignition engines working under the principles of Otto cycle (a, c), combustion occurs at constant volume. In compression ignition engines using the Diesel cycle (b, d), this process occurs at a constant pressure.

Process 3-4: Expansion. The assumptions regarding expansion stroke are the same as compression stroke.

Process 4-6: Exhaust stroke. In theoretical representations of both Otto and Diesel cycles, it is assumed that the working fluid is never exchanged and the fluid goes from state 4 to 1 due to a heat rejection process; however, the working fluid is exchanged for every cycle in a practical internal combustion engine. When this process is shown in the P-v diagram, the change of fluid state from 4 to 6 represents the exhaust stroke. During this stroke, the hot fluid is rejected from the engine. The exhaust valve is assumed to be opened at the bottom dead center and kept open until top dead center, during which the exhaust gas is completely rejected.

Process 6-1: Intake stroke: The assumptions are similar to the exhaust stroke. Additionally, the in-cylinder pressure is assumed to reach the supercharging pressure, if applied (c-d), as soon as the intake valve is opened at the top dead center; the only parameter that changes is the cylinder volume. The process from state 6 to 7 is omitted for naturally aspirated engines.
The thermal efficiency of a heat engine is evaluated by comparing the useful work output to the heat input. In an ideal system, useful work is the difference between the heat addition and heat rejection, and the supplied heat is the heat addition only. The correlation between the thermal efficiency and the heat exchange between the reservoirs is given as:

\[
\eta_i = \frac{Q_H - Q_L}{Q_H} \tag{2.9}
\]

In this equation, \( \eta_i \) refers to the thermal efficiency and \( Q_H \) and \( Q_L \) are the heat transfers from the reservoir with high temperature and to the reservoir with low temperature. Since the amounts of heat transfer into the system is measurable from the change of the fluid state, this correlation can be rewritten as:

\[
\eta_i = \frac{(T_3 - T_4) - (T_2 - T_1)}{(T_3 - T_2)} = 1 - \frac{(T_4 - T_3)}{(T_3 - T_2)} \tag{2.10}
\]
Since processes 1-2 and 3-4 are isentropic processes, the change of temperature from state 1 to 2 and 3 to 4 can be correlated to the change of cylinder volume, and re-written as

\[
\frac{T_2}{T_1} = \left(\frac{V_1}{V_2}\right)^{1-k} = CR^{1-k} = \frac{T_3}{T_4} = \left(\frac{V_3}{V_4}\right)^{1-k}
\]

2.11

In this equation, CR refers to the compression ratio: the ratio between the maximum cylinder volume at bottom dead center and the minimum volume at the top dead center positions of the piston. Finally, when equations 2.10 and 2.11 are combined, the theoretical thermal efficiency of the process becomes a function of compression ratio as:

\[
\eta_i = 1 - \frac{1}{CR^{1-k}}
\]

2.12

These two thermodynamic cycles define the limits of a process that can be attainable in a real engine; however a real process is more inclusive. First of all, the assumption of isentropic process is usually unattainable due to the temperature difference between the working fluid and the internal components of the engine. The engine components are made of metallic elements with naturally good heat transfer qualities, and are also cooled in order to ensure that these materials are strong and durable enough to withstand the conditions encountered during the process. A second source of inefficiency is the combustion mechanism itself: the combustion process is commonly a gradual process, and a fraction of the fuel is left unburned. In addition, combustion is typically initiated before the engine enters expansion stroke, and continues during this process as well. Finally, time scales in an internal combustion engine are barely enough to complete the combustion; therefore it is not possible to convert the whole portion of the heat provided in the fuel to work output. Finally, the engine uses a certain amount of energy in order to do pumping work on the intake charge and the exhaust gases during the fluid exchange process. This work focuses on the combustion aspect of the process; therefore the remaining types of inefficiencies will be handled as a bulk and won’t be mentioned in details.

### 2.3. Definition of engine performance based on pressure history and cylinder volume

In a real internal combustion engine, characteristics of a cycle can be obtained from the pressure history. The pressure history includes clues on heat release characteristics, power output and thermal efficiency, and reasons of inefficiencies up to a certain degree. In addition, pressure history is not influenced
by the mechanical energy losses of an engine, which can be considered favorable when the main objective is combustion. The performance characteristics obtained from the pressure history are called as “indicated” values.

The P-v diagram of a typical cycle is shown in figure 2.3. The difference between the ideal cycles and the real cycle can be understood at a first look, and the effects of inefficiencies explained at the end of the previous section can be seen as well. In addition, it is hard to determine the starting and end points of compression, heat addition, expansion, heat rejection and fluid exchange processes. Due to this reason, the process can’t be handled in sections; instead, it needs to be evaluated as a combination of consecutive volumetric processes that build a single cycle.

![Figure 2.2: Typical P-v diagram of a four stroke cycle in a real engine.](image)

In order to obtain the performance characteristics, the exact values of pressure and volume need to be obtained. In experimental works, the in-cylinder pressure is measured and recorded with respect to the position of the crank angle. The cylinder volume, on the other hand, is easily obtainable and does not vary from cycle to cycle. The dimensions of an engine are given by the manufacturer, or can be measured. When
these dimensions are known, the volume of the cylinder at a given crank angle can be obtained using equation 2.13. The parameters required for this correlation are given in figure 2.3.

\[
\frac{V}{V_{\text{min}}} = 1 + 0.5(CR - 1) \left[ \left( \frac{l}{a} \right) + 1 + \cos \theta - \sqrt{\left( \frac{l}{a} \right)^2 - \sin^2 \theta} \right]
\]

In this equation

\( V \): instantaneous volume

\( V_{\text{min}} \): Volume of the cylinder at top dead center position

\( l \): connecting rod length

\( a \): crank arm length, equal to half of stroke

\( \theta \): the instantaneous angular position of crank arm.

Figure 2.3: The dimensions required for obtaining instantaneous cylinder volume

Indicated mean effective pressure \( (P_{\text{mi}}) \) is a relative measure that describes the engine output as the work done by unit volume of the engine. When obtaining the indicated work from the pressure history, the definition of volumetric work is used as follows:
\[ W_{c,i} = \int p\,dV \]  

Where \( W_{c,i} \) is the indicated work per cycle, \( p \) is the pressure and \( dV \) is the rate of change of the volume. In this equation, the volume of the cylinder can be easily obtained based on the bore, stroke and crank arm dimensions. One particular consideration is, whether the work is obtained over compression or expansion strokes, or over entire four stroke operation. When the work is obtained over compression and ignition strokes, it is referred to as “gross indicated work per cycle”, or when entire 4 cycles are used, the work is called “net indicated work per cycle”. In this work, the performance characteristics are evaluated over entire four strokes. Once work is obtained, the indicated mean effective pressure can be obtained as follows:

\[ P_{mi} = \frac{W_{c,i}}{V_d} \]  

Where \( V_d \) refers to the swept volume. Additionally, thermal efficiency can also be obtained from the cyclic work: the amount of fuel delivered to the engine in every cycle is either a control parameter or can be measured, and the heating values of fuels are well-known. When comparing the amount of work to the total energy input of the fuel, thermal efficiency of the process can be described as how efficiently the fuel is converted to work as follows:

\[ \eta_i = \frac{W_{c,i}}{m_f Q_{HV}} \]  

Where \( m_f \) is the amount of fuel delivered to the engine per cycle and \( Q_{HV} \) is the heating value of the fuel.

Rate of heat release (ROHR) is a parameter that is useful for describing the rate of heat addition to the system. This parameter is also relatively informative when the discussing on combustion characteristics. Like cyclic work, rate of heat release can be obtained using the pressure history. The rate of change of heat in a system can be described as:

\[ Q_{ch} = mc_v dT + (h' - u) dm + pdV + dQ_{ht} \]  

In this equation, \( dQ_{ch} \) is the rate of change of total system heat, \( m \) is mass, \( c_v \) is constant volume heat capacity, \( h \) is enthalpy, \( u \) is energy, \( dQ_{ht} \) is rate of heat loss through cylinder walls. In this work, we are interested in
the combustion characteristics; therefore the heat release is obtained for the timings that combustion occurs. There is no change of mass; therefore the \( dm \) term is eliminated. In addition, it is not possible to measure the heat loss; therefore it needed to be neglected. Optionally, temperature is defined as a function of temperature and pressure in ideal gas equation; therefore its derivative can be obtained from these two parameters as well. After these arrangements, rate of heat release becomes:

\[
ROHR = \frac{k}{k-1} p \frac{dV}{d\theta} + \frac{1}{k-1} \frac{dp}{d\theta}
\]

In this equation, \( k \) refers to the specific heat ratio. The unit of ROHR is joules per crank angle (J/°CA). It is a convention to assume a constant specific heat ratio obtained at the intake condition. Additionally, rate of heat release can be integrated in order to obtain the Mass Fraction Burned (MFB). In this work, the heat loss through the cylinder is not accounted for; therefore the MFB values will always include the effects of heat loss, and the maximum values will be noticeably less than 100%.

### 2.4. Combustion mechanisms

Combustion is an irreversible exothermic chemical reaction between oxidizers and fuels. The oxidizer can be pure oxygen, or a gas mixture that includes oxygen, such as air, and the fuel is a matter that can react with oxygen. In the field of heat power engineering, the heat production holds a greater importance compared to the products of the chemical reaction, because it is possible to convert the heat to other types of energy, usually mechanical energy.

In internal combustion engine research, the oxidizer is air, consisting of 78.09% nitrogen (\( N_2 \)), 20.95% oxygen (\( O_2 \)) as other naturally occurring gases and water vapor. In combustion studies, composition of air is occasionally simplified as a mixture of 79% nitrogen and 21% oxygen. Using combustion of methane (\( CH_4 \)) as an example, a combustion reaction can be written as follows:

\[
CH_4 + 2(O_2 + 3.76N_2) \rightarrow CO_2 + 2H_2O + 7.52N_2
\]

In this example, 2 oxygen molecules are required for each methane molecule in order to consume both the air and the fuel completely, which also means that 9.52 units of air by moles is required for consuming 1 unit of methane. This particular condition is called the stoichiometric condition. The stoichiometric air to fuel (A/F) ratio is decided by the fuel type, and this parameter is usually given in either
molar or mass bases. The mixtures with excess air are referred to as “lean” mixtures and those with excess fuel are called “rich” mixtures. Additionally, equivalence ratio ($\phi$) is also used for describing whether a mixture is rich or lean. The definition of equivalence ratio is as follows:

$$\phi = \frac{(A/F)_{stoic}}{(A/F)}$$

Equivalence ratio of 1 refers to stoichiometric condition; equivalence ratio of less than 1 represents the lean condition. Unlike air to fuel ratio, equivalence ratio is not fuel specific. The reciprocal of equivalence ratio, the excess air ratio ($\lambda$) is also widely used; the choice between equivalence ratio and excess air ratio is only a matter of preference.

The rate at which the reaction occurs depends on the concentrations of the involved species and the conditions of the mixture. The governing equations for quantifying the rate of a reaction are:

$$r = A[CH_4][O_2]\exp(-E/RT)$$

$$k = AT^n\exp(-E/RT)$$

In this equation, $r$ is the reaction rate, $A$ is an arbitrary constant that replaces the gas kinetic collision frequency, the units in brackets are the concentrations of the reactants, $E$ is the activation energy, $R$ is the gas constant and $T$ is the temperature \[99\]. Arrhenius equation is an empirical relation between the temperature and the reaction rate. In order to increase the precision of the approximation, the original correlation is modified with additional temperature dependence term; the new form is called as improved Arrhenius equation, as seen in Equation 2.8. The parameters of this equation are found empirically by fitting the equation to the results of an experiment. In internal combustion engine research, three types of combustion mechanisms are commonly encountered: flame propagation, droplet combustion and autoignition. These three types of mechanisms will be explained in this section.

2.4.1. Premixed flames and flame propagation

In premixed flames, air and fuel are formed into a mixture prior to the start of combustion. Figure 2.4 shows a one dimensional graphical representation of the mechanism. After initiation of the chemical reaction, the reaction zone, also called as flame front, migrates towards the unburned mixture region. Flame front also
separates the burned and unburned mixture regions. The rate at which the flame front migrates towards the unburned region depends on the conditions in the system, such as the pressure, initial temperature, presence or absence of a fluid flow, the concentrations of air, fuel or diluents. Based on the magnitude flame propagation speed, the premixed flames can be classified as laminar premixed flames and turbulent premixed flames. In internal combustion engines, the most frequently occurring type of premixed is the turbulent type [98]. Flame propagation speed is the highest for mixtures of stoichiometric condition. The more the mixture is either on the lean or rich side, the slower the flame propagation speed will be, until a certain lower or upper limit. Flame propagation is typically terminated when the air/fuel ratio is too rich or too lean, or when the mixture is consumed completely.

**Figure 2.4: Graphical representation of a one dimensional flame propagation mechanism.**

### 2.4.2. Non-premixed (Diffusion) flames and droplet combustion model

In non-premixed flames, air and fuel are mixed simultaneously with the chemical reaction. In the past, non-premixed flames were used to be named as diffusion flames; this name is currently obsolete [98]. In internal combustion engine research, this model is commonly used for explaining the combustion of fuel droplets. In droplet combustion model, the stream of fuel spray breaks down to small droplets, after which air and fuel are mixed by diffusion. The graphical representation of droplet combustion model is given in figure 2.5. The fuel droplet core consists of the fuel only; the fuel droplet evaporates and mixes with the surrounding air by means of diffusion. As a result of diffusion, both fuel and air concentrations change gradually from the droplet surface towards the oxidizer. Combustion activity is sustained at the reaction zone, which has the most favorable air and fuel concentration levels. As the reaction continues, the reaction zone
shrinks towards the fuel droplet; when the oxidizer level becomes insufficient, chemical reaction becomes unable to sustain itself and the leftover fuel droplet forms into a soot particle. Soot formation usually produces yellow luminescence as a result of fuel-rich chemical reaction [98].

![Schematic representation of droplet combustion model.](image)

**Figure 2.5:** Schematic representation of droplet combustion model.

### 2.4.3. Autoignition phenomenon and knocking

In autoignition, air and fuel mixture ignites spontaneously without any need for any ignition source, such as spark discharge. This mechanism can be explained as follows: when the temperature of the mixture is above a certain level, which is defined as autoignition temperature, a long chain of chemical reactions begin automatically. If the temperature is preserved long enough, the chain of chemical reaction will be completed, and the mixture will ignite itself, releasing heat instantaneously. The duration that it takes from the start to the completion of the chemical reaction is predictable, and it is a function of mixture temperature, pressure and concentrations of the species that constitute the oxidizer and mixture. In the literature, this period is defined as ignition delay, and usually correlated to the aforementioned parameters in an Arrhenius type equation by adding pressure dependence, as given in equation 2.9.

\[
\tau = A \exp\left(-\frac{E}{RT}\right)p^n
\]  

In this equation, the ignition delay (\(\tau\)) is defined as a function of pressure and temperature. E is the activation energy of the fuel, A and n are empirical parameters that are obtained by fitting the equation to experimental data. Various ignition delay correlations are available in the literature for various types of fuels and mixture
conditions. Those equations may also include other parameters specific to a certain fuel blend. This mechanism is commonly observed in diesel engines and autoignition of premixed mixtures. In diesel engines, fuel droplets are ignited due to autoignition.

Heat release by autoignition occurs rapidly. In internal combustion engines, this scenario may yield to knocking, which is described as a combination of significantly fast rise of pressure rise and pressure oscillations accompanied by an audible knocking sound. Knocking is harmful for the engine components; therefore it needs to be avoided. Quantitative evaluation of knocking phenomenon will be revisited in oncoming sections.

2.4. The relation between combustion characteristics and exhaust emissions

Under ideal conditions, the reactants entering a chemical reaction are expected to be converted to the products with no leftovers; however combustion of fuels in a real engine always partially incomplete. A fraction of the fuel or the intermediate species are always left unburned. Secondly, all components of air and fuels may be involved in chemical reactions, regardless of their negligible concentrations. Apart from the common combustion products resulting from combustion of hydrocarbons, CO₂, H₂O and N₂, harmful species are commonly detected in exhaust gas due to incomplete combustion, excessively high combustion temperature and poor fuel quality. These species can be listed as carbon monoxide (CO), unburned hydrocarbons (HC) and oxides of nitrogen (NOₓ), soot and oxides of sulfur. In general, oxides of sulfur can be avoided by removing the sulfur content from petroleum products; however, the other species are produced when the combustion characteristics deviate from the favorable.

Carbon monoxide and unburned hydrocarbons are emitted as a result of incomplete combustion. In addition, unburned hydrocarbons can also be unburned fuel trapped in cold spots of an engine, such as the cylinder walls. A solution to reducing CO and HC emissions is increasing the reaction speed, which is possible by increasing the temperature of the in-cylinder mixture; however this solution has its limitations as well. First of all, the engine components can’t withstand the temperatures achieved during combustion; therefore they need to be cooled. Flame extinction at the cylinder walls is another contributor of unburned hydrocarbons, especially in spark ignition engines. It is noteworthy to mention that, both HC and CO will be emitted as a result of even the most efficient combustion. In order to keep their emission values below the allowable limit, manufacturers usually equip the engines with after treatment systems, such as catalytic converters.
The major source of NO\textsubscript{x} production in an internal combustion engine is the thermal NO\textsubscript{x}. NO\textsubscript{x} production is strongly dependent on the temperature: when the mixture temperature exceeds 1600°C, the rate of thermal NO\textsubscript{x} production reaches at significant levels. Both a higher temperature and a longer residence time will increase the rate of thermal NO\textsubscript{x} production drastically. NO\textsubscript{x} production is a significant problem in diesel engines; while the average temperature of in-cylinder mixture is typically lower in a diesel engine in comparison to a spark ignition engine, local temperature at a reaction zone, i.e. a droplet undergoing combustion, is typically in the vicinity of the adiabatic flame temperature, which commonly exceeds 2000K. A common NO\textsubscript{x} reduction is use of exhaust gas recirculation: introduction of non-reactive gases with both work as a diluent and keep the in-cylinder temperature lower due to their lower specific heat ratios.

Soot particles are formed by the unburned cores of fuel droplets. This issue is especially common for direct injection sprays with large droplet sizes. After injection, spray breakdown and atomization takes place, during which the droplet size is reduced due to evaporation of the fuel. If the droplet size is not small enough to fully evaporate until the end of the combustion, a fraction of the droplet kernel is left unburned and is converted to a soot particle. This is especially a prevalent issue in direct injection diesel engines. In order to eliminate emission of soot particles to the atmosphere, commercial and passenger cars are equipped with exhaust particulate filter. Another common measure for reducing soot emission is to reduce the droplet size by injecting the fuel at higher pressures; however, whether or not this is the right approach is widely discussed. Reducing the droplet sizes will influence the particulate size equivalently; modern diesel engines using high pressure injection systems produce nano-sized particles, which might be challenging to catch using a particulate filter.

2.5. Dual fuel gas engines and dual fuel combustion

The basic knowledge on internal combustion engines is given in the reference book written by Heywood, and the information given in this section is sourced from that work [97]. A well-established method for classification of internal combustion engines is the type of combustion that occurs during the heat addition stage. Two common types of internal combustion engines are spark ignition (SI) and compression ignition (CI) engines. In spark ignition engines, in-cylinder charge is a mixture of air and fuel; this mixture is ignited by a spark discharge, and the rest of the mixture is consumed by means of flame propagation under suitable conditions. This type of combustion starts at a single point; the duration of the combustion depends
on the flame propagation speed, which is decided by the reactivity of the mixture under given conditions. In compression ignition engines, the in-cylinder charge is commonly air; the temperature and the pressure of the air are increased during the compression stroke, into which the fuel is injected. In this mechanism, the fuel both autoignites during an ongoing air-fuel mixture formation process; therefore heat release occurs rapidly. Both combustion strategies have their own advantages and disadvantages in terms of a trade-off between combustion efficiency and exhaust emission characteristics.

A dual fuel engine refers to an internal combustion engine which uses two types of fuel for producing power. A dual fuel compression ignition gas engine is a type of dual fuel engine, which can be classified as an engine that uses a combination of compression ignition and flame propagation type combustion during heat addition stage. In these engines, the air-gaseous fuel mixture is formed to the desired homogeneity level prior to injection of the pilot fuel. The pilot fuel serves as the igniter of the premixed in-cylinder mixture; after injection, the pilot fuel sprays autoignite following a brief duration of ignition delay. The pilot fuel autoignition zones are also known as flame kernels. At this stage, the volumetric coverage of the flame kernels decides whether the premixed mixture is consumed instantly or after a comparatively longer duration of flame propagation. The compression ignition engines that are converted for dual fuel operation usually use the prior mechanism; however the amount of gaseous fuel that can be used in this method is limited by knocking due to rapid heat release [22-30, 38-42, 44-58]. The latter mechanism, which also forms the foundation of this research topic, relies on partial coverage of the combustion chamber by the flame kernels. Following the order of the pilot injection, pilot fuel autoignition and flame kernel formation, premix mixture is ignited at the flame kernels and flame propagation is initiated. Rest of the premixed mixture is consumed by the propagating flames. These three combustion mechanisms are graphically explained in figure 2.6.
Figure 2.6: Graphical explanation of spark ignition, compression ignition and dual fuel compression ignition combustion mechanisms.

These three combustion mechanisms show different performance characteristics, which also influences the exhaust emissions. Combustion in spark ignition engines occurs at a slower rate; a small fraction of the fuel or intermediate combustion species, namely unburned hydrocarbon (HC) and carbon monoxide (CO), is typically rejected during exhaust stroke. In return, in-cylinder temperature is not high enough to produce oxides of nitrogen (NO\textsubscript{x}), and the premixed intake charge ensures that soot emission is low. In diesel engines, combustion is almost an instantaneous process; therefore both HC and CO emissions are low; however high local temperature produces significant amounts of NO\textsubscript{x} and improper mixing yields measurable amounts of particulates. In dual fuel CI engines, exhaust emissions are typically a trade-off between CI and SI engines; however it is possible to improve exhaust emission characteristics by optimization of both in-cylinder mixture properties, use of suitable pilot injection strategies and advanced combustion mechanisms.

The advantages of a dual fuel gas engine over conventional engines can be listed as the flexibility of fuel choice, possibility of cleaner exhaust emissions due to lean-burn combustion and simplicity of fuel delivery components. Flexibility of fuel choice is recently gaining importance due to the increasing interest in biofuels. Conventionally, both internal components and the combustion control technologies of internal combustion engines are highly diversified in order to achieve the highest efficiency possible while restricting
the exhaust gas emission levels below defined standards; replacing the type of fuel used in these engines usually require complex modifications to both the components and control parameters. On the other hand, a dual fuel gas engine can successfully be operated using variety of gaseous fuels with minor adjustments to the control parameters. Lean-burn combustion capability is also an important quality of these engines; pilot fuel injection both eliminates misfiring problem and creates large flame kernels. In addition, NO\textsubscript{x} emissions are kept under control by reduction of in-cylinder temperature. Finally, due to low amounts of pilot fuel injection, the injection system does not require the complex and costly systems that are necessary for diesel engines.

2.6. PREmixed Mixture Ignition in the End-gas Region (PREMIER) combustion

A common problem regarding dual fuel CI combustion is the high emission levels of carbon monoxide and unburned hydrocarbon as a result of incomplete combustion at the end-gas regions. Propagating flames reach at the end-gas regions through the end of combustion process, and these regions might not have long enough duration to reach completion until the beginning of the exhaust stroke. While it is possible to keep the equivalence ratio of the gaseous fuel-air mixture higher in order to increase flame propagation speed and ensure complete combustion, this cancels most of the benefits of lean burn operation. In order to fully benefit from lean-burn operation without the drawbacks, the end-gas region needs to be treated separately. In recent years, autoignition based combustion technologies are commonly suggested for treating the issues related to the end-gas region. PREmixed Mixture Ignition in the End-gas Region (PREMIER) combustion is one of such technologies. PREMIER combustion mechanism is graphically explained in figure 2.7.

<table>
<thead>
<tr>
<th>Intake condition</th>
<th>Preparation for combustion</th>
<th>ignition</th>
<th>Heat release (flame propagation)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Premixed mixture</td>
<td>sprays</td>
<td>flame kernels</td>
<td>burned mixture</td>
</tr>
<tr>
<td></td>
<td>unburned mixture</td>
<td>End-gas autoignition</td>
<td></td>
</tr>
</tbody>
</table>

Figure 2.7: Mechanism of PREMIER combustion.
PREMIER combustion differs from the conventional dual fuel combustion, which will be referred to as normal combustion, by the behavior of the end-gas region. Combustion starts at the pilot fuel injection timing and forms the flame kernels. The air-gaseous fuel mixture is ignited by the flame kernels formed at the injection sites, triggering the flame propagation. As the air-fuel mixture is burned, heat release occurs, increasing the in-cylinder pressure and temperature. From this point onwards, the type of combustion depends on the characteristics of the unburned gas. If the propagating flames consume the unburned mixture before completion of the pre-ignition reactions of the premixed mixture, normal combustion is encountered; otherwise, the unburned mixture at the end-gas region will autoignite, yielding either PREMIER combustion or knocking. At this stage, the volume of end-gas region, the timing of end-gas autoignition and the heat release due to end-gas autoignition decide whether or not knocking occurs. During end-gas autoignition, heat release occurs quickly; due to this activity, the in-cylinder pressure rises quickly. Additionally, a larger end-gas volume will release a higher amount of heat and the pressure will rise higher. Typically, the engine is on the expansion stroke when the end-gas autoignition occurs. If the expansion rate of the piston is fast enough to overcome the effect of end-gas autoignition and keep the rate of pressure rise below knocking limits, PREMIER combustion can be achieved. PREMIER combustion does not include any signs of knocking, such as rapid pressure rise, pressure oscillations or the audible ringing sound. Due to occurrence of knock-free end-gas autoignition, it is possible to achieve higher combustion efficiency by reducing the unburned fuel sourcing from the end-gas region. This mechanism makes it possible to achieve both higher thermal efficiency and reduce CO and HC emissions; however higher in-cylinder pressure is sustained for a longer time, and NOx is increased as a result. Figure 2.8 gives examples of typical pressure histories and rates of heat release of normal, PREMIER and knocking conditions.
2.7. Properties of the fuels used in this work

In this work, three types of gaseous fuels and a single type of pilot fuel are used. The gaseous fuels are natural gas, methane and hydrogen; the pilot fuel is commercially available ultra-low sulfur content ULSC diesel fuel. Natural gas is sourced from a single manufacturer, and its composition is stated as 89.93% CH$_4$, 3.63% C$_2$H$_6$, 2.10% C$_3$H$_8$, 2.61% i-C$_4$H$_{10}$, 1.45% n-C$_4$H$_{10}$ and 0.27% N$_2$. Methane and hydrogen are over 99% purity according to the supplier; therefore they can be safely assumed as pure methane and hydrogen. The specifics of concentration of the diesel fuel are unknown; however it is safe to use the physical and chemical properties that are commonly available in the literature. It is necessary to mention that the pilot fuel used throughout this work is sourced from the same batch of production; therefore the properties will be consistent throughout this work. The properties of the test fuels that are used in analyses are given in Table 2.3.
<table>
<thead>
<tr>
<th></th>
<th>Diesel</th>
<th>Methane</th>
<th>Ethane</th>
<th>Propane</th>
<th>i-butane</th>
<th>n-Butane</th>
<th>Hydrogen</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Lower Heating value</strong></td>
<td>kJ/mol</td>
<td>-</td>
<td>802.34</td>
<td>1437.2</td>
<td>2044.2</td>
<td>2651.0</td>
<td>2659.3</td>
</tr>
<tr>
<td></td>
<td>kJ/kg</td>
<td>43.4</td>
<td>50.009</td>
<td>47.794</td>
<td>46.357</td>
<td>45.613</td>
<td>45.752</td>
</tr>
<tr>
<td><strong>Molecular weight</strong></td>
<td>kg/kmol</td>
<td>-</td>
<td>16.04</td>
<td>30.070</td>
<td>44.097</td>
<td>58.124</td>
<td>58.124</td>
</tr>
<tr>
<td><strong>Stoichiometric air-fuel ratio</strong></td>
<td>kg/kg</td>
<td>14.6</td>
<td>17.4</td>
<td>16.0</td>
<td>15.82</td>
<td>15.60</td>
<td>15.60</td>
</tr>
<tr>
<td></td>
<td>m³/m³</td>
<td>-</td>
<td>9.64</td>
<td>16.66</td>
<td>24.10</td>
<td>31.34</td>
<td>31.34</td>
</tr>
<tr>
<td><strong>Autoignition temp.</strong></td>
<td>°C</td>
<td>210</td>
<td>580</td>
<td>515</td>
<td>455</td>
<td>405</td>
<td>405</td>
</tr>
<tr>
<td><strong>Specific heat ratio</strong></td>
<td></td>
<td>-</td>
<td>1.32</td>
<td>1.18</td>
<td>1.13</td>
<td>1.19</td>
<td>1.18</td>
</tr>
<tr>
<td><strong>Boiling point</strong></td>
<td>°C</td>
<td>180-360</td>
<td>-161.5</td>
<td>-89</td>
<td>-42</td>
<td>-11.7</td>
<td>-1</td>
</tr>
</tbody>
</table>
3. Experimental setup

3.1. The test engine

3.1.1. Specifications of the test engine

The test engine used in this work is a single cylinder pilot fuel injected dual-fuel gas engine. The engine has a displacement of 781 cubic centimeters through $\phi96$mm bore and 108 mm stroke. The connecting rod length is 168mm. The engine has two intake and two exhaust valves. Both the piston and the equivalence ratio are changeable by using pistons of various geometries and cylinder head gaskets of suitable thicknesses. In visualization experiments, the cylinder head is offset from the block, and an extended block with optical access is installed. The test engine is shown in both metal engine and visualization settings in Figure 3.1(a) and 3.1(b) respectively.

Table 3.1: Engine specifications

<table>
<thead>
<tr>
<th>Engine type configuration</th>
<th>Water cooled, 4-stroke</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore×stroke</td>
<td>$\phi96$mm×108mm</td>
</tr>
<tr>
<td>Displacement</td>
<td>781cc</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>Changed throughout the work</td>
</tr>
<tr>
<td>Pilot fuel delivery</td>
<td>Common rail direct injection</td>
</tr>
<tr>
<td>Injector</td>
<td>Diesel direct injection, solenoid type</td>
</tr>
<tr>
<td>Gaseous fuel supply</td>
<td>Premixed charge through intake port</td>
</tr>
<tr>
<td>Natural gas flowrate control</td>
<td>Gas injector</td>
</tr>
<tr>
<td>Gaseous fuel flowrate control</td>
<td>Mass flow controller(Methane and hydrogen)</td>
</tr>
<tr>
<td>Air intake</td>
<td>Supercharged, adjustable intake pressure</td>
</tr>
<tr>
<td>Intake valve open/close</td>
<td>355°ATDC/135°BTDC</td>
</tr>
<tr>
<td>Exhaust valve open/close</td>
<td>130°ATDC/355°BTDC</td>
</tr>
</tbody>
</table>
3.1.2. Piston types, configurations and adjustment of compression ratio.

A shallow dish piston is used during experiments in metal engine settings, and two different compression ratios are used: 17.0:1 and 16.4:1. A shallow dish type piston is a type of piston geometry that can be found in gasoline engines, and they are suitable for flame propagation type combustion. Since this work primarily focuses on use of gaseous fuels, this is found to be a more suitable configuration compared the use of a diesel engine type piston, such as those with derby hat geometry. In visualization experiments, the extended cylinder block is installed between the main block and the cylinder head, which increases the distance between these two components by 295 millimeters. The extended piston is a 280 millimeters hollow extension, which attached to the top of a base piston using a spacer in between. In this configuration,
compression ratio is adjusted by switching between spacers of different thicknesses. In the given configuration, spacer thickness is 10mm. The extended piston is of flat top piston geometry. The configuration of the piston, cylinder head and the gaskets are shown for all types of equivalence ratio configurations in figure 3.2.

Figure 3.2: Simplified sketches of combustion chamber geometries of all experimental conditions.

3.1.3. Visualization parts

The optical setup is a modified version of the base engine, and consists of the extended block, the base piston, a spacer, the extended piston, 45° slanted mirror, the sapphire window and its retaining screw as the visualization components. These components are shown in figure 3.3. The modified system is designed based on offsetting the location of the cylinder head by 290 mm, between which a path for the optical access can be created. The extended block is used in order to offset the cylinder head from the block. A cylinder liner identical to the one on the engine block is inserted into this component in order to maintain the combustion chamber geometry as closely as possible. The extended piston can be described as a hollow cylinder, into which the sapphire window is attached using a hollow screw. Both the visible area of the sapphire window
and the central hollow section of the window retaining screw have a diameter of 62mm, as shown in figure 3.4., which also define the boundary of the visualization area. In order to stop leakage from this interface, an O-ring seals the interface where the round surfaces of these two components meet, and a copper ring is squeezed between the flange of the sapphire window and its corresponding seat on the extended window. The shape of the combustion chamber can be converted from flat top to derby hat geometry by replacing a copper ring of a higher thickness, which is also one of three methods for adjusting the equivalence ratio. The interface between the extended piston and the cylinder liner on the extended block is not lubricated; in order to compensate for the lack of lubrication and prevent from damaging these two components, the piston rings are replaced with Teflon counterparts. These Teflon rings need to be replaced during every engine rebuild or maintenance in order not to encounter compression leaks during the experiments. The extended piston is not connected to the crankshaft directly; this connection is provided via a base piston. The base piston is produced by tapping and drilling four screw holes and inserting an alignment pin to the center of the leveled piston top surface. The alignment pin matches a hole drilled into the extended piston and restrains uncontrolled movement of the extended piston. Four screws following M6x1.0 standard connect the base piston and the extended piston. The dimensions of both extended piston and the base piston are decided with the intention of making compression ratio adjustments possible. The second method for adjusting the compression ratio is insertion of a spacer of a suitable size is inserted these two pistons.
Figure 3.3: Imaging parts.

Figure 3.4: Visible area of the sapphire window.
3.2. Air induction and the supercharging systems

Intake charge is pressurized and stabilized by the supercharging system. This system relies on a screw type industrial compressor, two surge tanks, an electrically controlled valve, an absolute pressure transducer, a flowmeter and the air pressure PIV controller. The compressor pressurizes the ambient air and stores in the first surge tank at 7 atm pressure. The second surge tank serves as an air accumulator to the engine, onto which the pressure transducer is installed. The valve is installed between the surge tanks. The PIV controller reads the pressure value from the transducer, and operates the electrically controlled valve to maintain the second surge tank pressure at the desired level. The intake air flowmeter is installed to the exit of the second surge tank, and its output is used as an experimental data; this parameter is not involved in controlling the air flowrate in the system. An air heater and a k-type thermocouple are installed downstream from the air flowmeter, and another PIV controller governs the heating system; however the heater needs to be turned on or off manually before and after operating the engine, because the heating system requires constant flow of intake air through the port in order to measure its temperature. The outline of the supercharger system is given in figure 3.5.

![Figure 3.5: Outline of the supercharger and intake air heater systems](image-url)

37
3.3. Natural gas injection system

Natural gas is injected to the system by a gaseous fuel injector that is installed 250mm before the engine. Natural gas is a flammable substance; therefore several safety features are required in order to avoid any hazardous situations. The natural gas is obtained from the supplier in gas tubes. Two tubes of natural gas are connected to the first pressure regulator in order to ensure the stability of gas flow. In addition, a 5 liter surge tank is connected to the system. The surge tank is turned on during the calibrations and shut off during the experiments using a three-way valve. The first regulator is set to 1MPa. Following the pressure regulator is the panic purge valve system that provides the safety measure in emergency situations. The first valve is operated by air pressure, which is sourced from the high pressure surge tank of the supercharger system; this approach ensures that natural gas supply is interrupted when the engine is stopped. The second valve is a solenoid valve that is opened when the electric signal is interrupted, e.g. when the operation is terminated by using the panic button. Under standard operation situation, natural gas is delivered to the second pressure regulator located inside the experiment room, where fine pressure adjustment can be made. An accumulator is installed between the injector and the second pressure regulator, which stabilizes the supply pressure by acting as a buffer volume. The injector is connected to the timing control system and is operated by electric signals. Outline of the system is given in figure 3.6.
The supply rate of natural gas and homogeneity of air-natural gas mixture can be adjusted by controlling two parameters: natural gas supply pressure to the injector and injection timing characteristics. First of all, premixed mixture equivalence ratio is directly related to the supply rate of natural gas, which is decided by the natural gas supply pressure and the injection duration. In addition, the level of homogeneity is decided by these two parameters as well; however, the impact of these parameters is more complicated. Considering delivery of a fixed amount of natural gas, it is possible to use a higher gas supply pressure with a short injection signal, which will yield a mixture with more pronounced inhomogeneity; a fraction of the intake charge volume will have relatively higher natural gas concentration, and rest of the mixing process depends on the mixing process until start of combustion. On the other hand, delivering the natural gas at a lower pressure, and preferably as long as the intake valve is open, will yield a more homogeneous mixture before its introduction to the engine. In terms of the experimental aspects, the flexibility of natural gas delivery method is preferable.
Natural gas flowrate calibration process involves measuring the rate of change of surge tank pressure and temperature. The process begins by filling the surge tank and closing the valve that connects gas tubes to the supply system. When the fueling operation starts, the system is allowed to stabilize for 60 seconds, after which the first temperature and pressure measurements are taken. The readings are repeated for every 180 minutes. When determining the natural gas flowrate, Benedict-Webb-Rubin state of equation is preferred, because the relatively high pressure and low temperature inside the surge tank means that the properties of n-butane is significantly close to condensation in particular, and additionally, the mixture does not involve any monatomic gases on top of a minor fraction of nitrogen as diatomic gas. Under these circumstances, Benedict-Webb-Rubin equation is superior to alternative equation of state correlations. The pressure inside the tank is measured at a single point, and two k-type thermocouples that take readings of top and bottom locations of the surge tank volume ensure that the average temperature is obtained. Including the buffer volume inside the high pressure gas regulator and the pipes in the total reserve volume, the end result becomes 5.580 liters. In this system, supply pressure is always set to 900 kPa of absolute pressure; the flowrate is adjusted by changing the injection duration.

3.4. Gaseous fuel supply system

The main components in the gaseous fuel supply system are the mass flow controllers. These devices adjust the flowrate based on an input and do not require user calibration. In this work, the flowrate is continuously adjusted based on the air flowrate readings obtained from the flowmeter in order to maintain a fixed equivalence ratio during operation. A PLC controller reads the air flowrate signal from the intake air flowmeter, determines the flowrates of methane and hydrogen for the required methane/hydrogen ratio and equivalence ratio based on the mathematical definitions. The required flowrate is converted to 1-5V analog signal, where 1V and 5V refer to zero and maximum allowable gas flowrates respectively. Intermediate values are interpolated in between these limits. When the mass flow meter receives the required signal, it sends the gaseous fuel to the intake port. The intake port is equipped with curved pipes that direct the gas stream to the air flow direction, at the center of the pipe. These gas entries are installed approximately 3 meters upstream from the intake valves, which ensure that the premixed mixture is in a reasonably homogeneous condition. A certain prerequisite of these mass flow controllers is the pressure of the gas at the inlet: the manufacturer recommends around 100 kPa of pressure difference between the inlet and outlet of the mass flow controller for the most precise operation, which was carefully adjusted in this work. Additionally, a surge tank was required in order to stabilize methane flowrate; however the exact reason for the necessity of this
approach is not understood well. It is expected that certain types of impurities, such as water vapor, mixed into the methane bottle might cause poor pressure regulator performance, failing to provide methane at a constant pressure. Using two methane tube sat the same time solved this issue. The same issue was not observed for hydrogen. Additionally, the inlet and outlet pipe diameter was observed to restrict the flowrate as well; the mass flow controller requires a large enough inner pipe diameter for stable operation. Figure 3.7 shows the outline of the gaseous fuel supply system.

![Figure 3.7: Gaseous fuel supply system](image)

It is possible to increase flowrate control accuracy of the mass flow controllers by scaling down the maximum flowrate capacity by changing the internal settings of the device. The devices used in this work are Yamatake CMV-Q mass flowrate controllers, which have maximum flowrate capacities of 500 l/min for methane and 200 l/min for hydrogen. In comparison, the maximum flowrates required for these two gases were 40 l/min and 25 l/min respectively. As a result, both devices are downscaled to a maximum gas flowrate of 50 l/min, which is safely above the desired flowrates. An important consideration is to make the necessary input to the ladder code that the PLC controller uses.

### 3.5. Pilot fuel injection system
The pilot fuel used in this work is diesel fuel. Diesel fuel circulates in two fuel lines: the low pressure line and the high pressure line. Low pressure line connects the fuel returned from the pump, the injector and the common rail, and the fuel supplied from the tank. The high pressure line is fed by the diesel fuel pump and is connected to the fuel injector through the common rail. The outline of the pilot fuel injection system is given in figure 3.8.

In this system, the fuel pump is actuated by a 3 phase motor, speed of which can be adjusted by the dedicated knob on the main panel; based on which the pumping capacity can be adjusted. In this study, the pumping capacity is not a concern; therefore the motor speed is always kept at maximum. The pump belongs to a commercial diesel vehicle, and is capable of pressurizing diesel fuel up to 200 MPa. High pressure outlet of the pump is connected to the common rail. The fuel pump assembly consists of a solenoid needle valve,
which needs to be energized for enabling pressurization and restricting the pump flowrate. This valve is
directly connected to a power supply with voltage and current adjustability; however, the presence of this
valve is not critical in this experiment, so the voltage and current supply is usually adjusted high enough to
ensure that pressure loss can be avoided. The pump also has a return line, through which the accumulated air
bubbles and unused portion of the supplied fuel are rejected.

The common rail is used for three purposes: joining the high pressure lines from the fuel pump to the
pressure gage, the injector and the pressure relief valve. This component is made for withstanding high
hydrostatic pressures. The pressure relief valve is a detachable component of this component. The pressure
relief valve is an assembly that consists of a needle valve that is pushed by a mechanical spring. The stiffness
and preload of the spring stabilize the injection pressure. When adjusting the injection pressure, one of three
compression springs manufactured for rail pressure ratings of 40 MPa, 80 MPa and 140 MPa are inserted into
the pressure relief valve housing. Afterwards, the spring is preloaded to the desired pressure using a pusher
connected to the head cap of the relief valve by a screw. When the rail pressure exceeds the preset pressure,
fuel pushes the needle valve back and leaks towards the low pressure line until the required condition is
satisfied.

The injector is a solenoid type direct injection system component manufactured by Denso for use in
diesel engine equipped passenger vehicles. The injector requires both fuel pressure and an electrical signal for
allowing the fuel flow into the orifices. The injection signal determines the opening and the closing timing of
the nozzle. Once energized, the solenoid valve uses the fuel pressure to lift the nozzle spindle to allow
injection of the fuel, and the operation is reversed when the close signal is sent. Since fuel pressure is the
main force that manipulates the nozzle spindle, a small fraction of the fuel that enters the injector body is
sent back to the system after being depressurized. A bubble remover is installed between the injector and the
low pressure line. In this work, its nozzle is replaced by a purpose made nozzle that has three orifices; the
orifice diameter is $\odot 100\mu m$. The purpose of this nozzle is to make it possible to inject significantly low
quantities of diesel fuel. On the flat plane, the sprays are oriented 120 degrees from each other on the plane
normal to the central axis of the injector, and are separated by 70 degrees from the central axis. Orientation
of the sprays is shown in figure 3.9.
Both the diesel fuel supply and return fuel are collected on the low pressure line. A measuring pipette with a capacity of 3 milliliters is connected before the entrance of the fuel pump. When measuring the average injection rate, the fuel supply from the tank is closed using the valve attached after the filter, and the time it takes to consume a certain amount, typically 1 milliliter, is measured. The measuring pipette has indicators for every 0.1 milliliters, so it is possible to measure lower quantities during intermediate confirmations. Since the engine is operated at 1000 rpm, it is known that the fuel is injected 500 times in a minute. The density of diesel fuel is 0.832 g/ml. After rescaling the flowrate for 1 minute of fuel flowrate duration, the amount of fuel injection can be determined easily.

3.6. The main control panel

Measurement and control of a certain number of parameters are performed over the main control panel. This unit houses the electrical peripherals of the equipment that operate with 100V single phase AC and 200V three-phase AC electricity and follow the industrial standards. The components on this unit are shown in figure 3.10. The functions of the main control board are as follows:

1) Natural gas pressure indicator: The pressure is adjusted over a regulator; the display only informs about the pressure inside the natural gas accumulator that is installed before the injector. The units are in kilopascals
This indicator is referred to during the experiments in order to ensure that natural gas injection rate is constant.

2) (3) Exhaust gas temperature indicators: Exhaust temperature is measured in two locations using k-type thermocouples. The first measurement is taken 250 millimeters downstream from the engine head and displayed on indicator (2), and the other at the exhaust gas analyzer connection barrel and displayed on indicator (3).

4) Intake pressure PIV controller and indicator: this device controls the intake pressure based on the user input. The units are in kilopascals (absolute).

5) Intake air flowrate indicator: this device displays the air flowrate in cubic meters per hour normalized to 1 atmosphere of intake pressure.

6) Engine oil temperature indicator: this device displays the engine oil temperature measured at the bottom of the engine block by a k-type thermocouple.

7) Intake air temperature PIV controller: this controller governs the intake air heater based on the input parameters. The feedback mechanism is a k-type thermocouple that is installed downstream from the heater.

8) Coolant/heating fluid temperature controller: This device switches the recirculation water heaters on or off based on the water temperature readings. The temperature is adjustable

9) Supercharger on-off control

10) Recirculation water pump on-off control

11) Intake air heater on-off indicator (top) and switch (bottom)

12) Recirculation heater on-off indicator (top) and switch (bottom)

13) Diesel fuel pump motor speed governor knob (top) and on-off switch (bottom):

14) Panic button: When pressed, this button terminates the power connection into the control panel. When the panic procedure is triggered, the connection between the components installed on this panel and the electricity supply are terminated. This procedure stops diesel fuel pump, natural gas flow, shuts down all heating elements, the compressor, and purges the natural gas delivery system components that are located inside the experiment room. Additionally, the PLC controller used for other gaseous fuels is installed into this panel as well; therefore its operation is terminated, forcing the gaseous fuel flow to stop.
3.7. Data measuring, processing and recording devices

3.7.1. In-cylinder pressure measurement

Data evaluation process of this work relies on precise in-cylinder measurement. In-cylinder pressure was measured by a Kistler type 6052C high pressure transducer. This device has a measuring range of 0-250 bar, measurement error is less than 2% within a temperature range of 23 to 300 degrees Celsius and is optimized for use in internal combustion engines including the knocking condition. Under the tested conditions, a phenomenon called pressure drift was observed occasionally, which is treated during the data
analysis stage. A dedicated pressure sensor mounting hole was drilled to the cylinder head by the engine manufacturer in a way that the diaphragm of the sensor is exposed to the in-cylinder pressure. The signal produced by the piezo crystal of the sensor is sent to a Kistler type 5011 charge amplifier. This device amplifies the signal to a desired range based on user settings. During the experiments, the amplifier also applies a 20 KHz low-pass filter to the input signal. Output of the charge amplifier is calibrated on a dead weight tester once in every six months in order to ensure the correctness of the readings.

3.7.2. Crank angle, cam angle and top dead center sensors

The base engine does not have any electronic control units or sensors as original equipment. In order to understand the position of the piston in a four stroke cycle, crank angle position, camshaft top dead center position and cam full rotation signals are monitored using parallel infrared optical sensors. These sensors have an infrared LED and a phototransistor; the infrared light emitted by the LED is directed directly onto the semiconductor light sensor of the transistor, between which there is a 10 mm gap. If this gap is open, emitted infrared light triggers the transistors and electric current flow becomes possible; in case an opaque object is inserted in this gap, light transmission is interrupted and there will be no electric current flowing through the transistor. This process is similar to a switch turned on or off. On the mechanical side of the system, an encoder disc and a top dead center flag are connected to the flywheel of the engine, both of which pass through the gap of the optical sensor in each crank angle rotation. The encoder disc has 720 slits, meaning that the crank angle sensor will be triggered on and off 720 times in each rotation. The duration between two consecutive rising edges of sensor outputs is equivalent to 0.5 degrees of crank angle rotation. Top dead center flag interrupts the sensor once in every crank angle rotation, causing one digital on state per revolution. The top dead center sensor is positioned in such a way that its corresponding sensor creates the signal at the actual top dead center timing of the engine. A third flag is installed to the camshaft axis, which triggers the camshaft optical sensor once in every four cycles; however the output of this particular sensor is not used during the data processing stage; this component is required for the timer circuit to function properly. The generalized circuit diagram of the optical sensors is shown in figure 3.11. The circuit used in this work uses a generic 470Ω resistor for R1, another generic 10 KΩ resistor as the pull-up resistor R2, and a SG-206 photointerrupter made by Kodensha. The outputs of the sensors are connected to both the timer circuits and the data acquisition system. The use of the generated signals during data processing will be explained in chapter 4.
3.7.3. Data logger

The measurement made by the pressure sensor, crank angle, top dead center and injection timing signals are recorded by the data logger in this work. A Yokogawa DL750 ScopeCorder digital oscilloscope is used measuring and recording the pressure history data. This device is capable of measuring data from 16 separate channels; however only 4 channels were required in this work. This device is set to measure the signals at a sampling rate of 200 kilo samples per second (ksps) sampling rate during the work explained in chapter 5, and 100 ksps sampling rate during the work explained in chapters 6 and 7. Sampling period is set as 10 seconds; since the engine is operated at 1000 rpm engine speed throughout the work, which corresponds to 16.67 revolutions per second or 8.33 cycles per second, it is possible to record about 83 consecutive cycles under this setting. The results are always handled as a set of 80 cycles; therefore the presence of extra cycles ensures completeness of each data recording. After acquisition process and recording, the data is transferred to a PC for data analysis.

3.8. The timer circuit and auxiliary devices.

This work relies on precise control and parametric variation of all fueling parameters of the engine. A purpose built timer circuit and auxiliary devices answer for this need in this work. In order to simplify the process of changing fuel delivery parameters and sending trigger signal to the high speed camera, a TIME98 timing generator is used for synchronizing the engine position and output signals. Synchronization process requires two input signals: a trigger signal and a clock signal. The trigger signal is sourced from a combination

Figure 3.11: The generalized circuit diagram of photointerrupters.
of cam position and the top dead center sensors; both signals are converted to TTL level signals by passing through a 7414 hex inverter integrated circuit. In order to select the timing at which both of these signals rise, both are used as inputs of a 7400 TTL quad AND gate integrated circuit. When both signals are at digital level of 1, the AND gate of 7400 will produce the trigger signal. The other input, the clock signal, is produced by the cam angle sensor. The output of this sensor is rectified by passing through 7414 as well, and then used as inputs of a LM324 quad operational amplifier. This type of connection to an operational amplifier is typically used in driver circuits for improvement of signal quality, stability and noise reduction. The circuit provides 12 kHz of clock speed when the engine is operating at 1000 rpm. The circuit diagram of input signals are given in figure 3.12. Based on these signals, output signals are produced by the sequencer. TIME98 operates at TTL level signals, which is not suitable for operating an injector directly; therefore both the pilot fuel and the natural gas injectors have their dedicated injector drivers. Additionally, the length of the injection pulses can be changed at fixed intervals, which may not provide enough flexibility during adjustment of injection quantity. In order to add another level of flexibility to the adjustment of injection signals, the outputs of TIME98 are used as inputs of 74221 non-retriggerable monostable multivibrator integrated circuits. When triggered, 74221 can modify the length of the output signal, regardless of the input signal length. The duration of the output signal is a function of resistor and capacitor sizes; the pulse width is defined as f(ms)=0.7*R*C. The outputs of 74221 are connected to the relevant injector controller. If required, 74221 can be bypassed, which was the case for the experimental setup described in chapter 5. Circuit diagram of output signal conditioning stage is given in figure 3.13. TIME98 accepts the trigger signal as the start of a cycle and starts counting the crank angle signal inputs. Each crank angle corresponds to 0.5 degrees of crank angle rotation, and the counter increases until the value of 1440 at each cycle. Based on this system, the value of 720 is the top dead center position. The desired timings of both injection signals and camera trigger signal are adjusted on the scala from 0 to 1440 and sent to the device as the user input before starting its operation. Regardless of whether the engine is motored or halted, the timing generator does not send signals unless the process is started manually over the user interface on the computer. When the process start command is given, the timing generator reads the signal input and output parameters, based on which it performs its stand-alone operation. Please remember that it is not possible for the computer to control these signals using this device as an interface due to insufficient speed of the communication ports; therefore the stand-alone feature of this component is a key point. When the experimental data is collected and fueling needs to be stopped, the stop command is sent from the computer to the device. It is necessary to mention that, this approach also
requires attention in order not to send injection signals if the engine is not moving; injection of fuel at low engine speed is a well-known cause of mild-to-heavy knocking, which might cause damage to the engine.

Figure 3.12: Circuit diagram of TIME98 sequencer input signal conditioning.
Figure 3.13: Circuit diagram of TIME98 sequencer output signals and connection to auxiliary devices.
3.9. Exhaust gas analyzers

Exhaust emissions are measured using the combination of three devices: a Horiba MEXA 1170 HFD hydrocarbon gas analyzer, a Horiba PG240 exhaust gas analyzer and a Horiba MEXA 600-S opacimeter.

Dedicated hydrocarbon gas analyzer is categorized as a flame ionization detector. In this measurement process, concentration of unburned hydrocarbons during the decomposition process is correlated to the formation of hydrogen ions during in the exhaust gas stream. The device itself consists of flame ionization detector connected to a gas chromatography system, which requires constant stream of a test fuel, a sample gas and an air mixture of known composition. This device uses hydrogen as the fuel, a mixture of CH3, CH2 and CO as the sample gas and a synthetic air with 60% nitrogen, 39% oxygen and 1% argon in its composition. In order to ensure the precision of the measurement, the device is equipped with a heated sampling hose, which eliminates the possibility of precipitation of hydrocarbon species before the analysis is completed. In this experiment, the length of the sampling hose delays the measurement process for about 40 seconds; therefore this delay is compensated for during the data recording stage of the experiments.

The multi gas analyzer is capable of measuring NOx, carbon monoxide, carbon dioxide and oxygen concentrations. NOx measurement is based on chemiluminescence method; the reaction between NO molecule and ozone emits light, which is detected by a photo multiplier tube and converted to electrical voltage output. The output is proportional to the NOx concentration. In case of nitrogen oxides with more than a single oxygen atom, the molecules are introduced to a chemical reaction with carbon to reduce them to NO molecules. Carbon monoxide and carbon dioxide concentrations are measured by non-dispersive infrared absorption method. In this method, emission from an infrared light source passes through a filter, the measurement gas and the sample gas in a closed chamber, such as nitrogen. The sample gas absorbs certain wavelengths, according to Lambert-beer law. Attenuation of the absorbed light determines the concentration of the species. Oxygen measurement is performed in an electro-galvanic fuel cell. In this method, potassium hydroxide is placed between a lead anode and a gold plated cathode. When oxygen and potassium hydroxide come in contact, a chemical reaction occurs, producing electricity. Electrical current and oxygen concentration are proportional.
Opacimeter measures the amount of soot emissions based on the opacity of the exhaust gases. This device sends a light into a chamber of exhaust gases, and responds the returned light. The intensity of the returned light is compared to a reference intensity, typically taken during calibration process when the chamber is filled with clean air.

Exhaust gas samples are drawn from a chamber installed 3 meters downstream from the engine. In order to ensure that the exhaust gas temperature is suitably high, exhaust pipes are insulated. Measurement results are obtained from the displays of each individual device and recorded manually.

3.10. Imaging equipment and setup

The imaging setup consists of the high speed camera, metal-halide lamp, an optical lens, and the engine is required to be in visualization setup as explained in section 3.1.3. The outline of the imaging setup is shown in figure 3.14 and a picture of the actual setup is shown in figure 3.15. The in-cylinder images are captured by a NAC systems GX-1 high speed digital camera. This camera has a CCD type sensor, which is capable of measuring up to 100 kilo frames per second. In this device, there is a trade-off between the capturing speed and the frame size; therefore a higher capturing speed does not necessarily allow more detailed time series visualization. In order to correlate the time series images and the engine speed, it is decided to capture two images per one degree of crank angle rotation, which corresponds to 12 kilo frames per second speed, capturing images with dimensions of 412 pixels by 416 pixels. This is a reasonably fast recording speed and the images had sufficient level of detail. During the experiments, a Nikkor 50 mm f/1.2 lens is attached to the camera using the G-mount. Shutter of the camera is set to open intentionally, so that the maximum amount of light can be captured. The combination of a low f-number lens and removal of the exposure time limitation overcomes the problem of dimness of the images taken at high speed.

The work described in chapter 5 required the fuel sprays to be captured. Before combustion, fuel sprays do not emit light. One of the methods for capturing the sprays is providing external illumination by any light source. In this work, metal halide lamps are directed towards the combustion chamber through the visualization windows of the extended piston. This approach is chosen due to its simplicity. The background on the cylinder head is a dark color due to soot build-up. Fuel sprays are transparent yellow in their natural colors; when illuminated inside the combustion chamber, they appear in white color until they evaporate. It is not possible to detect the pilot fuel vapor with this particular approach; however the flame kernels emit read light emission during soot formation and blue light during combustion, the combination of which informs
about the extent of evaporation. Additionally, the intensity of the metal-halide lamp does not influence capturing of soot combustion; however it makes detection of weak blue flames harder. Image processing techniques are used in order to solve this issue, which will be explained in chapter 4.

Figure 3.14: Outline of the visualization setup.
Figure 3.15: The visualization setup.
4. Calibration of measurement devices, data acquisition and processing

4.1. Calibration of pressure data

The pressure sensor used in this work consists of a piezo crystal for pressure measurement, electrical charge of which is a function of the force applied on the crystal. The charge of the crystal is converted to electrical voltage by the charge amplifier. The charge amplifier is an off-the-shelf electrical component, characteristics of which need to be confirmed periodically. In our laboratory, pressure sensors are calibrated twice a year. During calibration, a dead weight tester is used for exerting known magnitudes of pressure on the pressure sensor. The pressure sensor is connected to the charge amplifier and the resulting voltage is always checked on DL750 data logger oscilloscope in order to keep measurement conditions similar. Pressures in the range of 0 to 18 MPa are tested in each calibration; In-cylinder pressure is known to reach or slightly exceed 16 MPa and the upper range of calibration pressure ensures that such conditions can be measured precisely as well. During a calibration session, testing starts at 0 MPa gage pressure, which is increased by 0.5 MPa intervals until 5 MPa gage pressure and 1 MPa intervals until 18 MPa. Once the peak calibration pressure is reached, the process is repeated by reducing the pressure down to 0 MPa gage pressure condition in order to confirm that the measurements are repeatable. At the end of measurement stage, measured pressure is correlated as a function of amplifier output voltage.

4.2. Calibration of natural gas flowrate.

Natural gas delivery system is designed for operation at various fueling conditions. Calibration of equivalence ratio depends on two parameters: intake air flowrate and the required equivalence ratio. Intake air flowrate is typically constant at a given supercharging pressure; using a different in natural gas flowrate does not change intake air flowrate measurably, unless the intake charge needs to be switched between a highly rich and lean one. When measuring natural gas flowrate, the natural gas accumulator is first filled from the tubes, after which the connection between the system and the fuel tubes is closed. At this point, the accumulator is the only source of natural gas. The combined volume of the accumulator, the buffer volume inside the high pressure regulator and the piping is 5.558 liters. Since the average pressure inside the accumulator in addition to the temperatures at the top and bottom regions can be measured at any time, the amount of natural gas can be obtained using the Benedict-Webb-Rubin equation of state. During the calibration process, the engine is fueled for about 60 seconds before the initial state of the accumulator is
recorded. After this, the state of the gas is recorded with 180 second intervals until the accumulator pressure drops below 1 MPa. This allows for around 12 consequent measurements depending on the desired equivalence ratio, if the accumulator was filled from a freshly connected gas tube with 11 MPa internal pressure. A high number of measurements allow confirmation of repeatability. After the pressure and temperature data is obtained and the change the amount gas inside the accumulator is determined, it is correlated to the air flowrate and timing intervals to obtain the equivalence ratio of the gas.

4.1.3. Calibration of amount of pilot fuel injection

As described in chapter 2, Pilot fuel injection system is equipped with a measuring pipette and strategically located valves that can turn on or off the pilot fuel flow into certain parts of the system. In this system, both the fuel supplied from the fuel tank and the returning fuel is connected on the low pressure diesel fuel line, which is fed to the high pressure fuel pump. A measuring pipette is also connected to this system, top side of which is used as a vent. The measurement pipette is also the accumulator of the system when the connection to the fuel tank is closed. Before the calibration process, the level of fuel inside the measuring pipette is the same as the fuel tank. Cutting the connection between the fuel tank and the system converts the measuring pipette into an accumulator. During calibration, the engine is fueled normally until the operation stabilizes. After the desired level of stability is ensured, connection to the fuel tank is closed. The measurement tube has markers for known amount of fuel volume. In this work, measurements were made over 1 ml of volume. Pilot fuel injection rate is correlated as:

$$m_{\text{inj}} = \frac{60nV_m\rho_{\text{diesel}}}{tN}$$  \hspace{1cm} (4.1)

where

- $m_{\text{inj}}$: injection quantity per cycle in milligrams
- $n$: stroke number, 2 for four stroke cycles
- $V_m$: measured volume of pilot fuel in milliliters
- $\rho_{\text{diesel}}$: density of diesel fuel
- $t$: the duration of measurement in seconds
- $N$: engine speed in revolutions per minute

If single injection strategy is applied using the 74221 multivibrator circuit, the duration of the signal is adjusted using the dedicated knob until the desired injection quantity is observed. Calibration of injection quantity is achieved by this method in the work described in chapters 6 and 7. If the signal duration is
controlled directly by the TIME98 as increments of the duration equivalent to 0.5 degrees of crank angle, two possible options are to design the experiment based on the achievable injection amounts or to change the injection pressure accordingly. Injection strategy in chapter 5 was designed around 0.3mg/cycle injection rate with 1.5°CA injection duration.

4.2. Continuous to cyclic data transformation

4.2.1. Recorded data file format

In-cylinder pressure, crank angle, top dead center and injection signals are recorded by Yokogawa DL750 Scopeorder data logger. In each session of performance tests, the engine is operated until the oil temperature stabilizes at 80°C, charge amplifier is reset and the engine is allowed to run for at least 10 seconds, during which the data is collected for recording. The screen on the data logger shows the properties of the complete range of all the signals ready for recording. When it is confirmed that the pressure data shown on the screen is a complete set, data logger is paused and the data is recorded. This device records the data in .wvf format, which is not native to any of the known operating systems. The manufacturer supplies the software required for conversion to known formats, such as a comma separated values format, which can be handled just like any file format native to excel. The converted files include several lines of device setting information, after which the actual data is given. In this file format, each channel is given in a single volume as a time series. When the device is set to work at 100 ksps sampling rate and record for 10 seconds, it records the values of slightly over one million sampling points. Charge amplifier output voltage, crank angle sensor level, top dead center sensor level and the injection signal sensor level and outputs of other connected measurement devices are given in a single row at a sampling point. In short, the file lists the data as a matrix with a size 1000199 rows and 4 columns.

4.2.2. Processing method of crank angle and top dead center signals

Crank angle and top dead center sensors circuitry are designed as standard digital circuits; however the on and off conditions are recorded simultaneously with the pressure sensor as analog signals. When handling these signals in a digital circuit, the values are thought to be either 5V during the state “1” and at the ground voltage level in state “0”. Since the data logger does not allow sampling of digital signals, both of these inputs needed to be recorded in analog mode. In analog sampling, the states are not clearly defined as on or off; even the shapes of the rising edges were measurable in the records. Additionally, the duration of on
or off states are of no concern for the analyses. In order to make the distinction, it was assumed that a voltage level of 0.5 V is the indicator of a rising edge, since the maximum possible level of an off state is lower than 0.3V, including the effect of signal noise. Once a rising edge is detected, its position on the time axis is recorded, after which the next rising edge was searched for. This process is applied for both top dead center timing and crank angle signals. As a result, only the rising edge of the signal is detected.

4.2.3. Determination of start of cycles and preparation of crank angle position data

It is known that a total of 167 top dead center signals are detected in each data record, which equates to at least 82 complete and 2 incomplete cycles in almost all cases. Since the engine is at the top dead center position twice in each cycle and camshaft position sensor is not recorded, start of a cycle is determined based on the pressure levels at each given top dead center signal timing. Pressure during intake stroke is always several times lower than the pressure at the end of compression stroke. Based on this knowledge, the first cycle starts from the timing of the second top dead center signal of a data set, is the pressure at the third top dead center signal timing is higher; otherwise the third top dead center is accepted as the start of the first full cycle.

Once starts of cycles are known, the list of crank angle timings can be prepared for 80 cycles. In this process, the crank angle signal that is the closest to the rising edge of top dead center signal is accepted as the reference point. After this, the data is shifted forward or backward as necessary: five crank angle signals are produced during the “on” state of the top dead center signal; it is essentially important to determine which one of these signals corresponds to the mechanical TDC timing. This decision is made based on the pressure characteristics of a motoring condition: the point of maximum pressure is the mechanical TDC timing, and the crank angle signal that is triggered at the timing closest to this point is designated as the actual TDC angle signal. This property never changes from an experimental session to another. In this study, this property is simulated by shifting back the timing by 1 degree of crank angle, or two crank angle signals. This point refers to 360 degrees before top dead center, and the following 1439 points belong to the same cycle. In general, 360 degrees after top dead center timing of a cycle is shared by the next cycle as its start. As a result, the crank angles are formatted into a matrix of 1441 by 80.

4.2.4. Cutting the time series pressure data into separate cycles
The crank angle matrix indicates precise locations of the pressure data in the time series by intervals of 0.5 degrees of crank angle. When the data is recorded at 100 ksp s sampling rate, each 0.5 degree of crank angle interval consists of 8 data points in average. In this work, pressure data is evaluated at a crank angle interval of 0.1, which means that 5 data points are required for each evaluation. At this point, it can be assumed that these 8 points are uniformly spaced. When handling the interval, pressure data is interpolated using these points. The final pressure data is in a matrix of 7201 by 80, the first data on each column referring to -360°CA, 3601’st data marking to TDC location and 7201’st data being the 360°CA position.

4.3. Filtering

The recorded pressure data consists of undesired instantaneous fluctuations due to a certain noise level introduced by the undesired charge deposition on the components or the signal conditioning electronics. Additionally, all data acquisition systems work at a specified level of analog-to-digital conversion resolution; if a signal level is at an uncertain level between two incremental conversion conditions, the least bit of the converted binary value might fluctuate between 1 and 0. This condition is described as least bit uncertainty. While it is not possible to eliminate these two undesired situations during data recording stage, it is possible to remove such characteristics from the data set using a set of filters. In contrast, inappropriate use of filters has negative impact on the quality data, such as extreme smoothness of the results, and eliminates valuable information on the characteristics of a measured signal together with the noise; therefore it is necessary to identify the right type of filter for each purpose and use with caution. This section introduces these filters and their intended uses.

4.3.1. Median filter

The digital representation of an analog signal fluctuates between a higher and a lower level, which is defined by the resolution of the analog-to-digital converter devices. If we assume that a device has a resolution of 10 bits for conversion of a voltage range of 0 to 10 volts, the smallest incremental step between two measurable voltage levels will be 9.76 mV; a time series record of a constant 5 V signal will fluctuate between 5.00976 V and 4.99024 V throughout the duration of measurement. This behavior can be minimized or completely removed when one dimensional version of median filter is applied. Median filter is based on comparing the values of a subset of the data and replacing the data point of concern with the median value of this range. When applying this filter, it is critical to choose an appropriate range for evaluating the median value; using an insufficiently short range of data as the subset for evaluation of the median value introduces
fluctuation of the recorded wave which does not exist in the unprocessed form, or using inappropriately long range of data for this purpose may shift the data or eliminate some of the valuable information. Quality and characteristics of the data needs to be confirmed before applying median filter. In this work, a median value filter of 11 point range is applied to the raw pressure data before further processing.

4.3.2. Moving average filter

Moving average filter is used for suppressing short term fluctuations in a data series in order to emphasize on the long term behavior. Similar to median filter, a subset of the data is used at each step of the method. In each step of the iteration, the average of a subset of the data with equal forward and backward range is assigned as the new value of a data point. It is formulated as:

\[ X_p = \frac{1}{2n+1} \sum_{i=-n}^{n} X_{p+i} \]

When a subset with an excessively long range is used, the resultant time series tends to be over-smoothed, masking intermediate term behavior. In this work, this filter is used in order to smooth the stepwise nature of the pressure history after applying median filter. In this work, correlation 4.1 is applied in a range of 5 consecutive data points, which equates to n=2.

4.3.3. Finite impulse response (FIR) filters

A finite impulse response filter is a digital signal processing method. In this method, a filter creates a signal response based on an impulse for a finite period of time. The impulse is one data point on the discrete time series, which creates a response with a length of N+1 for a discrete-time filter of size N. The output of a filter with a window size of N is the weighted sum of N+1 consecutive input values, which is mathematically described as:

\[ y[n] = b_0x[n] + b_1x[n-1] + \cdots + b_nx[n-N] \]

Where \( y[n] \) is the response, \( b_k \) is the impulse response of the filter at k'th instance, \( x[n] \) is the input signal. FFT filter works on the frequency domain; therefore the input signal needs to be converted to the frequency domain through Z-transform. In these filters, the values of \( b_i \) are correlated, typically denoted as \( h(k) \), and the inputs are evaluated as a series of Kronecker delta functions, such as \( x(n) = \delta(n) \). The impulse response of the filter \( h(n) \) can written as:
\[ h(n) = y(n) = \sum_{k=0}^{N-1} b_k \delta(n - k) \]

In frequency domain, this correlation is given as:

\[ Y(k) = H(k)X(k) \]

where \( k = \frac{2\pi k}{N} \). It is possible to perform the filtering on both time and frequency domains; the latter is used in this work. When handling the process in time domain, a time series representation of the frequency response is obtained by reverse Fourier transformation, which provides the coefficients \( b_k \); the result of convolution of \( b_k \) and \( x(n-k) \) is the \( n \)'th value of the filtered time series.

In this work, low pass and band-pass FIR filters are used. An ideal low-pass filter evaluates the signal in frequency domain; if the frequency is below the predetermined threshold, filter output is 1; otherwise the filter output is zero. Similarly, output of a band-pass filter is unity if the input is within the pass-band frequency. Additionally, when using a pre-recorded data set, it is possible to locate the data point at the center of the window, which is the approach used in this work. This approach causes a time shift of \( N/2 \) points on the time axis, which can be adjusted at the end of the application. Time domain representation of a low-pass filter is described as:

\[ h(i) = \frac{\sin(n\Omega_c)}{\pi n} \]

And a band-pass filter is defined as:

\[ h(i) = \frac{\sin(n\Omega_{c,h}) - \sin(n\Omega_{c,l})}{\pi n} \]

In both equations 4.6 and 4.7, \( \Omega_c \) is called the cutoff frequency; subscripts h and l indicate high and low limits of the band-pass frequency range in a band-pass filter. \( N \) refers to the \( n \)'th data point in a filter size \( N \); the index \( n \) starts from 0. Cut-off frequency ranges from 0 to \( \pi \) and formulated as

\[ \Omega_{c,h} = \pi \frac{f_{\text{pass}}}{f_{\text{samp}}} \]

In this correlation, the pass-band frequency \( (f_{\text{pass}}) \) or frequencies are correlated to the sampling frequency \( (f_{\text{samp}}) \).
4.3.4. FIR filter windowing and Dolph-Chebyshev window

A certain shortcoming of FFT filters is their behavior in the transition band range; frequency response of the filter to the impulses in the vicinity of the cut-off frequency has ripples. While it is not possible to eliminate the ripples completely, it is possible to reduce them using windowing techniques. This approach readjusts the frequency response in a way that it reduces the attenuation of unwanted ripples. In this work, Dolph-Chebyshev window is applied to the filter. In this window type, pass- and reject bands can be defined based on the demands of the application. Dolph-chebyshev window is defined on the time domain as:

\[ w(n) = \frac{1}{N} \left\{ \frac{1}{r} + 2 \sum_{n}^{N-1} T_{N-1} \left( x_0 \cos \left( \frac{i\pi}{N} \cos \left( \frac{2\pi n}{N} \right) \right) \right) \right\}, \quad n = 0 \ldots (N - 1)/2 \]

Where \( x_0 \) is

\[ x_0 = \cosh \left( \frac{1}{N - 1} \cosh^{-1} \left( \frac{1}{r} \right) \right) \]

\( T_n(x) \) is the Chebyshev polynomial of the first kind, which is defined as

\[ T_n(x) = \begin{cases} \cos(n \cos^{-1}(x)), & |x| \leq 1 \\ \cosh(n \cosh^{-1}(x)), & |x| \leq 1 \end{cases} \]

And \( r \) is band-pass bandpass ripple, correlated to the attenuation (A) as

\[ \frac{1}{r} = 10^{\frac{A}{20}} \]

A is selected based on the requirements; in this work, attenuation is selected as -160 in order to suppress the ripples as much as possible.

4.3.5. Savitzky-Golay filter

A savitzky-Golay filter, named after its publishers Abraham Savitzky and Marcel J.E. Golay, is a digital filter used for smoothing data by convolution process; a time series data is used for fitting a low degree polynomial by linear least squares method. During application, the least square method is repeated for each data point; therefore this filter has higher computational demands compared to other filter types mentioned so far. This filter is best suited for a signal with high noise intensity; signal-to-noise ratio can be improved significantly
without distorting the data. This method tends to over-smooth the data; therefore it was used only for smoothing the pressure data from the end-of combustion to the exhaust valve opening timing range in order to obtain a reasonable mass fraction burned profile.

4.4. **Specifics of the procedures for determination of performance characteristics**

4.4.1. **Numerical differentiation and integration**

Numerical differentiation is used for estimating derivative of a function when the values of the function are known at equally spaced intervals. In this work, 4'th order finite difference method is used, which correlates derivative of a point in a data series with respect to crank angle as given in equation 4.13.

\[
\frac{dx_n}{d\theta} = \frac{1}{\theta_n - \theta_{n-1}} \left( \frac{x_{n-4}}{280} - \frac{4x_{n-3}}{105} + \frac{x_{n-2}}{5} - \frac{4x_{n-1}}{5} + \frac{4x_{n+1}}{5} - \frac{x_{n+2}}{105} + \frac{4x_{n+3}}{280} \right) \tag{4.13}
\]

This procedure is used wherever derivative of pressure is required in a correlation, such as rate of heat release and temperature of the unburned mixture. Finite difference of crank angle (\(\theta\)) is constant throughout the process. Derivatives of other parameters, such as cylinder volume, are numerically correlated to crank angle; such parameters are differentiated by symmetric difference quotient as given in equation 4.14.

\[
\frac{dx_n}{d\theta} = \frac{x_{n+1} - x_{n-1}}{\theta_{n+1} - \theta_{n-1}} \tag{4.13}
\]

Unlike numerical derivation, numerical integration is not influenced by local fluctuations of the data. Additionally, integration procedure was applied in a short interval; which ensures that the numerical error is negligible. Trapezoidal rule is defined as:

\[
\int_{a}^{b} f(x) \, dx = (b - a) \left( \frac{f(b) + f(a)}{2} \right) \tag{4.13}
\]

4.4.2. **Rate of heat release and mass fraction burned (MFB)**

Formulation of rate of heat release was described in chapter 2, equation 2.18. In the analysis code written in the laboratory, the numerical procedure includes the following equations in a loop:
\[ \frac{\Delta P_n}{\Delta \theta} = \frac{1}{\Delta \theta} \left( \frac{P_{n-4}}{280} - \frac{4P_{n-3}}{105} + \frac{P_{n-2}}{5} - \frac{4P_{n-1}}{5} + \frac{4P_{n+1}}{5} - \frac{P_{n+2}}{105} + \frac{4P_{n+3}}{280} \right) \]  

4.14a

\[ \text{ROHR}_n = \frac{k}{k-1} p \frac{V_{n+1} - V_{n-1}}{\Delta \theta} + \frac{1}{k-1} V_n \frac{\Delta P_n}{\Delta \theta} \]  

4.14b

In this equation, \( k \) is the specific heat ratio; specific heat ratio is assumed constant at intake conditions amongst engine researchers. The unit of ROHR is Joule per degree of crank angle (J/°CA). It should be noted that the amount of gas inside the cylinder is constant only from the intake valve close to exhaust valve open timing range; therefore any timing outside this range does not comply with conservation of mass criterion and ROHR can’t be obtained for these intervals. In this work, ROHR is obtained from pilot fuel injection to exhaust valve open timing range. Mass fraction burned is obtained in this interval by integrating ROHR with respect to crank angle timing.

4.4.3. Unburned mixture temperature

The temperature of the in-cylinder mixture can be obtained using the correlations of polytropic process until start of combustion, after which this correlation will give the average temperature of the burned and unburned mixture. An alternative correlation is suggested by Livengood et.al, which is known as velocity of sound correlation. This correlation eliminates the dependency on the volume; when obtaining the temperature, it is critical that the exact amount of unburned mixture and its volume is required, which is not possible to estimate within reasonable accuracy. Instead, this correlation uses the density, pressure and speed of sound at given conditions for obtaining the temperature. It is a plausible assumption that both pressure and density will be reasonably uniform inside the cylinder. The correlation is given as:

\[ T = \frac{mc^2}{kR} \]  

4.15

In this equation, \( c \) refers to the velocity of sound at a given condition. When calculating temperature of air, in-cylinder mixture is treated as a real gas. Velocity of sound in a real gas is described as:

\[ c = \frac{K_s}{\sqrt{\rho}} \]  

4.16
Where $K_s$ refers to the bulk modulus of air at a given pressure, which can be obtained from the following equation:

$$K_s = -V \frac{dP}{dV}$$ \hspace{1cm} \text{(4.17)}$$

Unfortunately, this correlation is valid until start of combustion, because in-cylinder mixture conditions are never uniform from the start of combustion until the end of heat release. As an alternative solution, bulk modulus value of the in-cylinder mixture is obtained in the range from intake valve close timing to the start of combustion; bulk modulus of the unburned mixture is obtained by extrapolation of the prior conditions. Unburned mixture temperature is used for determining constant temperature ignition delay of end-gas regions, which was used in Livengood-wu integral method.

**4.4.4. Determination of end-gas autoignition timing by Livengood-Wu integral method**

Many constant pressure and temperature ignition delay studies have shown that ignition delays of fuels under given conditions can be correlated as an Arrhenius type equation. Livengood et.al. suggested that these correlations can be used for determining instantaneous pre-ignition reaction completion rates in an internal combustion engine. These values can be integrated until the result of integration reaches at 1, which indicates that the reaction is completed. The autoignition condition is described as:

$$\left( \frac{x}{x_c} \right) = \int_{t=0}^{t=t_c} \frac{dt}{\tau} = 1$$ \hspace{1cm} \text{(4.17)}$$

where $\tau$ refers to constant condition ignition delay of the air-fuel mixture. In recent years, constant pressure and temperature ignition delay correlations include additional parameters, such as equivalence ratio or molar fraction of reactants. This method was used in order to confirm whether the end-gas combustion activity is autoignition in nature.

**4.5. Image processing**

**4.5.1. Image recording and conversion**

The high speed camera used in this work is operated at frame speed of 12000 frames per second. Since the image is captured at a speed at which it is impossible to record the data to a hard drive; therefore
the camera uses built-in random access memory to store the video. After capturing, the video is downloaded to a hard drive in .mcf format, which allows changing camera settings even after capturing process. When the properties of the images are adjusted as required, it is exported as a sequence of .jpg images. In order to maximize the amount of information available in the images, jpeg compression is set to 0.

An image file consists of a three dimensional array as the relevant data; red, green and blue channel values of a pixel on 8 bit scale are given for all pixels in this array. Frame size of the captured images are 412 pixel by 416 pixel in this work; therefore each image visually represents a three dimensional matrix of 412x416x3 size. The entries on the third dimension from 1 to 3 refer to red, green and blue channels respectively.

4.5.2. Background subtraction

In-cylinder images were affected by undesired markings due to soot particle accumulation on the imaging window, known scratches and defects on the cylinder head, unwanted illumination around the valves, injector and inhomogeneity of the light source. Additionally, a high illumination level can also make it challenging to detect blue flames. In order to eliminate undesired characteristics of the images, background subtraction method was utilized. In this method, a reference image is captured before pilot fuel injection. The red, green and blue values of this image are subtracted from those of all following images. This method eliminates aforementioned background artifacts, which contains information on neither fuel delivery nor combustion characteristics. The leftover image mostly contains the desired characteristics.

4.5.3. Noise removal by median filter

After background removal, a small amount of salt-and-pepper noise is left in the images. The most commonly utilized method for removing such noises is the median filter, which replaces red, green and blue values of a cell by the median value of neighboring area. The size of the filter is selected by the user; however utilization of unsuitably large median filter results in saturation of edges in the image.

4.5.4. Image derivation

Image derivatives are calculated by using small convolution filters, such as a Sobel mask, Hast derivatives or Farid and Simoncelli derivatives. Generally, a larger convolution kernel gives a better
approximation of the derivatives, such as Gaussian filter. In this work, Farid and Simoncelli derivatives with a 7x7 kernel size was used. Farid and simoncelli convolution constants are given as;

\[
k = [0.004711 0.069321 0.245410 0.361117 0.245410 0.069321 0.004711];
\]
\[
d = [0.018708 0.125376 0.193091 0.000000 -0.193091 -0.125376 -0.018708];
\]

These arrays are used as the filter constants in a two dimensional convolution with the actual image. The resulting derivatives of the image usually require intensification of red, green and blue channels, which are multiplied by a factor of 5 for amplifying the values to a visible level.

5.1. Motivation

The research on characteristics of combustion in a dual fuel engine has been under investigation in our laboratory, and many important discoveries are made [87-95]. In these experiments, the main concern has been reduction the dependence on the pilot fuel; in order to realize this objective, a special injector nozzle with three orifices of less than 100μ diameters were used, which allowed reducing the energy contribution of diesel fuel below 2% mark when necessary [94]. This has also provided the conditions required for achievement of end-gas autoignition without knocking, which is named as PREmixed Mixture Ignition in the End-gas Region (PREMIER) combustion. So far, the effects of pilot fuel injection rate, equivalence ratio, use of EGR at different rates are investigated for different types of gaseous fuels. These studies have proven that PREMIER combustion can be implemented in a production engine, provided that certain issues can be solved. One of such issues is the limited operation range of the engine in PREMIER combustion mode. While it is possible to operate the test engine in this combustion mode by changing the injection timing by 1 or 2 degrees of crank angle from a certain base injection timing that is specific to the operating conditions and the fuel type, this may be inadequate considering the variety and intensity of cycle to cycle variations that occur in production engines. In order to overcome this challenge, it is necessary to have a better understanding of the PREMIER combustion mechanism and investigate the possibility of more advanced combustion control strategies. Autoignition of the end-gas autoignition depends on the combustion activity prior to its occurrence; therefore it is necessary to have a better control over the combustion activity from the beginning to the end. In pilot fuel injected dual fuel engines, start of combustion and flame kernel formation is one of the parameters that strongly influence the overall qualities of the combustion activity. One of the methods suggested to improve the control on flame kernel formation is use of split injection strategy [62]. In this work, the possibility of use of split fuel injection strategy as a means to widen PREMIER combustion operation range is evaluated, and the underlying mechanism is investigated based on engine output and in-cylinder visualization.
5.2. Specifics of the experimental setup, test procedure and data analysis

Outline of the performance test and visualisation experimental set-ups are shown in figure 5.1. The equivalence ratio selected for this experiment is 17.0:1 for both performance and visualization tests. During the performance tests, the metal engine is equipped with the shallow dish piston optimized for the selected compression ratio and the cylinder head gasket of 1.0mm thickness, as explained in Section 3.1.2 and figure 3.2. Natural gas was selected as the primary fuel only in performance tests; visualization experiments were carried out without addition of gaseous fuel, because at the time of the study it was not tested and confirmed whether the visualization components were strong enough to withstand the forces that will be applied during power tests. Intake pressure was 101.3 kPa; intake temperature was 40°C throughout the work. The combined equivalence ratio the gaseous fuel and the pilot fuel is set to 0.6 in power tests. Injection timing in the single injection experiments, and also both first and second injection timings in split injection experiments are varied as necessary, which will be discussed later. During the visualization tests, a metal halide lamp is utilized for illumination of fuel sprays prior to combustion. The experimental specifics of the test setup are given in table 5.1.

<table>
<thead>
<tr>
<th>Table 5.1: Configuration of the test engine and operating conditions</th>
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<tbody>
<tr>
<td>Bore x Stroke</td>
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<tr>
<td>Compression ratio</td>
</tr>
<tr>
<td>Piston type</td>
</tr>
<tr>
<td>Engine speed</td>
</tr>
<tr>
<td>Intake pressure</td>
</tr>
<tr>
<td>Equivalence ratio</td>
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<tr>
<td>Fuel delivery</td>
</tr>
<tr>
<td>Injection pressure</td>
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</tbody>
</table>
Figure 5.1: Experimental setup of (a) performance experiments and (b) visualization.
Natural gas is supplied at a rate of 26.7 mg/cycle in performance tests. The diesel fuel injection rate ($m_{inj}$) was 0.6 mg/cycle in both single and split injection experiments, corresponding to 2% of total energy input. This was decided based on system limitations; the minimum repeatable injection rates were 0.3 mg/cycle with 1.5°CA injection signal duration and 0.6 mg/cycle with 2°CA injection signal duration. Injection timing refers to the timing that the actuation signal is sent to the injector. The pilot fuel injector had a delay time of between 1.5 and 2°CA from the rising edge of the injection signal to the delivery of fuel. In single-injection experiments, injection timing ($\theta_{inj}$) was varied from 6°BTDC to 3°BTDC. In split-fuel injection experiments, the first injection timing ($\theta_{1}$) was varied in the range of 6°BTDC to 3°BTDC and the second injection timing ($\theta_{2}$) was varied from 3.5°CA after the first injection to $\theta_{2} = 15°$ATDC. Fuel supply strategies are tabulated in Table 2.

<table>
<thead>
<tr>
<th>Table 5.2: List of fuel delivery strategies</th>
</tr>
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<tbody>
<tr>
<td>Single</td>
</tr>
<tr>
<td>$	heta_{inj}$</td>
</tr>
<tr>
<td>Performance</td>
</tr>
<tr>
<td>5</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>3</td>
</tr>
<tr>
<td>Imaging</td>
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<tr>
<td>5</td>
</tr>
<tr>
<td>4</td>
</tr>
<tr>
<td>3</td>
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<tr>
<td>0.3</td>
</tr>
</tbody>
</table>

In this engine, pressure oscillations at 6.5 kHz, 10.5 kHz and 14 kHz frequencies are observed during knocking, and the pass-band frequencies of the FFT filters are selected accordingly [41]. A 4-20 kHz band-pass filter is applied to pressure history and the instantaneous differences are evaluated in order to obtain to
obtain knocking intensity. A low-pass filter with 6.5 kHz pass-band frequency was applied to the pressure history separately in order to obtain ROHR and performance characteristics. As an initial approach of systematic classification of operating conditions, it is decided that PREMIER combustion operating condition needs to exhibit end-gas autoignition in more than 50% of its cycles without knocking. When at least one knocking was observed within a data set, then that operating condition was classified as knocking. In absence of end-gas autoignition, the operating condition is a normal combustion. Pressure histories and rates of heat release are presented as averages of 80 consecutive cycles in the figure, unless labeled as “one cycle”. Pressure histories and rate of heat release characteristics of knocking conditions are represented by a single knocking cycle, having the closest pressure history and ROHR characteristics to the 80-cycle average. All engine performance characteristics derived from the pressure history and rate of heat release are presented as averages of 80 consecutive cycles. Performance tests were performed without imaging parts, due to their fragile nature under heavy load conditions. The engine has enough clearance to avoid spray and piston surface interaction at given injection timings; therefore flame kernel behaviour is expected to be similar in both performance and visualization experiments.

In this work, injection timing refers to the timing of the injection signal. The pilot fuel injector had a delay time of between 1.5 and 2°CA from the rising edge of the injection signal to the delivery of fuel. In single-injection experiments, injection timing ($\theta_{inj}$) was varied from 6° before top dead centre (°BTDC) to 3°BTDC. In split-fuel injection experiments, the first injection timing ($\theta_1$) was varied in the range of 6°BTDC to 3°BTDC and the second injection timing ($\theta_2$) was varied from 3.5°CA after the first injection to $\theta_2 = 15°$ATDC (after top dead centre). Fuel supply strategies are tabulated in Table 2.

The difference of combustion chamber geometry, lack of natural gas and difference of combustion chamber materials and the temperature of the engine components are common reasons for reduced in-cylinder temperature and pressure during visualization experiments. These differences will extend the ignition delay duration of the pilot fuel, due to which the flame kernels captured during visualization will possibly be larger; however the results of the visualization experiments are evaluated as clues that explain the effect of second injection timing, which can conceptually be applied to both situations within a reasonable degree of similarity. The cylinder was illuminated by metal halide lamps through visualization window of the extended piston in order to detect the spray patterns, and the image was reflected to the camera by a mirror. The reflection of light from the engine components does not affect the image quality, because they are concentrated outside the sapphire window boundaries. In-cylinder images were captured using a high-speed
camera at 12 kfps frame rate, which corresponds to two frames per crank angle. The first image of the sequence is captured at $\theta = 10^\circ$ ATDC and used for noise removal in background subtraction method. In addition, blue channels were not strong enough to distinguish the flame structure from the leftover; thus, Sobel mask is applied to the image in order to detect the boundaries of flame structures. The background images, the original images and the first derivatives after background subtraction are shown in Figure 2. The white circles in the processed images indicate the boundary of the sapphire window. Additionally, the flame kernels and fuel sprays are hard to distinguish in several images; therefore flame kernels are indicated in yellow circles and spray locations are indicated using small arrows. Additionally, raw image sequences are presented in figures 5.18-5.21 at the end of the chapter following the conclusions section.

Figure 5.2: Examples of background images, in-cylinder images and the first derivatives derived after background subtraction.

5.3. **Engine performance in single injection mode**

5.3.1. **Pressure history and rate of heat release**

Pressure history and ROHR of normal combustion, PREMIER combustion, and knocking operations with single injection are presented in figure 5.3. Both pressure history and ROHR of a single typical cycle are given for
only $\theta_{inj} = 6^\circ$BTDC to show the indicators of knocking clearly. In dual fuel combustion with pilot fuel injection, autoignition of the pilot fuel creates flame kernels and trigger flame propagation in the homogeneous gaseous fuel and air mixture. The rest of the in-cylinder mixture is consumed by the propagating flames. When the injection timing is sufficiently advanced, heat release from the propagating flames increase the in-cylinder pressure and provide the conditions for occurrence of autoignition in unburned mixture regions before being consumed by propagating flames. The strength of the end-gas autoignition is the factor that decides whether the cycle is knocking or PREMIER combustion operation. The difference between these two phenomena is distinguishable by the difference in pressure histories. If a cycle shows a rapid pressure rise and unwanted pressure oscillations that is detectable as audible knocking sound, it is a knocking cycle. Knocking is known to cause damage to the internals of the engine and must be avoided in practical engines. In contrast, PREMIER combustion occurs as a precursor to knocking, but the pressure rise is not as steep as in knocking and it does not have any pressure oscillations; therefore it does not have any drawbacks regarding its use. Unfortunately, PREMIER combustion occurred in a very limited operating range, only with the injection timing of $\theta_{inj} = 5^\circ$BTDC under the given operating conditions. Thus, the operation mode spanned from normal operation to knocking combustion when the injection timing advanced 2°CA from $\theta_{inj} = 4^\circ$BTDC to $\theta_{inj} = 6^\circ$BTDC.

Figure 5.3: Typical pressure histories and rates of heat release of normal combustion, PREMIER combustion and knocking operation.
5.3.2. Engine performance and operation stability

Indicated mean effective pressure and thermal efficiency are indicators of engine performance; results with higher numbers indicate a more efficient energy conversion at a given operating condition. Coefficient of variation of the indicated mean effective pressure (COV(P\text{mi})) is the indicator of operation stability; Comparatively, a more stable operation will show less variation of engine output on a cycle-to-cycle basis. These three characteristic of single injection operation are given in figure 5.4. The indicated mean effective pressure increased from $P_{\text{mi}} = 715$ kPa to $P_{\text{mi}} = 833$ kPa and thermal efficiency improved from $\eta_i = 41.7\%$ to $\eta_i = 48.6\%$ when the injection timing of $\theta_{\text{inj}} = 3^\circ\text{BTDC}$ was advanced to $\theta_{\text{inj}} = 6^\circ\text{BTDC}$. The highest performance characteristics are observed during knocking operation; therefore they do not represent a feasible condition. The indicated mean effective pressure and thermal efficiency observed during PREMIER combustion operation at $\theta_{\text{inj}} = 5^\circ\text{BTDC}$ were $P_{\text{mi}} = 809$ kPa and $\eta_i = 47.2\%$, both of which are significant improvements from $P_{\text{mi}} = 751$ kPa and $\eta_i = 43.8\%$ under normal combustion operation at $\theta_{\text{inj}} = 4^\circ\text{BTDC}$. This is a result of a combination of two scenarios: when combustion is triggered earlier, a larger fraction of the heat is released earlier, yielding a higher in-cylinder pressure. A higher fraction of the result can be converted to volumetric work during the expansion stroke. Secondly, end-gas autoignition occurs rapidly, consuming the in-cylinder mixture even faster and earlier, supporting the aforementioned scenario. The significant increase of both performance parameters indicate that the contribution of end-gas autoignition is indeed important. In addition, the stability of the engine output is performed as well. The lowest cyclic variation of engine performance is observed as less than 1\% in knocking operating condition. The coefficient of variation of indicated mean effective pressure in PREMIER combustion operating condition is in the vicinity of 1.5\%, which is superior to both normal combustion operating conditions tested in this work. Typically, a higher engine output yield more stable operation in internal combustion engines; therefore it is hard to determine whether occurrence of end-gas autoignition is a significant contributor to the improvement of the stability as observed in figure 5.4(c), or advancement of injection timing is the main factor. Comparing the characteristics of indicated mean effective pressure and its coefficient of variation, it can be suggested that occurrence of end-gas autoignition indeed affects the outcome; however a dedicated scientific study is required in order to come to a decisive conclusion.
Figure 5.4: Engine performance and operation stability with single injection: (a) indicated mean effective pressure, (b) thermal efficiency and (c) coefficient of variation of indicated mean effective pressure.
5.4. Effect of split injection on engine performance and operation range of PREMIER combustion

5.4.1. Pressure history, rate of heat release, and fraction of PREMIER combustion cycles

Pressure histories and rate of heat release characteristics of both single and split injection at $\theta_{inj} = 6^\circ$BTDC, $\theta_{inj} = 5^\circ$BTDC, $\theta_{inj} = 4^\circ$BTDC, and $\theta_{inj} = 3^\circ$BTDC are given in Figure 5.5(a) to 5.5(d) respectively. A wide range of second injection timings are tested for each first injection timing; the high number of data is not suitable for showing in a single graph because the results of some cases overlap; When such cases are encountered, only one representative set of the resembling pressures and rate of heat release characteristics are shown while the remaining ones are omitted. First of all, the effect of the first injection timing on engine output and heat release characteristics were similar for both single- and split injection experiments. Secondly, both in-cylinder pressure and rate of heat release showed significant levels of variation when the second injection timing is changed. Thirdly, the timing of the first injection has a more substantial influence on these characteristics compared to the second injection. Focusing solely on the effect of second injection timing, it can be seen that the pressure level of $\theta_{inj} = 6^\circ$BTDC/2.5$^\circ$BTDC was lower than the pressure level observed in $\theta_{inj} = 6^\circ$BTDC single injection. In contrast, this parameter was higher in $\theta_{inj} = 6^\circ$BTDC/1$^\circ$BTDC. It is known that the second injection timing in both cases were in the vicinity of autoignition timing of pilot fuel. Similarly, many cases in $\theta_{inj} = 4^\circ$BTDC and $\theta_{inj} = 3^\circ$BTDC split injection experiments had the same relation between the second injection timings and autoignition timings of their first injections. This observation is an indicator of a possible interaction between the second sprays and the flame kernels formed by the first sprays, and the autoignition timing of the latter decides whether or not the combustion activity will be faster. Another interesting phenomenon is observed for the cases with later second injection timings, which yielded a lower in-cylinder pressure and a slower heat release. This behavior is particularly clear for the second injection timing of $\theta_2 = 5^\circ$ATDC in $\theta_{inj} = 5^\circ$BTDC and $\theta_{inj} = 3^\circ$BTDC experiments. Two different scenarios can be suggested at this stage: the second spray might reduce the in-cylinder temperature for a certain duration and retard the heat release before its combustion, or it might change the combustion characteristics. In either case, it is safe to assume that the second spray interacts with the flames in an unusual manner, and the second injection timing of $\theta_2 = 5^\circ$ATDC might be the third critical timing. The clues of these assumptions will be searched in the in-cylinder images.
Figure 5.5: Pressure histories and rate of heat release characteristics of all experimental conditions with first injection timings of (a) $\theta_{inj}=6^\circ$BTDC, (b) $\theta_{inj}=5^\circ$BTDC, (c) $\theta_{inj}=4^\circ$BTDC, (d) $\theta_{inj}=3^\circ$BTDC.
The number of cycles with autoignition within an 80-cycle data set, and the corresponding percentage are obtained for each test condition and given in figure 5.6. The distinction between normal combustion and PREMIER combustion operating condition is made based on the results shown in this figure. In the conditions with typically low performance characteristics, end-gas autoignition may not be present in all conditions; the conditions with higher average engine output tend to have higher number of cycles with end-gas autoignition. Under the guidance of this knowledge, persistence of end-gas autoignition is chosen as the criterion for classification of an operating condition as PREMIE combustion. While the transition from normal- to PREMIER combustion has not yet been studied, the 50% threshold is chosen in this study. One of the reasons for this particular threshold value is the trend that this particular parameter changes: it is observed that the conditions with more than 50% end-gas autoignition cycles tend to be significantly over the threshold, with the exception of θᵢnj = 5°BTDC/5°ATDC. Secondly, the conditions that can’t meet this condition seem to preserve this particular characteristics throughout the second injection timing scale, except when a certain number of conditions are improved. Finally, 50% is a logical threshold value, which means that “more than half of the cycles have end-gas autoignition”. The results indicate that the lowest number of cycles with end-gas autoignition in single injection experiments are θᵢnj = 4°BTDC and θᵢnj = 3°BTDC cases, both of which had both lower in-cylinder pressure levels and performance characteristics. In contrast, all 80 cycles of θᵢnj = 6°BTDC and θᵢnj = 5°BTDC cases had end-gas autoignition; however the prior does not represent a usable condition due to knocking. When split injection strategy was applied, higher levels of in-cylinder pressures, better performance characteristics and quicker heat release were achieved with θᵢnj = 4°BTDC and θᵢnj = 3°BTDC. Based on the theoretical approach to heat release from propagating flames, it can be suggested that the observed improvement is a result of bigger flame kernels, due to which propagating flames can consume the mixture earlier. Another important observation that can be made from this figure is an unexpected reduction in the number of cycles with end-gas autoignition when the second injection timing is set as θ₂ = 5°ATDC; these were the lowest numbers in θ₁ = 5°BTDC and θ₁ = 3°BTDC, and the second lowest in θ₁ = 4°BTDC split injection experiment groups. The lowest number of end-gas autoignition cycles observed with the second injection timing of θ₂ = 5°ATDC also coincides with the lowest in-cylinder pressure levels in their respective data groups. The only exception was θ₁ = 6°BTDC; the number of cycles with end-gas autoignition never fell below 90% level throughout the second injection timing range; however it was possible to reduce the pressure levels and keep heat release characteristics under control. It can be suggested based on the agreement between these two parameters that a certain range of second injection timings decelerate or retard heat release substantially.
 Presence of end-gas autoignition is an indicator of either knocking or PREMIER combustion, and it is critical to make the distinction correctly. Knocking is undesirable due to its destructive nature. In addition, knocking is typically accompanied by in-cylinder pressure fluctuations, rapid pressure rise and significantly high levels of maximum in-cylinder pressure. In-cylinder pressure fluctuations mimic a cyclic structural load, the rapid pressure rise is equivalent to an impact, and unwantedly high in-cylinder load may yield to loading the engine components beyond their structurally allowable load limits. In order to discuss the difference between knocking and PREMIER combustion, knocking intensities and the maxima of in-cylinder pressures are given in figure 5.7. Knocking intensity is obtained from the in-cylinder pressure: a band-pass filter of with passband range of 4-20 kHz is applied to the pressure history, which eliminates the common characteristics of the cycles but removes the abnormalities, such as noise and the aforementioned in-cylinder fluctuations. On the next step, the difference between the levels of two consecutive peaks are obtained for the combustion period, the highest of which is chosen as the knocking intensity (KI). This method is suggested by Leppard [101]. It is observed that knocking intensities up to 0.1 MPa can be observed during motoring operation due to the noise level; any knocking intensity above this threshold is considered knocking. Based on this assumption, it is clear that $\theta_{inj} = 6^\circ$BTDC and the first three cases of split injection at $\theta_1 = 6^\circ$BTDC were above this threshold by a significant amount. The rest of the cases did not show any signs of knocking. The
conditions with significantly high knocking intensities also had the highest in-cylinder pressure records of all conditions. These four cases are labeled as knocking in the results.

Figure 5.7: Distinction of PREMIER combustion from knocking: (a) Knocking intensities and (b) maxima of in-cylinder pressures.
5.4.2. Engine performance and operation stability

Indicated mean effective pressure, thermal efficiency, and operation stability of both single and split injection operating conditions are presented in figure 5.8. The results showed that it is possible to suppress knocking with the first injection timing of \( \theta_{\text{inj}} = 6^\circ\text{BTDC} \); however, the range of the second injection timings is limited at TDC at the advanced end. While the highest indicated mean effective pressure and the thermal efficiency of knocking is higher than those of PREMIER combustion, the margin is not noticeably high; therefore, it can be stated it was possible to increase the engine performance characteristics to the levels that were previously observed during knocking operation. This trend continues until the second injection timing of until \( \theta_2 = 5^\circ\text{ATDC} \); however, further retardation of the second injection timing causes deterioration of engine performance. A similar trend was observed in the experimental group of \( \theta_1 = 5^\circ\text{BTDC} \), but the deterioration was observed earlier, at \( \theta_2 = \text{TDC} \), after which the performance characteristics plunge to the lowest value of their group at \( \theta_2 = 5^\circ\text{ATDC} \) and recover with even more retarded second injection timings. PREMIER combustion was not possible with single injection at \( \theta_{\text{inj}} = 4^\circ\text{BTDC} \); however, using split injection strategy with a second injection timing range of \( 1.5^\circ\text{BTDC} - 3^\circ\text{ATDC} \) both made achievement of PREMIER combustion possible and improved indicated mean effective pressure and thermal efficiency significantly. In addition, this is a significantly wide operating condition range. In contrast, the same approach did not improve normal combustion to PREMIER combustion in any split injection case of at \( \theta_1 = 3^\circ\text{BTDC} \); however, it was possible to improve engine output characteristics. The extent of improvement in terms of engine output is observed to be equally significant in both \( \theta_1 = 4^\circ\text{BTDC} \) and \( \theta_1 = 3^\circ\text{BTDC} \) split injection cases in comparison to their single injection counterparts, regardless of whether PREMIER combustion was achievable. The particular case of \( \theta_1 = 3^\circ\text{BTDC} \) showed a plunge of engine output and efficiency with the second injection timing of \( \theta_2 = 5^\circ\text{ATDC} \), similar to \( \theta_{\text{inj}} = 5^\circ\text{BTDC}/5^\circ\text{BTDC} \). Coefficient of variation of indicated mean effective pressure is an indicator of operation stability in terms of engine output; a lower result indicates better operation stability. As a result of these improvements, operation range of PREMIER combustion can be extended to an injection timing range of \( \theta_1 = 6^\circ\text{BTDC}-4^\circ\text{BTDC} \), as seen in figure 5.9. The coefficient of variation of the indicated mean effective pressure of \( \theta_1 = 6^\circ\text{BTDC} \) cases were lower than \( \text{COV}(P_{m_i}) = 1\% \) during both knocking and PREMIER combustion operation until the second injection timing was \( \theta_2 = 5^\circ\text{ATDC} \). After this injection timing, this value increased as high as 3\%, which is equivalent to the result observed during the least stable operation with later first injection timings. In addition, PREMIER combustion in \( \theta_1 = 4^\circ\text{BTDC} \) operation is in the vicinity of \( \text{COV}(P_{m_i}) = 2\% \) for PREMIER combustion operation, which is in the vicinity of \( \theta_1 = 5^\circ\text{BTDC} \) split injection cases.
Figure 5.8: Comparison of engine performance and operation stability of all experimental conditions: (a) indicated mean effective pressure, (b) thermal efficiency and (c) coefficient of variation of indicated mean effective pressure.
5.4.3. Effects of split injection on combustion characteristics

In order to explain the effect of split pilot fuel injection on the characteristics of PREMIER combustion, it is necessary to discuss the importance of flame kernels in this type of mechanism. In order to describe the progress of combustion from the injection timing to the end of combustion, rate of heat release of a typical PREMIER combustion cycle and its second derivative are produced based on the description given in a previous work, and presented in figure 5.10 [91]. In this figure, both curves are heavily filtered in order to reduce the effect of excessive unwanted noise and emphasize on their overall behavior. During injection stage, the pilot fuel is delivered into the cylinder. Pilot fuel undergoes autoignition after a brief ignition delay period, timing of which is detectable as the rising point of the first heat release peak, or as the first peak of the second derivative. This duration is decided by the in-cylinder temperature, pressure and concentrations of fuel, oxygen and other matters available in the in-cylinder mixture. Since the operating condition is kept constant throughout the work and there is no combustion activity prior to the ignition of pilot fuel, the effect of in-cylinder pressure can be ignored. Additionally, ignition delay of the pilot fuel is observed to show negligible variation throughout the work; therefore this parameter can be validated as constant. On the next stage, flame propagation starts from the pilot fuel ignition sites, which are referred to as flame kernels, and
spread towards the regions with unburned mixture. Heat release due to flame propagation reaches a detectable rate after the pilot-fuel heat-release peak and continues increasing as long as the rate of flame propagation heat release can overcome the volumetric expansion of the system during the expansion stroke. At this point, flame propagation speed and the size of flame kernels are two important parameters that influence the progress of combustion activity. Flame propagation speed depends on the turbulent burning velocity under the cylinder conditions, such as turbulence intensity, equivalence ratio, unburned gas temperature, and pressure, none of which can be influenced significantly without changing the operating condition or characteristics of the particular engine. Flame kernel size does not affect flame propagation speed measurably either; however, it determines how early the unburned mixture is consumed. A larger flame kernel ignites a larger volume, which shortens the distance that propagating flames are required to cover. When heat release occurs sufficiently fast to trigger end-gas autoignition, a third heat release peak appears in the ROHR. This is the indicator of end-gas autoignition in both PREMIER and knocking operations. All of these timings can also be obtained from the second derivative of rate of heat release.

![Diagram showing ROHR and its second derivative](image)

Figure 5.10: A typical rate of heat release in PREMIER combustion and its second derivative.
Visualisation on the effect of split injection on combustion is shown in figure 5.11. Figure 5.11(a) shows the images of flame kernel development in single injection at $\theta_{\text{inj}} = 5^\circ\text{BTDC}$. In this condition, the pilot fuel undergoes autoignition after completion of the ignition delay period and the initial forms of the flame kernels are formed. Due to the ongoing effect of in-cylinder mixture dynamics due to high pressure injection of the pilot fuel, the flame kernels begin migrating in the injection directions. When the split-injection strategy was applied with injection timings of $\theta_{\text{inj}} = 5^\circ\text{BTDC}/1^\circ\text{BTDC}$, the overall growth rate of the flame kernels became slower, as seen in figure 5.11(b). Expectedly, the amount of injection was reduced and the spray penetration length was shortened due to a shorter injection duration, the latter of which can be confirmed visually; therefore the sizes of the kernels were smaller than those observed with single injection until $\theta = 8^\circ\text{ATDC}$ and the flame kernels are formed closer to the injector. Flame kernels appeared at the same crank angle in both cases; however, both the location and the size of these kernels differed significantly in the two cases. Kernels of the single injection appeared instantly throughout the injection zones, and their sizes did not change significantly. In contrast, flame kernels for $\theta_{\text{inj}} = 5^\circ\text{BTDC}/1^\circ\text{BTDC}$ were small in the initial stage and their growth continued during the next 6.5°CA. Finally, the size of the flame kernels were not large enough in addition to their significantly delayed time of full growth, due to which the second injection did not have a significant contribution to flame propagation stage. Figure 5.11(c) shows the behavior of flame kernel growth in $\theta_{\text{inj}} = 5^\circ\text{BTDC}/5^\circ\text{ATDC}$, where engine performance and thermal efficiency showed significant deterioration. The flame kernels formed by the first injection reached their full size at a crank angle of 2.5°ATDC and showed no significant sign of growth until 8°ATDC. In order to capture the details of the mechanism that occurred with this particular second injection timing, the relevant area of the images are zoomed in using numerical methods and are given in figure 12 for all split injection cases with second injection timings of $\theta_2 = 5^\circ\text{ATDC}$. In all four sequences, the flame size did not show a measurable amount of growth until 7°ATDC. When the injection of the second spray started, kernel growth occurred towards the fuel injector starting at 7.5°ATDC. After a fraction of the second spray is consumed at the central region of the combustion chamber, the flame kernel growth continued towards the direction of injection. This mechanism makes it clear that the second spray partially supported the growth of the flame kernel. The growth of the flame kernel was slower and significantly delayed. Additionally, the second spray may have cooled the existing flame kernel during its evaporation stage; however this is not measured and needs to be confirmed in a future study. The same behavior is observed in all four cases, but the influence of this mechanism on the overall combustion characteristics was different in each case.
Figure 5.11. Flame kernel development at 5°ATDC: (a) $\theta_{inj} = 5°$BTDC single injection, (b) $\theta_{inj} = 5°$BTDC/1°BTDC, and (c) $\theta_{inj} = 5°$BTDC/5°ATDC.
Figure 5.12: Closeup view of inward kernel growth with second injection at $\theta_2=5^\circ$ATDC. (a) $\theta_{inj}=6^\circ$BTDC/5°ATDC, (b) $\theta_{inj}=5^\circ$BTDC/5°ATDC, (c) $\theta_{inj}=4^\circ$BTDC/5°ATDC and (d) $\theta_{inj}=3^\circ$BTDC/5°ATDC.
5.4.4. Suppression of knocking to PREMIER combustion by split fuel injection

To understand the extent of improvement that can be made by using split injection strategy, single injection at $\theta_{\text{inj}} = 6^\circ$BTDC with $m_{\text{inj}} = 0.3$ mg/cycle injection amount was tested and the results were compared with the results of single injection $\theta_{\text{inj}} = 6^\circ$BTDC with $m_{\text{inj}} = 0.6$ mg/cycle injection amount and split injection in $\theta_{\text{inj}} = 6^\circ$BTDC/TDC in figure 5.13. It is possible to suppress knocking in a single-injection strategy by reducing the injection amount and advancing the injection timing; however this approach may cause instability of engine operation. To maximise the efficiency, fast heat release is required without triggering knocking. This goal is achieved by controlling the timing of end-gas autoignition more precisely through use of split-injection strategy. After the first injection, the pressure history and ROHR of $\theta_{\text{inj}} = 6^\circ$BTDC/TDC and $\theta_{\text{inj}} = 6^\circ$BTDC single injection with $m_{\text{inj}} = 0.3$ mg/cycle were similar until $\theta = \text{TDC}$. Both in-cylinder pressure rise and heat release were delayed until $\theta = 2^\circ$ATDC in $\theta_{\text{inj}} = 6^\circ$BTDC/TDC due to later second injection. After this timing, the increases in both in-cylinder pressure and the ROHR at $\theta_{\text{inj}} = 6^\circ$BTDC/TDC were faster than those of $\theta_{\text{inj}} = 6^\circ$BTDC single injection with $m_{\text{inj}} = 0.3$ mg/cycle, because the second injection contributed to preparation of the conditions for end-gas autoignition. This allows end-gas autoignition to occur earlier without triggering knocking. In fact, it was confirmed that heat release in all split-fuel experiments at $\theta_{\text{inj}} = 6^\circ$BTDC was faster than the heat release observed in $\theta_{\text{inj}} = 6^\circ$BTDC single injection with 0.3 mg/cycle pilot fuel injection.

![Figure 5.13: Pressure histories and rates of heat release of $\theta_{\text{inj}}=6^\circ$BTDC single injection and $\theta_{\text{inj}}=6^\circ$BTDC/TDC split injection.](image)

90
Kernel development with $\theta_{\text{inj}} = 6^\circ$BTDC single injection with 0.6 mg/cycle pilot fuel injection, $\theta_{\text{inj}} = 6^\circ$BTDC/TDC and $\theta_{\text{inj}} = 6^\circ$BTDC/5°ATDC are shown in figure 5.14(a)-(c) respectively. The image sequence of $\theta_{\text{inj}} = 6^\circ$BTDC/5°ATDC is given in order to visually display the extent of delay flame kernel development encountered. Images taken at $\theta_{\text{inj}} = 6^\circ$BTDC single injection show that flame kernels appeared at 1°ATDC, grew rapidly, and their depth reached and surpassed the extent of the sapphire window until 4°ATDC with single injection, which is an expected behavior of the flame kernels. In the image sequence of split-fuel injection, the appearance of initial stages of the flame kernels were similar, and their sizes were comparable to those observed in single injection; however they do not grow as rapidly. Their growth occurs in a gradual manner and at a slower rate. Both the size and growth of the flame kernels at the time that the first injection autoignited is similar to the ones observed in $\theta_{\text{inj}} = 5^\circ$BTDC/TDC. Reviewing the parameters that influence flame propagation characteristics, it can be said that the smaller size of the flame kernel before the second injection was one of the major factors that retarded the heat release. The second sprays appeared at the crank angle timing of 2°ATDC, which is an expected occurrence for second injection timing of $\theta_2 = \text{TDC}$, remembering the fact that the response time of the injector is around 2°CA. At the time of injection, the spray zones already include the flame kernels, due to which it can be expected that the local temperature is high enough to reduce the ignition delay time of the second sprays significantly. After this timing, the flame kernels grew gradually at a noticeably slower rate, and they are contained in the visible region throughout the timing range shown in the sequence. In addition to their delay, these kernels could not reach as deep as the kernels that were formed in single injection, and their sizes were smaller in comparison. This outcome hints at the fact that the smaller flame kernels delayed the overall progress of combustion. First of all, propagating flames required a longer duration to consume the in-cylinder mixture until the end-gas autoignition occurred. This delayed the timing of the end-gas autoignition, and allowed it to occur later in the expansion cycle. It is a well-known fact that the velocity of the piston and the consequent increase in the rate of volumetric expansion is higher with a later timing in the first half of the expansion stroke. When the expansion rate of the piston is fast enough, it can overcome the rapid pressure increase due to autoignition of the end-gas mixture. In conclusion, it was possible to delay the growth of the flame kernels by using the split injection strategy with a suitable second injection timing, which also delayed the timing of end-gas autoignition activity long enough to suppress knocking.
Figure 5.14: Visual investigation of suppression of knocking: (a) $\theta_{\text{inj}}=6^\circ$BTDC single injection with $m_{\text{inj}}=0.6\text{mg/cycle}$ and (b) $\theta_{\text{inj}}=6^\circ$BTDC/TDC split injection. Additional reference graph on suppression of flame kernel growth at (c) $\theta_{\text{inj}}=6^\circ$BTDC/$5^\circ$ATDC.
5.4.5. Promotion of normal combustion to PREMIER combustion with split injection

Normal combustion can be promoted to PREMIER combustion by accelerating the progress of combustion by split injection, as seen in figure 5.15. In single injection at θ_{inj} = 4°BTDC, the heat release was not fast enough to trigger end-gas autoignition. The ROHR of the flame reached a peak value of about 10°ATDC, after which it slowed down due to the increasing rate of volumetric expansion. The behaviour of the split injection case was similar up to a crank angle of 10°ATDC; however, the initial peak of pilot fuel autoignition was slightly lower. After injection of the second sprays, the rate of heat release due to flame propagation became faster, having a higher peak value. As a result, this process increased in-cylinder pressure and temperature. The increase in the temperature is a well-known factor that improves rate of a reaction; this allows the fast flame propagation rate to be preserved for an even longer duration. Additionally, increase of both temperature and pressure shortened the ignition delay of end-gas mixture, due to which a larger number of cycles underwent autoignition with higher heat release peaks. Unfortunately, this mechanism has its limitations. Although split-fuel injection was applied with a first injection timing of θ_1 = 3°BTDC, PREMIER combustion could not be achieved.

Figure 5.15: Comparison of pressure histories and ROHR of single- and split-injection strategies at θ_{inj} = 4°BTDC and θ_{inj} = 4°BTDC/TDC.
Kernel development in $\theta_{\text{inj}} = 4^\circ\text{BTDC}$ single injection, $\theta_{\text{inj}} = 4^\circ\text{BTDC}/0.5^\circ\text{ATDC}$ and $\theta_{\text{inj}} = 4^\circ\text{BTDC}/5^\circ\text{ATDC}$ are shown in figure 5.16. The behaviour of the flame kernels in single-injection operation was similar to that of the $\theta_{\text{inj}} = 6^\circ\text{BTDC}$ single injection, but the event was delayed by 2°CA. This time, the timing difference between the first and the second sprays was shortened to 3.5°CA. In this approach, the end of delivery of the second injection and the appearance of flame kernels occurred simultaneously. These sequences show that, the first flame kernels appeared 1° of crank angle earlier with split injection; however, visual detection of flame kernels relies on their luminosity, which is not a reliable indicator of their presence. In particular, the sprays in single injection case are expected to mix with the in-cylinder charge better, reducing the soot production and luminosity of the flames at the same time. In contrast, second sprays in the split injection case are delivered onto the flames, leaving a significantly shorter time to mix with the in-cylinder charge, which is expected to produce a significantly stronger luminosity. Rate of heat release characteristics of both sequences indicated that the initiation of heat release from the pilot fuel was between $\theta = \text{TDC}$ and $\theta = 1^\circ\text{ATDC}$ and there was no noticeable difference between these two sequences; therefore it is safe to assume that ignition delay is not affected by changing the injection strategy. When the initial locations of flame kernels were compared with those observed in the split-injection sequences of figures 5.11 and 5.14, the kernels appeared farther from the injector tip in $\theta_{\text{inj}} = 4^\circ\text{BTDC}/0.5^\circ\text{ATDC}$. These two observations indicate that the second spray was not obstructed by the first flames in $\theta_{\text{inj}} = 4^\circ\text{BTDC}/0.5^\circ\text{ATDC}$; instead, spray penetration potentially increased the rate of kernel growth. Kernel growth in the $\theta_{\text{inj}} = 4^\circ\text{BTDC}/0.5^\circ\text{ATDC}$ split-injection operation was gradual, as was observed for $\theta_{\text{inj}} = 6^\circ\text{BTDC}/\text{TDC}$; however, the flame kernels in $\theta_{\text{inj}} = 4^\circ\text{BTDC}/0.5^\circ\text{ATDC}$ grew significantly faster. In fact, kernel growth in the single and split injection at $\theta_{\text{inj}} = 4^\circ\text{BTDC}/0.5^\circ\text{ATDC}$ sequences of figure 5.16 were comparable. While kernels of the single injection grew slightly faster towards the direction of penetration, kernels of the split injection grew larger. The characteristics of the flame kernels observed in $\theta_{\text{inj}} = 3^\circ\text{BTDC}$ were similar; however, the extent of improvement in the final flame kernel size was not as significant, and normal combustion could not be upgraded to PREMIER combustion under this operating condition. Instead, engine performance and operation stability improved significantly. From this observation, it can be suggested that the flame kernels were not large enough to increase the flame propagation heat release rate, due to which the end-gas conditions could not be improved sufficiently, or sustained long enough, in order to achieve a more substantial end-gas heat release.
Figure 5.16: Visual investigation of promotion of normal combustion to PREMIER combustion: (a) $\theta_{inj}=4^\circ$BTDC single injection, (b) $\theta_{inj}=4^\circ$BTDC/0.5$^\circ$BTDC.

Additional reference graph on suppression of flame kernel growth at (c) $\theta_{inj}=4^\circ$BTDC/5$^\circ$ATDC
Figure 5.17: Visual investigation improvement of heat release characteristics: (a) $\theta_{inj}=3^\circ$BTDC single injection, (b) $\theta_{inj}=3^\circ$BTDC/0.5$^\circ$ATDC. Additional reference graph on suppression of flame kernel growth at (c) $\theta_{inj}=3^\circ$BTDC/5$^\circ$ATDC.
5.5. Summary of observations

In this work, split pilot fuel injection strategy was used in a dual-fuel gas engine in the vicinity of the normal combustion/PREMIER combustion/knocking operation transition to assess the possibility of expanding the operation range of PREMIER combustion. The following conclusions can be made.

1. Split pilot fuel injection can be used to suppress knocking to obtain PREMIER combustion by delaying the growth of flame kernels and reducing their size. This increases the time required for propagating flames to consume unburned gaseous fuel and air mixture, and retards the overall progress of combustion. The maxima of feasible engine output and thermal efficiency are extended when knocking is suppressed and PREMIER combustion is achieved. The maximum values were similar to those observed during knocking operation.

2. Split pilot fuel injection can be used to promote normal combustion to PREMIER combustion by widening flame kernels and accelerating their rate of growth. As a result, a larger volume of gaseous fuel and air mixture is consumed earlier, which increases the unburned mixture pressure and temperature faster and earlier. Split injection significantly improves indicated mean effective pressure and thermal efficiency by converting normal combustion to PREMIER combustion. Additionally, it increases the probability of the occurrence of end-gas autoignition when a certain normal combustion operating condition is a precursor to PREMIER combustion.

3. The range of operating conditions that can be converted to PREMIER combustion by split fuel injection is limited. Heavy knocking or normal combustion with low engine output cannot be converted to PREMIER combustion.

4. When the end of delivery of the second injection coincides with the appearance of flame kernels, spray penetration supports flame kernel development by increasing both the sizes and growth speeds. When second injection starts before full development of flame kernels, the sprays and kernel initiation zones interact and produce larger flame kernels than is achievable with single injection. When the flame kernels are partially grown during injection, the final size and growth rate of the flame kernels are affected adversely. When the second injection occurs after full growth of the flame kernels formed by the first injection, a fraction of the second spray is consumed in the vicinity of the injector and the kernels grow towards the injector. Consequently, final size of flame kernels is restricted, and their growth is slower, and the fraction consumed around the injector does not provide any input to propagating flames.
5.6. Raw in-cylinder images of all recorded conditions

Figure 5.18: Unprocessed in-cylinder images of (a) $\theta_{\text{inj}}=6^\circ\text{BTDC}$ single injection, (b) $\theta_{\text{inj}}=6^\circ\text{BTDC/TDC}$ and (c) $\theta_{\text{inj}}=6^\circ\text{BTDC/5^\circATDC}$
Figure 5.19: Unprocessed in-cylinder images of (a) $\theta_{inj}=5^\circ\text{BTDC}$ single injection, (b) $\theta_{inj}=5^\circ\text{BTDC}/1^\circ\text{BTDC}$ and (c) $\theta_{inj}=5^\circ\text{BTDC}/5^\circ\text{ATDC}$
Figure 5.20: Unprocessed in-cylinder images of (a) $\theta_{\text{inj}}=4^\circ$BTDC single injection, (b) $\theta_{\text{inj}}=4^\circ$BTDC/0.5$^\circ$BTDC and (c) $\theta_{\text{inj}}=4^\circ$BTDC/5$^\circ$ATDC
Figure 5.21: Unprocessed in-cylinder images of (a) $\theta_{inj}=3^\circ$BTDC single injection, (b) $\theta_{inj}=3^\circ$BTDC/0.5$^\circ$ATDC and (c) $\theta_{inj}=3^\circ$BTDC/5$^\circ$ATDC.

6.1. Motivation

Both hydrogen and methane are obtainable from biological resources, and are promising fuels for the future. These two fuels have opposite characteristics. Hydrogen is a highly reactive fuel that has a very fast flame propagation speed and is easy to undergo autoignition. Due to these characteristics, it is challenging to use in internal combustion engines at high enough equivalence ratios that can provide reasonable power output. In contrast, methane is one of the least reactive bio-derivable gaseous fuels; its flame propagation speed is significantly slow and requires a long incubation period at significantly high temperatures in order to undergo autoignition. In recent years, blends of methane and hydrogen are suggested as a viable alternative fuel, because it is possible to achieve desirable characteristics by changing the fraction of these fuels in the mixture.

Due to the significant autoignition tendency, the research on usable autoignition characteristics of hydrogen has not been popular and the fundamental knowledge requires further attention. Occurrence of autoignition is the foundation of PREMIER combustion, which allows this combustion mechanism to excel at engine efficiency and exhaust emissions compared to normal combustion. The motivation of this section of the thesis intends to explain usable operation range of methane and hydrogen mixtures under PREMIER combustion based on in-cylinder pressure, heat release characteristics, engine performance and exhaust emissions. Additionally, end-gas autoignition characteristics will be evaluated based on average pressure histories, a brief introduction on the knocking resistance and end-gas autoignition characteristics will be provided in order to provide fundamental knowledge on autoignition characteristics of hydrogen fuel.

6.2. Specifics of the experimental setup, test procedure and data analysis

The experimental setup was explained in details in chapter 2; it will be briefly summarized in this section. Outline of the experimental setup is given in figure 6.1. A single cylinder, supercharged, micro-pilot fuel injected dual fuel gas engine is used. The swept volume of the engine is 781cc, bore and stroke are 96mm and 108mm, and the compression ratio is 16.4:1. The piston is a shallow dish type; this type of piston geometry is more favorable for flame propagation. The engine is connected to an electric motor which can govern the
engine at a fixed speed of 1000±1 revolutions per minute (rpm) during both motoring and loaded conditions. Intake air is pressurized by an industrial compressor. A surge tank and a heater are installed between the compressor and the engine for pressure and temperature stabilization. Mixtures of methane and hydrogen are used as the primary fuel and fed to the engine through the intake port as homogeneous air-fuel mixture, and their flowrate is controlled precisely by dedicated mass flow controllers governed by a PLC controller. Diesel fuel is injected by a solenoid type injector through a common rail. The injector has a purpose-built nozzle with 3 orifices of 0.1mm diameter. Injection timing and amount is controlled by a timing system, which reads signals from crank angle, top dead center (TDC) and cam sensors and sends injection signal. Specifications of the engine are given in table 6.1.

Figure 6.1: Outline of the experimental setup
Table 6.1: Engine and test bench specifications

<table>
<thead>
<tr>
<th>Engine type</th>
<th>Single cylinder, supercharged, 4 stroke, water cooled</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore × Stroke</td>
<td>96mm × 108mm</td>
</tr>
<tr>
<td>Volume</td>
<td>781 cc</td>
</tr>
<tr>
<td>Gas oil injection</td>
<td>3 hole injector, ∅0.1mm orifices</td>
</tr>
<tr>
<td>Injection system</td>
<td>Common rail with electronic injection timing control</td>
</tr>
<tr>
<td>Gaseous fuel delivery</td>
<td>Homogeneous air-fuel mixture through intake port</td>
</tr>
<tr>
<td>Gaseous fuel flowrate control</td>
<td>Mass flow controllers</td>
</tr>
</tbody>
</table>

An initial set of preliminary experiments were performed in order to discover the optimum equivalence ratio of pure methane. The equivalence ratio 0.6 was chosen as the basis because mixtures with higher methane concentration would undergo premature ignition. The equivalence ratio is reduced in steps of 0.02 until misfiring is encountered. Both the optimum equivalence ratio and the corresponding energy supply rate are kept constant throughout the next stage of the study. The injection conditions tested for both pure methane and methane-hydrogen mixtures are listed in table 6.2.

Table 6.2. List of injection timings at tested fueling conditions

<table>
<thead>
<tr>
<th>Test session</th>
<th>Injection timing (° BTDC)</th>
</tr>
</thead>
<tbody>
<tr>
<td>100% CH₄, φ=0.52</td>
<td>19, 18.5, 18, 17, 16, 15, 14, 12, 9</td>
</tr>
<tr>
<td>100% CH₄, φ=0.54</td>
<td>18, 17, 16.5, 16, 15.5, 15, 14.5, 14, 13.5, 13, 12, 9, 6</td>
</tr>
<tr>
<td>100% CH₄, φ=0.56</td>
<td>15, 14.5, 14, 13.5, 13, 12.5, 12, 9, 6, 3</td>
</tr>
<tr>
<td>100% CH₄, φ=0.58</td>
<td>12.5, 12, 11.5, 11, 10.5, 10, 9.5, 9, 6, 3</td>
</tr>
<tr>
<td>100% CH₄, φ=0.6</td>
<td>12, 11.5, 11, 10.5, 10, 9, 6, 3</td>
</tr>
<tr>
<td>100% CH₄, φ=0.56 (re-tested)</td>
<td>15.5, 15, 14.5, 14, 13, 12, 9, 6</td>
</tr>
<tr>
<td>CH₄ 90%-H₂ 10%</td>
<td>15, 14, 13.5, 13, 12.5, 12, 11, 10, 9</td>
</tr>
<tr>
<td>CH₄ 80%-H₂ 20%</td>
<td>13.5, 13, 12.5, 12, 11.5, 11, 10.5, 10, 9, 8, 6</td>
</tr>
<tr>
<td>CH₄ 70%-H₂ 30%</td>
<td>12, 11, 10, 9.5, 9, 8.5, 8, 7.5, 7, 6, 5, 4</td>
</tr>
<tr>
<td>CH₄ 60%-H₂ 40%</td>
<td>10, 9.5, 9, 8.5, 8, 7.5, 7, 6, 5, 4, 3</td>
</tr>
<tr>
<td>CH₄ 50%-H₂ 50%</td>
<td>8.5, 8, 7.5, 7, 6, 3, 0</td>
</tr>
<tr>
<td>CH₄ 40%-H₂ 60%</td>
<td>4, 3.5, 3, 2, 1, 0</td>
</tr>
</tbody>
</table>
Flowrates of methane and hydrogen are adjusted in order to constrain the total energy input at 2.6 kJ/cycle at any given hydrogen fraction during the second stage of the work, including the energy from the pilot fuel. This is achieved by controlling the intake pressure, which decides intake air flowrate. Intake temperature is constant at 40°C. Intake pressure is adjusted in order to maintain the total equivalence ratio (ϕ) constant at 0.56. Diesel fuel is used as the pilot fuel, and it is intended for only igniting the gaseous fuel-air mixture. It is injected at the injection pressure of 40 MPa and a rate of 0.8mg/cycle, which corresponds to 1.5% of the total energy input at 35.8 J/cycle. Injection timings are typically decided during experiments: typically late injection timings, always earlier than top dead center (BTDC) is chosen as a baseline, and are gradually advanced until knocking is confirmed audibly. The operating conditions are listed in table 6.3, and the tested injection timings are given in table 2.

<table>
<thead>
<tr>
<th>methane fraction</th>
<th>Vol%</th>
<th>100</th>
<th>90</th>
<th>80</th>
<th>70</th>
<th>60</th>
<th>50</th>
</tr>
</thead>
<tbody>
<tr>
<td>hydrogen fraction</td>
<td>Vol%</td>
<td>0</td>
<td>10</td>
<td>20</td>
<td>30</td>
<td>40</td>
<td>50</td>
</tr>
<tr>
<td>Common rail pressure</td>
<td>MPa</td>
<td>40</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pilot fuel flowrate</td>
<td>mg/cycle</td>
<td>0.8</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pilot fuel energy</td>
<td>J/cycle</td>
<td>33.6</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>total equivalence ratio</td>
<td>-</td>
<td>0.56</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Intake pressure</td>
<td>kPa</td>
<td>200</td>
<td>199.5</td>
<td>198.1</td>
<td>197</td>
<td>195.8</td>
<td>194.4</td>
</tr>
<tr>
<td>Air flowrate</td>
<td>mg/cycle</td>
<td>1630</td>
<td>1605</td>
<td>1592</td>
<td>1575</td>
<td>1556</td>
<td>1548</td>
</tr>
<tr>
<td>methane flowrate</td>
<td>mg/cycle</td>
<td>51.5</td>
<td>50.2</td>
<td>48.2</td>
<td>45.7</td>
<td>42.8</td>
<td>39.8</td>
</tr>
<tr>
<td>Methane energy</td>
<td>kJ/cycle</td>
<td>2.56</td>
<td>2.49</td>
<td>2.39</td>
<td>2.28</td>
<td>2.14</td>
<td>2.0</td>
</tr>
<tr>
<td>Hydrogen flowrate</td>
<td>mg/cycle</td>
<td>0</td>
<td>0.7</td>
<td>1.5</td>
<td>2.5</td>
<td>3.6</td>
<td>5.0</td>
</tr>
<tr>
<td>Hydrogen energy</td>
<td>kJ</td>
<td>0</td>
<td>0.08</td>
<td>0.18</td>
<td>0.29</td>
<td>0.43</td>
<td>0.57</td>
</tr>
</tbody>
</table>

In-cylinder pressure is measured by a pressure sensor installed to the cylinder head and combined with crank angle and TDC signals in order obtain the pressure history. Results of every test session pressure histories of 80 consecutive cycles. All performance and combustion characteristics discussed in this work are obtained from the pressure history; therefore all the results are the indicated values, such as indicated mean effective pressure ($P_{mi}$) or indicated thermal efficiency ($\eta_i$). Additionally, indicated mean effective pressure and thermal...
efficiency are obtained from 720 degrees of crank angle rotation and the results are reported as gross values. An FFT low-pass filter at 20 kHz is applied to the pressure history before further analysis in order to remove the noise. A second type of FFT filter, a 4-20 kHz band-pass filter is applied separately, only for obtaining knock intensities (KI) and power spectral densities in order to distinguish knocking and non-knocking cycles. Additionally, the pressure histories and ROHR that are given in the figures of this work are heavily filtered in order to provide a better presentation.

6.3. Preliminary experiments using methane

6.3.1. Pressure histories and rate of heat release characteristics of methane

A meaningful comparison between engine operation related characteristics of pure methane and methane-hydrogen mixtures requires correct identification of the optimum operating conditions in a preliminary experiment. Optimization of equivalence ratio was carried out by performing a series of performance tests in an equivalence ratio range of 0.52 to 0.6 with increments of 0.02. The 80 cycle averages of pressure histories and rate of heat release characteristics are given in Pressure histories and rate of heat release characteristics at most beneficial injection timing conditions are summarized in figure 6.2, and individual conditions are given in figures 6.3 to 6.7. During the performance tests, a retarded injection timing is selected as the baseline, which is advanced by 3 degrees of crank angle in each iteration until knocking is observed. Afterwards, the injection timing is retarded again by 0.5 degrees of crank angle in order to detect the cases with and without prevalent PREMIER combustion operation with more details. Pressure histories and rate of heat release characteristics are separated based on this procedure: injection timings with coarse and fine intervals are separated. According to the pressure histories, the transition between non-knocking operations to knocking operation was more abrupt when the equivalence ratio is increased; the most abrupt one was the case with equivalence ratio of 0.6. This trend also affects the maximum in-cylinder pressure that is attainable without knocking; the pressure histories with lower levels were observed with cases with higher equivalence ratios. Rate of heat release characteristics supported these observations as well: It is a well-known fact that faster heat release is synonymous with higher thermal efficiency; therefore a combination of faster flame propagation heat release and a more intense end-gas autoignition heat release is more desirable. At a first glance, it can be seen that end-gas autoignition heat release characteristics at equivalence ratios of 0.6 and 0.58 were inferior to the rest of the cases while flame propagation heat release was slightly faster for these cases. This outcome can be explained better when pressure histories and rate of heat release
characteristics of the most beneficial injection timings (MBT), the operating condition that occurs as a precursor to knocking, and the first condition with knocking are compared. The pressure histories of knocking conditions deviated from the most beneficial timing cases more significantly at higher equivalence ratios. Knocking occurs with earlier injection timings, due to which the start of combustion is advanced as well. Injection timings of all conditions shown in these figures were before the top dead center, so the start of combustion can be expected to occur during the compression stroke as well. When a higher fraction of heat release occurs during the compression stroke, the pressure and temperature will rise higher, yielding to autoignition of end-gas region. This behavior will be intensified for air-fuel mixtures of higher reactivity; increasing the equivalence ratio as long as maintaining it below unity, or using a fuel with higher reactivity will have the same effect. If the amount heat release from the end-gas region is high enough, knocking will occur, yielding to rapid pressure rise and oscillations in the pressure history. A mixture with a lower equivalence ratio also has lower energy density per volume of air-fuel mixture; therefore the intensity of end-gas autoignition will be lower as well, making it possible to maintain the PREMIER combustion operation for a wider range of injection timings. To sum up, the pressure histories and rate of heat release characteristics indicate that a lower equivalence ratio is more beneficial, because it becomes possible to increase the maximum in-cylinder pressure without knocking.

Figure 6.2: Pressure histories and rate of heat release characteristics at most beneficial injection timings
Figure 6.3: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.60.
Figure 6.4: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.58.
Figure 6.5: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.56.
Figure 6.6: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.54.
Figure 6.7: Pressure histories (a, b) and rate of heat release characteristics (c, d) in methane operation with equivalence ratio of 0.52.
6.3.2. Engine performance of methane

Engine performance characteristics are quantified as the indicated mean effective pressure and thermal efficiency and the operation stability is evaluated from the coefficient of variation of indicated mean effective pressure. These characteristics are given in figure 6.7(a)-(c) respectively. In these figures, the injection timings that yielded significantly poor characteristics were omitted, because such conditions deviate from usable conditions greatly and the remaining cases serve for comparison purpose adequately. The maximum indicated mean effective pressure was the highest with the equivalence ratio of 0.6 and the lowest for 0.52, as expected. Since all intake and compression conditions are preserved as much as possible, the amount of energy delivered by the fuel is expected to be higher when the equivalence ratio is increased. In addition, the higher reactivity of the gas with higher equivalence ratio meant that the earliest injection timings without knocking were later; therefore a large fraction of heat release occurred during the expansion stroke. As a consequence, the output of the engine is expectedly higher. In contrast, the maxima of thermal efficiencies were gradually higher as the equivalence ratio is reduced. The highest thermal efficiency was observed at equivalence ratio of 0.54 and injection timing of 14.5°BTDC ac 45.4%. Similarly, the lowest coefficient of variation of indicated mean effective pressure was observed for the cycles with the highest thermal efficiency as well, but it showed deterioration when the injection timing is retarded. This indicates that engine stability is significantly influenced by the stability of combustion: fuels with higher equivalence ratios show less combustion instability, which deteriorates when the equivalence ratio is reduced. The overall characteristics of the results show that there was a trade-off between engine output and thermal efficiency, which remarks the first criterion.
Figure 6.8: Performance characteristics of pure methane at tested equivalence ratios: (a) Indicated mean effective pressure, (b) thermal efficiency and (c) coefficient of variation of indicated mean effective pressure.
6.3.3. Exhaust emissions of methane

Nitrogen oxide (NO\textsubscript{x}), unburned hydrocarbon (HC) and carbon monoxide (CO) emissions of pure methane operation are given in figure 6.8(a)-(c) respectively. Exhaust emissions can be used for obtaining information on the qualities of combustion operation. Production rate of thermal NO\textsubscript{x} is typically high when the in-cylinder temperature rises above 1600°C; longer incubation period yields higher NO\textsubscript{x} production. Around 78 percent of air consists of nitrogen; therefore production of this type of emissions is more dependent on the combustion characteristics than the fuel type, and also it is possible to limit its production rate by constraining the in-cylinder mixture temperature below the threshold temperature. The emission results showed that the highest rates of NO\textsubscript{x} production were recorded at the earliest injection timings of each equivalence ratio condition. The mixtures with higher fractions of methane tended to produce more NO\textsubscript{x}, which also shows that the in-cylinder temperature was measurably higher, the duration that the in-cylinder temperature was preserved above thermal NO\textsubscript{x} production threshold was longer or a combination of both. Unfortunately, these conditions are also those that displayed the highest engine output and thermal efficiency. Unburned hydrocarbons (HC) and carbon monoxide (CO) are indicators of incomplete combustion. Unburned hydrocarbons can be detected in the exhaust gases when either intermediate species involving carbon or the unburned fuel is rejected in exhaust stream. Similarly, incomplete oxidation of carbon atoms cause rejection of CO molecules before CO\textsubscript{2} can be formed. While small amounts of both emissions are inevitable in any combustion activity, high emissions indicate unsuitable combustion characteristics regarding the application. Both were similarly low throughout the injection timing range at $\varphi=0.60$ and $\varphi=0.58$, which shows that the high reactivity of the air-fuel mixture compensated for the retarded injection timing and start of combustion. Early injection with the rest of the equivalence ratios yielded similar results. Due to poor efficiency, later injection timings do not represent a practically usable operating condition and are of minimum concern; however a wider range of usable injection timing is certainly favorable regarding practical operation. In the range of $\varphi=0.52$ to $\varphi=0.56$, both emissions deteriorate earlier and more significantly due to inferior reactivity of the air-fuel mixture. Within this group, only $\varphi=0.56$ can maintain comparably low emissions throughout a wide injection timing range. In conclusion, NO\textsubscript{x} emissions and high engine output are in a trade-off relationship across both injection timing and equivalence ratio ranges; in contrast, lower NO\textsubscript{x} emissions were observed for the fuel mixtures with lower equivalence ratios, which yielded increasingly higher thermal efficiencies at their most beneficial injection timings. $\varphi=0.60$ and $\varphi=0.58$ yielded superior HC and CO emissions, $\varphi=0.52$ and $\varphi=0.54$ have considerably poor emission characteristics; the fueling case with $\varphi=0.56$ had a wide injection timing range with reasonably low HC and CO.
Figure 6.9: Exhaust emission characteristics in pure methane operation: (a) Nitrogen oxide, (b) unburned hydrocarbon and (c) carbon monoxide emissions.
6.3.4. Determination of the optimum equivalence ratio

Engine performance and exhaust emissions at the most beneficial injection timing of each equivalence ratio case are summarized in figure 6.10. Based on the observations made in the previous sections, it was concluded that the $\phi=0.56$ is the optimum condition. This particular fueling condition showed the median value in all parameters. All these parameters are equally important for a practical engine and should be controlled. Under $\phi=0.56$ and $P_{in}=200$ kPa, it is found that the total amount of energy flow was 2.6 kJ/cycle. In order to compare the characteristics of methane-hydrogen mixtures on the oncoming section, equivalence ratio and the total energy input was kept constant; the air/fuel ratio was adjusted by controlling air flowrate, which was possible by changing the intake pressure.

Figure 6.10: Comparison of all engine performance and exhaust emission characteristics at most beneficial injection timing: (a) $P_{mi}$ (b) thermal efficiency, (c) COV($P_{mi}$); (d) NO$_x$ (e) CO and (f) HC emissions.
6.4. Methane-hydrogen mixtures

6.4.1. Pressure histories and rate of heat release characteristics of methane-hydrogen mixtures

During the research period, there was a noticeable seasonal difference between the experimental sessions of pure methane and methane-hydrogen mixtures; therefore the pure methane experiments at the equivalence ratio of 0.56 was performed again in order to ensure consistency of ambient conditions throughout this phase of the study. Please note that the effect of daily fluctuations of ambient conditions is less noticeable than seasonal changes. Pressure histories and rate of heat release characteristics of both methane-hydrogen mixtures and the updated pure methane at the most beneficial injection timing conditions are summarized in figure 6.11. Additionally, pressure histories and rate of heat release characteristics of wide ranges of injection timings at each fueling case are given in figure 6.12 and figure 6.13 respectively, which exclude knocking conditions and put little emphasis on the conditions that yielded poor combustion characteristics. Throughout the hydrogen fraction range, addition of hydrogen brought forth the necessity to retard the injection timing, which is an expected scenario due to high reactivity of hydrogen. Within the most beneficial injection timing conditions of all fueling cases, the highest in-cylinder pressure level was observed for pure methane; the maximum in-cylinder pressure decreased gradually with addition of hydrogen into the fuel mixture until 50%. The only exception of this group is the fueling case of 60%CH$_4$-40%H$_2$, the maximum pressure of which exceeded both 70%CH$_4$-30%H$_2$; however one of the reasons for this outcome is the change in ambient conditions between two experimental sessions. Additionally, injection timings can be changed in 0.5 degrees of crank angle intervals; the injection timing of 9.5 degrees before top dead center has a high probability of being the closest to the optimum condition as well. When the hydrogen fraction was increased to 60%, the maximum in-cylinder pressure dropped below 9 MPa level. It should be mentioned that 40%CH$_4$-60%H$_2$ fueling case is not suitable for practical operation. The underlying reasons will be discussed in details on the oncoming sections. Rate of heat release characteristics at the most beneficial injection timing show that, while the injection timings and start of injection was varied throughout the fueling condition range, many aspects of heat release characteristics converged to a common trend on the later stages of combustion activity, excluding the unique case of 40%CH$_4$-60%H$_2$ fueling case. First of all, the duration between the start of combustion to the heat release peak of flame propagation became gradually shorter as the hydrogen
concentration of the fuel is increased. Similarly, the maximum values of flame propagation heat release peaks were higher for the cases with higher hydrogen fraction as well. The end-gas autoignition timings that can be obtained from the 80 cycle average heat release characteristics was within a range of 8°ATDC to 12°ATDC. Furthermore, heat release characteristics also converged later in the cycle, around the timing of 35°ATDC; however it can be expected that there will be no significant combustion activity following this timing; it can be assumed that all zones in the combustion chamber are either consumed by end-gas autoignition or the reactions that are initiated by flame propagation are being finalized. Consequently, the delayed injection due to additional hydrogen did not retard the combustion activity as significantly. Finally, focusing on the special case of 40%CH₄-60%H₂, a phenomenon called super knocking, which occurs an uncontrollably violent heat release followed by extremely high in-cylinder pressures due to premature ignition of the in-cylinder mixture. This condition was observed at the injection timing of 4°ATDC, which is shown in figure 6.14. It can be assumed that this particular fuel mixture is sensitive to presence of hot spots inside the combustion chamber; therefore this fueling case is prone to knocking regardless of injection timing and is not suitable for operation under the operating conditions given in table 6.1. The deviation observed in figures 6.11-14 because of the fact that the most beneficial timing could not be identified for the fueling case of 40%CH₄-60%H₂. Due to this outcome, the distinction between PREMIER combustion and normal combustion operation will not be made for this particular fueling case.
Figure 6.11: (a) Pressure histories of and (b) rate of heat release characteristics at the most beneficial injection timings of all fueling cases.
Figure 6.12: Pressure histories of methane-hydrogen mixtures: (a) 100% CH₄, (b) 90% CH₄/10% H₂, (c) 80% CH₄/20% H₂, (d) 70% CH₄/30% H₂, (e) 60% CH₄/40% H₂, (f) 50% CH₄/50% H₂, and (g) 40% CH₄/60% H₂.
Figure 6.13: Rate of heat release of methane-hydrogen mixtures: (a) 100% CH₄, (b) 90% CH₄/10% H₂, (c) 80% CH₄/20% H₂, (d) 70% CH₄/30% H₂, (e) 60% CH₄/40% H₂, (f) 50% CH₄/50% H₂, and (g) 40% CH₄/60% H₂.
6.4.2. Engine performance of methane-hydrogen mixtures

Performance and operation stability characteristics of methane-hydrogen mixtures are given in figure 6.15. Despite reduced in-cylinder pressure levels of fuels with higher hydrogen fractions, indicated mean effective pressure of all fueling cases were similar at MBT conditions. Additionally, fuels with higher hydrogen fractions preserved the engine output at higher levels for a wider range of injection timings. This is a result of delayed injection and start of ignition, which reduced the fraction of fuel that was consumed during the compression stroke the top dead center; this energy is wasted while the engine did compression work. The amount of wasted work was lower for the mixtures of higher hydrogen fraction, which allowed a higher fraction of heat to be converted to useful work. This mechanism impacted the thermal efficiency as well. The maximum achievable thermal efficiency was 45.9% using pure methane; in contrast, the maxima of both 70%CH₄-30%H₂ and 50%CH₄-50%H₂ were 47.3%, which meant a 1.4% improvement in thermal efficiency by addition of hydrogen. The highest thermal efficiency was observed in 40%CH₄-60%H₂; however this particular needs to be omitted. Finally, the coefficient of variation of indicated mean effective pressure showed that addition of hydrogen to the fuel mixture improves the operation stability, regardless of its fraction. While operation with pure methane showed signs of deterioration as soon as injection timing was delayed beyond 12 degrees before top dead center timing, addition of hydrogen kept this parameter below 4% threshold throughout the tested injection timing range, which shows improved stability of operation with hydrogen.
Figure 6.15: Performance characteristics of methane-hydrogen mixtures at tested equivalence ratios: (a) Indicated mean effective pressure, (b) thermal efficiency and (c) coefficient of variation of indicated mean effective pressure.
6.4.3. Exhaust emissions of methane-hydrogen mixtures

Nitrogen oxide, unburned hydrocarbon and carbon monoxide emissions of methane-hydrogen mixtures are given in figure 6.16(a)-(c) respectively. Looking at the nitrogen oxide emissions, it can be seen that the response of the engine was not correlated to the amount of hydrogen in the fuel mixture; the maxima and the overall trend throughout the tested conditions were similar, excluding the fueling case of 60% hydrogen in the fuel mixture. Under these operating conditions, thermal NOx was the main source of NOx production. Based on this information, it can be suggested that the maxima of in-cylinder temperatures were equivalent throughout the cases. The reason for the deviation observed for the fueling case of 60% hydrogen is due to frequent occurrence of premature ignition regardless of injection timings; uncontrolled start of combustion elevated in-cylinder temperature and increased incubation period, promoting further production of thermal NOx. HC emissions showed that there were two noticeable differences between the methane-hydrogen mixtures and pure methane. First of all, the amount of HC was a function of injection timing in pure methane operation; advancing the injection timing consumed a higher fraction of the supplied fuel and reduced unburned hydrocarbon emissions. On the other hand, the amount of HC emissions was not correlated to how early the combustion started. Hydrogen is not a hydrocarbon fuel; therefore it was expected that replacing methane with hydrogen would proportionally reduce HC emissions; however the rate of improvement surpassed the expectations. The decrease of unburned hydrocarbon emissions was greater than the decrease of methane fraction. This is due to higher reactivity of hydrogen. It is well-known that the flame speed of hydrogen is significantly faster than those of hydrocarbon fuels that is preserved relevantly fast even under lean conditions, and also hydrogen is more susceptible to autoignition due to its lower ignition temperature, lower activation energy and shorter ignition delay time. Eventually, addition of hydrogen to the fuel mixture at any tested fraction had a positive impact on HC emissions. Investigating CO emissions, it is apparent that the scenario seen in HC applies to carbon monoxide emissions as well. Replacing a fuel that contains carbon atoms with hydrogen and a higher rate of reaction completeness allowed significant improvement. The biggest improvement was observed for the fuel mixture with 60% hydrogen concentration; unfortunately, this particular mixture is not suitable for practical operation under the given conditions due to the aforementioned reason. Summing up the observations on the exhaust emissions, it is apparent that addition of hydrogen does not introduce any trade-off relation of nitrogen oxides versus carbon monoxide and hydrocarbons. Addition of hydrogen reduces carbon monoxide and hydrocarbon emission levels without influencing nitrogen oxide emission levels.
Figure 6.16: Exhaust emission characteristics of methane-hydrogen mixtures: (a) Nitrogen oxide, (b) unburned hydrocarbon and (c) carbon monoxide emissions.
6.4.4. An overview of combustion characteristics of methane-hydrogen mixtures under PREMIEIR combustion operation

Higher reactivity of hydrogen compared to methane has been stated numerous times in section 6.4.1 and 6.4.2; therefore it is necessary to numerically introduce the statements. One of the convenient tools for evaluating the combustion development is mass fraction burned (MFB), which is an indicator of the ratio of the heat release at a given crank angle timing to the total amount of provided heat. 80 cycle average of mass fraction burned of all fueling cases are shown at the most beneficial injection timings in figure 6.17. The outcome seen in this figure supports several observations made earlier. First of all, the fraction of heat release before the top dead center timing was the highest during 100% methane experiments, which was reduced gradually as the fraction of hydrogen in the fuel mixture was reduced. Secondly, it was mentioned that the behavior of rate of heat release converged around the crank angle timing of 35°ATDC, which can be confirmed on this figure as well. It was also mentioned that the reason behind the improvement of thermal efficiency was faster heat release after the top dead center timing, which is another proposition that can be confirmed from mass fraction burned characteristics. Looking at the combustion characteristics past the crank angle timing of 35°ATDC, it can be seen that mixtures with higher hydrogen concentrations tended to rise higher. This is also another mechanism that is known to improve the efficiency of heat conversion. The reason behind the improvement of mass fraction burned characteristics due to addition of more hydrogen can be explained as a combination of two mechanisms. Higher reactivity of hydrogen consumed a higher fraction of fuel fed into the cylinder, bringing the chemical reaction to a higher completion level. The additional level of improvement in both hydrocarbon and carbon monoxide emissions can be related to the higher reactivity. Additionally, faster heat release also allowed less heat loss during the combustion activity.
Figure 6.17: Mass fraction burned characteristics of methane-hydrogen mixtures at the most beneficial injection timing

The duration of flame propagation heat release ($\Delta \theta_{Qf}$) and the timing of end-gas autoignition ($\Delta \theta_{ea}$) provide the information on individual characteristics of flame propagation and end-gas autoignition timing. Detailed discussion on the characteristics of end-gas autoignition phenomenon will be discussed on chapter 8; therefore this section provides only preliminary discussion in order to clarify the aspects regarding use of methane-hydrogen mixtures. The duration of flame propagation heat release from the end-of pilot fuel autoignition heat release to the occurrence timing of end-gas autoignition is described as flame propagation heat release duration and shown in figure 6.18. This result approves the aforementioned statement that flame propagation occurs faster for the mixtures containing a higher fraction of hydrogen. This duration had an average length of 16 degrees of crank angle for pure methane, and was gradually shortened to 13 degrees of crank angle at 40%CH$_4$-60%H$_2$ fueling condition; however the variation of the flame propagation duration was not a function of hydrogen concentration. It is highly possible that the characteristics of flame kernels affected the length of this duration; the injector is operated at a condition that it was not originally designed for, due to which the flame kernel size might show some fluctuations and the propagating flames may require a longer duration to bring the end-gas mixture to autoignition condition. This also influences the end-gas autoignition delay durations and their stability, as given in figure 6.19. Similar to the duration of flame propagation heat release, this parameter is also shortened as the fraction of hydrogen in the fuel mixture is
increased from 23 to 18 degrees of crank angle. Additionally, the magnitude of variation of end-gas autoignition delay is directly related to the variation observed for duration of flame propagation heat release; a higher variation of the latter amplifies the variation of the prior. In contrast, instead of the fact that pure methane showed the second least range of variation in terms of flame propagation heat release duration, it had the highest amount of end-gas autoignition delay duration variation. Based on these two observations, it can be stated that flame propagation characteristics of a methane-hydrogen mixtures are subject to a greater level of cyclic variation dependency compared to pure methane.

Figure 6.18: Flame propagation heat release duration of methane-hydrogen mixtures at the most beneficial injection timing.
6.4.5. Determination of change of combustion and knocking characteristics with addition of hydrogen

The fact that knocking occurred with earlier injection timings indicated that a fuel mixture with higher hydrogen fraction suffers from a lower knock resistance. Knocking is triggered when the intensity of end-gas autoignition is above a certain threshold, so that it causes rapid increase of end-gas region pressure, which creates a huge pressure difference between this region and its surroundings. This is called the shocked state, and is accompanied by pressure fluctuations, as it was shown in figure 6.14 for the super knocking case. In order to confirm whether this mechanism applied to the methane-hydrogen mixtures, the maxima of rate of change of heat release rates \( (\frac{d^2Q}{d\theta^2})_{\text{max}} \) of all presented fueling and injection timing conditions are given in figure 6.20. In this figure, the maxima might refer to the maximum inclination of rate of heat release during the flame propagation or end-gas autoignition heat release stages; however this should not cause any confusion. A typical rate of heat release observed during flame propagation or its inclination is not high enough to trigger knocking under the lean mixture conditions tested in this work, and such conditions will be
relevant to the experimental cases that yielded low engine output. Based on this information, it is safe to assume that the highest result of each fueling condition is related to the end-gas autoignition stage. Looking at the results, it can be seen that maxima of this parameter was below 6.78 J/°CA² level, which was marked by pure methane, as long as the hydrogen fraction was kept below 30%. After this point, the maxima of this parameter increased as 7.26 J/°CA², 7.53 J/°CA², 8.40 J/°CA² for 60%CH₄-60%H₂, 50%CH₄-60%H₂ and 40%CH₄-60%H₂ fueling cases respectively, however it can be expected that an experimental analysis with finer injection timing intervals might change the outcome towards gradually increasing trend. Another conclusion that can be drawn from this figure is, it is possible to benefit from a more intense end-gas autoignition heat release without encountering knocking with addition of hydrogen into the fuel blend.

Figure 6.20: Maxima of rate of change of heat release rates in all fueling and injection timing conditions.

6.5. Summary of observations

In this experimental work, pilot fuel injected a gas engine is operated using pure methane and various methane-hydrogen mixtures under supercharged intake condition. The results showed that

1. Addition of hydrogen into methane improves engine performance due to increased reactivity of the fuel mixture. Addition of hydrogen both increases flame propagation speed and shortens the end-gas autoignition duration. While maximum indicated mean effective pressures are almost identical for all
gaseous mixtures, thermal efficiency is higher when mixture gases are used. This is a combined effect of reduced combustion duration, reduction of the heat released during compression stroke and a higher level of combustion completeness.

2. In-cylinder pressure levels of methane-hydrogen mixtures were gradually lower for the fuel mixtures with higher hydrogen concentration; however neither heat release nor operation efficiency characteristics were affected adversely. This reduces the stress applied on internal components of the engine.

3. Presence of hydrogen in the fuel mixture reduces cyclic variations when end-gas autoignition is weak or inexistent, but has no distinguishable benefit when PREMIER combustion is achieved.

4. Addition of H\textsubscript{2} improves carbon monoxide and unburned hydrocarbon emissions systematically. This is due to reduced amount of hydrocarbon based fuel in the cylinder mixture. Additionally, a higher level of combustion completeness consumes an additional fraction of both emission types. \text{NO}_x emissions do not change significantly, which also shows that there is no trade-off of \text{NO}_x versus carbon dioxide and unburned hydrocarbon emissions.

5. Knocking resistance of hydrogen mixtures are strongly influenced by flame propagation speed and associated heat release; however no significant drawbacks regarding engine operation were observed. Mixtures with higher hydrogen concentrations required more retarded pilot fuel injection but the duration required for occurrence of end-gas heat release is observed to happen faster when H\textsubscript{2} concentration is increased.

6. There is a distinct hydrogen concentration limit, named as critical hydrogen concentration, above which PREMIER combustion is not achievable due to abrupt occurrence of super knocking. This threshold value is found to be 60\% under the tested operating conditions, at which the in-cylinder mixture was susceptible to ignition due to hot spots that form in the combustion chamber. The benefits that can be obtained thanks to PREMIER combustion are not achievable beyond this threshold hydrogen fraction.
7. Investigation of end-gas autoignition characteristics of PREMIER combustion using methane-hydrogen mixtures

7.1. Motivation

So far, differences between knocking, PREMIER combustion and normal combustion were not discussed thoroughly [95]. Additionally, it is necessary to introduce a systematic approach to the classification of an operating condition as PREMIER combustion. The methane-hydrogen mixtures reported in this work span in a methane number range of 100 to 50, and the abundance of experimental data is found to be suitable for comparison of end-gas autoignition characteristics of given fuel mixtures in addition to clarification characteristics of PREMIER combustion in both cumulative and cyclic bases.

7.2 Summary of pressure history, rate of heat release, performance and general combustion characteristics

80 cycle averages of Pressure histories and rate of heat release (ROHR) characteristics of all methane-hydrogen mixtures are given in figure 7.1; indicated mean effective pressure and thermal efficiency characteristics are given in figure 7.2. Figure 7.1 is identical to the figure 6.11 presented in chapter 6, except the fact that 40%CH₄-60%H₂ is removed because it will not be discussed in this chapter. Figure 7.2 on the other hand, includes performance characteristics of both all tested knocking and weak engine output conditions in order to explain the transition of operation from normal- to PREMIER and PREMIER- to knocking combustion operation. The observations made on pressure histories, rate of heat release characteristics, engine output can be summarized as:

1. The injection timings shown in this figure represent the most beneficial timings, which yielded the highest thermal efficiency without encountering knocking. These conditions were also precursors to knocking conditions at given hydrogen concentrations.
2. The pressure histories indicate that the maxima of knock-free in-cylinder pressures were lower for the fuel mixtures with higher hydrogen concentration. The maximum knock-free in-cylinder pressure became lower when the fraction of hydrogen up to 30%; increasing the hydrogen fraction further does not influence the maximum attainable in-cylinder pressure as significantly, because the maxima
of in-cylinder pressure in hydrogen-rich conditions are slightly higher than the peak pressure obtained during motoring operation, which is 8.1 MPa.

3. ROHR characteristics show that the maxima of end-gas heat release peak were similar throughout the hydrogen fraction scale, with a short but measurable retardation of end-gas autoignition timings as hydrogen fraction is increased.

4. Indicated mean effective pressures of most beneficial injection timing conditions were similar throughout the hydrogen concentration range. Due to the decreased heat release before top dead center, faster heat release past top dead center timings and a higher rate of combustion completeness allowed higher maxima of thermal efficiency in knock-free operating conditions when the fraction of hydrogen in the fuel mixture is increased.
Figure 7.1: 80 cycle averages of (a) In-cylinder pressure and (b) rate of heat release at the most beneficial injection timing conditions.
Figure 7.2: (a) Indicated mean effective pressure and (b) thermal efficiency of methane-hydrogen mixtures including low engine output and knocking operating conditions.
Mass fraction burned (MFB) is a convenient tool that describes the progress of combustion. When obtaining mass fraction burned, the total amount of heat released by the provided fuel needs to be obtained by integrating rate of heat release in a crank angle timing range of ongoing heat release. The ratio of the sum of heat release until a given crank angle timing to the total amount of provided heat is the mass fraction burned. A fraction of the heat release is always lost due to engine cooling, which reduces the heat release profile accordingly. In this work, it was not possible to obtain the exact amount of heat loss from the combustion chamber and could not be accounted for in the mass fraction burned characteristics; therefore the mass fraction burned values reported in the figures will involve a certain degree of deviation from the actual values. Mass fraction burned durations of MFB(0%-10%), MFB(10%-30%) and MFB(30%-75%) are in figure 8. MFB(0%-10%) duration is an indicator of initial flame kernel characteristics and beginning of flame propagation. First of all this parameter was minimally influenced by injection timing, because it is known that pilot fuel ignition delay was consistent with a cycle-to-cycle variation range of 0.5 degrees of crank angle throughout the tested range. The results show less than 2 degrees of crank angle excluding 50%CH₄-50%H₂ fueling condition, which indicates that flame kernel behavior was consistent throughout the experiments. Secondly, higher fraction of hydrogen in the gaseous fuel mixture yields shorter MFB(0%-10%) duration due to its higher reactivity. Mass fraction burned duration from 10% to 30% informs on mostly flame propagation characteristics of the tested fuels; end-gas autoignition typically occurred slightly later in a combustion cycle, which will be discussed later. Since the initial stage of the combustion was fairly stable, its effect was minimal on MFB(10%-30%). Conditions with later pilot fuel injection timings have a longer MFB(10%-30%) duration due to lower in-cylinder pressure and temperature as a result of delayed combustion activity. Fueling conditions with higher hydrogen content have shorter MFB(10%-30%) durations within a narrower duration range due to gradually increasing flame propagation speed. MFB(10%-30%) durations of knocking and PREMIER combustion were similar, and typically faster than normal combustion in each fueling case. Additionally, addition of hydrogen systematically shortened MFB(10%-30%) durations. The increase of MFB(10%-30%) durations of fuel mixtures with higher hydrogen concentrations were not as significant in general. In case of pure methane, MFB(30%-70%) duration strongly depended on progress of combustion activity until 30% of heat is released. Excluding pure methane fueling condition, the MFB(30%-70%) durations of normal combustion cases show minimal change within their respective fueling groups. In contrast, PREMIER combustion and knocking cases have significantly shorter MFB(30%-70%). This is a result of rapid heat release at end-gas region during autoignition.
Figure 7.3: Mass fraction burned durations of (a) 0%-10%, (b) 10%-30% and (c) 30%-75%
7.3. Distinction between knocking and non-knocking cycles and a quantitative approach to definition of PREMIER combustion operation range

The distinction between knocking and non-knocking cycles can be made based on pressure histories and rate of heat release characteristics, power spectral densities of pressure histories and band-pass filtered pressure histories. These properties are given in figure 7.4(a)-(c). The first indicator of a knocking condition is the oscillation that accompanies the pressure peak of the cycle. This condition resembles the shocked state of a fluid under detonation; however pressures of burned and unburned zones could not be measured separately and it is not possible to verify this statement numerically. This aspect needs to be investigated in future studies. Rate of heat release characteristics of knocking condition inform that an early and intense end-gas autoignition activity caused this occurrence, which supports the suggestion on the possibility of detonation. Power spectral density of the knocking cycles has a peak at 10.5 kHz, which is not present in non-knocking conditions. Based on Draper’s work, it is possible to calculate knocking frequency modes under given operating conditions [106]. This was performed by Azimov et.al. in the previous work and knocking frequencies of 6.5, 10.5 and 14 KHz were observed [91]. Additionally, the band-pass filtered pressure history shows that there was a noticeably strong instantaneous pressure difference between consecutive oscillation peaks and wells; the maximum instantaneous difference of the pressure history is also called as knocking (KI) intensity in the literature [102]. Due to the presence of a low level of noise in the recorded pressure histories, knocking intensity of any cycle will be higher than zero; therefore 0.1 MPa was selected as the knocking threshold; a knocking intensity above this threshold indicates knocking. The threshold value is selected based on the noise is consistently present in pressure histories of motoring data, when there is no combustion. It should be noted that knocking intensity might exceed the threshold value of 0.1 MPa during autoignition of the pilot fuel; however this occurrence does not cause spontaneous combustion of all in-cylinder mixture and trigger pressure oscillations. In light of this observation, knocking intensities were obtained in a timing range following pilot fuel autoignition to the end of combustion activity. Compared to knocking combustion condition, neither PREMIER nor normal combustion conditions show the aforementioned abnormalities. Power spectral density of both normal and PREMIER combustion cases were free of power peaks at the filtered frequency range and the knocking intensity of 0.1 was never exceeded in the relevant crank angle timing range, which indicate that PREMIER combustion is a type of knock-free combustion.
Figure 7.4: Comparisons of (a) pressure histories and rate of heat release characteristics, (b) power spectral densities and (c) knocking intensities of knocking, PREMIER combustion and normal combustion cycles.
Number of cycles with end-gas autoignition, 80 cycle maxima of knocking intensities and number of knocking cycles are given in figure 7.5. In these figures, cross shaped markers indicate knocking operation, which was concluded based on aforementioned methodology. First of all, the number of cycles with end-gas autoignition was obtained visually by investigating rate of heat release characteristics of all 80 cycles of each data set for presence of a confirmable end-gas heat release peak. The results showed that all cycles of knocking conditions had end-gas autoignition activity, but the rest of operating conditions had at least a single cycle that was normal combustion. Secondly, there were only three operating conditions which did not have any cycles with end-gas autoignition. Occurrence of end-gas autoignition was typical throughout the operating range, which is expected to be due to the ignition strategy; flame kernels appear at three distinct and evenly spaced locations, which also clearly define the boundaries of end-gas region, as it was discussed in chapter 5. It is highly possible that using a different pilot fuel injector nozzle that yields different flame kernel coverage characteristics might change the given outcome. Expectedly, number of cycles with end-gas autoignition became lower as the injection timing was retarded; however fuel mixtures with fractions of higher hydrogen concentrations, especially fueling cases of 60%CH₄-40%H₂ and 50%CH₄-50%H₂, sustained higher number of cycles with end-gas autoignition for a wider injection timing range, which indicates that addition of hydrogen increased the probability of occurrence of end-gas autoignition. Another interesting observation made on the number of end-gas autoignition cycles is about the behavior of the results in the fraction range of 50% to 25%; in three of the fueling cases, it was possible sustain this number for a wide range of injection timings before it dropped below 10% level. Additionally, this number typically plunged from a significantly high level into this range in 5 out of 6 fueling cases. In chapter 5, it was described that an operating condition is PREMIER combustion operating condition, if at least 50% of the cycles show end-gas autoignition and none of the cycles show signs of knocking. The observation on the 50% to 25% range informs that, there is an injection timing range, in which end-gas conditions are metastable and occurrence of end-gas autoignition is controlled by the magnitude of cycle-to-cycle variations. This observation also informed that, the fluctuation of number of end-gas autoignition in some fueling cases may be a result of cycle-to-cycle variations of the end-gas region conditions as well; though this needs to be confirmed in a future study. This range is defined as normal-to-PREMIER combustion transition range. In addition to the number of cycles with end-gas autoignition, maxima of knocking intensities and number of knocking cycles in each condition are used for describing the complete PREMIER combustion operation range. Any condition that had less than 25% end-gas autoignition cycles in the data set are discarded as normal combustion.
Figure 7.5: Distinction between combustion modes: (a) the number of cycles with end-gas autoignition, (b) the maxima of knocking intensities and (c) number of knocking cycles.
PREMIER combustion operation range and normal-to-PREMIER combustion transition ranges are shown in figure 7.6. The results showed that there was a variation of both PREMIER combustion operation and normal-to-PREMIER combustion transition ranges throughout the fueling range; however the combination of these two ranges showed a steady expansion as the fraction of hydrogen was increased. The narrow ones were 1 degree of crank angle injection timing range at 100%CH₄, 80%CH₄-20%H₂ and 70%CH₄-30%H₂ fueling cases while the rest of the fuel blends had a significantly wider PREMIER combustion operation ranges. While this range was between 1 and 2.5 degrees of crank angle, it was observed that PREMIER combustion occurred for an injection timing range of 8°BTDC to 3°BTDC in 50%CH₄-50%H₂ fueling case, defining a 5 degrees of crank angle PREMIER combustion operation range. This operating condition is the precursor to the unstable fueling condition of 40%CH₄-60%H₂, which was discarded due to frequent occurrence of premature ignition and super knocking. Based on that observation, it can be concluded that the fuel mixture consisting of 50% hydrogen is the most favorable fuel mixture for sustaining PREMIER combustion. Looking at the normal-to-PREMIER combustion transition range, it can be seen that increasing the fraction of hydrogen in the fuel mixture. Additionally, the cases with narrow PREMIER combustion operation ranges yielded wider normal-to-PREMIER combustion operation ranges. These observations indicated that increasing the fuel reactivity extended the range of injection timings with which end-gas autoignition can be achieved.

Figure 7.6: PREMIER combustion operation and normal-to-PREMIER combustion transition ranges
7.4. Difference between maximum pressures and maxima of rate of pressure rise rates of knocking and non-knocking cycles

The relation between maximum in-cylinder pressure \( (P_{\text{max}}) \) and the maximum of rate of change of in-cylinder pressure with respect to crank angle \( (dP/d\theta) \) are given in Fig 7.7(a)-(f) for the six earliest injection timing conditions of the complete range fueling range. It was initially expected that knocking cycles would have both high maximum in-cylinder pressures and its derivatives with respect to crank angle movement. The results showed that this expectation was correct; however the behavior can’t be explained as a proportional increase of these two parameters. This behavior can be seen in figure 7.6(d), which indicates the difference between knocking and non-knocking operation. In non-knocking conditions, maxima of in-cylinder pressures and pressure rise rates can be correlated as a logarithmic function in a certain range if needed. This range is also observed to match with PREMIER combustion operation range reasonably well. Normal combustion operation points, on the other hand, did not follow this trend. The results of operation at retarded injection timings showed that minima of pressure rise rates tended to saturate around 0.23 MPa/°CA range, which is the maximum pressure rise rate that can be observed during motoring condition. In these cases, a significant fraction of combustion activity occurred during expansion stroke and heat release rates were not high enough to cause a level of in-cylinder pressure increase that can exceed those observed during compression. When the fraction of hydrogen is increased, this behavior became more obvious. Due to this shift of characteristics, it became easier identify the cycles with end-gas autoignition in fueling case of 50%CH\(_4\)-50%H\(_2\): pressure rise rates of such cases can be correlated to the in-cylinder pressures. In knocking cases, the sudden change of pressure rise rate is an indicator of detonation, which was confirmable due to audible knocking during experiments. In detonation, pressure difference between the burned and unburned zones is higher than the level that can sustain combustion stability. Above this range, spontaneous ignition of the unburned mixture causes instant heat release shocks the mixture of the zone that was previously unburned, increasing its pressure. The combustion chamber of an internal combustion engine is a closed system, due to which the pressure wave created at the shocked region travels inside boundaries, causing transient high and low pressure levels, which can be suggested as the reason for the aforementioned pressure oscillation. It can also be expected that these non-correlated pressure rise rates are observed at one of the pressure oscillation points. The maximum pressure rise rate without knocking was 0.565MPa/°CA for pure methane, which is the highest of all test fuel mixtures. Addition of methane reduces maximum pressure rise rate without knocking. The non-knocking pressure rise rate limits are tabulated in table 4. Additionally, averages of maximum pressures vs maximum pressure rise rates is summarized and given in figure 7.8.
Figure 7.7: Maxima of in-cylinder pressures vs. maxima of rate pressure rise rates.
7.5. Confirmation of end-gas combustion behavior using Livengood-Wu integrals.

Livengood-Wu integrals method is approaches the problem of estimation of end-gas autoignition timing as a similitude of rate of chemical reaction, which is a convenient tool for discussing whether or not the end-gas combustion activity is actually autoignition; if observed end-gas autoignition timings and estimations made by Livengood-Wu integrals have good agreement, it can be used as an evidence [107]. In recent studies, constant temperature ignition delays ($\tau$) of fuels are correlated in certain pressure ranges as a function of temperature and molar concentration of species as:

$$\tau = A[fuel]^x [O_2]^y \exp(-E/RT)p^n$$  \hspace{1cm} (7.1)
Values of A, E and n are obtained from reference and given in table 7.2 [110-113]. We used three end-gas autoignition timings: the actual timings observed in rate of heat release characteristics, Livengood-Wu integral method estimates using the parameters suggested by Gersen et.al, and a second estimate using a database of constant temperature ignition delays obtained by CHEMKIN [108]. The correlation published by Gersen et.al is found to be the most suitable one for our work due to reasonably high applicable pressure range. Gersen et.al. correlate ignition delays of methane-hydrogen mixtures as:

\[ \tau = A \left( \frac{P_c}{T_c} \right)^n \exp \left( \frac{-E_a}{RT} \right) \]  
\[ \tau_{mix} = \tau_{H_2}^{\beta} \tau_{CH_4}^{1-\beta} \]

\( P_c \) and \( T_c \) refer to pressure and temperature prior to start of combustion and \( \beta \) is fraction of hydrogen in a methane-hydrogen mixture; A, n and \( E_a \) are empirically obtained at an equivalence ratio of \( \phi=0.5 \) in a rapid compression machine. The coefficients of equations 7.2 and 7.3 are given in table 7.3. Pressure levels in current work exceed those suggested by Gerber et.al as well; therefore a certain amount of deviation is expected. Autoignition delay times of the fuel compositions are obtained using CHEMKIN in the temperature range of 800K to 2200K with 50K of intervals and pressure range of 1MPa to 16MPa with 0.5MPa of intervals. This is used as a database, and intermediate values are obtained by linear interpolation. Actual end-gas autoignition timings are obtained from rate of heat release results by visual confirmation. In Livengood-Wu integral method, the differential time is divided by constant temperature ignition delay of end-gas mixture under given conditions, which gives instantaneous completion rate of pre-ignition reaction. These values are integrated until the resultant value reaches at 1, which indicates occurrence of autoignition. When obtaining unburned gas temperatures, it was assumed that the in-cylinder temperature increased by 20K and 60 K above the intake temperature using CHEMKIN database and Gersen's correlation respectively. These assumptions are reasonable, considering that intake valve close time is 135 degrees before top dead center. 80 cycle averages of actual end-gas autoignition timings, CHEMKIN database and Gersen's correlation estimates and the range of errors each estimate yielded are given in figure 7.9. Error bars given in the figures indicate the maxima of deviation of Livengood-Wu integral results from the actual end-gas autoignition timings, in degrees of crank angle. End-gas autoignition estimations based on CHEMKIN database and actual timings are in a good agreement. The maxima of deviation of this method are -2.2°CA and 2.1°CA, minus sign indicating underestimation. In average, CHEMKIN database underestimates end-gas autoignition timing by 0.55°CA. Ignition delays estimated based on the reference work and the actual values are in a reasonable
agreement for all cases with earlier injection timings and all cases using 100% methane; however later injection timing and higher fraction of hydrogen in the fuel mixture yield a larger deviation. Compared to CHEMKIN database, this method is inclined towards overestimating end-gas autoignition timings. The accuracy of estimations can't be commented on for the cases with low number of cycles with end-gas autoignition. The good agreement between estimation methods and actual timings for cases with earlier injection timings indicates that the end-gas activity is indeed autoignition, and it is possible to estimate its timing.

Figure 7.8: Average End-gas autoignition timings, their estimations and the deviation between actual and estimated errors.
### Table 7.2: Constant pressure ignition delay correlation parameters from the literature

<table>
<thead>
<tr>
<th>Reference work</th>
<th>Fuel type</th>
<th>Pressure Vol %</th>
<th>Temperature</th>
<th>x</th>
<th>y</th>
<th>A</th>
<th>$E_a$</th>
<th>x+y</th>
<th>kJ/mol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Petersen et.al. [110]</td>
<td>CH$_4$</td>
<td>4-26</td>
<td>&gt;1300</td>
<td>-0.2</td>
<td>-1.20</td>
<td>1.26E-14</td>
<td>32.7</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Petersen et.al. [110]</td>
<td>CH$_4$</td>
<td>4-26</td>
<td>&lt;1300</td>
<td>-0.38</td>
<td>-1.31</td>
<td>4.99E-14</td>
<td>19.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Cheng and Oppenheim [111]</td>
<td>CH$_4$</td>
<td>0.1-0.3</td>
<td>1600-2200</td>
<td>0.48</td>
<td>-1.94</td>
<td>1.19E-18</td>
<td>46.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Tsuboi and Wagner [112]</td>
<td>CH$_4$</td>
<td>0.2-0.3</td>
<td>1200-2100</td>
<td>0.32</td>
<td>-1.02</td>
<td>2.50E-15</td>
<td>53.0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>White and Moore [113]</td>
<td>H$_2$</td>
<td>0.4-1.0</td>
<td>800-2000</td>
<td>-0.33</td>
<td>-0.66</td>
<td>1.58E-11</td>
<td>17.19</td>
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<td></td>
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<tr>
<td>Cheng and Oppenheim [111]</td>
<td>H$_2$</td>
<td>0.1-0.3</td>
<td>800-2400</td>
<td>0.145</td>
<td>0.56</td>
<td>1.54E-14</td>
<td>17.20</td>
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</tr>
</tbody>
</table>

Table 7.3: Coefficients of Methane-hydrogen mixture ignition delays suggested by Gersen et.al. []

<table>
<thead>
<tr>
<th>Fuel</th>
<th>A</th>
<th>n</th>
<th>$E_a$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>s(cm$^3$/mol)</td>
<td>kJ/mol</td>
<td></td>
</tr>
<tr>
<td>CH$_4$</td>
<td>3.23E-2</td>
<td>-2.1</td>
<td>336</td>
</tr>
<tr>
<td>H$_2$</td>
<td>2.82E-13</td>
<td>-1.3</td>
<td>192</td>
</tr>
</tbody>
</table>

#### 7.6. End-gas autoignition characteristics of methane-hydrogen mixtures in PREMIER combustion

The parameters used for quantitative description of PREMIER combustion are shown in figure 7.10. Several of these parameters were suggested as indicators of end-gas autoignition in previous works [91, 96]. In this work, the range of parameters that can be obtained from rate of heat release characteristics is extended, based on which further discussion will be performed. In this figure, injection timing, pilot fuel ignition timing and end-gas autoignition timing can be obtained without any confusion: injection timing is a controlled parameter, and both pilot fuel ignition timing ($\theta_{inj}$) and end-gas autoignition timing ($\theta_{ea}$) can be derived from the inflection points seen in a typical rate of heat release curve. In contrast, it can occasionally be tricky to determine the exact timing of end of end-gas autoignition heat release, because these points are not as well-defined in weak PREMIER combustion cycles; therefore such conditions may contain a certain degree of error on the oncoming discussions. Pilot fuel ignition delay duration is conventionally accepted as the duration from the injection to the start of pilot fuel heat release. In this work, this parameter did not vary across the fueling range or injection timing range and no measurable influence on end-gas autoignition. 149
characteristics; therefore it will not be discussed. End-gas autoignition delay ($\tau_{ea}$) is defined as the duration from the start of combustion, which is ignition timing of the pilot fuel, to the timing of end-gas autoignition. Following is the end-gas autoignition duration ($\Delta \theta_{ea}$), which starts at the end-gas autoignition timing and continues until the end of end-gas heat release and during which the corresponding heat release takes place. The straight line that separates end-gas autoignition heat release region from the rest is assumed to be an imaginary flame propagation heat release profile, and is obtained by connecting the rate of heat release values at the start and the end of this duration; however this is an approximation and its precision needs to be discussed in a future study. The amount of heat release before occurrence of end-gas autoignition is also referred to as mass fraction burned (MFB) before end-gas autoignition. It should be noted that this parameter is not corrected for the amount of heat loss, since it is not possible to determine the amount of heat loss accurately. Finally, the amount of heat release by end-gas autoignition ($Q_{ea}$) is the parameter that will be used for discussing the end-gas region volumes comparatively.

Figure 7.10: Graphical representation of the parameters that describe PREMIER combustion.

Averages of mass fraction burned (MFB) until occurrence of end-gas autoignition is given in figure 7.10. The results reported in this figure include only the cycles with occurrence of end-gas autoignition; the remaining cases were omitted. There are two conclusions that can be drawn these results. First of all, it was not possible to achieve PREMIER combustion if the end-gas autoignition did not occur until 35% of the in-cylinder mixture was consumed, excluding 50%CH₄-50%H₂ fueling case. The occurrence of end-gas autoignition relies on the heat release from the prior combustion activity, which increases and sustains the pressure and temperature
of the unburned mixture. At this point, it is also possible that the conditions at the end-gas regions deteriorate due to decreasing pressure at a later stage of expansion stroke. It can be concluded that the mass fraction burned of 37% is an indirect indicator of such an occurrence. Focusing on 50%CH₄-50%H₂ fueling case, it was possible that the normal-to-PREMIER combustion transition range could have been sustained for a longer injection timing interval; however it was not tested because the cases with start of combustion timings of after top dead center typically yield unstable combustion activity. The lowest mass fraction burned before end-gas autoignition of mixtures with higher hydrogen fractions were gradually lower. Due to increased end-gas reactivity, it was possible to trigger autoignition at a lower temperature, which allowed occurrence of PREMIER combustion with a higher flexibility. In the literature, knocking resistance of a gaseous fuel is evaluated by its tendency to undergo autoignition under premixed conditions; however occurrence of usable end-gas autoignition in this system informs that this definition needs to be improved. It is true that hydrogen, one of the least knock-resistant gaseous fuels, undergoes knocking more easily; however it also undergoes knock-free autoignition in a premixed mixture for a wider range of operating conditions compared to methane. As a conclusion, it was observed that pure methane needed to be ignited earlier in order to achieve end-gas autoignition due to its high knocking resistance; addition of hydrogen improved autoignition characteristics of the mixture, widening the range of conditions that allow usable end-gas autoignition. While the effect of cyclic variations caused a noticeable degree of fluctuation, the fraction of hydrogen in the fuel mixture was typically proportional to the extent of mass fraction burned before end-gas autoignition range.

Figure 7.10: Mass fraction burned before occurrence of end-gas autoignition.
Cycle averages of end-gas autoignition timings (θ_{ea}) and end-gas autoignition delays (τ_{ea}) are given in figure 7.11. In this dual fuel gas engine, end-gas autoignition timing is typically decided based on the pilot fuel injection timing for a given operating condition. As stated previously, both the injection delay and the flame kernel properties are stable enough to state that the initial state of combustion is not a parameter that influenced the results of this works. Under the given circumstances, the earliest end-gas autoignition timings of PREMIER combustion operation were observed as 8.5°ATDC for pure methane, 9.5°ATDC for 90%CH₄-90%H₂ and 11°ATDC for the rest of the cases. The retardation of the earliest average end-gas autoignition timing without knocking and hydrogen concentration of the fuel mixture was proportional; however the effect of hydrogen composition had minimal influence. The earliest end-gas autoignition can be related to the cylinder volume expansion rate. It is known that the expansion rate of the volume and the increase of pressure due to quick heat release are two forces that counteract each other during the expansion stroke, regardless of the operating condition. When the expansion rate of the volume is fast enough to keep a possible pressure rise due to rapid heat release of the end-gas autoignition activity, knocking can be avoided. As shown in figure 7.10, a smaller fraction of premixed mixture is consumed during flame propagation in fuel mixtures with higher hydrogen concentrations, leaving a larger volume for autoignition. This scenario brings forth the requirement of a higher expansion rate in order to avoid knocking. Secondly, End-gas autoignition delay is shorter for mixtures with higher hydrogen fractions. This is a result of difference in the amount of heat release during flame propagation stage. Flame propagation speed of hydrogen is faster than methane; therefore the duration required for end-gas region mixture to reach autoignition state will be shorter for the fuel mixtures with higher hydrogen fractions. While the injection timing needed to be retarded to prevent the engine from knocking, enhanced reactivity of the fuel mixtures with higher hydrogen concentrations yielded systematically shorter end-gas autoignition delay times. Additionally, the range of end-gas autoignition timing is wider for fuel mixtures with higher hydrogen concentrations. This outcome can be commented as a combination of higher reactivity of hydrogen and a larger unburned end-gas volume later in the cycle. Improved heat release characteristics of hydrogen due to higher reactivity means that it is possible to overcome a higher volumetric expansion rate and preserve the conditions required for occurrence of end-gas autoignition long enough to allow end-gas autoignition. While increasing expansion rate will slow down the heat release measurably, mixtures with higher hydrogen fractions can sustain the required condition until a later timing. Since the end-gas volume is slightly larger, a longer duration is required for the propagating flames to consume this region, which will require gradually longer times at the later stages of the expansion stroke.
Figure 7.12: End-gas autoignition timings and delays
Currently, there is a need for quantification of PREMIER combustion based on its end-gas heat release characteristics. In order to achieve this goal, a new scale, named as PREMIER combustion index (PI) is introduced as:

\[
P_I = \frac{100 \times (Q_{ea}/Q_{total})}{\Delta \theta_{egai}}
\]

In this formula, the \( Q_{total} \) refers to the total energy input of fuels based on their higher heating values. The relation between the percentage of heat released by end-gas autoignition and end-gas autoignition heat release duration is used due to its resemblance of indicated mean effective pressure, as this parameter indicates the amount of heat released per unit time during this combustion activity. Averages of end-gas autoignition heat release durations, end-gas autoignition heat release amounts and PREMIER combustion indices are given in figure 7.13. End-gas autoignition heat release duration was typically longer than 10 degrees of crank angle for all cases, and between 12 to 16 degrees of crank angle for the most intense PREMIER combustion cases tested in this work. Theoretically autoignition is defined as an instantaneous phenomenon; however practical cases indicated a rather gradual behavior. The first reason is the geometrical aspect of the combustion process in this particular set-up: the sprays create three flame kernels, and the areas between these kernels are the three end-gas regions. Minute differences between flame propagation characteristics will cause variation between the temperatures in these regions, which will alter their separate autoignition timings. Once one site autoignites, the average pressure and temperature will increase, promoting autoignition at the other sites as well. This short timing difference extended end-gas heat release duration and suppressed knocking. The second reason is a possible temperature gradient at the end-gas regions. The temperature of end-gas regions can safely be expected to be the highest in the vicinity of the flame front and the lowest around cylinder walls. This gradient also dictates that the autoignition reaction completion rate is different throughout an end-gas region as well. Additionally, one can expect a certain degree of inhomogeneity and local variation of equivalence ratio. When autoignition occurs at single spot, it triggers the rest of the region. This behavior resembles flame propagation; however it occurs at a significantly faster speed. The combination of these conditions extended the end-gas autoignition heat release duration, which is also one of the reasons knocking can be avoided. The amount of heat release without knocking increased gradually from 466 J for pure methane to 567 J for 50%CH\textsubscript{4}-50%H\textsubscript{2}. Values of this parameter decreased almost linearly in their respective groups as injection timing is retarded. End-gas autoignition heat
release duration was longer for the fuel mixtures with higher hydrogen fractions. Heating value of methane is more than 3 times of heating value of hydrogen; therefore a mixture with higher hydrogen concentration will occupy a bigger volume for the same heat content; a larger volume will take longer heat release duration until heat release is completed. End-gas autoignition heat release duration is typically longer and the amount of heat release is lower when injection timing is retarded, because the reactivity of the mixture will be slower during a faster rate of volumetric expansion. If the end-gas autoignition conditions are satisfied even later, then the majority of the premixed mixture will be consumed by propagating flames, leaving a smaller portion to be autoignited. In this particular case, the duration of end-gas autoignition heat release will be shorter due to smaller end-gas volume. This might also indicate that not all of the three end-gas regions undergo autoignition. This behavior is especially significant for operating conditions with less than 25% of its cycles showing PREMIER combustion behavior. In these cycles, the end of end-gas autoignition is not an indicator of a definitive end of combustion activity. Combining these two parameters in PREMIER intensity index in figure 7.13(c), it can be seen that the aforementioned weak PREMIER combustion cases display the lowest values in their respective groups, excluding pure methane fueling condition. In addition, the cases that include more than 50% of end-gas autoignition cycles in its data set show a higher PI value, which increases almost exponentially as the number of PREMIER combustion cycles increase. Knocking cycles allocate the peak values in their respective data set. Premier combustion indices of the operating conditions cases that were precursors of knocking were in the vicinity of 1.6 for the fueling cases of case of 100%CH₄, 90%CH₄-10%H₂ and 50%CH₄-50%H₂, which shows that this value can be used as a threshold. The rest of the cases showed poor engine output due to experimental uncertainties, which also reflected to the end-gas autoignition characteristics. The similarity between PREMIER combustion indices of the three cases of the prior cases showed that, occurrence of knock is irrelevant to the fuel type; instead, the intensity of end-gas autoignition, its duration and the expansion rate of the cylinder decide whether or not knocking occurs. It should be noted that the range of expansion rate of the combustion chamber is 1.5 cm³/°CA for the most intense knocking cases, in the range of 2.25 to 3.5 cm³/°CA for PREMIER combustion cases and between 3.5 to 6.5 cm³/°CA for the rest of the cases throughout the work.
Figure 7.13: End-gas autoignition characteristics: (a) end-gas autoignition heat release durations, (b) end-gas autoignition heat release and (c) PREMIER combustion indices.
7.7. Summary of observations

In this work, a pilot fuel ignited dual fuel engine is operated with methane-hydrogen mixtures with methane numbers spanning from 100 to 50. A detailed data analysis is performed in order to investigate end-gas autoignition characteristics. The following observations are made:

- The reasonable agreement between Livengood-Wu integral using two different ignition delay estimation methods and actual timings of start of rapid heat release support the proposition that this combustion activity is autoignition in the end-gas region. The absence of rapid pressure rise and pressure oscillations during PREMIER combustion operation indicates that it is distinctive from knocking.
- Heat release occurs faster for cycles with end-gas autoignition. A higher number of cycles with end-gas autoignition in an operating condition yield a higher thermal efficiency due to shorter combustion duration.
- The earliest end-gas autoignition timing without knocking is not influenced by fuel type significantly. Higher flame propagation characteristics of fuel mixtures with higher hydrogen fractions reach at end-gas autoignition condition faster; therefore later start of combustion is required. Faster flame propagation and heat release is the reason behind the increase of thermal efficiency for fuel mixtures of higher hydrogen contents.
- Lower heating value of hydrogen extends the duration of end-gas autoignition heat release by increasing the end-gas mixture volume. This also allows a larger fraction of the in-cylinder mixture to be consumed by autoignition without encountering knocking.
- While fuel mixtures with higher hydrogen fractions have inferior knock resistance in terms of maximum in-cylinder pressure and its derivative, the operation range with usable end-gas autoignition is wider. The end-gas volume of such fuel mixtures is larger and the amount of end-gas heat release is higher. Due to these advantages, thermal efficiency can be improved while maintaining the engine output.
8. Conclusions

In this study, a pilot fuel injected dual fuel gas engine is operated using various gases. Engine performance, exhaust emissions and combustion characteristics are evaluated by the results of performance tests and visualization studies. The following conclusions are drawn:

1. Split pilot fuel injection can be used to suppress knocking to obtain PREMIER combustion by delaying the growth of flame kernels and reducing their size. This increases the time required for propagating flames to consume unburned gaseous fuel and air mixture, and retards the overall progress of combustion. The maxima of feasible engine output and thermal efficiency are extended when knocking is suppressed and PREMIER combustion is achieved. The maximum values were similar to those observed during knocking operation.

2. Split pilot fuel injection can be used to promote normal combustion to PREMIER combustion by widening flame kernels and accelerating their rate of growth. As a result, a larger volume of gaseous fuel and air mixture is consumed earlier, which increases the unburned mixture pressure and temperature faster and earlier. Split injection significantly improves indicated mean effective pressure and thermal efficiency by converting normal combustion to PREMIER combustion. Additionally, it increases the probability of the occurrence of end-gas autoignition when a certain normal combustion operating condition is a precursor to PREMIER combustion.

3. The range of operating conditions that can be converted to PREMIER combustion by split fuel injection is limited. Heavy knocking or normal combustion with low engine output cannot be converted to PREMIER combustion.

4. When the end of delivery of the second injection coincides with the appearance of flame kernels, spray penetration supports flame kernel development by increasing both the sizes and growth speeds. When second injection starts before full development of flame kernels, the sprays and kernel initiation zones interact and produce larger flame kernels than is achievable with single injection. When the flame kernels are partially grown during injection, the final size and growth rate of the flame kernels are affected adversely. When the second injection occurs after full growth of the flame kernels formed by the first injection, a fraction of the second spray is consumed in the vicinity of the injector and the kernels grow towards the injector. Consequently, final size of flame kernels is restricted, and their growth is slower, and the fraction consumed around the injector does not provide any input to propagating flames.
5. Addition of hydrogen into methane improves engine performance due to increased reactivity of the fuel mixture. Addition of hydrogen both increases flame propagation speed and shortens the end-gas autoignition duration. While maximum indicated mean effective pressures are almost identical for all gaseous mixtures, thermal efficiency is higher when mixture gases are used. This is a combined effect of reduced combustion duration, reduction of the heat released during compression stroke and a higher level of combustion completeness.

6. In-cylinder pressure levels of methane-hydrogen mixtures were gradually lower for the fuel mixtures with higher hydrogen concentration; however neither heat release nor operation efficiency characteristics were affected adversely. This reduces the stress applied on internal components of the engine.

7. Presence of hydrogen in the fuel mixture reduces cyclic variations when end-gas autoignition is weak or inexistent, but has no distinguishable benefit when PREMIER combustion is achieved.

8. Addition of H₂ improves carbon monoxide and unburned hydrocarbon emissions systematically. This is due to reduced amount of hydrocarbon based fuel in the cylinder mixture. Additionally, a higher level of combustion completeness consumes an additional fraction of both emission types. NOₓ emissions do not change significantly, which also shows that there is no trade-off of NOₓ versus carbon dioxide and unburned hydrocarbon emissions.

9. Knocking resistance of hydrogen mixtures are strongly influenced by flame propagation speed and associated heat release; however no significant drawbacks regarding engine operation were observed. Mixtures with higher hydrogen concentrations required more retarded pilot fuel injection but the duration required for occurrence of end-gas heat release is observed to happen faster when H₂ concentration is increased.

10. There is a distinct hydrogen concentration limit, named as critical hydrogen concentration, above which PREMIER combustion is not achievable due to abrupt occurrence of super knocking. This threshold value is found to be 60% under the tested operating conditions, at which the in-cylinder mixture was susceptible to ignition due to hot spots that form in the combustion chamber. The benefits that can be obtained thanks to PREMIER combustion are not achievable beyond this threshold hydrogen fraction.

11. The reasonable agreement between Livengood-Wu integral using two different ignition delay estimation methods and actual timings of start of rapid heat release support the proposition that this combustion activity is autoignition in the end-gas region. The absence of rapid pressure rise and
pressure oscillations during PREMIER combustion operation indicates that it is distinctive from knocking.

12. Heat release occurs faster for cycles with end-gas autoignition. A higher number of cycles with end-gas autoignition in an operating condition yield a higher thermal efficiency due to faster heat release.

13. The earliest end-gas autoignition timing without knocking is not influenced by fuel type significantly. Higher flame propagation characteristics of fuel mixtures with higher hydrogen fractions reach at end-gas autoignition condition faster; therefore later start of combustion is required. Faster flame propagation and heat release is the reason behind the increase of thermal efficiency for fuel mixtures of higher hydrogen contents.

14. Lower heating value of hydrogen extends the duration of end-gas autoignition heat release by increasing the end-gas mixture volume. This also allows a larger fraction of the in-cylinder mixture to be consumed by autoignition without encountering knocking.

15. While fuel mixtures with higher hydrogen fractions have inferior knock resistance in terms of maximum in-cylinder pressure and its derivative, the operation range with usable end-gas autoignition is wider. The end-gas volume of such fuel mixtures is larger and the amount of end-gas heat release is higher. Due to these advantages, thermal efficiency can be improved while maintaining the engine output.
References


171