On the combustion of premixed natural gas/gasoline dual fuel blends in SI engines

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On the Combustion of Premixed Natural Gas-Gasoline Dual Fuel Blends in SI Engines

Sotiris Petrakides

A Doctoral Thesis

Submitted for the Degree of Doctor of Philosophy

Faculty of Aeronautical and Automotive, Chemicals and Materials Engineering
Loughborough University

October 2016

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Executive Summary

The continuous update of challenging emission legislations has renewed the interest for the use of alternative fuels. The low carbon content, the knocking resistance, and the abundance reserves, have classified natural gas as one of the most promising alternative fuels. The major constituent of natural gas is methane. Historically, the slow burning velocity of methane has been a major concern for its utilisation in energy efficient combustion applications.

As emphasized in a limited body of experimental literature, a binary blend of methane and gasoline has the potential to accelerate the combustion process in an SI engine, resulting in a faster combustion even to that of gasoline. The mechanism of such effects remains unclear. This is partially owned to the inadequate prior scientific understanding of the fundamental combustion parameters, laminar burning velocity ($S_{u0}$) and Markstein length ($L_b$), of a gasoline-natural gas Dual Fuel (DF) blend. The value of $L_b$ characterises the sensitivity of the flame to stretch. The flame stretch is induced by aerodynamic straining and/or flame curvature.

The current research study has therefore being concerned on understanding the combustion mechanism of premixed gasoline - natural gas DF blends both on a fundamental as well as practical SI engine level. The understanding on the contribution of $S_{u0}$ and $L_b$ to the velocity of a stretched laminar propagating flame has been extended through numerical analysis. A conceptual analysis of the laminar as compared to the SI engine combustion allowed further insights on the effect of turbulence to the mass burning rate of the base fuels.

On a fundamental level, the research contribution is made through the quantification of the response of $S_{u0}$ and $L_b$ with the ratio of methane to PRF95 (95%vol liq iso-octane and 5%vol liq n-heptane) in a DF blend. Methane has been used as a surrogate for natural gas and PRF95 as a surrogate for gasoline. Constant volume laminar combustion experiments have been conducted in a cylindrical vessel at equivalence ratios of 0.8, 1, 1.2, initial pressures of 2.5, 5, 10 Bar, and a constant temperature of 373 K. Methane was added to PRF95 in three different energy ratios 25%, 50% and 75%. Spherically expanding flames visualised through schlieren photography were used to derive the values of $L_b$ and $S_{u0}$. It has been concluded that for pressures relevant to SI engine operation (>5bar) and stoichiometric to lean Air Fuel Ratios (AFRs), there is a positive synergy for blending methane to PRF95 due to the convergence of $L_b$ of the blended fuel towards that of pure gas and $S_{u0}$ towards that of pure liquid.

In an SI engine environment, the research contribution is made through the characterisation and scientific understanding of the mechanism of DF combustion, and the importance of flame-
Executive Summary

stretch interactions at various engine operating conditions. Optical diagnostics have been integrated with in-cylinder pressure analysis to investigate the mechanism of flame velocity and stability with the addition of natural gas to gasoline in a DF blend, under a sweep of engine load (Manifold Absolute Pressure = 0.44, 0.51, 0.61 Bar), speed (1250, 2000, 2750 RPM) and equivalence ratio (0.8, 0.83, 1, 1.25). Consisted with the constant volume experiments, natural gas was added to gasoline in energy ratios of 25%, 50% and 75%. It has been concluded that within the flamelet combustion regime the effect of $L_b$ is dominating the lean burn combustion process both from a flame stability and velocity prospective. The effect of $S_u^0$ on the combustion process gradually increases as the AFR shifts from stoichiometric to fuel rich values.

For stoichiometric to fuel lean mixtures, the effect of turbulence on the increase of the mass burning rate is on average 13% higher for natural gas as compared to gasoline. The higher turbulence sensitivity of natural gas is attributed to its lower $L_b$ value.
I would like to express my honest appreciation to my Ph.D supervisor, Prof. Rui Chen for his support, advice and encouragement throughout my research. The privilege of conducting an independent research would not be possible without the confidence that Prof. Chen showed to my face, and the financial support from the department of Aeronautical and Automotive Engineering at Loughborough University. I would also like to express my thanks to Prof. Martin Passmore for his contribution on securing my departmental private studentship.

It is amazing what you can accomplish by having such family and friends. Parents, this work would never being possible without your immeasurable support at all levels. Most importantly, thank you for giving me values and ideals. I am grateful to you. Brother, I admire you, just that. I will make anything necessary to pay the faith you have shown to me.

I am feeling so blessed having true friends like you by my side.

To my Chinese colleagues, in particular to Dongzhi Gao, thanks for spending endless hours in the lab with me back in Tianjin, China. I really appreciate it.

And to the one and only, Evanthia thank you for bringing love and happiness into my life. You have everything that I ever dreamed of. This work is dedicated to you…
Journal Publications

The following journal publications have been achieved in relation to the present research in the current thesis.


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<td>Dual Fuel</td>
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<td>SI</td>
<td>Spark Ignited</td>
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<td>PRF</td>
<td>Primary Reference Fuel</td>
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<td>RPM</td>
<td>Revolutions Per Minute</td>
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<td>AFR</td>
<td>Air to Fuel Ratio</td>
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<td>MFB</td>
<td>Mass Fraction Burned</td>
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<td>Green House Gas Emissions</td>
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<td>OEM</td>
<td>Original Equipment Manufacturer</td>
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<td>BMEP</td>
<td>Brake Mean Effective Pressure</td>
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<td>Standard Temperature and Pressure</td>
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<td>Brake Specific Fuel Consumption</td>
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<td>MAF</td>
<td>Mass Air Flow</td>
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<td>m/s</td>
<td>Stretched Burning Velocity</td>
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<td>Pressure</td>
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<td>-</td>
<td>Specific Heat Ratio</td>
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<td>$T_{ad}$</td>
<td>K</td>
<td>Adiabatic Temperature</td>
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<tr>
<td>$T_u$</td>
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<td>Unburned Gas Temperature</td>
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<tr>
<td>$c_p$</td>
<td>J/kgK</td>
<td>Specific Heat at Constant Pressure</td>
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<td>Molar Fraction</td>
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<tr>
<td>$D$</td>
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<tr>
<td>$A_T$</td>
<td>m$^2$</td>
<td>Turbulent Flame Surface Area</td>
</tr>
<tr>
<td>$u_t$</td>
<td>m/s</td>
<td>Turbulent Burning Velocity</td>
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List of Symbols

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<thead>
<tr>
<th>Symbol</th>
<th>Unit</th>
<th>Description</th>
</tr>
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<tr>
<td>$\rho_u$</td>
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<td>Unburned Gas Density</td>
</tr>
<tr>
<td>$\rho_b$</td>
<td>Kg/m$^3$</td>
<td>Burned Gas Density</td>
</tr>
<tr>
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<td>-</td>
<td>Turbulent Stretch Factor</td>
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<tr>
<td>$Y_T$</td>
<td>-</td>
<td>Turbulent Instability Factor</td>
</tr>
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<tr>
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<td>Kg</td>
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<tr>
<td>$\tilde{\omega_R}$</td>
<td>m/s</td>
<td>Scaled Burned Gas Velocity</td>
</tr>
<tr>
<td>$\tilde{\sigma}$</td>
<td>m/s</td>
<td>Average standard deviation</td>
</tr>
<tr>
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<tr>
<td>$R_w$</td>
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</tr>
<tr>
<td>$dQ_{ch}$</td>
<td>J/s</td>
<td>Heat Release Rate</td>
</tr>
<tr>
<td>$K_{Turb}$</td>
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</tr>
<tr>
<td>H/C</td>
<td>-</td>
<td>Hydrogen to Carbon Ratio</td>
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Chapter 1

1 Introduction

The current chapter introduces the principal cause and the ultimate purpose of undertaking a research on natural gas and gasoline dual fuelling in SI engines. Besides, the novel contributions and the outline of the current thesis are presented.

1.1 Motivation

Environmental impacts of greenhouse gas emissions (GHG), as well as future air quality, are forcing governmental bodies to continuously updating their legislations adapting challenging emission standards. In particular, according to the official records published by the international council of clean transportation presented in Figure 1.1 [1], the global CO₂ emissions have to be reduced on average by about 30% from the last enacted targets.

At present, the global growing interest for clean, energy efficient transport solutions has been highlighted numerous times. This is inherently linked with the ability of OEM’s to develop, manufacture and sell powertrains [2]. The compliance with strict emission standards, in parallel with further enhancements of fuel efficiency and overall performances seems a challenging yet critical milestone for the internal combustion engine research.
Alternative fuels have a central contribution towards compliance with future emission legislations. It is not accidental that the use of natural gas has shown an exponential increase in recent years. From a combustion prospective, the low carbon content and the superior anti-knock characteristics have classified natural gas as one of the most promising alternative fuels. In addition, natural gas is an abundant hydrocarbon. With the recent discoveries of shale gas, there is an increasing number of nations that tend to be characterised as oil-short and gas-rich [3]. In the majority of those nations the gas prices are held low as a matter of public policy and the use of natural gas in domestic applications and public transport are mandatory for energy security purposes. Consequently, the shift towards the utilisation of natural gas in future energy efficient combustion applications is further enhanced especially within oil short and gas rich nations.

Following the prior discussions, it is obvious that there is a positive synergy towards the use of natural gas in the future transportation sector. In the short to medium term, natural gas is expected to expand and establish as a clean alternative fuel in the automotive market with more than 65 million natural gas vehicles out in the roads by 2020 [4]. However, the slow burning velocity of natural gas in parallel with the reduction in volumetric efficiency from its port injection in SI engines are still challenges to be faced for its efficient utilisation in future internal combustion engines.
In a normal driving scenario, substantial reductions in fuel consumption can be achieved by engine downsizing philosophy. The main philosophy relies on an increased power density of a lower capacity engine through excessive inlet charging. That leads to an improved mechanical efficiency and indirect reductions in the overall pumping losses over its higher capacity naturally aspirated counterpart. Due to the effects of unburned gas auto-ignition, commonly called knock, the extent at which SI engines can be downsized is combustion limited. Besides, as a consequence of momently low volumetric efficiency, transient performances and low speed torque are also distinct challenges to be faced by a downsized engine.

A Dual Fuel (DF) strategy of natural gas and gasoline is intended to mitigate knock at high loads while minimizing the momently low volumetric efficiency and thus maintaining the transient and low speed performances of the engine. The main principle is to exploit the knocking resistance of natural gas, and the density as well as the latent heat of vaporization of gasoline. Consequently, a positive synergy can be generated between the two fuels for optimizing the downsized engine operation.

Interestingly, as pointed out from a limited body of experimental literature [5][6], during dual fuel operation, the burning rate in an SI engine increases even in comparison to that of gasoline. This is a critical experimental finding as it can partially solve the historic problem of the slow burning velocity of natural gas. However, the combustion mechanism that governs the mentioned experimental findings still remains unclear. Consequently, a comprehensive research on the combustion mechanism of natural gas and gasoline dual fuel blends is presented in the current thesis on a fundamental and practical SI engine level.

1.2 Aim & Objectives

The current thesis aims to establish a structured scientific understanding on the basis of fundamental combustion characteristics for the combustion mechanism of binary blends of natural gas and gasoline in SI engines. The objectives of this research are listed below:

- Constant volume premixed laminar combustion experiments needs to be undertaken to derive the fundamental combustion characteristics, burning velocity ($S_u^0$) and Markstein Length ($L_b$), of the blended as well as the base fuels. Besides, the mass burning rate of the tested fuels has to be initially investigated through pressure analysis in laminar combustion conditions.
Introduction

- Extend the understanding on the contribution of $S_0$ and $L_0$ to the velocity of a stretched propagating flame through a numerical analysis at various simulated conditions.
- The derived fundamental knowledge has to be applied to scientifically understand the dual fuel combustion mechanism in SI engines. The dual fuel combustion mechanism needs to be analysed through an extensive experimental campaign in an SI engine.
- The transition mechanism characterising the difference in burning rate from the constant volume to the engine combustion needs to be investigated especially with the addition of gasoline to natural gas at different equivalence ratios. Such investigation can provide further insights for the effect of turbulence on the mass burning rate.

Following the outcomes of this research, some recommendations for future work in the area of dual fuel combustion both on a fundamental as well as SI engine level are provided.

1.3 Novel Contributions

The key novel contributions arising from the current research study are listed below:

- The fundamental combustion characteristics of the blended as well as the base fuels have been quantified through a an experimental campaign in a constant volume combustion vessel. The derived combustion characteristics of the blended fuels were lacking from literature.
- A computationally inexpensive yet reasonable accurate scientific model has been reconstructed for stretched flame velocity predictions. The model can track the effect of stretch on the flame propagation velocity. Thus, it can be used to extend the understanding and provide further insights on the contribution of laminar burning velocity and Markstein length on the velocity of a propagating flame.
- Motivated from the inadequate available knowledge, the current research establishes a global scientific understanding on the premixed dual fuel SI engine combustion mechanism. As the mechanism is based on the fundamental combustion characteristics of a combustible mixture, it is believed to be globally applicable to different operating conditions and fuels within the flamelet premixed SI engine combustion regime.
- The current research presents the first direct comparison of the burning rates of natural gas and gasoline dual fuel blends in a constant volume and an SI engine environment. Such comparison reveals the difference in the dominant combustion
parameters involved in each experimental environment. For the base fuels, the sensitivity of the burning rate to the presence of turbulence due to a transition from laminar to engine combustion is conceptually evaluated.

1.4 Thesis Outline

Chapter 2: A Literature Survey on Dual Fuelled SI Engine Combustion. This chapter outlines the synergies for a natural gas and gasoline dual fuelling strategy in modern downsized SI engines, while underlining the open challenges for natural gas implementation in future energy efficient combustion applications. A background is given on the flame fundamentals that are essential for a scientific understanding of the SI engine combustion. Summarizing the literature review, important areas where the current knowledge requires progress are identified. Such areas motivate the current research.

Chapter 3: Research Methodology. The experimental apparatuses and the adapted experimental techniques for the constant volume and the SI engine combustion are presented. The numerical methodology for the prediction of the stretched flame propagation velocity and the burning rate definitions in the two experimental environments are also documented. The contributors to the transition mechanism characterising the difference in burning rate from constant volume to the SI engine combustion are identified.

Chapter 4: Constant Volume Combustion. The post processing methodology of the raw flame images for deriving the fundamental combustion parameters, laminar burning velocity ($S_{u0}$) and Markstein Length ($L_b$) is addressed at the start of the current chapter. The response of the fundamental combustion characteristics with the dual fuel ratio is comprehensively discussed in all investigated conditions. Through pressure analysis, the mass burning rate is investigated. From a fundamental combustion prospective, the synergies for blending gasoline with natural gas are identified.

Chapter 5: Numerical Analysis on Stretched Flame Velocity. A reconstructed scientific model has been used to extend the understanding on the contribution of $S_{u0}$ and $L_b$ to the
velocity of a stretched propagating flame. A numerical analysis has been performed at various simulated conditions.

Chapter 6: Dual Fuelled SI Engine Combustion. Optical diagnosis has been integrated with in-cylinder pressure analysis in an optically assessed SI engine to investigate the mechanism of flame velocity and stability with the addition of gasoline to natural gas in a dual fuel blend. Experiments are performed under a sweep of engine load, speed and equivalence ratio. The mechanism of the dual fuelled SI engine combustion is identified and discussed based on the prior knowledge of the fundamental combustion characteristics of the mixtures.

Chapter 7: On the Transition from Constant Volume to Engine Combustion. The transition mechanism characterises the difference in burning rate from the constant volume to the SI engine combustion. The response of the transition mechanism with the DF ratio is evaluated in the present chapter. The influential parameters involved at each tested condition will be comprehensively discussed. For the base fuels, the sensitivity of the burning rate to the presence of turbulence will be assessed through a conceptual analysis of the burning rate definitions and associate experimental results.

Chapter 8: Concluding Remarks and Open Challenges. The results presented in the main body of the thesis are summarised and key conclusions are derived. Areas to expand the progress made by the current research are identified under open challenges.
Chapter 2

2 Literature Survey on Dual Fuelled SI Engine Combustion

This chapter details the recent advancements on the use of natural gas and gasoline dual fuelling in SI engines. In addition, a background is given on the flame fundamentals with particular reference to the combustion of natural gas, gasoline, and their binary blends. Ultimately, the presented material adds more details on the reasons that motivated the current research and forms the foundations for the rest of the thesis.

2.1 Engine Downsizing

Harmonization with the latest emission legislations whilst improving fuel consumption and engine performances has been the driver in passenger vehicle powertrain technology over recent years. The reliability of internal combustion engines is proven for decades. They form a cost effective yet reliable and straight forward way for chemical to kinetic energy conversion. Downsizing philosophy is seen as a key technology for the future of the Spark Ignition (SI) engine [7],[8],[9].

The downsizing philosophy implies an increase in power density through excessive inlet charging of a lower capacity engine. That leads to an improved mechanical efficiency over its higher capacity naturally aspirated counterpart. An indirect reduction in pumping losses for a typical driving scenario can be also obtained for the downsized compared to its naturally
aspired variant. In particular, an engine with smaller capacity will operate in a higher specific load for a given torque demand, hence a reduction in pumping work can be obtained. Consequently, for a typical driving scenario the operating point of a downsized engine shifts to a more fuel efficient area of the fuel consumption map in comparison to its naturally aspired variant.

On the other hand, as reported by Fraser et al. [10] if a comparison of thermal efficiency is made at the same BMEP then the highly turbocharged downsized engine will be worse when compared to its naturally aspired variant. The difference is increased with the increase of engine load. This is mainly attributed to the reduced compression ratio of a downsized engine, and the retarded ignition timing as well as excessive fuel enhancement performed at high loads as a knock mitigation strategy. Indeed, the extent at which SI engines can be downsized is limited by undesirable knocking and pre-ignition phenomena [11], [12], [13]. The AFR map versus engine speed and load for the Ford three cylinder 1L downsized engine as officially reported by Ford motor company [7] is presented in Figure 2.1. The AFR is mostly stoichiometric although the fuel enhancement in high load conditions is clearly evident.

Steady state low speed torque and transient response are critical if any level of engine downsizing is going to be considered as an acceptable concept. However, the performance of a conventional charging system is going to be restricted by the availability of exhaust energy at low engine speeds. Consequently, the maximum allowable volumetric efficiency of the engine is limited and hence the overall steady state and transient performances are degraded. Particular measures including sophisticated charging systems [10] [14], particular scavenging strategies, and cooling effect measures introduced by liquid fuel evaporation [15] have been implemented in order to eliminate the undesired lag of the charging system and increase the low speed volumetric efficiency of a downsized engine.
2.1.1 Dual Fuelling Synergies

The concept of natural gas-gasoline dual fuelling has been mainly motivated from the current challenges of a downsized engine. In order to appreciate the purpose of a dual fuelling strategy in a downsized engine, the physical properties of natural gas and gasoline are summarised in Table 2.1. The main constituent of natural gas is methane. The physical properties of methane have been used to reflect those of natural gas. Typical refinery gasoline consists of hundreds of hydrocarbons. The strict composition of gasoline may differ in different continents. Indicative values are presented in Table 2.1. Where applicable values are taken according to the European fuel certification [16].

<table>
<thead>
<tr>
<th>Fuel Properties</th>
<th>Natural Gas</th>
<th>Gasoline</th>
</tr>
</thead>
<tbody>
<tr>
<td>H/C Ratio</td>
<td>4</td>
<td>≈1.89</td>
</tr>
<tr>
<td>Molecular Weight [kg/kmol]</td>
<td>16</td>
<td>≈98</td>
</tr>
<tr>
<td>Density at STP [kg/m³]</td>
<td>0.67</td>
<td>≈720</td>
</tr>
<tr>
<td>Lower Heating Value [kJ/kg]</td>
<td>50000</td>
<td>≈44000</td>
</tr>
<tr>
<td>Octane Number</td>
<td>125</td>
<td>≈95</td>
</tr>
<tr>
<td>Stoichiometric AFR</td>
<td>17.2</td>
<td>≈14.7</td>
</tr>
</tbody>
</table>

Table 2.1. Main physical properties of natural gas and gasoline

The natural gas molecule contains around 53% lower carbon as compared to gasoline. Consequently, natural gas allows a theoretical 25% decrease in CO₂ emissions if the same
thermal efficiency is assumed between the two fuelling modes. In addition, the compression ratio of an SI engine fuelled with natural gas can be increased as compared to gasoline, due to its superior anti-knocking characteristics, enhancing the thermal efficiency. Directly related to the high octane number of natural gas is the absence of any fuel enrichment as a way of knock mitigation during natural gas SI engine operation. Furthermore, a full range Maximum Brake Torque (MBT) spark timing can be applied for natural gas fuelled engines. However, owning to the gaseous state of natural gas and its low density, injecting natural gas in the inlet plenum of an SI engine leads to a direct volumetric efficiency reduction as compared to gasoline fuelling. On top, the absence of the evaporative effect from the injection of the gaseous fuel is also adversely affecting the volumetric efficiency in an SI engine.

The implementation of natural gas in an SI downsized engine as a way to extend its auto-ignition limits, hence power density, sounds an interesting potential scenario. However, unless direct injection is adapted, gaseous injection decreases volumetric efficiency, impacting directly the peak engine torque especially at low speed-loads where the charging system is out of its operational map [17].

From an engine operation prospective, the mitigation of auto-ignition phenomena without compromising the thermal efficiency, whilst maintaining low speed volumetric efficiency has motivated the implementation of a natural gas-gasoline dual fuelling strategy. The main principle is to exploit the high octane number of the gaseous fuel and the density as well as latent heat of vaporization of the liquid fuel, in order to generate a positive synergy for optimizing the downsized SI engine operation [18]. In a dual fuel mode, the optimisation of the downsized SI engine operation is achieved through,

- Absence of fuel enrichment.
- Maintain MBT spark timing.
- Adapting higher compression ratio
- Operate at higher boost pressures.

In comparison to the base fuels, the research and development on natural gas-gasoline dual fuelled SI engines is very limited. The first experimental study in an SI single cylinder carburettor engine fuelled with premixed binary blends of natural gas and gasoline was conducted back in the early 90s by Gu et al [19]. At stoichiometry, with 60% natural gas energy fraction, they reported 7.9% power improvements, and 1% better thermal efficiency as compared to dedicated natural gas fuelling. The experimental findings were credited to an improved volumetric efficiency during dual fuel operation, and to an increased flame velocity of the blended fuel as compared to that of natural gas. As it was stated, the increase of flame
velocity with the addition of gasoline to natural gas did not follow a simple energy weighted average between the two fuels.

The next reported study performed by Pipitone and co-workers [20] back in 2009. Stoichiometric natural gas-gasoline dual fuelling has been applied to a port fuel injected naturally aspirated SI engine. As compared to dedicated gasoline operation, they experimentally achieved up to 27% better BSFC at Wide Open Throttle (WOT) using a natural gas mass fraction of 50% credited to the absence of fuel enrichment and the constant MBT combustion phasing. The absence of fuel enrichment and the MBT timing were possible due to the higher knock resistance of natural gas in comparison to gasoline. There was no reduction in engine power during dual fuel operation as compared to dedicated gasoline operation. That was attributed to the counterbalance of the reduction in volumetric efficiency with the addition of natural gas, from an improved IMEP induced by an optimised combustion phasing on dual fuelled as compared to gasoline operation.

Understanding the need of turbocharging to exploit the full potential of dual fuelling, Delpech et al. [18] were the first back in 2010 to conduct a study concerning a port fuel injected turbocharged SI engine optimised for dual fuel operation. The engine was fuelled with indirect injection of methane and gasoline. For a 55% methane mass fraction, they have reported over 26.5 Bar of BMEP on stoichiometric operation with thermal efficiency rising up to 36% at WOT. The maximum attainable BMEP on dual fuel mode was 14% higher as compared to dedicated gasoline operation. In dual fuel operation, fuel consumption could be reduced by more than 25% if similar BMEP as compared to dedicated gasoline operation was maintained. No further explanation was given for the observed phenomena apart from the implementation of MBT Spark timing and the absence of fuel enrichment on dual fuel mode.

Following the work of Delpech et al.[18], Obiols and co-workers [21] applied direct injection of gasoline with port injection of methane on a turbocharged SI engine. They implement two different strategies during DF operation. Firstly, they experimentally obtained the potential fuel consumption benefit and secondly the increase in power density as compared to each single fuel taken alone. Consisted with the two previous mentioned studies, the experimental study of Obiols et al. [21] was also constrained in stoichiometric fuel-air mixtures. On a dual fuelled stoichiometric WOT operation with methane mass fraction of 70%, the BMEP was increased up to 23% compared to the dedicated gasoline fuelling. As stated by Obiols et al. [21] and illustrated in Figure 2.2, the improved volumetric efficiency combined with an increase in flame velocity during DF operation allowed the cBSFC ( c: “corrected” by considering the Lower Heating Value of methane) to be reduced by about 3% even compared to pure methane operation.
There were no further insights on the contribution of an increased flame velocity to the reduction in fuel consumption during dual fuelling operation.

An excellent trade-off between engine performances, fuel consumption, THC, CH$_4$ and NOx emissions was achieved for a methane mass fraction of about 60% as summarised in Table 2.2. Values are directly derived from the study of Obiols et al. [21].

On the initiative of overcoming problems associated with bi-fueled SI engines, Movahed et al. [22] performed natural gas-gasoline dual fuelling in a turbocharged SI engine. Both fuels were port injected in the inlet plenum. The study of Movahed et al. [22] supports the already reported experimental findings that for an increase in thermal efficiency whilst maintaining overall engine performances, dual fuel operation is a synergetic strategy in comparison to a dedicated single fuel operation.

<table>
<thead>
<tr>
<th></th>
<th>Difference compared to 100% methane operation</th>
<th>Difference compared to 100% gasoline operation</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum BMEP</td>
<td>+16%</td>
<td>+20%</td>
</tr>
<tr>
<td>cBSFC</td>
<td>+1%</td>
<td>-13%</td>
</tr>
<tr>
<td>Specific THC emissions</td>
<td>-85%</td>
<td>-64%</td>
</tr>
<tr>
<td>Specific CH$_4$ emissions</td>
<td>-89%</td>
<td>Not Applicable</td>
</tr>
<tr>
<td>Specific NOx emissions</td>
<td>-34%</td>
<td>-48%</td>
</tr>
</tbody>
</table>

Table 2.2. Overview of dual fuelled engine performances [21].
Having appreciated the potentials of natural gas-gasoline dual fuelling for energy efficient combustion applications, Genchi and co-workers.[23],[24] quantified the increase in Motor Octane Number (MON) with the addition of natural gas (86% vol methane) to gasoline in a cooperative fuel research engine. The results showed that commercial super quality gasoline (100 RON) can be achieved by a natural gas mass fraction of 25%. The results of the test confirmed that the addition of natural gas to gasoline considerably raises the knock resistance of the blended fuel.

2.2 Burning Rate Characteristics

Historically, as a stoichiometric fuel-air mixture was mainly used in production SI engines, for the same combustion phasing an increase of negative work was experienced during natural gas as compared to gasoline fuelling. That was credited to an overall slower combustion process on natural gas fuelling and the need of extra ignition advance [19] [25] [26] [27]. An increase in negative work deteriorates the thermal efficiency of an SI engine.

The overall slower combustion of natural gas in comparison to that of gasoline at stoichiometric conditions has been experimentally justified by a number of studies. A late study has been performed by Sevik and co-workers [28] in an SI engine fuelled with premixed natural gas(94% vol methane) and gasoline air mixtures at stoichiometric, WOT conditions. The engine speed and load were held constant at 1500 RPM and 3.2 Bar IMEP and ignition timing was set to MBT for each fuelling mode. The combustion of premixed natural gas was found to be on average 8% and 24% slower as compared to that of gasoline in the 0-10% Mass Fraction Burned (MFB) regime and in the 10-90% respectively. The experimental findings were credited to the slower laminar burning velocity of natural gas.

The experimental study of Catania and co-workers [29] quantified the burning rate of natural gas (88.3% vol methane) in comparison to that of gasoline in a bi-fuel SI engine operated under different AFRs. The engine speed was set to 4600 RPM and the load was near 4.4 bar BMEP. The ignition timing was set to MBT and premixed mixtures were implemented for each fuelling mode. For rich to stoichiometric AFRs, the burning rate of gasoline was consistently faster than that of natural gas. At lean conditions (Φ=0.77), as compared to gasoline, the burning rate of natural gas was found to be faster in the 0-10% MFB regime and slower in the 10-90%. There was no justification as for the mechanism of the reported experimental phenomena.
The recent optical study of Aleiferis et al. [30] and the study of Serras-Pereira et al. [31] have been conducted in the same SI engine. The engine was fuelled with premixed alcohol and hydrocarbon fuel-air mixtures. The spark timing was fixed for all tested fuels. At 1500RPM and relatively low loads, both studies reported a faster burning rate for methane as compared to gasoline in the initial stages of combustion from stoichiometric to lean ($\Phi=0.83$) mixtures. For the lean mixtures ($\Phi=0.83$), the faster combustion of methane over gasoline preserved for the whole combustion process. The studies of Aleiferis [30] and Serras-Pereira [31] performed at a lower engine load and speed in comparison to the study of Catania et al. [29]. As it has been stated by Aleiferis et al. [30] there is a trend of lower Markstein lengths for those fuels whose flames produced faster burning velocities in the SI engine environment. The Markstein length is a fundamental combustion characteristic. It characterises the sensitivity of a flame to stretch. Flame stretch is induced by flow aerodynamics and/or flame curvature. The Markstein length is mainly governed by the thermo-diffusive properties of a combustible mixture, the so-called Lewis number effect. The concept of flame stretch and Markstein length will be comprehensively discussed in the next sections of the thesis.

The effects of flame and stretch interactions on the combustion process of an SI engine have been experimentally investigated following a novel technique, for iso-octane and methane air mixtures by the research group of Brequigny [32], [33], [34]. In the particular studies [32], [33], [34], the considered fuel-air mixtures in the SI engine were examined at different equivalence ratios to present similar laminar burning velocities at ignition timing, and therefore allow for the effect of the flame stretch sensitivity of a particular fuel on the flame velocity to be investigated. Methane being the least sensitive fuel has shown the fastest combustion, in contrast to iso-octane being the most stretch sensitive fuel shown the slowest. It has been reported [34], that the phasing of 5%, 10% and 50% mass fraction burned in an SI engine is linearly linked to the Lewis number and therefore to the Markstein length of the combustible mixture. It has been also reported by the same research group that the flame of a low stretch sensitive fuel such as methane is more sensitive to turbulence wrinkling than the flame of a high stretch sensitive fuel such as iso-octane. As has been concluded, the flame stretch sensitivity observed in the laminar regime directly impacts the combustion process in an SI engine.

Although the importance of flame-stretch interactions in an SI engine have been also pointed out by another late publication of Aleiferis et al. [35], there is still a limited understanding on such effects in an SI engine environment especially with respect to a natural gas-gasoline DF blend.

Motivated from the low burning velocity of methane and the reduction in volumetric efficiency from its port fuel injection in SI engines, Di Iorio and co-workers performed the first optical
studies in an SI engine fuelled with direct methane injection and port gasoline [5] [6]. Prior to the current research thesis, the optical studies performed by Di Iorio et al. [5] [6] were the only available experimental studies concerned with the burning rate of natural gas and gasoline dual fuels in SI engines. The experimental studies were aiming to improve the burning rate of methane through the addition of gasoline whilst minimising the volumetric efficiency reductions at stoichiometric and lean conditions (\(\Phi = 0.83\)). The injection duration of methane was adjusted to minimise the CoV of IMEP at each tested condition whilst that of gasoline was held constant at the firing TDC to promote a homogeneous gasoline air mixture. The spark timing was held constant for all tested conditions. As experimentally justified by Di Iorio et al. [5] [6], the blended fuels attained a faster flame propagation rate even compared to that of gasoline. This is a critical finding as it can partially solve the historic problem of a slow propagating natural gas flame. The mechanism for the increased flame propagation rate of the blended as compared to the base fuels was attributed to the chemical interactions of methane and gasoline and to a better mixture stratification during the dual fuel operating mode. However, supporting experimental evidence or further explanations have not been reported to justify the arguments. The same research group reported experimental findings on the air assisted natural gas-gasoline dual fuel combustion performed in the same SI engine as their prior experimental studies [36]. The findings have been consisted with the previous comments, supporting the faster flame propagation velocity of the blended as compared to the base fuels. The experimental findings have been attributed to the same hypothetical mentioned reasons.

In contrast to natural gas as well as gasoline and its surrogates, the flame behaviour of gasoline - natural gas DF blends has not been adequately investigated in an SI engine. There is still a limited understanding with regards to the mechanism of a faster DF flame in comparison to the base fuels. A comprehensive understanding of the fundamental mixture parameters, laminar burning velocity and Markstein length, is essential for evaluating the dual fuel combustion mechanism in SI engines. A background on the laminar burning velocity and Markstein length of natural gas, gasoline and their binary blends will be given in the following sections.

2.3 Flame Fundamentals

2.3.1 Laminar Burning Velocity

The fundamental laminar burning velocity \(S_u^o\) of a combustible mixture is defined as the velocity at which a one-dimensional unstretched, adiabatic and isobaric flame travels through a
flammable quiescent, homogenous unburned gas mixture. The laminar burning velocity depends only on the unburned mixture composition, initial temperature as well as pressure. Thus, the laminar burning velocity is a fundamental property of a combustible mixture. Consequently the burning velocity being a fundamental property of a combustible mixture makes it an important target for combustion modelling, in particular the validation of chemical kinetic mechanisms.

Laminar burning velocities of hydrocarbon fuels have long been the subject of extensive experimental [37] and theoretical investigations [38]. The timeless interest on the investigation of the laminar burning velocity in part reflects its important role in the performance of SI engines. As it is experimentally justified, the fuel’s burning velocity affects the burn rate in an SI engine. Subsequently, the overall engine performances including fuel consumption and emissions are also affected by a change in burning velocity [39], [40].

As reported by Andrews and Bradley [41], significant discrepancies can be observed between the burning velocities obtained from earlier measurements which utilised different experimental techniques. It is now understood [42] that these discrepancies are due to the varying degree of flame stretch in the different experimental techniques. In earlier studies, the flame stretch that will be discussed in the next section, was not systematically considered for deriving the unstretched burning velocity. Consequently, only relatively late experimental studies concerned with the derivation of laminar burning velocities from outwardly propagating spherical flames are referenced within the current thesis. In addition, the referenced studies are concerned only with elevated pressures due to their relevance on engine combustion.

Substantial efforts have been devoted over the years to improve the understanding on the fundamental combustion characteristics of methane as well as gasoline. Typical refinery gasoline consists of hundreds of hydrocarbons. Iso-octane as well as binary blends of primary reference fuels have been widely adopted as convenient gasoline surrogates. Studies reporting values of laminar burning velocities at elevated pressures have been conducted for gasoline [43],[44] [45], and its surrogates [46],[47],[48],[49] as well as methane [50], [51], [52], [49], [53].The tested conditions of the referenced studies are presented in Table 2.3.

In all the aforementioned studies, the reported laminar burning velocity of methane is consistently lower compared to that of gasoline and its surrogates under similar tested conditions for all Air to Fuel Ratios (AFRs). Using appropriate literature data, at lean conditions (Φ=0.8) the burning velocity of methane is on average 5%, 13% and 25% lower as compared to that of gasoline and its surrogates at 2.5, 5 and 10 bar respectively whereas at stoichiometry is
lower by 5%, 13% and 23% at the respective pressures. At rich conditions ($\Phi=1.2$), the burning velocity of methane is on average 24% lower than the burning velocity of gasoline at 5 bar.

An increase in pressure decreases the burning velocity of both fuels. However, as reported by Gu et al. [50] methane-air mixtures are more sensitive by an increase in pressure than iso-octane air mixtures. This fact is also evident by the percentage differences between the burning velocity of the gaseous and the liquid fuel as reported in the previous paragraph. On the other hand, an increase in temperature increases the burning velocity of both fuels and iso-octane air mixtures are less responsive to temperature variations than methane air mixtures [50].

<table>
<thead>
<tr>
<th>$T$ (K)</th>
<th>$P$ (bar abs.)</th>
<th>$\Phi$</th>
<th>Composition</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>358</td>
<td>$\leq 6$</td>
<td>0.8-1.6</td>
<td>75,85,95 RON</td>
<td>[43]</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td>Gasoline, Iso-octane, PRF85</td>
<td></td>
</tr>
<tr>
<td>373</td>
<td>10-25</td>
<td>0.7-1.2</td>
<td>Gasoline, PRF87, Iso-octane</td>
<td>[44]</td>
</tr>
<tr>
<td>373</td>
<td>10-25</td>
<td>0.7-1.2</td>
<td>90 RON Gasoline, PRF87</td>
<td>[45]</td>
</tr>
<tr>
<td>373</td>
<td>10</td>
<td>0.8-1.3</td>
<td>Iso-octane</td>
<td>[46]</td>
</tr>
<tr>
<td>323-473</td>
<td>1-10</td>
<td>0.6-1.6</td>
<td>Iso-octane</td>
<td>[47]</td>
</tr>
<tr>
<td>358-450</td>
<td>$\leq 10$</td>
<td>0.8-1.6</td>
<td>Iso-octane</td>
<td>[48]</td>
</tr>
<tr>
<td>360</td>
<td>5</td>
<td>0.8,1,1.2</td>
<td>Iso-octane</td>
<td>[49]</td>
</tr>
<tr>
<td>360</td>
<td>5</td>
<td>0.6-2</td>
<td>Iso-octane</td>
<td>[53]</td>
</tr>
</tbody>
</table>

Gasoline - Gasoline surrogates

<table>
<thead>
<tr>
<th>$T$ (K)</th>
<th>$P$ (bar abs.)</th>
<th>$\Phi$</th>
<th>Composition</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>300-400</td>
<td>$\leq 10$</td>
<td>0.8,1,1.2</td>
<td>Methane</td>
<td>[50]</td>
</tr>
<tr>
<td>298K</td>
<td>0.5-4</td>
<td>0.6-1.35</td>
<td>Methane</td>
<td>[51]</td>
</tr>
<tr>
<td>298K</td>
<td>$\leq 20$</td>
<td>0.6-1.4</td>
<td>Methane</td>
<td>[52]</td>
</tr>
<tr>
<td>360</td>
<td>5</td>
<td>0.8,1,1.2</td>
<td>Methane</td>
<td>[49]</td>
</tr>
<tr>
<td>360</td>
<td>5</td>
<td>0.6-1.3</td>
<td>Methane</td>
<td>[53]</td>
</tr>
</tbody>
</table>

Methane

<table>
<thead>
<tr>
<th>$T$ (K)</th>
<th>$P$ (bar abs.)</th>
<th>$\Phi$</th>
<th>Composition</th>
<th>Ref.</th>
</tr>
</thead>
<tbody>
<tr>
<td>363</td>
<td>1</td>
<td>0.85-1.2</td>
<td>Methane + Iso-octane</td>
<td>[54]</td>
</tr>
<tr>
<td>368-448</td>
<td>1-5.5</td>
<td>0.85-1.2</td>
<td>Methane + Iso-octane</td>
<td>[55]</td>
</tr>
</tbody>
</table>

Binary Blends

Contrary to the base fuels, it appears that there is very limited prior experimental work reporting the laminar burning velocity of a natural gas-gasoline dual fuel blend. The authors are only aware about the two recent studies published in December 2014 and December 2015 by Baloo and co-workers [54], [55]. The experimental studies report the laminar burning velocities and
Markstein lengths of methane-isoctane fuels blended in 70% and 95% methane volumetric fraction. The first experimental study [54], conducted at atmospheric pressure, a temperature of 363 K and at equivalence ratios ranging from 0.85 to 1.2. As far as the laminar burning velocity is concerned, it has been reported that the addition of methane to iso-octane increases the burning velocity at lean conditions in comparison to the base fuels. In contrast, at rich conditions the burning velocity of the blended fuels is found to be lower than the burning velocity of the base fuels. In their later study, Baloo and co-workers [55] examined the same fuels and AFRs at pressures up to 5.5 bar and temperatures ranging from 368 to 448 K. It has been found that the phenomenon of a higher burning velocity of the blended fuels in comparison to the base fuels deteriorates as pressure increases. For the blended fuels, the sensitivity of the burning velocities to the temperature is found to be between the sensitivity of the base fuels. It is clear that further experimental work is needed to reliable derive the complex response of burning velocity with the addition of gaseous to the liquid fuel at elevated pressures.

2.3.2 Markstein Length

Although the laminar burning velocity is a fundamentally important combustion parameter, even in laminar well controlled combustion experiments actual flames are not propagating with a rate equal to the laminar burning velocity. That is credited to the effect of flame stretch. It is well acknowledged that the characteristics of premixed flames can be greatly affected by aerodynamics [56],[57].

2.3.2.1 The Concept of Flame Stretch

In the majority of real combustion applications like in SI engines, a flame propagates in a nonuniform and unsteady flow field. It is therefore expected that the flame velocity and stability will be affected by the effect of the aerodynamics on the flame, the so-called stretch rate effects. Even in well controlled laminar combustion experiments assuming perfectly quiescent conditions, the outwardly propagating spherical flame will be subjected to stretch due to the curvature of the flame as will be further discussed.

The general situation of a wrinkled flame in a nonuniform flow is conceptually depicted in Figure 2.3, with arbitrary flow vectors also known as streamlines moving towards the flame. The influence of stretch rate on the flame response can be considered in two levels as illustrated in Figure 2.3. On the hydrodynamic level, the flame is simply an interface separating unburned and burned mixtures. Transport of heat and mass can be assumed to have no effect on the flame.
The flame collapses into a flame sheet with no preheat zone. The flame propagates with a flame velocity \( (S_b) \) which is normal to the flame surface and can differ from the fundamental burning velocity \( (S_u^0) \).

![Diagram](image)

Figure 2.3. The concept of flame stretch [57]

The presence of tangential straining, induced by the flow field on the flame, changes the flame surface area and consequently the volumetric burning rate. Whether the tangential straining increases or decreases along the surface of the flame, the local volumetric burning rate can also increase or decrease. Apart from the unsteady flow field, the extent at which tangential straining is varying along the flame surface is also dependent on the local curvature of the flame. The role of the normal straining is to allow adjustment of the flame location in the normal direction so that the flame situates where the local flame velocity balances the local flow velocity. Thus, on a hydrodynamic level, the combined effects of the tangential and normal straining are the displacement of the flame surface, distortion of its geometry, and modification of the volumetric burning rate.

Actual flames are transport depended, in the basis of which a preheat zone exist where heat and mass diffusion are main contributors for controlling the combustion process. Such flame configuration is shown in Figure 2.3b. In this level of consideration, the tangential straining can modify the temperature and concentration profiles in the preheat zone through interactions with heat and mass diffusion. Consequently the velocity and stability of the flame will be affected. The stretch at this level will be referred to as flame stretch. The normal straining affects the residence time of the unburned mixture within the preheat and the reaction zone. The flame temperature and completeness of the reaction is therefore affected. The direct influence of normal straining in the reaction zone is expected to be small because of the secondary importance of convective transport in this zone [57].
The hydrodynamic and flame stretch are strongly coupled, in that the hydrodynamic imposes the flame stretch while the flame stretch has a critical influence on the flame velocity as well as stability.

### 2.3.2.2 The Stretch Rate

The generally accepted definition of the flame stretch rate was first suggested by Williams [58] and is given as,

\[ a = \frac{1}{A} \frac{dA}{dt} \]  \hspace{1cm} (2.1)

The stretch rate corresponds to the fractional area change of a flame surface element (A) which moves with the flame velocity. The stretch rate has units of 1/s. As proved later by Matalon [59] and Chung and Law [60] the simple definition in eq. 2.1 can collectively describe the various influences due to flow nonuniformity, flame curvature and flame/flow unsteadiness on the surface of a propagating flame. Matalon [59] deduced a coordinate-invariant formulation of the stretch rate based on the results of Buckmaster [61]. Subsequently, Chung and Law [60] derived a more concise expression for the stretch rate using the invariant formulation of Matalon [59], while Candel [62] finalise the expression to:

\[ a = S_u \nabla_n - (v \cdot n) \nabla_n + \nabla_t v_t \]  \hspace{1cm} (2.2)

Where \( S_u \) is the stretched burning velocity, \( n \) is a unit vector normal to the flame surface, and \( v \) the flow velocity in the tangential direction. The normal and tangential gradient operators at the flame surface are given by the symbols \( \nabla_n \) and \( \nabla_t \) respectively. The stretched burning velocity \( (S_u) \) is derived if the flow velocity normal to the flame surface is subtracted from the flame velocity \( (S_b) \). For an infinitesimal thin flame and a weak hydrodynamic stretch [63], \( S_u \) can be well approximated as the ratio of \( S_b \) to the expansion factor (\( \sigma \)) [64]. The expansion factor is defined as the ratio of unburned to burned gas density. The first term on the right-hand side of eq. 2.2 represents the contribution to flame stretch by the flame curvature, the second corresponds to the contribution of normal straining and the third to the tangential straining.

### 2.3.2.3 Nonequidiffusion Flames

To define what a nonequidiffusion flame is, and demonstrate the influence of flame stretch on nonequidiffusion flames, the parameters Lewis number and preferential diffusion have to be introduced. The Lewis number (Le) is the ratio of thermal to mass diffusivity of a combustible
mixture, whereas the preferential diffusion is defined as the ratio of mass diffusivity of the deficient to the excess reactant. For a lean mixture the deficient reactant is the fuel while for a rich mixture is the oxidizer. A non-unity Lewis number and/or preferential diffusion indicate a nonequidiffusion flame. The majority of practical flames are actually nonequidiffusion both from a Lewis number as well as preferential diffusion prospective and they are continuously subject to stretch.

The temperature of a stretched flame depends on the Lewis number of the combustible mixture. If Le = 1, the total energy of the flame is conserved as the diffusive heat loss from the reaction zone to the unburned mixture is counterbalanced by the chemical energy gain due to mass diffusion of the deficient reactant from the unburned mixture to the reaction zone. However, if Le > 1 heat loss exceeds the mass gain resulting in a drop of flame temperature from its adiabatic value and subsequently a reduction of flame velocity from its unstretched value. Contrary, for Le < 1 mass gain exceeds the heat loss and the flame temperature is increased beyond the adiabatic value while the stretched flame velocity is higher than its unstretched value.

As far as preferential diffusion is concerned, for a stretched flame if the leaner reactant is also the more diffusive one the reactant concentration in the reaction zone will become more stoichiometric with an increase of stretch rate such that the flame temperature is higher and the flame velocity is increased. The inverse holds if the leaner reactant is the less diffusive one [57]. In particular, for methane being more diffusive than air, and gasoline being less diffusive than air, the effect of preferential diffusion on the reactant concentration just ahead of the flame is shown in Figure 2.4. It has been reported by Muppala et al. [65] and Dinkelacker et al. [66] that the positively curved (concave) part of the flame highlighted within the dotted circle governs the characteristics of the combustion process while the convex part is of secondary importance. Practical experimental phenomena of preferential diffusion effects as well as non-unity Lewis number effects have been documented in [67], [68], [69].

The precise derivation of Lewis number and preferential diffusion during a combustion process is extremely challenging. There are many intermediate species produced with different diffusivities that continuously altering the effective diffusivity of the combustible mixture. A more direct approach is to derive a global parameter to represent the effect of stretch on the flame response. Such parameter is the Markstein length to be considered in the next section.
2.3.2.4 Stretched Flame Velocity

In quite early years, Karlovitz et al. [70] proposed the concept of flame stretch to explain phenomena of flame extinction in non-uniform flow fields, followed by the pioneer work of Markstein [71] that allowed the flame velocity to vary in response to the flame stretch induced by curvature to describe phenomena of cellular instability. The response of the flame to stretch has been further analyzed by Clavin and Williams [72], Pelce and Clavin [73], and Matalon and Matkowsky [74] on the basis of an asymptotic analysis, assuming that the flame preserves its laminar structure under moderate flow perturbations. Considering the mentioned earlier studies, Clavin P. [75] shows that the stretched laminar burning velocity \( S_u \) differs from that of the corresponding unstretched velocity \( S_{u0} \) such as,

\[
S_u = S_{u0} - La
\]  

(2.3)

In the proposed model, the response of the unstretched burning velocity \( S_{u0} \) to the stretch rate \( (a) \) is represented by the unburned gas Markstein length \( (L) \). The Markstein length is considered as a characteristic length in the order of the thickness of the flame. As mentioned previously in section 2.3.2.2 on the assumption of an infinitesimally thin flame and moderate stretch rate, the stretched burning velocity multiplied by the expansion ratio equals to the flame velocity. On this consideration, the flame velocity can be simply derived as,

\[
S_b = S_u \sigma = S_{u0} \sigma - L \sigma a = S_{b0} - L_b a
\]  

(2.4)
where the value of burned gas Markstein length ($L_b$) is used to characterise the response of the propagating flame velocity ($S_b$) to the stretch rate. The burned gas Markstein length is of more practical importance to the current study than the unburned gas Markstein length. In the current study as will be further discussed in section 3.4.5, $L_b$ equals to $L_\sigma$. The burned gas Markstein length includes the influence of the thermal expansion ($\sigma$) on the response of the flame to stretch. For the rest of the study, the term Markstein length will be referred based on its burned gas ($L_b$) value unless otherwise stated.

The burned gas Markstein length is effectively the stretch sensitivity of a particular flame and can be precisely derived as will be explained in section 4.2. For $L_b > 0$ the flame velocity will be increased under stretch, whereas for $L_b < 0$ it will be reduced. The flame is insensitive to stretch if $L_b = 0$.

For outwardly propagating spherical flames, the derivation of the Markstein length ($L_b$) is necessary in order to obtain the value of the laminar burning velocity at a particular test condition. Consisted with the literature concerning the laminar burning velocity as presented in Table 2.3, the Markstein length is well studied for methane as well as gasoline surrogates in contrast to a natural gas-gasoline dual fuel blend.

In particular, a part of the study of Gu et al. [50] and Mandilas et al. [49] directly compared the burned gas Markstein length of iso-octane and methane air mixtures at different equivalence ratios. As emphasized, these two fuels responded to flame stretch in an opposite manner with respect to the equivalence ratio. These findings are also supported by the experimental study of Lawes et al [53]. The Markstein length of iso-octane increases with equivalence ratio whereas that of methane decreases. At lean conditions ($\Phi=0.8$), methane has on average 4.2, 4.1 and 1.6 times lower Markstein length as compared to that of iso-octane at 2.5, 5 and 10 bar respectively. The Markstein length of methane attains negative values at 5 and 10 bar, implying an increase in flame velocity with stretch under lean burn conditions. In contrast, at rich conditions ($\Phi=1.2$) the Markstein length of methane is on average 2 times higher than that of iso-octane.

As pressure increases, the Markstein length of both fuels exponentially decreases for all equivalence ratios, and it reaches a plateau at a pressure higher than about 4 to 5 bar. The Markstein length of iso-octane shows a higher proportional decrease by an increase in pressure in comparison to methane. The effect of temperature on Markstein length is found to be very weak as compared to the effect of pressure for methane and iso-octane air mixtures [50], [47].

Besides, the response of the Markstein length for iso-octane air mixtures with various levels of CO$_2$ dilution is quantified in the study of Zhou and co-workers [76]. As reported, the Markstein length is slightly affected by CO$_2$ dilution. In comparison to the effect of pressure, the CO$_2$
dilution effect is also found to be very weak. It can be therefore stated that the Markstein length of a hydrocarbon air mixture is mostly depended on pressure, equivalence ratio and fuel composition.

There is very limited literature information available with regards to the Markstein length of the blended fuels. The limited literature information are reported by Baloo et al [54] [55] only at 1 and 2.5 bar. The Markstein length of the two blended fuels (70% and 95% methane volume fraction) is found to be between those of the base fuels although they did not follow a simple volume fraction weighted average. It is clear that the available literature information for the Markstein length of the blended fuels is not adequate to allow for a scientific understanding on the dual fuel SI engine combustion. The Markstein length of the blended fuels needs to be further investigated especially at higher pressures and fuel lean to rich conditions.

2.3.3 Flame Instability

The presence of flame instability manifested as cellular structures, cross cracks and wrinkles on the flame surface is probably one of the most fascinating and at the same time scientifically challenging phenomenon for the combustion community.

It has been long acknowledged that nonequidiffusion flames are prone to phenomena of flame instability. As illustrated in Figure 2.5 for Le > 1 and hence Lb > 0, the burning is intensified at the concave part of the flame due to the concentration of heat fluxes just in front of the flame, and weakened in the concave part due to the higher thermal energy loss as compared to the mass energy gain. Such flame is diffusively stable. Consequentially, on the same reasoning for Le < 1 and hence Lb< 0, flame is diffusively unstable as the burning will be intensified at the convex part of the flame and weakened at the concave. The phenomenon of cellular instability can be also interpreted on the basis of the different diffusivities of the deficient and abundant reactants, as discussed in the previous section and indicated in Figure 2.4. It can be then concluded that the flame is diffusively unstable if it is deficient in the more mobile reactant.
As firstly proposed by Markstein [71], the burning velocity can be also altered by pure curvature effects without the need of nonequidiffusion flames. The burning will be intensified at the concave part of the flame due to pure curvature effects as the heat fluxes are focussed just ahead of the flame, and at the same logic it will be reduced on the convex flame part. The stabilising effect due to pure curvature is expected to shift the stability boundary based on nonequidiffusive considerations away from \( \text{Le}=1 \) to a smaller value of \( \text{Le} \). We shall refer to this mode of instability as thermodiffusive instability. A chronological set of a thermodiffusively unstable flame is illustrated in Figure 2.6.

In certain occasions, although the flame propagates with \( \text{Le} > 1 \), it can still show wrinkles and cross cracks in the later stages of flame evolution. As reported by Aldredge and Zuo [77], such mode of flame instability is discovered independently by Darrieus and Landau, and is attributed to the coupling between flame and flow-field dynamics. This mode of instability is commonly known as hydrodynamic instability also called Landau-Darrieus instability.
The mechanism of hydrodynamic instability considers an infinitesimally thin flame as a density discontinuity and involves the interaction of the hydrodynamic disturbances generated by the flame and the actual flame itself. Due to such interactions, the flow streamlines respectively diverge and converge in approaching the convex and concave parts of the flame as shown in Figure 2.5. Thus, for the convex segment of the flame, the widening of the streamtube causes the flow to slow down. However, since the flame velocity remains unaffected as specified by definition, the local velocities of the approach flow and the flame can no longer balance each other, hence resulting in further advancement of this flame segment into the unburned mixture [57]. A similar argument for the concave segment implies that the flame will further recede into the burned mixture. Thus, the hydrodynamic mode of instability is inherently unstable. It has to be noted that in the presence of finite flame thickness as in every realistic flame, the curvature stabilisation mechanism as discussed in the previous paragraph is also operative due to the presence of diffusive fluxes. It can be then concluded that the hydrodynamic instability is promoted with decreasing flame thickness. In addition, the intensity of the hydrodynamic instability increases with the increase of the expansion ratio.

The onset of flame instability can be predicted knowing the Pectel number ($\text{Pe}_c$), [50] [78]. The Pectel number is defined as the ratio of the critical flame radius where instability occurs to the flame thickness ($\delta$). Thus, multiplying $\text{Pe}_c$ with $\delta$ the critical flame radius is given by,

$$\text{Pe}_c \delta = R_{\text{inst}} = \left[ A e^{B \frac{(L_b-L)}{(\sigma-1)\delta}} \right] \delta \quad (2.5)$$

The empirical constants $A$ and $B$ are derived by Bradley et al. [78] and correspond to 1809 and 103.

Appreciating the fact that the flame can be stabilised by a sufficiently high curvature manifested as hydrodynamic stretch on the flame, Bradley and co-workers [78] develop a more rational criterion for flame instability than the Pectel number. Based on the Pectel number, they have developed a relationship to calculate a critical stretch rate. For stretch rates higher than the critical value, flame instability should be absent. In its natural form, the critical stretch rate is given by,

$$a_{cl} = 0.0075 e^{-0.123 \frac{(L_b-L)}{(\sigma-1)\delta} \frac{S_0}{\delta}} \quad (2.6)$$
Thermodiffusive instabilities occur both in laminar and turbulent combustion [79] [80]. A number of experimental studies exist with particular emphasis on quantifying the role of flame instability to the increase of turbulent mass burning rate [79] [81]. However, there is no final quantitative agreement of the effect of flame instability on the mass burning rate [82]. Consequently, solid well agreed models of such effect are currently missing from literature.

2.4 Literature Summary

The necessity for compliance with future emission legislations has renewed the interest for the use of alternative fuels. The low carbon content, the knocking resistance, and the abundance reserves, have classified natural gas as one of the most promising alternative fuels. The synergies for improving the performances of an SI downsized engine through natural gas-gasoline dual fuelling have been presented through the current literature review. It follows that the slow burning velocity of natural gas remains an open challenge for its utilisation in energy efficient combustion applications. It has been experimentally observed that the addition of gasoline to natural gas has the potential to improve methane’s combustion, leading to a faster flame velocity even compared to that of gasoline. The mechanism behind the observed experimental phenomena still remains unclear. A comprehensive understanding of the fundamental combustion parameters, laminar burning velocity and Markstein length is essential for evaluating the dual fuel combustion mechanism in SI engines. It appears that there is very limited prior experimental work reporting the fundamental combustion parameters of a natural gas-gasoline dual fuel blend. The current thesis aims to establish a structured scientific understanding on the basis of fundamental combustion characteristics for the combustion mechanism of binary blends of natural gas and gasoline in SI engines.
Chapter 3

3 Research Methodology

3.1 Overview

The laminar burning velocity and Markstein length of natural gas-gasoline dual fuel blends need further investigation especially at elevated pressures where there are no available literature data. In that end, constant volume combustion experiments have been conducted to derive the fundamental combustion characteristics of the blended as well as the base fuels. A numerical analysis is then followed to improve the understanding on the contribution of burning velocity and Markstein length to the stretched flame propagation velocity at various simulated conditions. The derived knowledge has been used to explain the dual fuel combustion mechanism analysed through an experimental campaign performed in an optically assessed SI engine. The transition mechanism characterising the difference in burning rate from constant volume to engine combustion is investigated in the last chapter of the current thesis. The experimental apparatuses and the implemented experimental techniques are fully documented in the current chapter. In addition, the numerical methodology and the burning rate definitions in both experimental environments are presented. The post-processing technique of the raw experimental data is discussed separately in the specific chapters to follow for each experimental environment.
3.2 Constant Volume Experiments

3.2.1 Constant Volume Combustion Vessel

The constant volume combustion vessel is a closed cylindrical cavity with an inner diameter of 100 mm and a volume of 2.2 L. It is made of number 45 steel and is placed horizontally as shown in Figure 3.1.

![Figure 3.1. Constant volume combustion vessel](image)

The full optical capability of the combustion vessel includes optical access through three windows mounted on the front, back and left walls of the combustion vessel. The windows are made of high-quality quartz glass. The front window is of a racetrack-shape with a length of 230 mm, a width of 80 mm, and a thickness of 100 mm. The back as well as the left window is of circular shape with a diameter of 80 mm and a thickness of 50 mm. On the right part of the vessel there is an access for mounting the liquid fuel injector whereas at the top there is access for the location of pressure and temperature transducers as shown in the right schematic of Figure 3.1. The combustion vessel is capable of withstanding a maximum transient pressure of 10 MPa.

3.2.2 Schlieren Optical Diagnosis

The schlieren technique with knife-edge has been widely used to visualize flame fronts. The classical implementation of an optical schlieren system uses light from a collimated light source where rays are parallel, to shine on or from behind a target object. A knife-edge placed at the
focal point is intended to block about half of the light. Variations in the refracted light caused by density gradients in the fluid distort the collimated light beam. This distortion creates a spatial variation in the intensity of the light. The result is a set of lighter and darker patches corresponding to positive and negative fluid density gradients in the direction normal to the knife-edge. The changes in density are often more relevant to the underlying chemical and thermal processes than the flame’s light emission. The optics used in the current research to allow for the application of the schlieren method are illustrated in Figure 3.2.

Figure 3.2. Optics necessary for the schlieren method. A: Concave Mirrors (Collimators), B: Focusing Lens, C: Knife Edge, D: Flat Mirror, E: Slit, F: Light Source with Focussing Lens

Early applications of schlieren technique was made by Toepler in 1866 [83]. The advantages and limitations of this method in combustion visualisation were previously studied [84], [85], [86]. It has been found that for flames concave to the burnt gas, as in the present study, the schlieren edge consistently lies within the preheat zone of the flame at an isotherm of 850 to 900 K depending on flame radius [86]. In contrast to a direct flame imaging approach, the observed flame location using the schlieren method is minimally affected by changes in flame thickness. Thus, the schlieren technique has been used by the majority of the studies in literature to derive the laminar burning velocity of a combustible mixture [50] [48] [87] [44]. However, the flame area based on the schlieren image will be consistently smaller than the actual value. The consistently lower flame area does not affect the derivation of the visualised flame velocity as the schlieren edge maintains a constant location within the preheat zone of the flame.
3.2.3 System Integration

For the needs of the current research, optical access to the cylindrical combustion vessel was possible through the opposing back and front windows. A schematic of the experimental setup is illustrated in Figure 3.3. The entire vessel was uniformly preheated by a set of electrical heating elements totaling 3.2 kW. One of the heaters was fully inserted inside the vessel to induce a transient temperature difference only during the filling process. The temperature difference evoked natural convection to stir the mixture enhancing the mixing of fuel and air. Similar technique has been used by Jerzembeck et al. [44]. The interior air temperature was controlled within 3 K using a closed-loop feedback controller set to 373K. The temperature could also be observed manually from a second temperature sensor mounted on the top of the bomb. The particular temperature has been selected to allow reference with available literature information. Three initial absolute pressures have been tested corresponding to 2.5, 5 and 10 bar. The particular pressure conditions have been selected to approximately reflect idling, part and high load conditions in a turbocharged engine at the point of spark. The pressure rise during the combustion process was obtained using a Kistler 6113B pressure transducer. The mixture was ignited using a slightly modified standard ignition plug with extended electrodes of 1.35mm in diameter. The spark plug was centrally fitted at the left wall of the combustion vessel. The left window was replaced with a spark plug mounting cap specifically design for the needs of the current research. The ignition system generated a spark with duration of 0.7 ms. A vacuum pump was used to scavenge the combustion vessel after each combustion event. For safety reasons, a 6 MPa pressure release valve was installed on the combustion vessel.

The flame progress recorded at 6000 frames per second with a resolution of 512X512 pixels by high speed schlieren photography arranged in a Z configuration. A 245W halogen lamp was used as the light source. The light was focused onto a slit using a focusing lens in order to generate the spotlight for the schlieren technique. Passing through a group of mirrors, the light path was then cut by a knife-edge which is essential for the schlieren method. Two different high speed cameras have been used for the current experimental work. A Photron Fastcam SA5 was used for the experimental work at an initial pressure of 5 Bar, instead of a Photron Fastcam SA-X2 that was used at 2.5 and 10 bar. The high speed cameras were synchronized with the spark timing and the interior pressure rise recording.
3.2.4 Dual Fuel Mixture Preparation

To allow for a direct comparison with available experimental data whilst still reflect the combustion characteristics of gasoline, PRF95 (95%volliq iso-octane and 5%volliq n-heptane) was used as a gasoline surrogate. High purity (99.9%) methane was used as a surrogate for natural gas. The dual fuel blends consist of methane and PRF95 in three different energy ratios (25%, 50%, 75%). A blend with 25% of its energy contributing from methane as defined in eq.3.1 was labelled as DF25, with 50% DF50, and for 75% DF75.

\[
DF_{\text{Ratio}} = \frac{M_{CH_4} \times LHV_{CH_4}}{M_{PRF95} \times LHV_{PRF95} + M_{CH_4} \times LHV_{CH_4}}
\]  

Figure 3.3. Schematic diagram of the experimental setup.

At each initial pressure, three different equivalence ratios have been examined. The examined equivalence ratios correspond to 0.8, 1 and 1.2. For all test conditions summarised in Table 3.1,
the air to fuel ratio was calculated using the method of chemical balance and assuming products of complete combustion. High purity technical air was used with an oxidizer concentration \([O2/(O2+N2)]\) of 0.2 ± 0.01. In Table 3.1, the term DF100 represents pure gaseous fuel (methane) and DF0 the liquid fuel (PRF95).

<table>
<thead>
<tr>
<th>Fuel</th>
<th>CH₄ Mole Fraction</th>
<th>CH₄ Mass Fraction</th>
<th>Pressure (Bar)</th>
<th>Temperature (K)</th>
<th>Equivalence Ratio (Φ)</th>
</tr>
</thead>
<tbody>
<tr>
<td>DF100</td>
<td>1</td>
<td>1</td>
<td>2.5,5,10</td>
<td>373</td>
<td>0.8,1,1.2</td>
</tr>
<tr>
<td>DF75</td>
<td>0.95</td>
<td>0.728</td>
<td>2.5,5,10</td>
<td>373</td>
<td>0.8,1,1.2</td>
</tr>
<tr>
<td>DF50</td>
<td>0.86</td>
<td>0.470</td>
<td>2.5,5,10</td>
<td>373</td>
<td>0.8,1,1.2</td>
</tr>
<tr>
<td>DF25</td>
<td>0.68</td>
<td>0.228</td>
<td>2.5,5,10</td>
<td>373</td>
<td>0.8,1,1.2</td>
</tr>
<tr>
<td>DF0</td>
<td>0</td>
<td>0</td>
<td>2.5,5,10</td>
<td>373</td>
<td>0.8,1,1.2</td>
</tr>
</tbody>
</table>

Table 3.1. Summary of experimental conditions

In every experimental condition, the air to fuel ratio was prepared inside the vessel using the partial pressure method. The followed methodology for deriving the partial pressures of the fuel-oxidizer is shown in Appendix A. The necessary amount of liquid and gaseous fuel was determined depending on the targeted dual fuel ratio, equivalence ratio, and the associate pressure and temperature as it is also indicated in Appendix A. The vessel was uniformly preheated to the desired temperature (373 K). Whilst the heater mounted inside the vessel was turned on, the liquid fuel was injected into the combustion vessel using a multi-hole gasoline direct injector with an injection pressure of 12 MPa. The targeted fuel mass was supplied inside the combustion vessel by individual injections using pre-calibrated data. The pre-calibration process involves the determination of the mass of liquid per single injection. After the injections were completed, two minutes were given to allow for the complete evaporation of the liquid fuel. Considering the correct increase of pressure change caused by the evaporation of the liquid fuel compared to the thermodynamic ideal-gas law calculations, methane and then air were slowly introduced in the combustion vessel using a fine needle valve and a pressure transducer to control the filling process. The technical air was heated by an external heater before flowing into the combustion vessel to better approximate an isothermal filling process. After the filling process was completed the interior heater was turned off, and three minutes of quiescence were given to minimize any flow structures and/or temperature stratifications inside the vessel. The quiescence time also promotes the homogeneous mixing of fuel and air.

For each tested condition, the described experimental procedure that allowed the evaluation of the fundamental laminar burning velocity as well as burned gas Markstein length was carried out at a minimum of three times. The average values are reported in chapter 4 as well as error bars evaluated based on standard error.
3.3 SI Engine Experiments

3.3.1 Optical Research Engine

A single cylinder optical SI engine designed by Lotus engineering specifically for the application of optical diagnostics has been used to analyse the dual fuel combustion process. The geometrical characteristics of the engine are summarised in Table 3.2. In its full optical capability, the engine features a full length silica cylinder liner and a sapphire window of 60mm in diameter pressed into the crown of an elongated hollow designed piston. The upper piston crown was made from titanium due to the similar thermal expansion coefficients of titanium and sapphire. The engine can also be fitted with an equivalent cylinder liner made of steel to facilitate safe engine operation at relatively higher loads. The optical engine is shown in Figure 3.4.

<table>
<thead>
<tr>
<th>Displaced Volume</th>
<th>0.5 L</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore</td>
<td>88 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>82.1 mm</td>
</tr>
<tr>
<td>Connecting-Rod Length</td>
<td>142 mm</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>10:1</td>
</tr>
<tr>
<td>Chamber Type</td>
<td>Pent-Roof</td>
</tr>
<tr>
<td>Piston Type</td>
<td>Flat</td>
</tr>
<tr>
<td>Piston offset</td>
<td>0.8 mm</td>
</tr>
</tbody>
</table>

Table 3.2. Geometrical characteristics of the engine

A curved profile was machined at the top of the liners, the inverse of which has been machined into the cylinder head. A hydraulic ram applying 10 bar of pressure was used to secure the liner to the cylinder head on a silicon gasket. The setup allows for the liner to be removed, cleaned, and refitted in less than 20 minutes without the need of removing the cylinder head.

The elongated hollow designed piston allows a plane view of the pent-roof combustion chamber through a 45° mirror mounted within the hollow piston, between the upper and the lower crown. The upper crown contains a carbon fibre piston ring which runs unlubricated in the cylinder liner to maintain in-cylinder pressures without oil fouling the window. The lower piston crown contains two compression rings and one oil control ring to prevent oil from escaping the crankcase. The engine has both primary and secondary balance shafts to allow operation at elevated speeds and it was driven by a 15 kW Brook Hansen© induction motor.
The pent roof cylinder head is designed with a centrally located liquid injector, a near central spark plug typical of a spray guided configuration, and a pressure transducer located between the intake and exhaust valves, on the intake side of the engine. The four overhead poppet valves are actuated by means of a fully variable electro-hydraulic valve system presented in Figure 3.5. The system allows different lift and/or duration profiles to be operated at each individual valve. A hydraulic power pump provides the flow of hydraulic fluid to the servo valves at a pressure of 280 bar. Linear displacement transducers allow the instantaneous position of the valves to be monitored. The servo valves where control by a Lotus controller connected to a PC that allows a user interface for the system.
3.3.2 Inlet and Exhaust System

The intake system as shown in Figure 3.6 was designed by Lotus engineering to emulate the flow dynamics of a commercial parent engine. At the start of the intake system an automotive equivalent air filter is fitted to a Cussons\textsuperscript{\textcopyright} P7200 air flow meter. Downstream of the mass flow meter a 60L plenum is mounted to minimize the bulk airflow structures entering the inlet port. The 60L plenum was connected to a throttle plate of 40 mm in diameter through a pipe of 650mm in length. The throttle body is connected to a smaller 2.5L intake plenum designed to minimize any pressure oscillations returning from the intake valves. The intake runner where the gaseous and liquid port fuel injectors are mounted, are 49 mm in diameter and 250 mm in length.
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The exhaust port led to an exhaust plenum with a volume of 1.1L. An oxygen sensor, a pressure transducer, and a thermocouple are all mounted in the exhaust plenum. The exhaust plenum connects to a 3.1 m steel pipe with 49 mm internal diameter which led to a standard automotive silencer and a weak extraction system that vends the exhaust gases to the atmosphere.

### 3.3.3 Optical Flame Diagnosis

Visualisation methods have been historically an invaluable diagnostic tool that has proven critically useful for understanding combustion phenomena in SI engines. In particular, the flame radius can reveal details very early in the combustion process, a period that is not typically well resolved by thermodynamically derived MFB data [30]. Various studies have been concerned with the application of optical diagnostics for combustion analysis in internal combustion engines. The most common techniques include natural light imaging, schlieren imaging, and Mie-scattering tomography. A symbolic comparison of the various techniques is illustrated in Figure 3.7. Simultaneous flame images of the three different techniques are illustrated at the upper part of the figure. A magnification of the captured flame fronts is shown in the lower part of the figure. The flame resides between an outer envelope of radius \( R_u \), outside which there is no burned gas, and an inner envelope \( R_b \) inside which there is no unburned gas [88]. An actual experimental comparison of the schlieren and the mie-scattering techniques can be found in the publication of Gillespie and co-workers. [88]

Mie-scattering technique allows for a 2D planar imaging at a set point across the flame. It has been particularly useful in the characterisation of turbulent flame tomography. As shown in Figure 3.7 and discussed in [88], [35], the Mie-scattering technique is able to obtain planar details of the flame structure, including an accurate representation of the wrinkled flame front. Such tomographic analysis is not feasible by natural light or schlieren imaging. Schlieren and natural light photographs give a 2D projection of the 3D flame. Both of these techniques suffer from an overlap of images from different planes (as with a view of a mountain range in which only the mountain peaks are visible to the observer while the valleys between are obscured) [88]. On the other hand, due to the continuous movement of the flame within the cylinder, the Mie-scattering being a planar technique is unable to capture the global flame growth. The actual flame growth can be obtained with natural light and schlieren imaging. As discussed in section 3.2.2 the location of the schlieren images will lie just behind the location of the natural light images as shown in Figure 3.7.
For the purpose of the current research, and considering the simplicity of the natural light photography, the technique has been selected to analyse the initial (0-5% MFB) flame evolution of the dual fuel mixtures. Flame visualisation was performed using an intensified CCD camera, LaVision© NanoStar, capable of acquiring 8 frames per second and equipped with a 105mm Nikon© focussing lens. The CCD chip has an array size of 1280 x 1024 pixels with a pixel size of 6.7 x 6.7μm. In the current experiments, the array size corresponds to a spatial resolution of 0.07 mm per pixel. The camera was triggered by a LaVision© timing unit synchronised with the engine’s encoders and controlled by the LaVision© Davis software. The actual frame rate is synchronised by the Davis software with respect to the engine speed, and corresponds to 1 image per 3 cycles at 1250RPM, per 6 cycles at 2000RPM and 7 cycles at 2750 RPM. At each test condition, 5 acquisitions at each crank angle were recorder starting from the spark timing up and until TDC.

### 3.3.4 System Integration

The actual engine configuration as used in the present experimental study is illustrated in the upper part of Figure 3.8. For the purpose of the current optical study, the metal liner was used and flame visualisation allowed through the sapphire window located at the flatted top piston crown as shown in the lower schematic of Figure 3.8. The CCD camera was located at an appropriate supporting bracket to minimize vibrations, opposite the 45° mirror. The camera was focused at the spark plug location. A typical valve timing and lift as used in the parent Lotus
production engine was set for all tested conditions. The valve timings are summarised in Table 3.3. The spark timing was fixed at 35° CA BTDC.

The engine position is provided by two Leine & Linde© optical encoders, one mounted on the end of the crankshaft and one with 2:1 drive representing the camshaft, providing 360 and 3600 pulses per revolution respectively. The electronic control signals to the injectors and ignition drivers were generated by an AVL© 4210 engine instrument controller which was referenced to the engine’s shaft encoders with a resolution of 0.2° Crank Angle (CA). Thus, injection duration and timing as well as ignition dwell period and timing were manually controlled with the AVL© 4210 unit.

Two data acquisition systems were utilized for the current work. A slow speed acquisition system was used to monitor temperatures at a low sample rate (1Hz) via K-type thermocouples. Ambient, cylinder head, air intake and exhaust temperatures were closely monitored and recorded throughout the experiments on a desktop computer equipped with an in-house Labview© software. An Omega© OS102 infra-red temperature sensor was focussed at the cylinder liner to measure the outer cylinder wall temperature.

High speed (°CA resolved) acquisition was achieved using an AVL© Indiset Advanced system which also allowed real-time display of various operating parameters, as well as calculated performance parameters such as IMEP, CoV_{IMEP}, and DF ratio. Pressures in the intake and exhaust manifolds as well as gas injection pressure and in cylinder pressure were obtained; the latter using a water-cooled Kistler© 6043A60 transducer fitted in the cylinder head.

The AFR was monitored via an ECM© 1200 AFR recorder which uses a heated zirconia-based high speed oxygen sensor in the exhaust and allows for a custom H/C ratio to be set according to the particular fuel under investigation. This is essential for accurately monitoring the AFR of the different DF mixtures. The mass flow rate of natural gas was measured using the FMA-1600A mass flow meter from Omega©, with an accuracy of 0.8% of the actual reading. The Cussons© P7200 air flow meter mounted just after the air filter was integrated with an NI© CompactDAQ to measure the gravimetric air flow into the engine with an accuracy of ± 1% of the actual reading. The above measurements were fed to the AVL© Indiset system to facilitate the real-time derivation of the DF ratio as will be explained in the next section.
Figure 3.8. Experimental setup of the optical research engine (Upper Plot) - Schematic of the engine’s optical configuration (Lower Plot)
3.3.5 Dual Fuelling Strategy

The engine was fitted with a natural gas port fuel injector, Bosch© NGI-2, upstream the intake at about 200 mm from the intake valves. The injector was supplied with compressed natural gas (92-96% CH₄ mass content) via a two-stage regulator set to 4bar for all test conditions. Fuel injection pressure was chosen in order to be within the linear operating range of the injector. The injection timing of the gaseous fuel was set to TDC (start of intake) resulting in an open valve injection strategy. In comparison to other injection strategies, the open valve injection strategy allowed for the lowest CoV of IMEP and the fastest burning rate to be achieved during a dedicated natural gas operation. Similar findings have been reported in literature [89], [28]. It was therefore adapted throughout the experimental study as the preferred injection timing for the gaseous fuel. Pump-rated 95 RON gasoline was injected at the back of the intake valves at 45° ABDC (IVC timing), to allow for heat transfer effects onto the fuel and therefore enhanced vaporisation. The injection pressure was set to 3.5 bar. The settings of the engine are summarised in Table 3.3.

<table>
<thead>
<tr>
<th>Intake Valves Open / Close / Lift</th>
<th>15° BTDC / 45° ABDC / 9.35 mm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Exhaust Valves Open / Close / Lift</td>
<td>45° BBDC / 15° ABDC / 9.35 mm</td>
</tr>
<tr>
<td>Natural Gas PFI Timing</td>
<td>TDC (Start of Intake Stroke)</td>
</tr>
<tr>
<td>Natural Gas Injection Pressure</td>
<td>4 bar</td>
</tr>
<tr>
<td>Gasoline PFI Timing</td>
<td>45° ABDC (IVC timing)</td>
</tr>
<tr>
<td>Gasoline Injection Pressure</td>
<td>3.5 bar</td>
</tr>
<tr>
<td>Spark Timing</td>
<td>35° CA BTDC</td>
</tr>
</tbody>
</table>

Table 3.3. Experimental engine settings

The DF ratio is defined in the same manner as in the constant volume experiments and corresponds to the energy ratio of NG (Eₙg) to the total (Eₜot) energy in the DF blend as shown in eq. 3.2.

\[
DF_{\text{Ratio}} = \frac{E_{\text{NG}}}{E_{\text{TOT}}} = \frac{E_{\text{NG}}}{E_{\text{NG}} + E_{\text{Gasol}}} = \frac{M_{\text{NG}} \times \text{LHVNG}}{M_{\text{NG}} \times \text{LHVNG} + M_{\text{Gasol}} \times \text{LHVGasol}}
\]  

(3.2)

The only difference between eq 3.1 and 3.2 is the fuel composition. Natural gas was added to gasoline in three different energy ratios, 25% (DF25), 50% (DF50), and 75% (DF75). Using the measured mass flow rate of air (MAF) and natural gas (Mₙg), as well as the relative AFR (λ), the DF ratio has been derived as depicted in the diagram of Figure 3.9, and displayed in real-time on a cycle-to-cycle basis during an experimental engine run. In Figure 3.9, the measured
values are shown with a thick arrow, the information provided by the user as ellipsoidal shapes and the mathematical operators as rectangular shapes.

Figure 3.9. Real-time derivation procedure for obtaining the dual fuel ratio

The hydrogen to carbon ratio (H/C) of gasoline has been set according to the European certification [16] whilst its stoichiometric AFR was set to 14.7. Due to the lack of consistent data on the lower heating value (LHV) of gasoline, its value was set to that of PRF95 (95% volliq iso-octane and 5% volliq n-heptane) and corresponds to 44.66 (MJ/kg). The characteristics of methane have been used as equivalent to those of natural gas. The LHV of methane corresponds to 50 (MJ/kg). For the calculation of the stoichiometric AFR of a particular DF blend, PRF95 has been used as a surrogate for gasoline and methane as a surrogate for natural gas. The stoichiometric AFR has been calculated using the method of chemical balance and assuming products of complete combustion. For the different DFs, the calculated H/C ratios and stoichiometric AFRs (AFR\textsubscript{stoich}) are summarised in Table 3.4, with DF100 representing pure gas (natural gas) and DF0 pure liquid (gasoline).

<table>
<thead>
<tr>
<th>Fuel</th>
<th>H/C ratio</th>
<th>AFR\textsubscript{stoich.}</th>
</tr>
</thead>
<tbody>
<tr>
<td>DF100</td>
<td>4</td>
<td>17.2</td>
</tr>
<tr>
<td>DF75</td>
<td>3.48</td>
<td>16.52</td>
</tr>
<tr>
<td>DF50</td>
<td>3.02</td>
<td>15.87</td>
</tr>
<tr>
<td>DF25</td>
<td>2.62</td>
<td>15.27</td>
</tr>
<tr>
<td>DF0</td>
<td>1.89</td>
<td>14.7</td>
</tr>
</tbody>
</table>

Table 3.4. Fuel properties as used for the derivation of the dual fuel ratio
3.3.6 Operating Conditions

Engine experiments have been conducted under a sweep of engine load, speed and AFR. For the AFR sweep the engine was run at 2000 RPM with a Manifold Absolute Pressure (MAP) of 0.44 bar. Four different equivalence ratios ($\Phi = 0.8, 0.83 1, 1.25$) were tested at that particular load and speed. To reveal the effect of the fuel characteristics on the combustion process, it was deemed necessary to hold the spark timing (35°C BTDC) as well as throttle position constant for the various runs of the different DFs during the AFR, load, and engine speed sweep. Even though a drop in volumetric efficiency is expected as DF ratio increases, the throttle position was kept constant in order to expose all DFs to the same in-cylinder flow characteristics at the point of spark.

A MAP of 0.44 bar with a spark timing of 35°C BTDC, corresponds to 2.7 bar IMEP for NG at $\Phi=1$. As suggested by Stanfield [90] and supported by the authors, this has been a common industry test condition and typical of the NEDC test. In the current engine, and at the same load conditions, Stanfield [90] has quantified the bulk in-cylinder air motion reporting values of the tumble and swirl ratio.

For the engine load sweep, the equivalence ratio was set to 0.8 and MAP was increased from 0.44 to 0.52 and 0.61 bar respectively. For the engine speed sweep, the equivalence ratio was kept at 0.8. The same load was targeted as for pure natural gas fuelling at 2000 RPM, corresponding to 1.7 bar IMEP. As the breathing capability of the engine is changing with the engine speed, throttle has been tuned to achieve the same IMEP throughout the engine speed sweep. Starting from 1250 RPM, the engine speed was increased to 2000 RPM and finally to 2750 RPM. For the engine speed sweep only DF0, DF50 and DF100 have been tested. The experimental test matrix is summarised in Table 3.5.

<table>
<thead>
<tr>
<th>Engine Parameter</th>
<th>Equivalence Ratio (Φ)</th>
<th>Engine Load</th>
<th>Engine Speed (RPM)</th>
<th>Fuels</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFR</td>
<td>0.8, 0.83, 1, 1.25</td>
<td>MAP : 0.44 (bar)</td>
<td>2000</td>
<td>All</td>
</tr>
<tr>
<td>Load</td>
<td>0.8</td>
<td>MAP : 0.44, 0.52, 0.61 (bar)</td>
<td>2000</td>
<td>All</td>
</tr>
<tr>
<td>Speed</td>
<td>0.8</td>
<td>1.7 bar IMEP on NG Fuelling</td>
<td>1250, 2000, 2750</td>
<td>DF0, DF50, DF100</td>
</tr>
</tbody>
</table>

Table 3.5. Experimental test matrix
As there is no cooling for the cylinder liner, typical for fully accessible optical engines, the time during a particular experimental run was limited to less than 2 minutes. The process for each test condition required the engine head to first be heated using the lubricating oil to a temperature of 50 °C. The lubricating oil was heated with a 9 kW industrial electric heater and circulated with a Brook Hansen© electric pump. The engine was then motored before activating the ignition coil and injectors. Whilst the engine was heated up to a liner temperature of 70 °C, the AFR and DF ratio was fine tuned to the desired values. At a liner temperature of 70 °C the flame imaging was initiated and at a temperature of 90 °C the recording of in-cylinder pressures. The maximum allowed temperature of the cylinder liner was limited to 100 °C. The ambient temperature for all test conditions was 17 ± 2 °C. For each test condition, 250 engine cycles were recorded for analysis, that allow for an average cycle to be calculated and analysed as will be explained in section 6.2.1.

### 3.4 Numerical Methods

#### 3.4.1 Flame Velocity Model

Following the work of Karlovitz et al. [70] and Markstein,[71], Clavin [75] developed a model to account for the effects of flame stretch on the development of a laminar flame. As discussed in section .3.2.4, the model correlates linearly the stretched flame velocity \( S_b = \frac{dR_f}{dt} \) with the fundamental burning velocity \( S_u^0 \) and the effects of stretch such as for an infinitesimally thin flame [63],

\[
S_b = S_u^0 \sigma - L_b a
\]  

(3.3)

Equation 3.3 is the same as equation 2.4 although for the reader’s convenience is repeated in this section. The flame stretch rate is an additive contributor of the aerodynamic strain, and the flame curvature [59] ,[60],[62]. In a quiescent flow necessary for laminar combustion, an outwardly spherical flame propagates normal to its surface implying that the tangential staining is zero [57]. Thus, the global flame stretch can be simply defined as [57],

\[
a = \frac{2}{R_f} S_b
\]  

(3.4)
where $R_f$ is the flame radius.

The model presented in eq.3.3 has been successfully used by other researches in an effort to predict either the laminar [91] or turbulent [92], [93] flame velocity in real combustion applications. In particular, Dahms et al. [94] proposed a model where the turbulent flame velocity in an SI engine is computed from the stretched laminar burning velocity calculated by the model of Clavin as illustrated in eq.3.3.

In the context of the current analysis, eq.3.4 was substituted to eq.3.3 and the model has been solved with respect to the stretched flame velocity such as,

$$S_b = \frac{S_{u0} \sigma}{R_f + 2L_b} R_f$$  \hspace{1cm} (3.5)

The model is intended to predict the stretched flame velocity of a premixed outwardly propagating spherical, infinitesimally thin, isobaric, and stable flame in a quiescent flow.

At a given flame radius ($R_f$) the stretched flame velocity of a particular fuel can be predicted only if reliable sub-models of the laminar burning velocity ($S_{u0}$), Markstein length ($L_b$) and expansion ratio ($\sigma$) are available. Such models are fully documented in the following sections.

### 3.4.2 Chemical Kinetics

Chemical Kinetics has long being used in literature for the prediction of laminar burning velocity and flame structure [51], [38],[46]. Of particular engineering importance is the consumption and production of species during a flame propagation process that controls the release of heat. Chemical kinetics is the science of chemical reaction rates. While thermodynamics provides steady state information of the combustion process, chemical kinetics describe the transient state of the system during the combustion process [95].

A chemical reaction process can be generally described by a global chemical equation such,

$$\text{Fuel} + \text{Oxidizer} = \text{Products}$$

A global reaction indicates that the oxidation process of the fuel is an instantaneous one - step process. However, chemical kinetics during a combustion process rarely proceeds in this simple manner. In reality, a combustion process is a much more complex and sequential process including multiple intermediate products.
The use of global reactions to express a chemical reaction system is frequently a “black box” approach. Global reactions provide the input-to-out perspective to the chemical process, which is not capable to characterise the actual path that reactants followed in order to form products. Therefore, a global equation is unable to describe a chemical process in detail. A group of elementary reactions is essential to reliably characterise a combustion process.

### 3.4.2.1 Elementary reactions

An elementary reaction is a chemical reaction in which one or more species react directly to form products in a single reaction step with no reaction intermediates. It represents the actual change that take place at a molecular level during the reaction. Based on the number of molecules involved in an elementary reaction, there are three major types of elementary reactions briefly summarised in table 3.6.

<table>
<thead>
<tr>
<th>Type of reaction</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Unimolecular</td>
<td>Rearrangement or Dissociation of a single molecule</td>
</tr>
<tr>
<td>Bimolecular</td>
<td>Collision and Reaction of two molecules</td>
</tr>
<tr>
<td>Termolecular</td>
<td>Collision of three molecules</td>
</tr>
</tbody>
</table>

Table 3.6. Types of elementary reactions

Most elementary reactions of interest in combustion are bimolecular and can be generally expressed as,

\[
aA + bB \rightarrow cC + dD
\]  

(3.6)

where \(a, b, c, d\) are stoichiometric coefficients. The rate of an elementary reaction \(w\) has the same value whether you consider the rate of consumption of reactants or the rate of formation of products and is expressed as,

\[
w = -\frac{1}{a} \frac{d[A]}{dt} = -\frac{1}{b} \frac{d[B]}{dt} = \frac{1}{c} \frac{d[C]}{dt} = \frac{1}{d} \frac{d[D]}{dt} = -k [A]^a[B]^b
\]

(3.7)

Where \([X]\) denotes the molar concentration of species, and \(k\) the rate constant which is applicable for all types of reactions. Negative rates indicate that the species are consumed.

### 3.4.2.2 Rate Constant

The rate constant is given by an exponential function of temperature in the so-called Arrhenius form,
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\[ k = A'T_u^b e^{\frac{-E}{RT}} \]  \hspace{1cm} (3.8)

where \( A' \) is the pre-exponential factor defining the frequency of colliding molecules, \( E \) is the activation energy needed to bring reactants into a reactive state, \( T_u \) is the unburned temperature, \( R \) is the gas constant, and \( b \) is the temperature exponent.

### 3.4.2.3 Chain Reactions

A combustion process is a series of reactions leading to a self-amplifying self-sustaining chain of chemical events, initiated by the formation of highly reactive molecules called radicals. The sequence of a reaction chain can be typically divided into four major stages such as:

- Initiation, involves the formation of radicals from stable species.
- Branching, allows more radicals to be produced than consumed.
- Propagation, in which number of radicals does not change.
- Termination, in which radicals are destroyed and reactivity ceases.

A kinetic model for reactants-to-products conversion is a group of elementary reactions resulting to an overall fuel’s reaction mechanism. The mechanism contains all elementary reactions in the mentioned chain reaction types relevant to the fuel and oxidizer under consideration.

In parallel with the conservation equations of mass and energy, the laminar burning velocity of a particular fuel-oxidizer mixture can be numerically predicted if for all species involved in the reaction mechanism the net production and destruction rates are summarised into a system of ordinary differential equations using the same methodology as in eq. 3.7. The system of equations can be solved using computerised methods.

For the purpose of the current research, Cantera [96] an open source software tool for problems involving chemical kinetics, thermodynamics, and/or transport processes has been used as the kinetic solver.

The conservation equations used by the Cantera software package governing a steady, isobaric, one dimensional unstretched flame are fully documented in the PREMIX manual [97]. The model of a freely propagating flame in the Cantera software package is equivalent to that of PREMIX [97]. PREMIX has been developed by CHEMKIN\(^\text{©}\) for modelling laminar flames. The correctness of such models for laminar burning velocity simulations has been proved over the years through their wide usage in literature [51] [38][46]. Thus, further discussion of the applied conservation equations is not attempted in this thesis.
To enable the prediction of laminar burning velocity, Cantera has to be integrated with a purposely valid reaction mechanism which will be considered in the following section.

### 3.4.3 Reaction Mechanisms

A comprehensive reaction mechanism aims to include all elementary reactions that are involved in a reacting system. The construction of such mechanism requires accurate reaction rate, thermodynamic, and transport data for each species. Many of those species have never been determined experimentally. Theoretical methods have been used in many cases to determine the reaction rates of such species [98]. Reduced kinetic models are derived from the comprehensive mechanisms by means of sensitivity analysis, as well as steady state and partial equilibrium assumptions. Many of the intermediate species during a combustion process are present only in very low concentrations. By assuming that these species are unimportant and/or they are at steady state, the number of reactions and species can be significantly reduced, resulting in a simplified system of differential equations to be solved.

Since the first attempts in kinetic modelling of hydrogen have been made in the early 1970s, the development of comprehensive mechanisms for other practical fuels has rapidly progressed. In an attempt to model the combustion of natural gas, a team of kinetics experts have developed the GRI mechanism back in 2000 [99]. The mechanism is suited for application in high temperature oxidation processes including laminar burning velocity simulations. It consists from 325 elementary reactions and 53 species. The GRI mechanism was then followed by the Leeds mechanism [100] developed by a group of European kinetics based on the studies of Miller and Bowman [101] and Glaborg et al. [102]. The mechanism consists of 357 reactions and 37 species and it was also intended for simulation of high temperature oxidation processes of light hydrocarbons up to C₂. Over the years, several other groups followed with the development of reaction mechanisms for light hydrocarbon oxidation including Ranzi [103], San Diego [104] and USC II [105] mechanisms.

A late comprehensive reaction mechanism concerning the oxidation of C₁ -C₄ hydrocarbons was developed by the National University of Ireland (NUI) [106] and includes the latest reaction rates as well as thermodynamic and transport properties of species involved. The mechanism builds on earlier work performed by NUI [107],[108]. It was given the name AramcoMech and contains 253 species and 1542 reactions.

An extensive validation of the laminar burning velocity of methane computed with the AramcoMech is reported in the study of Metcalfe et al. [106] with temperatures scaling from
295K to 600K, pressures from 1 bar to 10 bar and equivalence ratio from 0.4 to 2.2. Figure 3.10 [106] illustrates the validation of the mechanism against various experimental data at pressures of 1, 5 and 10 bar and 298 K. Apart from the Leeds mechanism, a comparison of the performance of the already mentioned mechanisms versus the AramcoMech is also indicated in Figure 3.10. The AramcoMech is providing well validated results over the range of tested equivalence ratios especially if the scattered between the various sets of experimental data is considered.

Figure 3.10. The performance of various mechanisms in predicting the burning velocity of CH₄. Experimental data are derived from the studies of, W.Lowry [109], Y.Kochar et al. [110], Rozenchan et al [52], Gu et al [50] Hassan et al. [51], Vagelopoulos et al. [111], Vanmaaren et al. [112], Vagelopoulos & Egofoopoulos [113], Taylor [114], Egofopoulos et al [115], Hidaka et al. [116]

In general, the reaction mechanism of a hydrocarbon fuel is hierarchical [117]. Thus, the reaction mechanism of a given fuel is made up by the mechanisms of all possible smaller molecule fuels. The reaction mechanism derived by Lawrence Livermore National Laboratory (LLNL) is suited to gasoline kinetic modelling and is one of the most comprehensive mechanisms available in literature including 1389 species and 10481 reactions [118]. It is also capable of modelling general multi-component hydrocarbon mixtures. Its core structure is based on the C₁-C₄ AramcoMech mechanism. As the correctness of the LLNL mechanism has been proved over the years, researches have used the mechanism as a starting point for the development of practical reduced mechanisms to simulate the combustion of gasoline surrogates [119], [120],[44].

The mechanism of Jerzembeck et al. [44] was derived based on the LLNL mechanism, with the essential prerequisites of modelling the laminar burning velocity of binary blends of primary
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reference fuels as well as shorter alkanes including methane. As clearly stated by Jerzembeck et al. [44] all significant reactions related to laminar flames have been maintained in the reduced mechanism. A set of validation data for the computed laminar burning velocities of PRF87 as reported by Jerzembeck et al. [44] is presented in Figure 3.11. For lean and stoichiometric mixtures, the mechanism attains a very good validation with the experiments. At rich mixtures and especially at pressures higher than 15 bar the computations underestimate the experimental results. The burning velocity of gasoline is reasonable reproduced by the PRF mixture at all tested AFRs. Hence, PRF mixtures can be used as valuable surrogates for gasoline. For a comprehensive validation of the mechanism the reader is referred to the study of Jerzembeck et al. [44].

![Figure 3.11. Validation of Jerzembeck mechanism against experimental results [44]](image)

For the purpose of the current research, the Jerzembeck mechanism [44] has been selected to assess the performance of the currently available kinetics in predicting the laminar burning velocity of PRF95 and methane fuel blends. The mechanism has been integrated with the Cantera software package to enable such numerical predictions.

### 3.4.4 Expansion Ratio

The expansion ratio or as it is also commonly called the expansion factor is defined as the ratio of unburned to burned gas density. The calculation of the expansion ratio requires the chemical equilibrium of the burned products to be obtained in order to derive the burned gas density. In Cantera, chemical equilibrium has been computed with the elements potential method, similar to that used in Stanjan [121]. The method of elements potential relates the mole fractions of each species to quantities called element potentials and then solves for the chemical equilibrium of the system. On the other hand, if one uses the method of equilibrium constants it is necessary to identify the exact set of reactions that take place in the chemical system. Thus, the advantage of the element potential method is that the exact reactions involved in the system are not
necessary to be obtained. For further information on the method the reader is referred to the work of Reynolds [121]. Computations of the chemical equilibrium with the method of elements potential are widely used in literature.

### 3.4.5 Markstein Length Model

An updated theoretical model for predicting the burned gas Markstein length has been reconstructed based on the studies of Bechtold and Matalon [122] and Peters and co-workers [123]. Following the work of Matalon and Matkowsky [74], Bechrold and Matalon [122] derived an analytical expression for the unburned gas Markstein length as,

\[
L = \delta \left[ y_1 + \frac{1}{2} \beta \left( L_{eff} - 1 \right) y_2 - \left( \sigma - 1 \right) \gamma_1 / \sigma \right]
\] (3.9)

Where \( \delta \) is the flame thickness, \( \sigma \) is the expansion factor, \( \beta \) is the Zeldovich number which characterises the sensitivity of the reaction rate to the flame temperature, and \( L_{eff} \) is the effective Lewis number of the combustible mixture.

After evaluating three common assumptions of thermal conductivity (\( \lambda_c \)) namely \( \lambda_c = 1, T^{1/2}, T \), Bechtold and Matalon [122] concluded that assuming \( \lambda_c = T^{1/2} \), values of Markstein length could be predicted which agreed best with experimental data. As such, using \( \lambda_c = T^{1/2} \) the final expressions of \( \gamma_1 \) and \( \gamma_2 \) become [122],

\[
\gamma_1 = \frac{2\sigma}{\sqrt{\sigma} + 1}
\] (3.10)

\[
\gamma_2 = \frac{4}{\sigma - 1} \left[ \sqrt{\sigma} - 1 - \ln \left( \frac{1}{2} \left( \sqrt{\sigma} + 1 \right) \right) \right]
\] (3.11)

Based on the work of Clavin [75], Rogg B and Peters [124] also developed a theoretical model for predicting the unburned gas Markstein length similar to the one derived in [72]. The model was finalised by Peters and co-workers [123] to include an effective Zeldovich number sub-model such as,

\[
L = \delta \frac{1 + \Delta}{\Delta} \left[ \ln (1 + \Delta) + \frac{\beta}{2 L_{eff}} \left( L_{eff} - 1 \right) \int_0^\Delta \frac{\ln (1 + x)}{x} dx \right]
\] (3.12)

The constant \( \Delta \) is expressed as
and the Zeldovich model is defined as,

$$\beta = 4 \frac{T_{ad} - T_u}{T_{ad} - T_0} \quad (3.14)$$

where $T_{ad}$ is the adiabatic and $T_u$ the unburned gas temperature outside the preheat zone. As justified by Taylor [114] and Gottigens et al. [125], to better represent the thermodiffusive properties of the combustible mixture, thermodynamic and transport properties such as thermal and mass diffusivity, thermal conductivity and specific heat should be evaluated at a temperature ($T_0$) corresponding to the point of transition between the preheat and the reaction zone. Such analysis has not been considered by Betchmod and Matalon [122]. A model for calculating the inner layer temperature ($T_0$) of hydrocarbon flames as well as the flame thickness has been used from the work of Gottinges et al. [125]. Assuming an exclusive dependence on the pressure ($P$) [123] [125], the inner layer temperature is calculated as,

$$T^0 = \frac{-E}{\ln(P/B)} \quad (3.15)$$

The activation energy ($E$) and the constant B for methane and iso-octane fuels are taken from the work of Gottigens et al. [125] and Muller et al. [123] respectively. The values for iso-octane are taken to be representative for those of PRF95. Such values are currently unavailable for a methane-PRF95 binary blend.

The flame thickness ($\delta$) has been evaluated as,

$$\delta = \frac{T_{ad} - T_u \left( \frac{\lambda_c}{c_p} \right) T^0}{\rho_u \cdot S_u^0} \quad (3.16)$$

The parameter $\left( \frac{\lambda_c}{c_p} \right) / \rho_u$ is effectively the thermal diffusivity of the mixture. For hydrocarbon fuels, as reported by Gottigens et al. [125] the constant $c$ is near to unity without any exclusive dependence on the fuel and it was therefore set to unity throughout the current numerical analysis.
The difference between the unburned and burned gas Markstein length is attributed to the existence of a finite flame thickness [56]. Flame thickness decreases with the increase of pressure and attains a minimum value at near stoichiometric mixtures. In the range of equivalence ratios that this numerical study is concerned (\(\Phi = 0.6-1.2\)), and for pressures higher than atmospheric, as reported by Sun et al. [56] and supported by Taylor [114] the burned gas Markstein length can be confidently derived by multiplying \(L\) with the expansion ratio ratio such as,

\[
L_b = L \sigma
\]  

(3.17)

### 3.4.5.1 Lewis Number

The described Markstein length models have been developed based on the asymptotic theory. The asymptotic theory [74] considers the combustible mixture to be well away from stoichiometry so that the resulting Markstein length depends only on a single Lewis number that of deficient reactant. Predictions based on this theory are clearly not valid at near stoichiometric conditions. Following the study of Joulin and Mitani [126] an effective Lewis number model has been developed by Betchold and Matalon [122] that exhibits an exclusive dependence on equivalence ratio and is therefore valid for near stoichiometric conditions such as,

\[
Le_{eff} = 1 + \frac{(Le_E - 1) + (Le_D - 1) A}{1 + A_i}
\]  

(3.18)

with

\[
A_i = 1 + \beta (\Phi' - 1)
\]  

(3.19)

and

\[
\Phi' = \frac{Y_{E_a}/\nu_E W_E}{Y_{D_a}/\nu_D W_D}
\]  

(3.20)

The Lewis Number of the excess and deficient reactant is represented by \(Le_E\) and \(Le_D\) respectively. The symbol \(\Phi'\) represents the excess to deficient reactant mass ratio in the unburned mixture. Similar expressions for an effective Lewis number as in eq. 3.18 have been used in other research studies [127],[128].
As pointed out by Bourgine et al. [129] the definition of the Lewis number of a multicomponent fuel mixture is a challenging task. A number of works have been dedicated to the formulation of this parameter [130], [65], [66]. The study of Dinkelacker et al. [66] have assessed the existing available approaches, concluding that the Lewis number of a multicomponent fuel mixture can be best approximated as,

\[
Lef = \sum \frac{\lambda_c}{X_{fi} D_{fi}}
\]

(3.21)

with \(X_{fi}, D_{fi}\) being the molar fraction and the mass diffusivity of the individual fuel components in the fuel mixture. The thermal conductivity (\(\lambda_c\)) is only slightly affected by the fuel composition as it is a property of the whole fuel-air mixture, and thus it is dominated by the large nitrogen content [66]. The mass diffusivity of each fuel component has been evaluated based on the diffusivity of the particular fuel component within air. The mass diffusivity of oxygen is calculated against the diffusivity of the multicomponent fuel and nitrogen mixture. Thermochemical and transport properties of the individual species have been derived using Cantera, integrated with the reaction mechanism of Jerzembeck et al. [44]. The prescribed methodology for predicting the Lewis number of a multicomponent fuel-air mixture has not been adapted in either of the mentioned studies concerning the derivation of Markstein length [122], [123].

The contributions made to the core models as documented in the current and previous section are aiming to extend their numerical capabilities and performances. The performance of the models will be evaluated in chapter 5.

### 3.5 Burning Rate Definitions

The mass burning rate in any given combustion application can be defined as,

\[
\dot{m}_b = \rho_u u_t A_f
\]

(3.22)

where \(\rho_u\) is the unburned gas density, \(A_f\) is the total flame surface area of the wrinkled flame front, and \(u_t\) is the mean turbulent burning velocity of the flame front. The basic concept of laminar flamelet combustion [131], [132], implies that the turbulent flame consists of thin reacting interfaces between reactants and products and that these interfaces have the structure of
strained laminar flames. Thus in the context of flamelet combustion, the turbulent burning velocity of the flame front equals to the stretched laminar burning velocity ($S_u$). The definition of the stretched laminar burning velocity is given in section 2.3.2.4.

### 3.5.1 SI Engine Environment

In the context of flamelet combustion, the mass burning rate in a homogeneous SI engine can be defined as,

$$\dot{m}_{b,Eng} = \rho_{Eng} S^0_{u,Eng} I_{0,T} A_T Y_T$$  \hspace{1cm} (3.23)

where $S^0_{u,Eng} I_{0,T}$ is the mean turbulent burning velocity of the spatial flame front along the flame surface. The mean turbulent stretch factor ($I_{0,T}$) represents the effect of flame stretch on altering the unstretched laminar burning velocity ($S^0_{u,Eng}$) of the combustible mixture ($I_{0,T} = S^0_{u,Eng} / S^0_{u,Eng}$). It is mainly depended on the Markstein length of the mixture. A value of $I_{0,T}$ higher than unity indicates an increase of burning velocity due to flame stretch and vice versa. The mean turbulent flame surface area ($A_T$) can be increased by the wrinkling of the flame due to a turbulent flow field. In addition, the flame surface area can be further increased by flame cellularity induced by phenomena of flame instability as discussed in section 2.3.3. Solid well agreed models quantifying the effect of flame instability on the mass burning rate are currently unavailable in literature [82]. Thus, an empirical turbulent flame instability factor ($Y_T$) is introduced in the burning rate equation to track any further increase of the flame surface area due to phenomena of flame cellularity induced by flame instability. For nonequidiffusion flames, the higher localised flame curvature induced by flame cellularity implies that the flame will experience a higher localised flame stretch. The higher localised flame stretch will alter the burning velocity in comparison to a stable flame. The effect of a localised increase of stretch upon the burning velocity can be tracked by the spatial change of the stretch factor ($I_{0,T}$) along the surface of the flame. High localised stretch values will increase the mean stretch experienced by the flame and consequently the mean stretch factor.

In the current analysis, the parameters involved in the derivation of the mass burning rate are kept in rather simple and fundamental terms in order to aid the understanding of the reader on the influential parameters involved. To derive the influential parameters involved the burning rate is written as,
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\[ \dot{m}_{p,Eng} = \rho_{u,Eng}S_{u,Eng}^0 I_0 Y_T A_L \frac{A_T}{A_L} \]  

(3.24)

From the ideal gas law, the unburned gas density (\(\rho_{u,Eng}\)) is defined as,

\[ \rho_{u,Eng} = \frac{P}{(RT_u/W_u)} \]  

(3.25)

where \(W_u\) is the molecular weight of the unburned mixture and \(R\) is the ideal gas constant. The unburned gas density is depended on pressure (\(P\)), unburned gas temperature (\(T_u\)), equivalence ratio (\(\Phi\)) and composition (\(c_i\)),

\[ \rho_{u,Eng} = f(P, T_u, \Phi, c_i) \]  

(3.26)

The unstretched laminar burning velocity (\(S_{u,0}\)) is only depended on the thermochemical properties of the combustible mixture as discussed in section 2.3.1,

\[ S_{u,Eng}^0 = f(P, T_u, \Phi, c_i) \]  

(3.27)

A stable unstretched laminar flame is propagating with a rate equal to its unstretched flame velocity (\(S_{u,0}\)). For such a flame, its surface area (\(A_L\)) is an exclusive function of the thermochemical properties of the combustible mixture,

\[ A_L = f\left(S_{u,Eng}^0\right) \]  

(3.28)

Thus,

\[ A_L = f(P, T_u, \Phi, c_i) \]  

(3.29)

Using Fractal geometry [133] the ratio of turbulent to laminar flame surface area (\(A_T/A_L\)) can be modelled as,

\[ \dot{m}_{p,Eng} = \rho_{u,Eng}S_{u,Eng}^0 I_0 Y_T A_L \left[ \left( \frac{L_{Max}'}{L_{Min}'} \right)^{D_T-2} \right] Y_T \]  

(3.30)
Where \((L'_{\text{Max}}/L'_{\text{Min}})\) is the ratio of the flame wrinkling scales, \(D_T\) is the fractal dimension, and \(Y_T\) is the non-dimensional empirical constant aiming to track the increase of flame area due to phenomena of flame instability in turbulent flames.

The ratio of the flame wrinkling scales can be well approximated by the ratio of integral length scale \(I_i\) to the Kolmogorov scale \(\eta\) \[133\] as,

\[
\frac{L'_{\text{Max}}}{L'_{\text{Min}}} \approx \frac{I_i}{\eta}
\]  

(3.31)

The ratio of the flame wrinkling scales will be affected by the turbulence levels inside the engine. Therefore,

\[
\frac{L'_{\text{Max}}}{L'_{\text{Min}}} = f(u)
\]

(3.32)

Where \(u\) symbolises the turbulence characteristics. According to Liou et al. \[134\] the fractal dimension \((D_T)\) which characterizes the roughness or degree of wrinkling of the flame surface is defined as,

\[
D_T = 2.35 \frac{u'}{u' + S^0_{u_{\text{Eng}}}} + 2 \frac{S^0_{u_{\text{Eng}}}}{u' + S^0_{u_{\text{Eng}}}}
\]  

(3.33)

Where \(u'\) is the turbulence intensity. Thus,

\[
D_T = f(P, T_u, \Phi, c_i, u)
\]

(3.34)

As discussed in section 2.3.3 the onset of flame instability can be predicted knowing the thermochemical properties of the mixture and the stretch experienced by the flame. Turbulence intensity is directly affecting the stretch experienced by the flame. Thus, in an SI engine environment the onset of flame instability is depended on the turbulence characteristics in addition to the thermochemical properties of the combustible mixture.

The stretch factor equals to the ratio of stretched \((S_{u_{\text{Eng}}})\) to the unstretched \((S^0_{u_{\text{Eng}}})\) laminar burning velocity. Considering the model developed by Clavin \[75\] (eq 3.3), and knowing (section 2.3.4) that \(S_u = S_b / \sigma\), and \(L = L_b \sigma\), the stretch factor can be defined as,
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\[ I_{0T} = \frac{S_{u_{Eng}}}{S_{0u_{Eng}}} = 1 - \frac{L_p \sigma}{S_{u_{Eng}}} a_{Eng} \]  

(3.35)

The turbulent stretch rate \( a_{Eng} \) is constituted from the additive contributions of the flame curvature, the normal and the tangential straining. The stretch induced by the flame curvature and the normal straining is defined as the geometric stretch \( a_g \) and that induced by the tangential straining as turbulent stretch \( a_t \) such as,

\[ a_{Eng} = a_g + a_t = \frac{2}{R_f} S_{p_{Eng}} + \frac{u'}{\lambda_T} \]  

(3.36)

The tangential straining is approximated as the ratio of turbulent intensity \( u' \) to the Taylor micro scale of turbulence \( \lambda_T \) following the work of Abdel-Gayed and co-workers [135].

Thus \( I_{0T} \) is dependent on,

\[ I_{0T} = f(P, T_u, \Phi, c_i, u) \]  

(3.37)

It is therefore concluded that the mass burning rate in an SI engine is depended on the in-cylinder pressure \( P \), unburned gas temperature \( T_u \), equivalence ratio \( \Phi \), composition \( c_i \), and turbulence characteristics \( u \), as shown in eq. 3.38. The dependence of burning rate on the mentioned parameters is highly nonlinear.

\[ \dot{m}_{b,Eng} = f(P, T_u, \Phi, c_i, u) \]  

(3.38)

The parameters that affect the burning rate (eq. 3.38) in an SI engine are also dependent variables. For example, a change in composition will affect the unburned gas temperature. To help the reader appreciate the mentioned phenomena, a simplified engine compression stroke is simulated with an adiabatic variable volume model, and a compression ratio of 10:1. Three different fuels have been considered at stoichiometric conditions. The fuels consist of CH₄, PRF95 (95% vol. of iso-octane and 5% vol. of n-heptane), and a dual fuel blend (DF50) with half of its energy contributing from CH₄ and half from PRF95.
Figure 3.12. Effect of piston compression on the unburned gas temperature during different fuelling modes

As can be observed from Figure 3.12 at identical initial conditions and for the same compression, a change in fuelling mode will lead to different compressive temperatures attributed to the different specific heat ratios among fuels. For completeness, the compressive temperature of pure air is also shown in Figure 3.12.

3.5.2 Constant Volume Environment

Experiments in the Constant Volume Combustion Vessel (CVCV) allow for the same initial pressure and hence temperature among the different tested fuels due to the nonexistence of piston compression.

The mass burning rate inside the CVCV can be defined as,

\[
\dot{m}_{b,CVCV} = \rho_{u,CVCV} S_{u,CVCV}^{0} \dot{I}_L A_L Y_L
\]

In the constant volume vessel, there is no turbulence effect involved as the mixture is initially quiescent. With the nonexistence of turbulence, there is only a contribution from the geometric stretch. Hence, the stretch factor can be derived as,

\[
\dot{I}_L = 1 - \frac{L_b \sigma}{S_{u,CVCV}^{0}} a_g = 1 - \frac{L_b \sigma}{S_{u,CVCV}^{0}} \frac{2}{R_f} S_{b,CVCV} = 1 - \frac{L_b \sigma^2}{S_{u,CVCV}^{0} R_f} S_{u,CVCV}
= \frac{1}{1 + \frac{2 L_b \sigma^2}{R_f}}
\]

(3.40)
Thus inside the CVCV, $I_{0L}$ is depended only on thermochemical properties,

$$I_{0L} = f(P, T_u, \Phi, c_i)$$  \hspace{1cm} (3.41)

It has to be noted that flame instabilities manifested as cellular structures on the flame surface can lead to a self-turbulirizing effect in the combustion vessel [50]. In contrast to the SI engine environment, the onset of flame instability in the constant volume environment is only depended on the thermochemical properties of the mixture. There is no effect from the flow field as the mixture is initially quiescent.

With the nonexistence of turbulence, the flame surface area is only affected by the stretched burning velocity ($S_{u0}^{CVCVI0L}$) and by the phenomena of flame instability ($Y_L$). In a CVCV both stretched burning velocity and flame instability are thermochemical parameters of the combustible mixture, thus $A_L$ is depended on,

$$A_L = f(P, T_u, \Phi, c_i)$$  \hspace{1cm} (3.42)

Following the previous analysis, it can be concluded that the mass burning rate during the experiments in the constant volume combustion vessel is depended only on the thermochemical parameters of the combustible mixture.

$$\dot{m}_{b,CVCV} = f(P, T_u, \Phi, c_i)$$  \hspace{1cm} (3.43)

For the constant volume combustion and in contrast to the SI engine environment, the influential parameters of the mass burning rate are independent variables. At the time of ignition, three out of four parameters that affect the burning rate in the constant volume combustion vessel (eq. 3.43) can be constrained and the effect of the fourth parameter on the overall burning rate can be explicitly investigated.

### 3.5.3 Transition Mechanism

For a homogeneous mixture of the same equivalence ratio and composition, the transition mechanism characterizing the difference in burning rate from the constant volume to the engine combustion can be revealed considering the derivation of the equations 3.38 and 3.43.
For a particular fuelling mode, the contributors of the transition mechanism as indicated in eq. 3.44 are the effects of turbulence on the burning rate as well as the difference in the temperature and pressure due to piston compression.

\[ \dot{m}_{b,\text{CV CV}} - \dot{m}_{b,\text{Eng}} = f \left( (P_{\text{CV CV}} - P_{\text{Eng}}), (T_{\text{CV CV}} - T_{\text{Eng}}), u \right) \]  

(3.44)

Where \( P_{\text{CV CV}} \), \( T_{\text{CV CV}} \) is the pressure and temperature inside the Constant Volume Combustion Vessel (CVCV) and \( P_{\text{Eng}} \), \( T_{\text{Eng}} \) is the pressure and temperature in the engine environment.

In comparison to the constant volume environment, the turbulent flow field experienced in the SI engine directly affects the flame surface area and the stretch experienced by the flame. Subsequently the burning velocity will be affected by the flame stretch through the stretch factor and the onset of flame instability will be altered.

In addition to the effect of flame compression on the unburned gas mixture, the piston compression induces a further increase on the initial pressure and temperature experienced by the combustible mixture in the SI engine as compared to the constant volume experiments. Consequently, the laminar burning velocity and the Markstein length can differ between the two experimental environments.

The effect of the transition mechanism will be discussed in chapter 7 based on the burning rate characteristics experienced in the constant volume as compared to the engine combustion.

### 3.6 Chapter Summary

The present chapter outlined the experimental technique for the constant volume and the SI engine experiments. An overview of the instrumentation used for both types of experiments and in particular the integration of optical diagnostics was presented. The dual fuel mixture preparation and the control of the AFR in both experimental apparatuses were comprehensively explained. The post-processing technique of the raw experimental data is discussed separately in the specific chapters to follow for each experimental environment. Besides, the numerical methodology for the prediction of the stretched laminar flame propagation velocity and the burning rate definitions in the two experimental environments were documented in the present chapter.
Chapter 4

4 Constant Volume Combustion

4.1 Introduction

Practical combustion phenomena are critically affected by the fundamental laminar burning velocity \( (S_u^0) \) of the fuel-oxidizer mixture. Since all realistic flames are curved and/or travel through a strained flow field, the Markstein length \( (L_b) \) quantifying the flame stretch sensitivity, is also necessary to completely characterise the flame evolution [136].

Substantial efforts have been devoted for improving the understanding on methane as well as gasoline combustion. It appears that there is inadequate prior experimental work reporting the fundamental combustion parameters, laminar burning velocity and Markstein length, of a natural gas-gasoline dual fuel blend. The laminar burning velocity and Markstein length of the blended fuels need further investigation especially at elevated pressures. Thus, the experimental work presented in the current chapter aims to investigate the relationship between laminar burning velocity and Markstein length, with the ratio of gas to liquid in a dual fuel blend at elevated pressures. In the current experimental work a binary blend of primary reference fuels commonly known as PRF95 (95% v/o of iso-octane and 5% v/o n-heptane) is used as a gasoline surrogate. Methane is used as a surrogate for natural gas. Values of laminar burning velocities and Markstein lengths are measured at equivalence ratios of 0.8, 1, 1.2, initial pressures of 2.5, 5, 10 Bar and a temperature of 373 K.
4.2 Post-processing Methodology

The experimental apparatus and the filling technique for the constant volume combustion experiments were presented in chapter 3. The post processing procedure of the raw flame images for deriving the fundamental combustion parameters, laminar burning velocity and Markstein Length is addressed in the current section. Besides, the thermodynamic analysis of the acquired pressure traces in the combustion vessel used to infer the mass burning rate of the tested fuels will be also documented.

4.2.1 Flame Theory

A common approach of measuring burning velocity and Markstein length in a combustion vessel has been the constant pressure outwardly propagating spherical flame method [137],[52],[49],[44]. The method is suitable for extrapolation of measured stretched flame velocities to their fundamental non-stretched values and the associate Markstein lengths, due to the well-defined stretch rates of an outwardly spherical flame. The constant pressure outwardly propagating spherical flame method in combination with the theory given by Strehlow and Savage [63] have been used by most of the studies in literature [137],[52],[49],[44][48]. The theory of Strehlow and Savage derived on the assumption that the burned gas is coming to rest after crossing an infinitesimally thin flame.

In the present experimental work, the use of a cylindrical combustion vessel instead of a spherical one imposes non-symmetrical (cylindrical) confinement on the outwardly flame evolution. The non-symmetrical confinement disrupts the induced flow field from the symmetrically confined (spherical) case, causing the motion of burned gases within the burned zone even for a constant pressure in the combustion vessel[136] [138]. Significant deviations from the commonly applied flame theory can be introduced, leading to substantial errors (>15%) in the flame velocity measurements and subsequently in the derivation of laminar burning velocity.

In a cylindrical vessel, the observed propagation velocity $S_{observed}$ recorded by schlieren photography can be related to the flame velocity $S_b$ and the flow velocity of burned gas behind the flame front ($U_b$, positive in the inward direction) through [136] [138],

$$S_{observed} = S_b - U_b$$

(4.1)
Direct application of the conventional constant pressure flame method assuming zero burned gas velocities will yield erroneous flame velocities. It has been shown that the induced error increases exponentially with the ratio of flame radius ($R_f$) to the vessel’s wall ($R_w$) radius for $R_f > 0.3R_w$ [136]. In the current analysis, a flow-corrected flame velocity has been derived based on the model developed by M.P. Burke et al. [136],

$$S_b = \frac{S_{observed}}{\left(1 + \frac{\sigma - 1}{\sigma} \bar{\omega}_r \right)} \quad (4.2)$$

where $S_b$ is the corrected flame velocity, $\sigma$ the thermal expansion factor and $\bar{\omega}_r$ is a scaled burned gas velocity. The model accounts for the actual induced burned gas motion within the burned zone due to the non-symmetrical confinement of the flame. A detailed description of the model can be found in the publication of M.P. Burke et al. [136].

The flame stretch rate ($\alpha$) can collectively describe the various influences due to flow nonuniformity, flame curvature, and flow/flame unsteadiness on the surface of an outwardly propagating spherical flame. In a quiescent flow, an outwardly spherical flame propagates normal to its surface implying that the tangential staining is zero [57]. Thus, the stretch rate in the laminar constant volume experiments can be defined as shown in eq.3.4.

For the Markstein theory to be satisfied exactly, it requires an unwrinkled, spherical, infinitesimally thin, weakly stretched, adiabatic, quasi–steady flame with a constant expansion factor in a zero gravity, unconfined environment [136]. These assumptions are not satisfied in practical applications, even in well-controlled experiments.

The validity of the linear relation (eq. 3.3) starts to be questionable when the Lewis number of a mixture significantly deviates from unity. As reported by Kelley and Law [139] a nonlinear extrapolation between stretched flame velocity and stretch rate should be used for mixtures with Lewis numbers appreciably different from unity. According to Halter et al. [140], the use of a nonlinear methodology is only required when the burned gas Markstein length ($L_b$) reaches or surpasses the unity value (in mm). As will be illustrated in section 4.3.3 the maximum value of $L_b$ measured in the current experimental study corresponds to...
0.9 mm. Following the correlation derived by Halter et al. [140] for evaluating the relative percentage difference between linear and non-linear extrapolation methodology, the maximum difference in the current experimental study corresponds to 2%. It was therefore concluded that in the current study a linear extrapolation methodology can still be used with confidence.

Despite its limitations, the extrapolation of a spherical outwardly propagating flame to its zero stretch using the Markstein method and the model of Clavin as shown in eq.3.3 is widely accepted and used in literature [137],[52],[49],[44],[48],[50]. The Markstein theory has been used in the present study in order to allow for a comparison with the existing related literature information.

On the assumption of an infinitesimally thin flame, the fundamental laminar burning velocity \( S_0 \) can be obtained by dividing the unstretched flame velocity \( S_b \) with the thermal expansion ratio \( \sigma \) such as,

\[
S_u = \frac{1}{\sigma} S_b
\]  

(4.3)

The required expansion ratios have been computed using the model for a freely propagating flame in the Cantera software package as discussed in section 3.4.4.

### 4.2.2 Flame Radius Definition

An in-house image processing code specifically developed for the current experimental setup was used to track the flame radius over time. The flame radius was tracked along the Y-axis as shown in Figure 4.1, as it is the only direction at which the adjacent walls of the vessel are symmetrical. The flame was visualized with the schlieren method. The chronological change in flame radius determined from the gradient of a first-order least squares fit through four radii adjacent to each point under consideration, allow for the calculation of the observed flame propagation velocity \( S_{\text{observed}} \). A similar technique has been used in [44] [48]. Data processed in this manner without any explicit smoothing technique, allow the most of the consistency with the raw data.
4.2.3 Upper Boundary of Optical Analysis

The flow corrected ($S_b$) and uncorrected ($S_{b,unc}$) flame velocities versus stretch rate are presented in Figure 4.2 for a stoichiometric PRF95-air mixture at an initial pressure of 5 bar. The normalized flame radius by the vessel’s wall radius (50 mm) is also presented at the top of the figure as a secondary x-axis. The flame velocity is initially increasing attributed to the effect of a decreasing stretch for a mixture of positive Markstein length. The flame appears relatively unaffected by confinement for $R_f < 0.2 R_w$. For larger radius the non-symmetrical confinement induced the burned gas motion and the two velocities start to deviate. However, for $R_f < \approx 0.36 R_w$, a distinct drop in flame velocity can be observed even for the corrected case. The phenomenon was consistently occurring at a flame radius of about 18 mm for all the experimental conditions and fuels. The relative pressure increase at that point was not higher than about 6%. Therefore the drastic drop in flame velocity cannot be explained by the direct effect of pressure on the reactivity of the fuel.

The radiation-induced reduction in laminar burning velocity has been quantified using the correlation proposed by Yu et al. [141]. The maximum reduction for the current experiments calculated to be lower than 4%. It was also concluded that radiative heat loss could not explain the drastic drop in flame velocity.
As illustrated in the schematic of Figure 3.3, the asymmetry in the x-axis with the presence of a wall much closer to the flame at the right side of the cylindrical vessel, is thought to promote high levels of flow field asymmetries for $R_f < \approx 0.36 R_w$, that distort the flame from its spherical shape.

To help the reader visualize the mentioned phenomenon, a symbolic illustration is presented in Figure 4.3. The figure presents indicative flame surface contours as experienced during the current experimental work (solid lines), as compared to contours that would correspond to an unconfined flame evolution (dotted lines). At the early stages (i.e a,b), the burned gas is relatively motionless and the flame shape remains similar to that of the unconfined case. However, in contrast to the unconfined case, as the flame develops (i.e c-d-e), the burned gas deviates from its motionless state causing a non-similar flame propagation velocity along the X as compared to the Y direction. For large flame radii (i.e d-e), high levels of flow field asymmetries significantly distort the flame from its spherical shape.

As suggested by M.P.Burke et al. [136], the accuracy of the model is expected to be questionable in a strongly disrupted flow field. It was therefore necessary to limit the analysis of flames up to a maximum radius of 18 mm ($0.36 R_w$) to avoid high levels of induced flow field asymmetries that degrades the accuracy of the flow-correction mode.
4.2.4 Lower Boundary of Optical Analysis

The early stage of flame evolution is influenced by ignition transients that affect the measured value of flame velocity. The effects are more prominent for mixtures of high Lewis number [142]. In the current experimental conditions, DF0 (PRF95) is having the highest Lewis number. As suggested by Bradley et al.[48], the sharp fall in flame velocity with stretch rate indicates that in this regime a fully developed flame is not yet established. Following the previous comments, data have been excluded for radii below 7 mm at 2.5 Bar, 6 mm at 5 Bar, and 5 mm at 10 Bar. The resulted values are consistent with literature, as different researches [44], [48],[51],[47] suggest that ignition transients diminish at flame radii between 5 -10 mm. Consequently, having defined the upper and lower boundaries, the smallest range of analysis (11mm) corresponds to a pressure of 2.5 bar. Within this range there is a minimum of 21 data points available for the extrapolation technique to be applied. Similar amount of data points as the minimum amount in the current experimental work have been successfully used by Kelley and Law [139] for their extrapolations of $S_b$ to zero stretch.
4.2.5 Extrapolation Technique

The unstretched flame velocity ($S_b^0$) and the corresponding Markstein length ($L_b$), can be determined using a linear extrapolation through the largest possible range of radii where there is no spark influence and where the curve of $S_b$ versus stretch rate is reasonably linear [48]. Historically, the choice of data range has been somewhat arbitrary. Different researchers made different choices without giving quantitative justification [142]. In an effort to derive the values of $S_b^0$ and $L_b$ with a consisted approach a sensitivity analysis has been performed through the selected reasonably linear range of radii. The overall methodology is depicted in Figure 4.4, whereas the axes have been magnified to point out the oscillatory trend of $S_b$ purely for presentation purposes. The observed oscillations of $S_b$ are induced by the unavoidable acoustic disturbances inside the vessel [44] [48]. The lower boundary of the sensitivity analysis is defined as the first point of the selected reasonably linear range. An extrapolated line is fitted starting from the lower boundary and moving with increments of 0.5 mm in radius towards the upper boundary. The upper boundary is defined as the point at which $L_b$ changes sign compared to its initial sign at the lower boundary. Each extrapolated line within the range of sensitivity analysis is giving a value of $S_b$ at zero stretch ($S_b^0$). The selected $S_b^0$ is defined as the average within one standard deviation of all the resulted values. The intersection of the extrapolated line giving the closest value to the derived $S_b^0$ (dotted red), is used to define the value of $L_b$.

![Figure 4.4. Extrapolation technique and sensitivity analysis definition.](image)
For each investigated pressure and equivalence ratio, five different fuels have been tested with a minimum of three repeats per fuel. A sensitivity analysis has been performed for each investigated point to determine the value of $S_b^0$. At each pressure, the average standard deviation ($\sigma'$) and average $S_b^0$ of all tested fuels is calculated at each equivalence ratio. The induced uncertainty on $S_b^0$ due to the extrapolation technique presented in Figure 4.5 is defined as,

$$\Delta S_b^0 = \left(1 - \frac{\bar{S}_b^0 - \sigma'}{S_b^0}\right) \times 100 \quad (4.4)$$

The trend of the induced uncertainty due to the extrapolation procedure appears to increase with the decrease of pressure attributed to a reduced amount of available data points for extrapolation within the selected linear range.

**4.2.6 Thermodynamic Analysis**

The rate of heat release (HRR) in the constant volume environment can be obtained by considering the instantaneous pressure and volume within the vessel as well as the value of the specific heat ratio of the combustible mixture. For a comparison of different fuels within the same environment and similar thermodynamic conditions, models representing heat transfer and blow-by are often omitted leading to the eq. 4.5.

$$dQ_{ch} = \frac{1}{\gamma - 1} V dP \quad (4.5)$$
The pressure (P) in the vessel is recorded at each sampling point. The specific heat ratio (γ) must be calculated as it is a function of temperature pressure and composition. Prior to combustion, the pressure as well as temperature is constant in the CVCV. Knowing the composition of the combustible mixture, and using ideal gas law, the trapped mass of fuel and air can be obtained (Appendix). From the time of spark, the average charge temperature at each sampling point can be calculated by considering an ideal gas with mass according to the total trapped mass (fuel + air), volume as the total volume of the vessel and a pressure as recorded. Cantera is used within an in-house Matlab© code to calculate the specific heat ratio at each sampling point from a given pressure, temperature and fuel/air composition. Equation 4.5 is then evaluated at each sampling point within the same Matlab© code to give the HRR. The HRR is then integrated from time of spark and normalized to allow MFB rates to be evaluated. Error bars evaluated based on the standard error of the different repeats are superimposed on the average durations of MFB for all tested conditions.

4.3 Results – Discussion

4.3.1 Flame Evolution and Morphology

The evolution of a stable laminar flame defined as the flame radii over time is governed by the laminar burning velocity (S₀) of the fuel-oxidizer mixture, and the sensitivity of that flame to stretch characterised by the Markstein length (Lₘ). At a pressure of 5 Bar, the mean flame evolutions selected among the different repeats of each fuel, at each tested equivalence ratio, are presented in the left plots of Figure 4.6. The flame evolutions, are presented on a logarithmic scale up to a radius of 15mm along with the time elapsed from the point of spark. At respective time steps up to 6.7 ms, the percentage difference of the flame radius of each fuel in comparison to that of the pure liquid fuel (PRF95) has been calculated and shown in the right plots of Figure 4.6. A Dual Fuel (DF) ratio of 0% corresponds to the pure liquid fuel (PRF95) whereas 100% corresponds to the gaseous fuel (CH₄).
At lean conditions ($\Phi = 0.8$), it has been observed that at 0.8 ms after spark, the flame radius is increased with the addition of methane to PRF95 in a dual fuel blend. There is 41% difference between the radius of DF100 in comparison to that of DF0. The characteristic $S$ shape corresponding to the flame evolution of DF0 is due to the phenomenon of flame reverse. The phenomenon is found to be most prominent in mixtures of relatively high Lewis numbers [142]. Flame reverse phenomena are observed for DF0 and to a much lower extend DF25 only at lean conditions. At 3.3 ms after spark, the flame radius of DF50 is larger than

Figure 4.6. Flame Evolution of all fuels at $P_{\text{initial}} = 5\text{Bar}$ (Left plots). Sensitivity of the flame’s radius to DF ratio (Right plots).
double the radius of DF0. From 3.3 ms onwards, the flame evolution of the DF50 and DF25 is similar. The flame evolution of DF75 and methane are diverging from the one of DF50 whereas that of DF0 is converging towards DF50 up to 10 ms, and then gradually starts to diverge. As far as flame evolution is concerned, similar phenomena is observed at 2.5 Bar, whereas at 10 Bar all DFs including methane are having a faster evolution than DF0 at the early stages of combustion and slower in the developed flame regime.

At lean conditions, the effect of dual fuelling in the flame evolution is of particular practical importance. To allow for the visualization of flame evolution, chronological schlieren images of three selected fuels CH₄, DF50 and DF0 are presented in Figure4.7. There are no signs of flame wrinkling or any indication of cellular structures up to the maximum radius of analysis. The shape of the flames looks smooth independently of the fuel. Although particular attention has been applied on minimizing the effect of the electrodes on the morphology of the flame by adjusting their diameter and inter distance, the effect could not be totally eliminated. Similar visual effects owning to the electrode and flame interactions have been reported in other experimental studies in literature [44],[49],[143]. As far as flame morphology at lean conditions is concerned, flames at a pressure of 2.5 Bar and 10 Bar shown consisted behavior as in the 5 Bar case.

At stoichiometric conditions (Φ = 1), the qualitative response of flame evolution to the DF ratio at 0.8 ms after spark, is the same as in the lean conditions. From 1.7 ms onwards, the flame evolution of the DF50 mixture forms a medium between the tested fuels. The flame evolution of DF0 and DF25 are converging towards DF50 in contrast to DF75 and methane that are diverging. Similar trends in flame evolution could be observed at a pressure of 2.5 Bar. At a pressure of 10 Bar, the flame evolution of the DF75 mixture resulted to be considerably faster compared to the rest of the fuels. The response was consistent for all of its repeats.
Figure 4.7. Chronological schlieren images at $\Phi = 0.8$, $P_{\text{initial}} = 5\text{Bar}$
The morphology of stoichiometric DF flames at a randomly selected radius of about 10 mm is illustrated in Figure 4.8. The wrinkling on the flame surface is increased with the DF ratio, although cellular structures could not be observed up to the maximum radius of analysis. This is in contrast to the observations of flame stability at 2.5 and 5 Bar where flames are relatively free of wrinkles.

![DF ratio (%)](image)

Figure 4.8. Schlieren flame images of all DF flames at $\Phi = 1$, $P_{\text{initial}} = 10$ bar at a randomly selected radius of 10 mm.

As proposed by Rozenchan et al. [52] and supported by Qiao et al. [144] at the absence of cell cracking to smaller scales (cellularity) the linear relationship between flame velocity and stretch still holds. The considerably faster flame evolution of DF75 at a pressure of 10 Bar and $\Phi = 1$ is thought to be caused by phenomena of flame instability.

At rich conditions ($\Phi = 1.2$), the response of the flame evolution to the DF ratio is totally different compared to the lean conditions. At 0.8 ms after spark, the flame radius is decreased with the addition of methane to PRF95 in a dual fuel blend. All DFs have a slower flame evolution compared to DF0. As the flame develops, the flame evolution of DF50 and DF75 becomes slower even compared to that of methane. The trend in flame evolution with respect to the DF ratio is similar at 2.5 Bar. However, at a pressure of 10 Bar cellular structures have been observed for all DFs altering the flame evolution and leading to faster flames even compared to those of DF0. Rich flames at a pressure of 10 Bar have been excluded from further analysis for the derivation of $S_a^0$ and $L_b$.

With the addition of methane to PRF95 is evident that flame evolution is altered at all equivalence ratios. In the present study, the evaluation of laminar burning velocity and Markstein length will enhance the understanding on the mechanism behind the response of flame evolution with the DF ratio. For all tested conditions, the effects of methane addition to PRF95 on both fundamental combustion parameters will be quantified in the next sections.


4.3.2 Stretch Effects

Using the same data as for the plots of flame evolution in the previous section, the stretched flame velocity versus flame stretch is plotted in Figure 4.9 for DF100, DF50 and DF0 at three different equivalence ratios, and a pressure of 5Bar. The presented flame velocities correspond to flame radii between 6 to 15 mm. The influence of flame stretch on the flame velocity is characterised by the value of burned gas Markstein length ($L_b$). The fitted lines resulted from the extrapolation technique, and used for calculating $L_b$, are also presented.

At lean conditions ($\Phi = 0.8$), as flame stretch increases, the flame velocity of DF0 is decreased attributed to a positive $L_b$ whereas that of methane is increased due to a negative $L_b$. The flame velocity of DF50 remains relatively unaffected by flame stretching. For the whole range of flame stretch, DF50 has a faster flame velocity than DF0. The difference gradually increases with flame stretch. Following the extrapolated lines, the flame velocity of methane becomes faster than that of DF0 at a flame stretch of about 600 1/s. At stoichiometric conditions ($\Phi = 1$), the flame velocity of all fuels is decreased with the flame stretch. However, as the DF ratio is increased, the sensitivity of the flame velocity to the flame stretch is reduced. As flame stretch increases, the flame velocity of methane and DF50 converges and eventually becomes faster as compared to the velocity of DF0. The flame velocity of the DF50 blend becomes faster than that of DF0 at a flame stretch of about 300 1/s. At rich conditions ($\Phi = 1.2$), methane’s flame is having the largest sensitivity to stretch followed by DF0 and DF50. All fuels are having a positive $L_b$ although DF50 has a value close to zero. For the whole range of flame stretch the flame velocity of DF0 is higher than the velocity of methane and DF50. It is evident from Figure 4.9 that the response of flame velocity to the flame stretch characterised by $L_b$ is depended both on the equivalence ratio and on the particular fuel under consideration.
Figure 4.9. Stretched flame velocity versus stretch rate, $P_{\text{initial}}$: 5Bar.
4.3.3 Markstein Length ($L_b$)

The response of $L_b$ with respect to the DF ratio as well as pressure is depicted in Figure 4.10, for each tested equivalence ratio. At each investigated point, error bars are evaluated based on the standard error of all the repeated tests. The uncertainty of the extrapolation procedure and the repeatability of the tests at each investigated point are contributing to the extent of the error bars. Available literature data are also presented in Figure 4.10 for the base fuels. It appears that there is no prior work reporting values of $L_b$ for different ratios of methane addition to PRF95 at the current tested pressures. For presentation purposes, some of the literature data are slightly shifted on the x-axis. At each test pressure, the data are correlated with a suitable fit (solid lines) aiming to present the overall trend of $L_b$ versus DF ratio. A quadratic relationship has been applied for lean and rich conditions and a linear relationship for stoichiometry. The coefficients of the resulted fits are presented in Table 4.1.

Methane being the lightest hydrocarbon among the tested fuels is found to have the lowest $L_b$ at lean and stoichiometric conditions, and the highest at rich conditions. In contrast, PRF95 being the heaviest hydrocarbon, shown opposite response to that of methane. Similar phenomena have been reported in literature [50],[49]. At lean conditions, with the increase of DF ratio the values of $L_b$ are reduced following a quadratic relationship in the form of $a \text{DF}_{ratio}^2 + b \text{DF}_{ratio} + c$. At a pressure of 2.5 Bar, the values of $L_b$ for all DFs are converging to that of methane. As pressure increases, the reduction in $L_b$ with the DF ratio gradually becomes more linear. At stoichiometric conditions, with methane addition to PRF95 there is a linear decrease in $L_b$ for all tested pressures. Following the fitted lines of the form $a \text{DF}_{ratio} + b$, with a 25% increase in DF ratio, the value of $L_b$ is reduced by 16%, 20%, 28% at a pressure of 2.5, 5, and 10 Bar respectively. At rich conditions, the response of $L_b$ with DF ratio is contrary to the stoichiometric and lean conditions, with DF75 and methane being more sensitive to flame stretch than PRF95 at a pressure of 2.5 Bar. At 5 Bar all DFs found to have lower values of $L_b$ as compared to PRF95 and to larger extend methane.

For the three tested equivalence ratios, the response of $L_b$ is not only affected by a change in fuel but is also affected by a change in pressure. As pressure increases the value of $L_b$ is reduced for all fuels as can be clearly observed in Figure 4.10. For a given fuel-air mixture, the absolute value of $L_b$ decreases with an increase in pressure attributed to the reduction of flame thickness [56]. Due to the reduced flame thickness, the stretch induced on the flame by its curvature and flow straining is reduced, and therefore the flame become less sensitive to stretch manifested by a lower value of $L_b$. 
Figure 4.10. Burned Gas Markstein Length for all investigated conditions with available literature data. Crosses: [48] Squares: [49] X markers: [50] Stars: [52]
Available literature data are also presented in Figure 4.10. Bradley et al. [48] reported values of $L_b$ for an iso-octane-air mixture at different pressures, temperatures and equivalence ratios. Appropriate values from that study are illustrated in Figure 4.10 (+ markers) for a comparison to the values of PRF95 resulted from the current study. Mandilas et al. [49] reported values of $L_b$ for both methane and iso-octane air mixtures at 5Bar and 360K. Values from this study are reported with squares. Also for methane, the reported values of $L_b$ from the experimental studies of Rozenchan et al. [52] (star markers), and Gu et al. [50] (x markers), are presented. Considering the reported discrepancies of the measured Markstein lengths by different researchers that can be even larger than 300% [145], it can be concluded that the reported values of $L_b$ from the current experimental work are in satisfactory quantitative and qualitative agreement with the selected values from literature.

### 4.3.3.1 Mass Diffusivity

The response of $L_b$ with the equivalence ratio for all tested fuels at a pressure of 5 Bar is illustrated in Figure 4.11. As discussed in section 2.3.2 the Markstein length is depended on thermodynamics and transport properties of the combustible mixture. In particular, $L_b$ is found to be mainly governed by the thermo-diffusive properties, the so-called Lewis number effect. In general, for a mixture of Lewis number higher than unity, $L_b$ is expected to be positive and for Lewis number lower than unity negative. As stated by Law and Sung [57] this argument still holds even if only the relative mass diffusivities of the fuel and oxidizer species are considered. For a sufficiently off stoichiometric mixture where its mass diffusivity ($D$) can be approximated as that of the deficient reactant (fuel for lean and oxidizer for rich conditions); If the diffusivity of the fuel is higher/lower than the diffusivity of the oxidizer, $L_b$ is expected to be negative/positive. As proposed by Law and Sung [57] based on molecular weight considerations, as the fuel molecule becomes lighter, the
diffusivity of the fuel relative to air increases. Following the mentioned reasoning, the
diffusivity of the fuel relative to that of air increases with the DF ratio.

![Graph showing Markstein length versus equivalence ratio for all fuels at P_initial = 5Bar](image)

Although an equivalence ratio of 0.8 does not reflect a sufficiently off-stoichiometric mixture, the diffusivity of the fuel can be reasonably assumed representative to that of the mixture. As can be observed from Figure 4.11, L_b is inversely scaled with the mass diffusivity of the fuels. The mass diffusivity of the fuel is increased with DF ratio leading to a reduction in L_b. It has been found that the relative values of L_b for all DFs converge to that of methane at lean conditions. The mass diffusivity of the base fuels in a DF mixture is considerable different (for example, D_{CH_4} = 21.9 mm^2/s and D_{C_8H_18} = 6.6 mm^2/s [122]). Considering the difference of the mass diffusivity of the base fuels as well as their mole fractions in the different DFs shown in Table 3.1, the effective diffusivity of the DF mixtures is believed to be proportionally biased towards that of methane. Similar phenomena have been discussed for a mixture of methane and hydrogen in the study of Dinkelacker et al. [66].

For stoichiometric conditions, the diffusivity of the mixture is expected to depend on both the diffusivity of air and fuel. In contrast to PRF95, for methane and all DFs the value of L_b at stoichiometric conditions is increased compared to the lean conditions. As the DF ratio decreases the increase in L_b is lower. This response supports our thoughts that the effective diffusivity of a DF mixture is proportionally biased towards that of methane. At rich conditions, the deficient reactant is air and all fuel air mixtures are expecting to converge to a single diffusivity, that of air. As can be observed from Figure 4.11, the values of L_b seem to be relatively converge for all investigated fuel air mixtures.
It has to be pointed out that at lean conditions and a pressure of 2.5 Bar although the reduction of $L_b$ with the DF ratio can be qualitatively explained by the proposed theory, methane does not show a negative value of $L_b$. It can be concluded that the effective mass diffusivity is definitely a major contributor to the response of $L_b$ with equivalence ratio for the different DFs, however it is not adequate for a quantified explanation.

4.3.4 Laminar Burning Velocity ($S_u^0$)

Following the evaluation of $L_b$, values of the laminar burning velocity ($S_u^0$) for all investigated conditions are presented in Figure 4.12 with available literature data. Similar to the analysis of $L_b$, suitable fits (solid lines) are also presented with their coefficients reported in Table 4.2. At stoichiometric conditions and a pressure of 10 Bar, the value of $S_u^0$ for the DF75 blend is considerably higher compared to the rest of the fuels. As discussed in section 4.3.1, DF75 is thought to be affected by phenomena of flame instability therefore its velocity is not taken into consideration for the linear fit correlation.

Methane resulted to have a lower $S_u^0$ than PRF95 at all investigated conditions. Interestingly, at lean conditions it has been found that by blending methane with PRF95 the resulted $S_u^0$ of all DFs is larger even compared to that of pure liquid fuel at a pressure of 5 Bar and to less extent 2.5 Bar. The only exemption corresponds to the DF75 blend at 2.5 Bar. At a pressure of 10 Bar, with the increase of the DF ratio the value of $S_u^0$ is reduced. However the burning velocity of all DFs converges to that of liquid fuel. At stoichiometric conditions, with the increase of DF ratio there is a linear decrease in $S_u^0$ for all tested pressures. Following the fitted lines, with a 25% increase in DF ratio, the value of $S_u^0$ is reduced by 2%, 4%, 5% at a pressure of 2.5, 5, and 10 Bar respectively. At rich conditions the response of $S_u^0$ with DF ratio is contrary to that at lean conditions. All DFs resulted to have a lower $S_u^0$ even compared to that of methane.

The recent study of Baloo et al.[54], conducted at atmospheric pressure reported similar findings on the response of $S_u^0$ with the DF ratio as in the current study. Consisted with the current experimental findings, the later experimental investigation of Baloo and co-workers [55] reported that the phenomenon of a higher burning velocity for the blended as compared to the base fuels decreases with pressure. However, they have reported that at a pressure of 5.5 bar the burning velocity of the blended fuels is between the base fuels.
The chemical paths leading to the initiation and/or recombination reactions during the combustion of a DF blend can explain the response of $S_{u0}$ with the DF ratio. However, as stated by Baloo et al. [54] [55] and supported by the authors (section 5.2.1), detailed chemical kinetics of the blend fuel that will develop the understanding on the response of $S_{u0}$ with the DF ratio are currently unavailable.

The adverse effect of pressure on $S_{u0}$ is clearly shown in Figure 4.12. As pressure increases the value of $S_{u0}$ is decreased for all investigated conditions. According to Galmiche et al. [47] at high pressures the recombination reaction $H + O_2 + M \rightarrow HO_2 + M$ reduces the H atom concentration and thus competes with the initiation reaction $H + O_2 \rightarrow O + OH$ producing free radicals O and OH. This process tends to reduce the overall oxidation rate and to inhibit the combustion reaction. This finding is also supported by C.K. Law [57], although he is suggested that the increase of the unburned gas density with pressure is the main contributor for the reduction in burning velocity.

Available literature data are also included in Figure 4.12. For DF100, data are taken from the work of Gu et al. (x marks) [50] and Mandilas et al. (rectangles) [49]. For DF0, data are taken from the work of Bradley et al. (+ marks) [48], Jerzembeck et al. (triangles) [44], Beeckmann et al. (circles) [46] and Mandilias et al. (rectangles) [49].
Figure 4.12. Laminar burning velocity for all investigated conditions with available literature data. Crosses : [48] Squares : [49] X : [50] Triangles : [44], Circle : [46]
It appears that there is no prior literature study reporting values of $S_0^0$ for methane-PRF95 dual fuel blends at the current experimental conditions. At a pressure of 2.5 Bar, the experimental values of $S_0^0$ for PRF95 obtained in this work are on average 22% higher compared to those reported in literature. For the rest of the experimental tests, there is a maximum deviation of 12% between the values of $S_0^0$ obtained in this work as compared to the ones reported in literature at the same temperature.

### 4.3.5 Flame Instability

As explained in section 4.2.3 due to the non-symmetrical flame restriction there is a distinct drop in flame velocity at a radius of about 18mm. Thus, for flame radius larger than 18mm the flame velocity is directly affected by the non-symmetrical flame restriction. Consequently, the quantification of the effect of flame instability on the flame velocity could not be evaluated. However, on a phenomenology prospective the response of flame instability with the DF ratio can be assessed from direct flame visualisation and explained based on the instability mechanism discussed in section 2.3.5. For these purposes, typical flames for all DFs are presented in Figure 4.13 for the three tested equivalence ratios at a pressure of 5bar. The flames are presented up to their maximum visualisation point just before they exit the optical window.

The propensity of the flame to instability is linked with the associate value of Markstein length. According to the instability mechanism explained in section 2.3.5, the lower the Markstein length the higher the propensity of the flame to develop thermodiffusive instability. Initially, the thermodiffusive instability is manifested as cross cracks and small scale wrinkles on the flame surface that in a later stage develop into cellular structures. At $\Phi=0.8$ and $\Phi=1$, the Markstein length is reduced with the DF ratio. As illustrated in Figure 4.13, as DF ratio increases the flame gradually becomes more wrinkled although cellular structures have not been observed up to the maximum visualisation point. The flame wrinkling is more evident at $\Phi=0.8$.

As compared to $\Phi=0.8$ and $\Phi=1$, at $\Phi=1.2$ the Markstein length is reduced for DF0, DF25, and DF50 although is increased for DF75 and DF100. Consequently, flame cellularity is observed for DF0, DF25, and DF50 in contrast to DF75 and DF100. It has to be mentioned that the Markstein length of DF0 and DF75 are about the same at $\Phi=1.2$ and 5bar. However, DF0 shows a clear cellular flame whereas DF75 appears to be more stable. That is attributed to the curvature stabilisation mechanism. As presented in Figure 5.6, the flame thickness of pure gaseous fuel is larger than the liquid fuel. Hence, it is expected that the flame thickness...
of DF75 is larger than DF0 at 5 bar and $\Phi=1.2$. Subsequently the effect of curvature stabilisation mechanism on the flame is stronger for the DF75 as compared to the DF0 flame.

<table>
<thead>
<tr>
<th>DF Ratio (%)</th>
<th>0</th>
<th>25</th>
<th>50</th>
<th>75</th>
<th>100</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Phi=0.8$</td>
<td><img src="image1.png" alt="Image" /></td>
<td><img src="image2.png" alt="Image" /></td>
<td><img src="image3.png" alt="Image" /></td>
<td><img src="image4.png" alt="Image" /></td>
<td><img src="image5.png" alt="Image" /></td>
</tr>
<tr>
<td>$\Phi=1$</td>
<td><img src="image6.png" alt="Image" /></td>
<td><img src="image7.png" alt="Image" /></td>
<td><img src="image8.png" alt="Image" /></td>
<td><img src="image9.png" alt="Image" /></td>
<td><img src="image10.png" alt="Image" /></td>
</tr>
<tr>
<td>$\Phi=1.2$</td>
<td><img src="image11.png" alt="Image" /></td>
<td><img src="image12.png" alt="Image" /></td>
<td><img src="image13.png" alt="Image" /></td>
<td><img src="image14.png" alt="Image" /></td>
<td><img src="image15.png" alt="Image" /></td>
</tr>
</tbody>
</table>

Figure 4.13. The response of flame instability to the equivalence ratio $P_{\text{initial}}=5$ bar.

Having evaluated the response of the flame instability at different equivalence ratios, the effect of pressure can now being discussed. The response of the flame for all DFs at $\Phi=1$ is presented in Figure 4.14 for all tested pressures. It is evident that an increase in pressure promotes the effect of flame instability. In addition to the reduction of the Markstein length with pressure that will promote the thermodiffusive instability, the hydrodynamic instability is also influencing the stability of the flame. As pressure increases, the flame thickness is reduced for the base fuels as illustrated in Figure 5.6. The flame thickness of all DFs is expected to be reduced with pressure similar to the base fuels. As pressure increases the effect of hydrodynamic instability becomes more prevalent due to the gradual reduction of the stabilising effect of curvature with the decrease of flame thickness.
The above phenomenological findings are in close agreement with the flame instability mechanism as discussed in section 2.3.3 and verify the dependence of flame instability to the Markstein length. The effect of flame instability on the flame velocity with the addition of gaseous to liquid fuel remains a distinct research gap that requires further analysis.

### 4.3.6 Mass Burning Rate

Through thermodynamic analysis of the pressure traces acquired in the combustion vessel, the response of mass burning rate with the DF ratio has been investigated. The mean pressure traces of all fuels at an initial absolute pressure of 5 bar are shown in Figure 4.15.

The peak pressure of all fuels increases from lean to rich mixtures. The highest peak pressure corresponds to pure liquid fuel at $\Phi = 1.2$ and the lowest to pure gaseous fuel at $\Phi = 0.8$. The pressure traces of the base fuels at $\Phi = 0.8$ are clearly separated from those of the blended fuels. At $\Phi = 1$, the highest peak pressure was achieved by DF25 and the lowest by DF100. The DF50 and DF0 have similar peak pressures followed by DF75. The pressure of DF50 is initially higher than DF0. However as the combustion proceeds the pressure trace of DF0 cross the one of DF50. At $\Phi = 1.2$, the location of peak pressure of the pure liquid fuel and DF25 appeared to be more advanced compared to the rest of the fuels.
Figure 4.15. Average recorded pressure traces at $P_{\text{initial}} = 5$ bar
The phasing of the various percentages of MFB illustrates similar trends with the mean pressure traces. For an efficient presentation of the extensive experimental results, only the duration of 0-10 % MFB and 10-90 % MFB is illustrated for the rest of the tested conditions.

In the current study, the duration of 0 -10 % MFB has been used as an indication of the overall burning rate during the initial flame development regime. Similarly, the duration of 10-90 % MFB is indicative of the overall burning rate during the developed flame regime. At a pressure of 5 bar, the MFB durations for the development and the developed flame regime are shown in Figure 4.16 for the five tested fuels.

At lean conditions (Φ = 0.8), all DFs resulted in a faster burning rate (lower MFB durations) as compared to PRF95 and to a higher extent methane in both regimes. In the developing flame regime the average burning rate of all DFs is 22% and 37% higher compared to the liquid and gaseous fuel respectively. Among DFs, DF50 was found to be the fastest and DF25 the slowest. In the developed flame regime, the average burning rate of all DFs in comparison to liquid as well as gaseous fuel is higher by 27% and 53% respectively. Among DFs, DF75 was found to be the slowest and DF50 the fastest.

At stoichiometric conditions (Φ = 1), DF50 and DF25 are 5% faster than DF0 in the development flame regime. DF75 is marginally slower than DF0 and DF100 is the slowest of all. During the developed flame regime all DFs have faster burning rates in comparison to gaseous but only DF25 is 7% faster than the liquid fuel.

At rich conditions (Φ = 1.2), the difference in burning rate for DF75, DF50 and DF100 is within 4% in the developing flame regime. DF25 is faster than DF100 and slower than DF0.
In the developed flame regime, the burning rate of DF75 and DF50 is even slower than that of DF100 whereas DF0 showed the fastest burning rate.

As far as the liquid fuel is concerned, at similar initial conditions (5Bar – 373K), the value of $S_u^0$ is found to be similar at $\Phi = 1$ as compared to $\Phi = 1.2$. This is not reflected in the measured MFB durations. The duration of MFB 0-10% is 16% higher at $\Phi = 1.2$ in comparison to $\Phi = 1$ for a PRF95-air mixture. Moreover, at $\Phi = 0.8$ the value of $S_u^0$ is 30% lower compared to that at $\Phi = 1.2$, whereas the difference in MFB 0-10% is 48%. Similar trends can be observed in the developed flame regime. It is clear that the mechanism behind the phenomena cannot be solely explained by the laminar burning velocity. During the initial stages of combustion, due to the inverse proportionality of the flame stretch rate to the flame radius, the flame will experience the highest levels of stretching. As the flame develops and the flame radius is increasing, the stretch rate is reduced. Therefore, it is expected that the value of Markstein length is having a higher influence on the burning rate during the initial stages of combustion for all fuels. It has to be noted that phenomena of flame instability is also affecting the burning rate.

As far as methane is concerned, during the developing flame regime the burning rate at stoichiometric conditions is 4% and 41% faster than in rich and lean conditions respectively. During the developed flame regime stoichiometric and rich equivalence ratios resulted to give the same overall burning rates.

During the developing flame regime, the burning rate of both DF75 and DF50 is similar under lean and rich conditions. In the developed flame regime, the overall burning rate of both DF75 and DF50 is on average 20% faster under lean conditions as compared to the rich operation whereas its 19% slower as compared to the stoichiometric conditions.

At stoichiometric and rich conditions, DF25 resulted in the same burning rates in the developing flame regime. Under lean conditions, the burning rate is 27% slower compared to the stoichiometric and rich conditions. In the developed flame regime, DF25 showed the fastest burning rate at stoichiometry, and the slowest at lean conditions.

Summarizing the effects of the various fuels and different AFRs on the burning rate, it has been found that the slowest burning rate corresponds to DF100 at lean conditions whereas the fastest to DF0 at rich conditions. All DFs give their fastest burning rate at stoichiometric conditions. Interestingly, at lean conditions all DFs are faster than the liquid and to larger extent gaseous fuel in both regimes. At rich conditions, DF0 is the fastest of all whereas DF75 and DF50 are even slower than methane.
Having evaluated the dependence of fuel and AFRs on the burning rate, the effect from a different initial pressure can now be evaluated. At stoichiometric conditions, the burning rates in both the developing and developed flame regime are illustrated in Figure 4.17 for the three tested pressures.

It can be observed that in both flame regimes the duration of MFB is increased with pressure for all fuels. When the initial pressure is increased from 2.5 to 10 bar, the burning rate during the developing flame regime is decreased by 46% for DF100 as well as for DF50 and 40% for DF0. In the developed flame regime, the percentage decrease in burning rate is similar as in the developing regime.

In both flame regimes, the burning rate of all tested fuels at 2.5 bar follows a similar trend to the already discussed trend at 5 bar. On the other hand, when the initial pressure is increased to 10 bar, the response of the burning rate is substantially different from the two lower pressures. The unusually fast burning rate of DF75 at 10 bar is likely to be due to an unstable flame as discussed in section 4.3.1. The propensity of a flame to instability as experimentally justified in section 4.3.5 is increased with pressure especially for combustible mixtures of low Markstein lengths. For lean to stoichiometric AFRs, the Markstein length of DF100 is lower than DF0 whereas at rich conditions is higher than DF0.

At lean conditions, the burning rates corresponding to the three different initial pressures are depicted in Figure 4.18. It has to be noted that due to the unnoticed inaction of the acquisition system only two repeats have been captured for the DF25 and DF0 fuels at lean conditions (Φ = 0.8) and a pressure of 10 bar. Although error bars could not be calculated for
these two fuelling modes, the maximum percentage difference between their two repeats for MFB 0-10% and MFB 10-90% was less than 2%. Similarly to the stoichiometric conditions, in both flame regimes the burning rate of all tested fuels at 2.5 bar follows a similar trend with that at 5 bar. The negative effect of pressure on the burning rate is also evident at lean conditions. The only exception corresponds to methane at an increase in pressure from 5 to 10 Bar. At a pressure of 10 bar the flame is affected by phenomena of flame instability. Flame instability results in an increase in burning rate that will mask the effects of pressure. When the initial pressure is increased from 2.5 to 10 bar the percentage decrease in burning rate is higher than that at stoichiometric conditions, implying a stronger effect of pressure on the burning rate.

Figure 4.18. Effects of pressure on the MFB rates at \( \Phi = 0.8 \)

The burning rates at rich conditions (\( \Phi = 1.2 \)) are illustrated in Figure 4.19 for the three tested pressures. Similarly to lean and stoichiometric conditions, in both flame regimes the burning rate of all tested fuels at 2.5 bar is following a similar trend with that at 5 bar. As can be observed from Figure 4.19 in the developing flame regime, methane as well as all DFs have a faster burning rate at 10 bar as compared to 5 bar. For DF75 and DF50 the burning rate at 10 bar is even faster than at 2.5 bar. It seems that all fuels are affected by flame instability at a pressure of 10 bar. During the developed flame regime all DFs showed their fastest burning rate at a pressure of 10 bar. For the liquid fuel the fastest burning rate corresponds to 2.5 bar and the slowest to 10 bar in both flame regimes. This is mainly credited to the fact that at rich conditions the DF0 flame is highly unstable even at low pressures.
It can be summarized that at each equivalence ratio, the burning rate of all tested fuels showed a similar trend at 2.5 and 5 bar in both flame regimes. At a pressure of 10 bar and especially at rich conditions, all five fuels are likely be affected by phenomena of flame instability that can mask the effects of pressure on the burning rate. It can be reasonably assumed that the effect of flame instability on the burning rate is stronger than the effect of pressure.

![Figure 4.19. Effects of pressure on the MFB rates at Φ = 1.2](image)

### 4.4 Dual Fuelling Synergies

With the evaluation of both fundamental combustion parameters $L_b$ and $S_u^0$, the mechanism of the flame evolution as discussed in section 4.3.1 can now be explained. For convenience, due to the linear fitted correlations, the discussion will be related to the stoichiometric mixtures although is applicable to both lean and rich conditions. At a pressure of 5 Bar, with a 25% increase in the DF ratio, the values of $S_u^0$ and $L_b$ are reduced by 4% and 20% respectively. As already discussed, at the very early stages of combustion the flame radius is increased with DF ratio. It is clear that the mechanism behind this phenomenon is attributed to the decrease of $L_b$ as the dual fuel ratio increases. As the flame develops and flame radius increases, stretch rate is reduced. This implies that the effect of $L_b$ on the flame velocity is decaying. Therefore $S_u^0$ will start to dominate the flame evolution. As a result, an increase in the DF ratio will delay the flame evolution. Indeed at stoichiometric conditions, the flame evolution of PRF95 becomes faster and that of methane slower as the combustion process.
progress. From a Markstein length prospective, methane seems a suitable fuel for real combustion applications whereas from a laminar burning velocity prospective, PRF95 has a distinct advantage over methane.

At lean conditions, it has been found that there is a distinct synergy in blending methane with PRF95 as the advantages of the light and heavy hydrocarbon fuels are combined to form a suitable fuel blend for future lean burn energy efficient combustion applications. For a DF blend, the Markstein length that dominates the early stages of combustion has been found to converge to that of methane, whereas the laminar burning velocity that governs the developed flame propagation regime is even higher than that of PRF95. The synergy for Methane-PRF95 dual fuelling arise from the advantageous combination of these two fundamental combustion parameters $L_b$ and $S_u^{0}$ that allows for the flame evolution of DF50 blend to be up to 1.2 times faster compared to that of PRF95 at lean conditions.

### 4.5 Chapter Summary

The effects of methane addition to PRF95 (95%vol$_{liq}$ of iso-octane and 5%vol$_{liq}$ n-heptane) on the fundamental combustion parameters, laminar burning velocity ($S_u^{0}$) and Markstein length ($L_b$), were experimentally investigated in a cylindrical combustion vessel at equivalence ratios of 0.8, 1, 1.2, initial pressures of 2.5, 5, 10 Bar and a constant temperature of 373 K. Methane is used as a natural gas surrogate and PRF95 as a gasoline surrogate. Methane was added to PRF95 in three different energy ratios 25%, 50% and 75%. Spherically expanding flames were used to derive the flow corrected burning velocities, from which the corresponding $L_b$ and $S_u^{0}$ were obtained. The flame velocities were corrected for the motion of burned gas induced by the cylindrical confinement. It has been found that at stoichiometric conditions there is a linear decrease in $L_b$ and $S_u^{0}$ with the DF ratio in all investigated pressures. At rich conditions, all DFs resulted to have lower $S_u^{0}$ as compared to gaseous and to a larger extend liquid fuel. The values of $L_b$ for all DFs were lower than methane and comparable to that of PRF95. At lean conditions, the values of $L_b$ for all DFs are biased towards those of methane whereas the values of $S_u^{0}$ found to be higher than those of PRF95 at pressures of 2.5 and 5Bar. At 10 Bar both $L_b$ and $S_u^{0}$ reduce with DF ratio although $S_u^{0}$ of all DFs coverage to that of PRF95. The findings of the current study indicate a distinct synergy in the utilization of dual fuelling in future lean burn energy efficient combustion applications.
Chapter 5

5 Numerical Analysis on Stretched Flame Velocity

5.1 Introduction

The fundamental understanding of the combustion process is essential for the development of energy efficient combustion applications. Of primary importance is the flame velocity that directly affects the efficiency of a combustion process [39]. The fundamental laminar burning velocity \( S_{\infty} \) is a very important physicochemical property of the mixture commonly used in Computational Fluid Dynamic (CFD) as well as thermodynamic combustion simulations [92], [146], [147]. However, as reported in the previous chapter, methane having the lowest burning velocity at \( \Phi = 1 \) and \( \Phi = 0.8 \), attained the fastest flame evolution at the initial stages of combustion. That was attributed to the effect of Markstein length on the flame velocity. Thus, a reliable flame velocity model needs to account for the effect of flame stretch on the flame velocity. That is mandatory in order to reliably predict the stretched flame propagation velocity of a particular fuel under different operating conditions.

In the present chapter, the performance of the current numerical models on predicting the burning velocity and Markstein length of methane-PRF95 DF blends will be firstly assessed. The contributions made by the current research aiming to extend the numerical capabilities of the models and enhance their performances will be fully documented. A conceptual analysis is then presented to improve the understanding on the contribution of burning
velocity and Markstein length to the stretched flame velocity at various simulated conditions.

5.2 Numerical Predictions

5.2.1 Laminar Burning Velocity

The computed laminar burning velocities of the experimentally tested PRF95 and methane DF blends are shown in Figure 5.1 against their already reported experimental values (section 4.3.4) as well as literature data at a pressure of 5 bar and 373K. Throughout the numerical analysis an oxidizer concentration \([O_2 / (O_2 + N_2)]\) of 0.2 has been used in order to allow direct comparisons with the experiments. Apart from methane at \(\Phi = 1.2\), the computed burning velocities of the base fuels are well validated with the results obtained from the current experimental campaign. The maximum deviation corresponds to 12%. The experimentally measured value of methane’s burning velocity at \(\Phi = 1.2\) is higher than the available literature. Considering the scattered between the three experimentally derived points, the extent at which the actual experimental value of burning velocity deviates as compared to the computed value cannot be confidently stated.

In contrast to the base fuels, the mechanism is unable to predict the experimentally derived burning velocities of the dual fuel blends at \(\Phi = 0.8\) and \(\Phi = 1\). The computed values predict a near monotonic decrease of burning velocity at all AFRs. However, at \(\Phi = 0.8\) the experimentally obtained burning velocity of all DFs is higher than the base fuels. The kinetic mechanism is unable to predict even the qualitative trends of burning velocity for the dual fuel blends at \(\Phi = 0.8\). The same conclusions can be derived at 2.5 bar whereas at 10 bar there is only a qualitative agreement between computations and experiments.

It is therefore concluded that the chemical paths leading to the initiation and/or branching reactions during the combustion of a DF blend are missing from the currently available kinetic mechanisms. As stated by Baloo et al. [54] and supported by the author, detailed chemical kinetics of the blend fuel that will develop the understanding on the response of burning velocity with the DF ratio are currently unavailable. Further numerical analysis on the burning velocity is therefore constrained to the base fuels.
Figure 5.1. Computed burning velocities of all tested fuels against experimental data from chapter 4 and available literature data. Crosses : [48] Squares :[49] X marker : [50]
The computed burning velocities of the base fuels for a sweep of equivalence ratio, pressure and temperature are shown in Figure 5.2. Where applicable, experimental data from the current research are superimposed in the figure. Selected values from literature are also illustrated only at points where the current experimental data deviate from those of literature.

At all simulated conditions PRF95 attains a higher burning velocity than methane. The burning velocity peaks at $\Phi = 1$ for both fuels. That is mainly attributed to the higher adiabatic flame temperature for near stoichiometric mixtures. There is a near monotonic decrease in burning velocity with pressure for both fuels, although PRF95 mixtures are less
affected by pressure than methane mixtures. There is 14% difference between the burning velocity of the base fuels at 2.5 bar and 57% at 40 bar of pressure. An exponential increase in the burning velocity with temperature was computed for both fuels, since the burning velocity depends on the chemical reaction rates. The burning velocity of methane is more affected than that of PRF95 by an increase in temperature. There is 26% difference between the burning velocity of the base fuels at 400 K and 14% at 800K. The numerical results are in close agreement with the experimental data. As discussed in section 2.3, the experimental study of Gu et al. [50] directly compared the burning velocity of iso-octane and methane air mixtures and the qualitative findings have been the same with the current numerical analysis.

5.2.2 Expansion Ratio

The expansion ratio or as it is also commonly called expansion factor is defined as the ratio of unburned to burned gas density. It is necessary not only for the derivation of the flame velocity but also for the calculation of the Markstein length. The computed expansion ratios of the base fuels for a sweep of equivalence ratio, pressure and temperature is shown in Figure 5.3.

For all simulated conditions, the expansion factor of PRF95 is consistently higher than that of methane owning to the different molecular weights of the fuels. The expansion factors peak at stoichiometry for both fuels. That is mainly attributed to the reduction of the burned gas density as the AFR approaches stoichiometry. There is a very weak dependence of the pressure on the expansion factors. However, the expansion factors are exponentially decreased with temperature for both fuels due to a reduction of the unburned gas temperature. The computed expansion factors agree well with the published data of Gu et al. [50] and Bradley et al. [48].
As justified in section 3.4.5, the Markstein length is depended on the Lewis Number indicative of thermodiffusive effects, Zeldovich Number indicative of the underlined chemistry, flame thickness and expansion ratio.

The computation of the Markstein length for the blended fuels has not been possible due to the lack of available activation energies for deriving the Zeldovich number and kinetic models for deriving the flame thickness. However, the Lewis number of the blended fuels can be used as an indication for the Markstein length of the blended fuels.

Figure 5.3. Computed Expansion Ratios versus AFR, Pressure and Temperature for the base fuels.
The computed Lewis number of PRF95 and methane dual fuels versus equivalence ratio is depicted in Figure 5.4 at a pressure of 5 bar and 373 K. In a recent study, Aleifreris et al [35] reported values of Lewis number for iso-octane to be 2.79/0.92 for lean and rich mixtures sufficiently of stoichiometry whereas Dinkelar et al. [66] and Muppala et al. [65] reported values of 0.955 and 0.89 respectively for lean methane-air mixtures. In the current numerical study, the computed Lewis numbers of the base fuels are in close agreement to the reported values. There are no available solid literature data as for the Lewis number of PRF95 and methane dual fuels.

As can be observed from Figure 5.4, the Lewis number of PRF95 (DF0) showed contrary trends in comparison to that of methane (DF100). The Lewis number of PRF95 decreases with the equivalence ratio whereas that of methane increases. The Lewis numbers of the dual fuel blends are converging to the values of methane. Considering the molar concentrations of methane in the various dual fuel blends (DF75→95%, DF50→86%, DF25→68%) as shown in Table 3.1, it can be concluded that the diffusivity of the multicomponent fuel mixture is dominated by that of methane. Recalling from section 4.3.3, the experimentally derived Markstein length of the dual fuel blends also converge to that of methane although the phenomena are not as prevalent as with the computed values of Lewis number. Nevertheless, a strong dependence of the Markstein length on the Lewis number can be concluded.

The burned gas Markstein length of the base fuels has been computed with the updated model of Peters and co-workers, that will be referred to as model A, and Betchold and
Matalon that will be referred to as model B. Figure 5.5 illustrates the computations with both models against experimental results from the current research.

In contrast to the experimental values and computations with model A, the model B predicts a minimum value of methane’s Markstein length at stoichiometry. Such trend has not been reported in any of the referenced literature [50],[52],[49]. In contrast, model A predicts the experimental results quite well showing a decrease of Markstein length with leaner mixtures. As for the PRF95, both models quantitatively agree with the experimental data. In contrast to methane, the Markstein length of PRF95 shows an increase with leaner mixtures.

Figure 5.5. Computed burned gas Markstein length versus AFR, Pressure, and Temperature. Experimental values are reproduced from chapter 4. Model A : Dotted lines with symbols, Model B : Solid lines, X markers : Experimental Data.
As reported by Gu et al. [50], the Markstein length of methane-air and iso-octane-air mixtures shows an exponential decrease with pressure, and effectively reaches a plateau at pressures higher than about 4 bar. Although the underlined trends are well captured with both models, the experimentally derived negative values of methane’s Markstein length are not predicted. Nevertheless, model B overestimates the Markstein length of methane as compared to model A. The decrease of Markstein length with pressure is attributed to the reduction of flame thickness as shown in Figure 5.6.

![Figure 5.6](image_url)

Figure 5.6. Effect of pressure on the flame thickness of base fuels

At pressures above atmospheric, it has been reported in literature that the Markstein length is a weak function of temperature for both methane and iso-octane air mixtures [50] [47]. As predicted by model A, the Markstein length of methane is quite insensitive to temperature variations. However, the computed Markstein length of PRF95 shows higher dependence on temperature than methane. Model B shows a higher dependence of temperature on the Markstein length of both fuels.

Both models have been derived based on the asymptotic theory without detailed chemistry involved. In contrast to model B, the qualitative and in some instances quantitative trends of Markstein length for the base fuels can be satisfactory captured with model A. Since model A contains no detailed chemistry, the fact that it can make reasonable predictions demonstrates that transport effects dominate the response of Markstein length as suggested by the phenomenological analyses of section 3.4.5. This conclusion supports the previous discussion on the Markstein length of the dual fuel blends considered on the basis of Lewis number.

Model A being a computationally efficient yet reasonable accurate model has been integrated in the stretched flame velocity model to facilitate further analysis on the propagating laminar flame velocity.
5.2.4 Stretched Flame Velocity

To assess the performance of the flame model itself as shown in eq. 3.5, empirical values of burning velocity and Markstein length have been used at $\Phi=0.8$ and a pressure of 5 bar. The performance of the model is shown in Figure 5.7 against experimental data. The experimental flame propagation velocity of the base fuels is derived from their average flame evolutions as reported in Figure 4.6 of chapter 4.

![Flame Velocity Graph](image)

Figure 5.7. Simulated flame velocity of the base fuels versus experimental data derived in chapter 4 at $\Phi=0.8$ and $P_{\text{initial}}=5\text{bar}$.

It is clear from the definition of flame stretch eq.3.4, that peak value of stretch is expected at the very initial stages of combustion implying a dominant effect of Markstein length on the flame velocity. As the flame develops, the flame stretch is reduced, and the propagating flame velocity approaches the value of the unstretched flame velocity. The unstretched flame velocity is defined as the burning velocity multiplied by the expansion factor ($\sigma S_u^0$).

As can be observed from Figure 5.7 the response of the flame velocity is contrary for methane as compared to PRF95 at the initial stages of combustion. Methane having a negative Markstein length shows an initial increase of flame velocity compared to its later values, in contrast to PRF95 that has a positive Markstein length and shows an initial decrease in flame velocity. The model can capture well the response of the flame velocity to stretch, although in the very initial stages ($R_f<2.5\text{mm}$) there is a deviation between the computed and experimental values. As discussed in the study of Bradley et al. [148], the deviation is attributed to the assumption of an infinitesimally thin flame thickness. Consequently, at the very initial stages of combustion where flame stretch attains peak values the assumption of an infinitesimally thin flame results in an underestimation of the effect of flame stretch on the flame velocity.
Integrating the sub-models of burning velocity and Markstein length to the flame model, the response of the stretched flame velocity against different equivalence ratios at a pressure of 5 bar and 373 K is computed and shown in Figure 5.8. It is clear that as the equivalence ratio is reduced, the stretched flame velocity of methane attains a clear advantage over that of PRF95 in the initial stages of combustion. That is attributed to the effect of Markstein length. As the flame develops and stretch rate is reduced, PRF95 becomes faster than methane due to its higher burning velocity. The extent at which methane is faster than PRF95 is increased with a lower equivalence ratio. The crossing point between the two velocities can be thought as a turning point at which the burning velocity gradually starts to have a stronger effect than that of Markstein length on the stretched flame velocity. The crossing point is extended into a larger flame radius as the mixture becomes leaner. For rich mixtures PRF95 is always faster than methane although for presentation clarity simulations are not presented.

Figure 5.8. Simulated stretched flame velocity ($S_b$) versus equivalence ratio for the base fuels. $P = 5$ bar, $T = 373$ K

The ratio of the stretched over the unstretched flame velocity as derived from the flame velocities of Figure 5.8 at $\Phi=0.6$, is illustrated in Figure 5.9. As the ratio of the two velocities approaches unity the effect of flame stretch on the flame velocity decays. As can be concluded from Figure 5.9, the flame velocity of methane can be increased by 48% compared to its unstretched value whereas that of PRF95 is reduced by over 80% at the start of the flame propagation process. Even at a flame radius of 10 mm, the flame velocity of PRF95 is 24% lower than its unstretched value owning to a relatively high positive value of Markstein length.
The effect of pressure on the stretched flame propagation velocity as computed by the flame model at $\Phi=0.8$ is illustrated in Figure 5.10. As expected from the trend in Markstein length, at low pressures methane has a significantly faster flame velocity than PRF95 at the initial stages of combustion. As pressure increases, the Markstein length of both fuels relatively converge to a single value as shown in Figure 5.5. It is therefore expected that the burning velocity will have a greater effect on the flame propagation as pressure increases. Consequently, for pressures above 10 bar PRF95 is faster than methane throughout the combustion process.

It has to be noted that as pressure increases the flame can become unstable due to combined phenomena of thermodiffusive and hydrodynamic instability. As discussed in section 2.3.3., mixtures with low Markstein lengths are more prone to instabilities, implying that methane is more likely to become unstable than PRF95 under lean burn conditions. Thermodiffusive and hydrodynamic instabilities can greatly increase the velocity of a propagating flame. The current flame model does not account for the effects of flame instability on the flame velocity.
In the context of turbulent flamelet combustion, the turbulent flame front preserves the structure of a laminar flame and is propagating with a stretched laminar flame velocity ($S_b$) [132]. The effect of turbulence on combustion is solely reduced to wrinkling of the inherently laminar flame front increasing its surface area. Under such conditions, the effect of Markstein length, is expected to be of crucial importance to the combustion process especially for lean burn combustion. An experimental campaign on a single cylinder optical SI engine has been undertaken to investigate such phenomena as will be considered in the next chapter.

### 5.3 Chapter Summary

A numerical model has been developed aiming to predict the stretched laminar flame propagation velocity of PRF95 and methane dual fuels whilst extending the understanding on the influential parameters involved. Due to the lack of chemical kinetics and activation energies of the blended fuel, the predictive model has been constrained to the base fuels.

The burning velocity has been predicted using Cantera kinetic solver integrated with the reaction mechanism of Jerzembeck et al. [44]. Through current numerical contributions on the basis of Lewis number, an optimised Markstein length model based on [123] has been reconstructed and validated with experimental results.

It has been found that the effects of flame stretch quantified through the Markstein length, can drastically change the response of flame velocity especially at lean burn conditions. The transport effects dominate the Markstein length.

It has been suggested that in the context of turbulent flamelet regime, the effect of Markstein length is expected to be of crucial importance to the SI engine combustion. To address these issues and to allow further insights on the engine combustion of the blended fuels, an experimental campaign in an optically assessed SI engine has been undertaken. The analysis is presented in the following chapter.
Chapter 6

6 Dual Fuelled SI Engine Combustion

6.1 Introduction

Historically, for SI engine combustion, the fundamental laminar burning velocity ($S_u^0$) of the fuel-oxidizer mixture has been used as a major performance criterion. However, in an SI engine environment, the flame is actually continuously stretched by its curved nature and its propagation through a strained turbulent flow field. Consequently, the Markstein length ($L_b$), which quantifies the response of the flame velocity to stretch, is critically essential to completely characterise the development of an expanding flame in an SI engine both from a stability and velocity prospective.

In the context of turbulent flamelet regime, whereas the current experimental work is located (section 6.3.1), the turbulent flame front preserves the structure of a laminar flame and is propagating with a stretched laminar flame velocity ($S_b$) [132]. Under such conditions, as shown in the experimental and numerical analysis presented in the two previous chapters, the effect of Markstein length ($L_b$) is of crucial importance to the combustion process. It is therefore expected that that SI engine combustion will be critically affected by the effect of Markstein length.

In contrast to natural gas as well as gasoline and its surrogates, the flame behaviour of natural gas-gasoline DF blends has not been adequately investigated in an SI engine. As
discussed in section 2.2, there is still a limited understanding with regards to the mechanism of a faster DF flame in comparison to the base fuels in an SI engine. The importance of flame-stretch interactions with the ratio of gas to liquid in a DF blend at various engine operating conditions is still a distinct research gap. The research contribution of the experimental study presented in the current chapter is made through the characterisation and scientific understanding of the mechanism of DF combustion, and the importance of flame-stretch interactions under a sweep of engine load, speed and AFR.

6.2 Post-Processing Methodology

A comprehensive explanation of the engine experimental apparatus and the integration of optical diagnostics is presented in section 3.3. Besides, the dual fuelling strategy and the rational for the operating conditions implemented in the current experimental campaign have been also documented in that section.

6.2.1 Thermodynamic Post-Processing Technique

Whilst in-cylinder pressures were recorded using the AVL© Indiset system as discussed in section 3.3, post-processing analysis was carried out using an in-house MATLAB© code. The purpose of the in-house code is to allow for the change of the specific heat ratio ($\gamma$) both as a function of in-cylinder temperature and pressure as well as DF ratio.

The rate of heat release in the engine was derived with a single zone model, using the instantaneous in-cylinder pressure and volume as well as the value of the specific heat ratio of the combustible mixture as documented by Gatowski et al [149]. For a comparison within the same engine and similar operating conditions, models representing heat transfer and blow-by are often omitted leading to eq.6.1.

$$dQ_{ch} = \frac{\gamma}{\gamma - 1} PdV + \frac{1}{\gamma - 1} VdP$$  \hspace{1cm} (6.1)

The average pressure (P) is obtained at each crank angle from the measured data. A crank slider model taking into account the current piston offset (0.8 mm) is used to calculate the in-cylinder volume (V). From the time of Inlet Valve Closure (IVC), the average charge temperature at each crank angle can be calculated by considering an ideal gas with mass
according to the total trapped mass (fuel + air) and a pressure and volume as obtained. The mass of trapped air is evaluated from the MAF meter, whilst the intake valves are open. The specific heat ratio ($\gamma$) has to be calculated as it is a function of temperature pressure and composition. A chemical kinetics solver, Cantera [43] is used within the Matlab© code to calculate the specific heat ratio at each crank angle from a given pressure, temperature and a fuel/air composition. The composition was assumed free of exhaust residuals. The kinetic solver has been integrated with the kinetic mechanism of Jerzembeck et al [44]. To calculate the in-cylinder temperature at the IVC timing, and to approximate the exhaust residual fraction within the cylinder, the model developed by Heywood has been used [150]. For all current experimental test conditions, the maximum mass fraction of exhaust residuals was calculated to be 7%.

The Heat Release Rate (HRR) is then evaluated at each crank angle from eq. 6.1. The HRR is then integrated from time of spark and normalized to allow for the Mass Fraction Burn (MFB) to be evaluated. In the current study, the duration of 0-10% MFB has been used as an indication of the overall burning rate during the flame development regime, and the duration of 10-90% MFB as the an indication of the overall burning rate in the developed flame regime. The flame establishment regime is defined as the duration of 0-5% MFB. The burning rate of each fuel within the flame establishment regime is inferred from the duration of 0-5% MFB. The duration of 0-5% MFB is derived following an analysis of the optical data as will be explained in the next section.

### 6.2.2 Optical Post-Processing Technique

The derivation of the flame evolution involves the calculation of ‘enflamed’ areas through binarisation of each image and identification of its outlined. An in house Matlab© code was developed specifically for the current experimental setup to track the chronological change of flame radius. A typical chemiluminescence image with a superimposed flame outlined as automatically identified by the code is shown in Figure 6.1. At each crank angle five flame acquisitions were performed, each one at a different engine cycle. The mean flame radius at each crank angle was derived from averaging the equivalent flame radius calculated through the flame area of each individual cycle based on a circle with the same area. Similar technique has been used by Aleifreris et al. [30]. The Coefficient of Variation of the flame radius (CoV$R_{\text{Flame}}$) that allows for the cycle to cycle variability to be evaluated at the flame establishment regime was also calculated at each crank angle from the five acquired images.
As pointed out by Hamai et al. [151] and supported by Aleiferis et al. [152] the CoV of the flame radius within the flame establishment regime is a strong indicator of the CoVIMEP.

In order to isolate the flame only, avoiding picking up reflected light from external sources, masking and filtering of the image as well as variable thresholding was applied. Masking has been applied on the image, in order to isolate the region of interest avoiding reflections from the metal housing of the elongated piston. After masking the image, a 5x5 median filtering was applied to minimize any spatial noise on the image. A low value of threshold was necessary in order to track the flame just after the spark event where the flame is small and light intensity is low. However, as the flame develops the emission of light continuously increases. Using the same initial threshold value, reflected light from the valves or the near flame region was evident. It was therefore necessary to increase the threshold value with respect to the development of the flame. Following its initial value, the threshold was first increased for a flame radius above 3 mm and a second increase occurred for radius above 9 mm for all test conditions. Variable threshold was also used by other researchers in their optical studies due to similar reasons [153].

A sensitivity analysis was performed in order to quantify the change of flame radius with the threshold value. The dimmest flames correspond to natural gas at $\Phi = 0.8$ representing a ‘worst-case’ scenario and therefore were selected for the analysis. It has been found that there is a decrease of 1.8% in flame radius per 10% increase in threshold value at a flame radius of 3 mm, 0.44% at a radius of 9 mm and 0.37% at a radius of 13 mm.

Using the formulation of Beretta et al. [154] the MFB can be linked to the volume occupied by a flame such as,

$$ MFB = \left[ 1 + \frac{\rho_u}{\rho_b} \left( \frac{1}{y_b} - 1 \right) \right]^{-1} $$

(6.2)
where \( y_b \) is the volume fraction burned evaluated based on an equivalent sphere with the same flame radius as that of the flame, \( \rho_u \) is the unburned gas density and \( \rho_b \) the burned gas density. The ratio of unburned to burned gas density is commonly called the expansion ratio. The expansion ratio was evaluated at the point of spark for each fuel. The unburned gas temperature \( (T_u) \) was calculated using the isentropic relationship,

\[
T_u = T_{IVC} \left( \frac{P}{V_{IVC}} \right)^{\gamma-1} \gamma
\]

(6.3)

For a particular fuel, Cantera was used to obtain both \( \rho_u \) based on the calculated temperature and measured in-cylinder pressure, as well as \( \rho_b \) through the thermodynamic equilibrium of the burned mixture as explained in section 3.4.4. The MFB in the flame establishment regime (0-5% MFB) has been calculated using the optical data and eq 6.2.

### 6.2.3 Calibration of the Spark Dwell Period

The spark dwell period refers to the charging duration of the ignition coil. As it has been well acknowledged in literature [152] long spark durations can mask the effects of fuel characteristics and in-cylinder variations on the flame propagation, especially in the initial stages of combustion. It is a primary aim of present study to evaluate the effect of fundamental fuel characteristics on the flame propagation. It is clear that within the context of the current study, any masking of the phenomena is detrimental. It was therefore necessary to choose the spark dwell period such as ignition window was minimised whilst still supplying the minimum required energy to allow for a consistent ignition of all fuels.

The work of Gardiner et al. [155] investigated the spark voltage requirements for ignition of natural gas and gasoline in an SI engine, and concluded that natural gas needed consistently higher spark voltage and hence energy to initiate ignition as compared to gasoline. That was attributed to the direct effect of fuel type on ionization voltage levels. For both fuels, leaner mixtures increase the ignition voltage requirements.

Following the work of Gardiner et al. [155], in the current experimental work natural gas at \( \Phi = 0.8 \) needs the highest levels of spark energy in order to ignite. Thus, the spark dwell period was reduced down to levels that still allow a consistent ignition of natural gas at \( \Phi = 0.8 \), although masking of the effects of fuel characteristics on the flame propagation were
minimised. The optimised spark dwell period resulted to be 1 ms. At ambient conditions this corresponds to a spark duration of 1 ms measured with a Tektronix© TDS 2002 oscilloscope.

In the flame establishment regime, the effect of an increase in spark duration on the burning rate is shown for all fuels in Figure 6.2 at $\Phi = 0.83$, 2000RPM and a MAP = 0.44 bar. The location of the 5% MFB After Ignition Timing (AIT) is presented versus the DF ratio for a long spark dwell period (4 ms) and hence duration versus the optimised case (1 ms). As an overall trend, the burning rate is increased with the DF ratio for both cases evident by a reduction in the 5% MFB location. However, for the long spark duration the increase in burning rate with the DF ratio is considerable flatter in comparison to the optimised case. Thus, an increase in spark duration can mask the magnitude of the effects of fuel characteristics on the burning rate but not their overall trend. At lean burn conditions ($\Phi = 0.83$), as DF ratio increases the burning rate becomes less sensitive to the spark duration.

![Figure 6.2. Sensitivity of burning rate to the spark duration.](image)

As it has been reported in literature and experienced in the current study, a reduction in spark duration has an unavoidable effect on the combustion stability [152]. The sensitivity of the CoV\_IMEP of all DFs versus the spark duration is presented in Figure 6.3, at $\Phi = 0.83$, MAP : 0.44 bar and 2000 RPM. It can be clearly observed that with a decrease in spark duration, the sensitivity of the CoV\_IMEP to the DF ratio is increased. At a spark dwell of 1ms, there is a strong exponential increase of the CoV\_IMEP with a reduction of the DF ratio. As will be comprehensively discussed in the next section, this is mainly attributed to the fuel characteristics and their effect on the combustion process. The effect of fuel characteristics on the combustion process is a primary aim of the current study. It was then concluded that a spark dwell of 1 (ms) was essential in terms of fulfilling the aim of the current study, and not a matter of debated discussions on the statistical quality of the experiments.
A spark dwell of 1 ms was applied for the rest of this experimental study unless otherwise stated.

6.3 Results – Discussion

6.3.1 Operating Combustion Regime

Before attempting to discuss the burning rates at the different test conditions, it is particularly useful to place the present experimental work into the context of combustion diagrams and clearly define the combustion regime under investigation. To facilitate such analysis, all relevant combustion parameters are calculated at the spark timing and presented in Table 6.1, for a MAP of 0.44 bar and a speed of 2000 RPM. As there is no available chemical kinetics to predict the burning velocity of the blend fuel, only the thermodynamic parameters of the DF50 blend have been evaluated. These parameters will be necessary in the discussion of forthcoming sections. Methane has been used as a surrogate for natural gas, and PRF95 as a surrogate for gasoline. For the computed thermodynamic conditions at the point of spark as discussed in section 6.2.1, the laminar burning velocity \( S_{u0} \) of the surrogate fuels is calculated with the model of a freely propagating unstretched flame in the Cantera software package [96]. Pure fuel-air mixtures free of exhaust residuals have been considered. Cantera was integrated with the kinetic mechanism of Jerzembeck et al. [44]. The mechanism is validated against experimental values of burning velocities for both methane as well as PRF95 mixtures [44]. The laminar flame thickness \( \delta \) is defined as the ratio of kinematic viscosity \( \nu \) to the burning velocity \( \delta = \nu / S_{u0} \). The kinematic viscosity \( \nu \) and the
expansion ratio \((\sigma = \rho_u / \rho_b)\) at spark timing conditions were also evaluated using Cantera. The turbulence intensity \((u')\) and integral length scale \((l)\) at the point of spark are derived based on the rapid distortion theory as commonly used in literature [156], [157] such as,

\[
\begin{align*}
  u' &= 0.375u_p \\
  l &= 0.2h_{cl}
\end{align*}
\]  

(6.4)  
(6.5)

where \(u_p\) is the mean piston velocity and \(h_{cl}\) is the clearance height. The clearance height is defined as the distance from the top of the piston crown to the top of the pent-roof head. As experimentally shown by Liou et al. [158] and supported by Stone [159], the coefficient for calculating the turbulence intensity in an SI engine is in the range of 0.25 to 0.5. The average value of 0.375 is used in the current study. As derived by Heywood [150], and supported by the recent experimental findings of Aleiferis et al. [35], the turbulent length scale is about 20% of the clearance height. At the point of spark (35°CA BTDC) and an engine speed of 2000 RPM, turbulence intensity was calculated to be 2.05 m/s and the integral length scale 4.9 mm. These values have been used for all AFRs.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>(T_{Spark}) (K)</th>
<th>(P_{Spark}) (bar)</th>
<th>(\sigma)</th>
<th>(\delta) (mm)</th>
<th>(S_u^0) (m/s)</th>
<th>(L_b) (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>(\Phi = 0.8)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DF100</td>
<td>548</td>
<td>4.1</td>
<td>3.99</td>
<td>0.023</td>
<td>0.494</td>
<td>-0.12</td>
</tr>
<tr>
<td>DF50</td>
<td>536</td>
<td>4</td>
<td>4.2</td>
<td>-</td>
<td>-</td>
<td>0.16</td>
</tr>
<tr>
<td>DF0</td>
<td>529</td>
<td>3.89</td>
<td>4.4</td>
<td>0.019</td>
<td>0.548</td>
<td>0.63</td>
</tr>
<tr>
<td><strong>(\Phi = 1)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DF100</td>
<td>550</td>
<td>4.2</td>
<td>4.39</td>
<td>0.017</td>
<td>0.658</td>
<td>0.09</td>
</tr>
<tr>
<td>DF50</td>
<td>541</td>
<td>4.1</td>
<td>4.62</td>
<td>-</td>
<td>-</td>
<td>0.27</td>
</tr>
<tr>
<td>DF0</td>
<td>527</td>
<td>3.9</td>
<td>4.92</td>
<td>0.014</td>
<td>0.72</td>
<td>0.42</td>
</tr>
<tr>
<td><strong>(\Phi = 1.25)</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DF100</td>
<td>553</td>
<td>4.2</td>
<td>4.31</td>
<td>0.021</td>
<td>0.523</td>
<td>0.19</td>
</tr>
<tr>
<td>DF50</td>
<td>536</td>
<td>4</td>
<td>4.65</td>
<td>-</td>
<td>-</td>
<td>0.05</td>
</tr>
<tr>
<td>DF0</td>
<td>525</td>
<td>3.9</td>
<td>5</td>
<td>0.014</td>
<td>0.649</td>
<td>0.12</td>
</tr>
</tbody>
</table>

Table 6.1. Combustion parameters evaluated at spark timing

As has been reported in literature [50] [47], and discussed in section 5.2.3 the value of Markstein length is mainly a function of pressure, fuel and AFR. The effect of temperature and exhaust residuals can be assumed negligible compared to the mentioned contributors.
Values of the Markstein length for the selected fuels have been directly used from the constant volume experimental study presented in section 4.3.3 at an absolute pressure of 5 bar. An absolute pressure of 5 bar is very close to the pressures experienced at the spark timing during the current experimental investigation as shown in Table 6.1.

The combustion regime of the base fuels is shown in the Peters-Borghi diagram [160] of Figure 6.4. Blue color represents natural gas and red gasoline. Triangles represent $\Phi = 0.8$, circles $\Phi = 1.25$ and rectangles represent stoichiometry. All points lie within the corrugated flame regime. As mentioned in the introduction, within the flamelet regime, the turbulent flame front preserves the structure of a laminar flame, propagating with a rate equals to the stretched laminar flame velocity ($S_b$). In this combustion regime, the effect of Markstein length ($L_b$) is expected to be of crucial importance to the combustion process.

![Figure 6.4. Regimes of Turbulent Combustion at 2000RPM. Triangles $\Phi=0.8$, Rectangles $\Phi=1$, Circles $\Phi=1.25$. Natural Gas: Blue, Gasoline: Dotted Red, $u' = 2.05$ m/s, $l = 4.9$mm.](image)

The effect of exhaust residuals on $S_n$ as well as an increase in $u'$ through an increase of engine speed, will move the combustion regime towards the distributed reaction zone. In the distributed reaction zone the smaller turbulent eddies can penetrate into the preheat zone of the flame structure, and thereby enhance the heat and mass transfer rates [132]. The heat and mass transport is therefore critically influenced by turbulence, and the effect of flame stretch on the flame response is expected to decay.

It is important to underline that such fundamental analysis can only be made on an order of magnitude basis and transitions between different regions in the diagram should not be taken to indicate a step change in the characteristics of the combustion process [30].
6.3.2 In-cylinder Thermodynamic Analysis

The mean in-cylinder pressures and the associate curves of MFB for all DFs are shown in the subplot of Figure 6.5 at $\Phi = 0.8, 1, 1.25$, 2000 RPM and a MAP = 0.44 bar. The mean pressures as well as the MFB values are shown from the point of spark ($35^\circ$CA BTDC) and onwards. At lean burn conditions ($\Phi = 0.8$), natural gas gives the highest peak in-cylinder pressures and gasoline the lowest. All DFs are scaling in between the two fuels although DF50 attains a higher peak pressure compared to DF75. At stoichiometric conditions all DFs found to give higher peak pressures than the base fuels. In contrast to the lean conditions, at a rich AFR ($\Phi = 1.25$), gasoline has a considerable higher peak pressure in comparison to natural gas, with all DFs sitting in between the base fuels.

Figure 6.5. Thermodynamic Analysis: Mean In-cylinder pressures to MFB rates. Spark Timing = 145 $^\circ$CA ABDC.
At the point of spark, and for all tested AFRs, the in-cylinder pressure increases with DF ratio. This is a direct consequence of the effect of the specific heat ratio ($\gamma$). The specific heat ratio increases with the DF ratio, implying a higher in-cylinder pressure for the same compression. Despite not adjusting the throttle position to account for the air displacement as DF ratio increases, the phenomenon is consistently appearing in all AFRs. This underlines the importance of altering the value of $\gamma$ for the calculation of the MFBs of the various DFs. On average, the difference in pressure at the point of spark for natural gas as compared to gasoline is 0.25 bar, resulting in an increase of temperature of 23 K. The difference is reduced as the AFR gets leaner due to the heat capacity of the fuel-air mixture approaching that of pure air independently of the fuel.

The consistent scaling of in-cylinder pressure with the DF ratio at the point of spark indicates a well-controlled fuelling of the engine. The phenomena form an indirect validation of the overall procedure for adjusting the DF ratio during the engine experiments.

For a more efficient presentation, and to allow a direct comparison between the burning rates of the different DFs at all tested AFRs, the duration of 0-10% MFB and 10-90% MFB was derived for all fuels and tested AFRs as illustrated in Figure 6.6. The duration of 0-10% MFB has been used as an indication of the overall burning rate within the flame development regime, and the duration of 10-90% MFB as an indication of the overall burning rate in the developed flame regime. At each AFR, the data are correlated with a suitable fit shown as a line passing through them, aiming to illustrate the trend of the overall burning rate versus the DF ratio.

It has been found that at lean conditions ($\Phi = 0.8, 0.83$), the burning rate is linearly increased with the DF ratio in both the development as well as the developed flame regime. That is evident by a linear decrease in the duration of the MFBs. At stoichiometric conditions, all DFs including natural gas are faster than gasoline in the flame development regime. However, in the developed flame regime gasoline catches up and is marginally faster than natural gas. Although all DFs are still faster than gasoline in the developed flame regime, the differences are reduced as compared to the development flame regime. Similar findings with regards to the burning rate of the base fuels at lean and stoichiometric AFRs are reported by Aleiferis et al. [30]. Contrary to the lean mixtures, at a rich AFR ($\Phi = 1.25$), the burning rate is linearly decreased with DF ratio. Overall, and more evident in the developed flame regime, there is a tendency for the burning rates to diverge as DF ratio decreases for rich as compared to lean mixtures. Rich mixtures give the fastest burning rates. On the other hand, the burning rates at all AFRs relatively converge as DF ratio increases with stoichiometric mixtures resulting in the fastest burning rates.
At $\Phi = 0.83$, the burning rate in both flame regimes has been derived for a spark dwell of 4 ms to evaluate the consistency of the already reported experimental findings with a longer charging period of the ignition coil and hence longer spark duration. As can be observed from Figure 6.7, an increase in spark duration can mask the magnitude of the effects of fuel characteristics on the burning rate, evident by a reduction in the slope of the fitted line, but not their overall trends. The same conclusions derived within section 6.2.3 in the flame establishment regime, are still applicable in the initial as well as developed flame regime.

Following the previous discussion, it is clear that the burning rate is altered with the DF ratio. The response of burning rate with the DF ratio is contrary between lean and rich mixtures with DFs being faster than the base fuels on stoichiometry. To reveal the mechanism behind the observed experimental phenomena, the optical data from the flame establishment regime with a parallel discussion of the fundamental combustion parameters $S_a$ and $L_b$ are necessary.
6.3.3 Optical Analysis of Flame Evolution

A set of typical chronological combustion images for gasoline (DF0), DF50 and natural gas (DF100) are shown in Figure 6.8 at $\Phi = 0.8$, 2000RPM, and a MAP = 0.44 bar. Natural light photography as equipped in the current optical study allows for a two dimensional projection of the three dimensional flame. The combustion images represent a typical average cycle of the selected fuels. Although an effort has been made to show representative images of the acquired cycles, the cyclic variation in the flame development is unavoidable.

As the DF ratio decreases the flame intensity appears to be higher and more spatially homogeneous. There are no luminous spots over the images, and the actual flames appear reasonable circular indicating a well-mixed fuel-air mixture absent of fuel rich zones. There is a tendency of flame development towards the upper part of the combustion chamber.
where the exhaust valves are located. The phenomenon is consisted for all tested conditions. It is believed to be attributed to the higher temperatures exhibited by the exhaust valves.

The flame evolution becomes faster as DF ratio increases, although the difference between DF50 and natural gas is gradually reduced as the flame develops. The presented combustion images are well correlated to the derived flame radius shown in Figure 6.9 at $\Phi = 0.8$.

![Figure 6.8. Typical flame images at 15°, 20°, 25°, 30°, and 35° CA AIT ($\Phi = 0.8$, MAP : 0.44 bar, 2000 RPM)](image_url)

The mean flame evolution of all DFs as evaluated from the optical analysis at $\Phi = 0.8$, 1, 1.25, 2000 RPM, and a MAP = 0.44 bar is shown in Figure 6.9. At each crank angle, the
CoV of the flame radius (CoV_{R_{\text{Flame}}}) evaluated from the 5 flame acquisitions as explained in section 6.2.2 is also illustrated in a subplot included in the main plot. The red shaded area highlights the region at which an occasionally visible spark kernel is jumping around the ground electrode. This phenomenon is causing an arbitrary high CoV_{R_{\text{Flame}}} that does not belong to the actual behaviour of the flame, and is therefore omitted from further discussions. At a flame radius higher than about 16 mm, flames start clipping out of the piston crown window, and therefore data beyond this radius has to be discussed with caution. At each crank angle, error bars are evaluated based on the standard error for all DFs. For presentation clarity, error bars are plotted only for the base fuels, in order to give a direct indication of the experimental error experienced in the current study.

At lean conditions (\( \Phi = 0.8 \)), even though the laminar burning velocity (\( S_{u0} \)) at the point of spark is higher for gasoline compared to natural gas as shown in Table 6.1, the flame evolution is found to get faster as natural gas was added to gasoline evident by a larger flame radius. The difference in flame radius between the base fuels is preserved through the flame evolution. At stoichiometry, as the flame develops, DF50 and DF75 are diverging from the flame evolution of natural gas, whereas DF25 and gasoline are converging. At rich conditions (\( \Phi = 0.8 \)), and in contrast to the lean AFR, the flame evolution gets faster with the decrease of DF ratio although DF50 and DF75 resulted to have about the same flame evolution.

In the initial stages of flame evolution, whereas the integral length scale is larger than the flame size, the flame will sense only the high frequency fraction of the turbulent spectrum [135] [147]. There is a characteristic time scale which is required for turbulence to wrinkle the flame surface altering the near laminar flame evolution. Within this period, the flame exhibits a near laminar flame propagation with a rate equals to the stretched laminar burning velocity (\( S_{b} \)). As the flame develops, although the turbulent flame front will still propagate with a rate equals to the stretched laminar flame velocity, turbulence will wrinkle the flame surface increasing its overall area as well as the stretch experienced by the flame. The increase of the flame surface area gives rise to the turbulent flame velocity, being considerable higher than the stretched laminar flame velocity. These phenomena are evident in Figure 6.9 as a progressive change in the slope of the flame evolution. The phenomena are more obvious for natural gas at \( \Phi = 1.25 \).

Having illustrated and discussed the flame evolution of the various DFs in the different AFR conditions, the mechanism behind the observed phenomena can now be analysed.
Figure 6.9. Flame evolution and stability at lean (Φ = 0.8), stoichiometric and rich (Φ = 1.25) AFRs.
6.3.4 The Mechanism of Flame Behaviour

6.3.4.1 AFR Sweep

In an effort to clearly reveal the mechanism of flame evolution, the location of 5% MFB has been derived to illustrate the effect of DF ratio on the burning rate within the flame establishment regime. On the same logic, the average CoV of flame radius in the range of 10 to 25°CA AIT has been calculated to clearly illustrate the effect of DF ratio on the flame variability. The lower boundary (10°CA AIT) has been selected in order to be well absent of any spark effects, and the high boundary (25°CA AIT) to avoid any clipping of the flame out of the window.

The location of 5% MFB is calculated directly from the flame evolutions of the previous section using eq. 6.2, and it is presented in Figure 6.10. The 5% MFB location for $\Phi = 0.83$ is also calculated and presented in the same figure. For gasoline at $\Phi = 0.8$, the 5% MFB location has been extrapolated from its flame evolution as even at 35°CA AIT the 5% MFB was not achieved. At each AFR, the data are correlated with a suitable polynomial fit. The combustion parameters derived in Table 6.1, as well as the fundamental combustion characteristics of the DF blends derived in chapter 4 will be particularly referenced in an effort to clearly characterise and scientifically understand the mechanism of DF combustion.

![Figure 6.10. Burning rate versus DF ratio – AFR Sweep.](image)

Figure 6.10. Burning rate versus DF ratio – AFR Sweep.

It is apparent from Figure 6.10 that in the flame establishment regime, and lean burn conditions ($\Phi = 0.8, 0.83$), there is a linear increase in burning rate with the DF ratio evident by an advanced 5% MFB location. The phenomena are in contrast to the fact that natural gas (DF100) has a lower burning velocity than gasoline at the point of spark as shown in Table 6.1. At $\Phi = 0.8$, with 25% increase in DF ratio the burning rate increases by 8% in
comparison to that of pure gasoline (DF0). At spark timing, the average absolute in-cylinder pressure is 4 bar. In chapter 4, under similar pressure conditions (5 bar) and $\Phi = 0.8$, the burning velocity of all DFs has been reported to be even faster than that of gasoline. It is therefore evident that the burning velocity is not adequate in order to explain the response of the burning rate with the DF ratio at lean burn conditions. As shown in chapter 5, the other critical combustion parameter influencing the flame velocity is the Markstein length. As experimentally justified in chapter 4, at an absolute pressure of 5 bar and $\Phi = 0.8$, the Markstein length decreases with DF ratio. Natural gas and DF50 have about 6.5 and 4 orders of magnitude lower Markstein length than gasoline respectively. It worth noting that at $\Phi = 0.8$ and 5 bar, natural gas has a negative value of $L_b$ implying an increase of flame velocity under stretch.

As discussed in section 2.3.2.2 the stretch rate is an additive contributor of aerodynamic strain, and flame curvature. For an outwardly propagating spherical flame and a weak effect of the tangential straining compared to the sum of normal straining and flame curvature, the global stretch rate can be defined as in eq 3.4. The statement of a weak effect of tangential straining compared to the sum of normal straining and curvature in an SI engine environment is justified up to a turbulent intensity of 2.57 m/s by the experimental studies of Chaudhuri et al. [93] and Renou et al. [161]. In the study of Renou et al. [161], due to the thermal expansion of the flame, the velocity vectors in the fresh gases just ahead of the flame front are found to remain normal to that front implying a low tangential strain rate. As reported [161], within the flamelet combustion regime and for low-turbulence conditions, the local flame characteristics are governed by the curvature effects. At the same track, the recent study of Chaudhuri et al. [93] with turbulence intensities rise up to 2.57 m/s concluded that the stretch induced by pure curvature exceed that due to tangential straining by at least a factor of two. Their findings are supported by Breugny et al. [34], Aleiferis et al. [30] and Dahms et al. [94]. In particular Breugny et al. [34] and Aleiferis et al. [30] used eq 3.4 to obtain the global stretch rate in an SI engine assuming a weak effect of tangential straining as compared to the sum of normal straining and flame curvature. A similar methodology was adapted in the current study. It is clear from the definition of flame stretch (eq. 3.4) that peak value of stretch is expected at the very initial stages of combustion. As the flame develops and flame radius increases flame stretch is reduced.

In the current tested conditions, the global flame stretch peaks at $\sim$5000 1/s for natural gas at $\Phi = 0.8$. As the flame develops, stretch rate is reduced and eventually stabilises to a value of $\sim$1250 1/s. At the initial stages of flame establishment, the global flame stretch of gasoline is $\sim$1000 1/s lower than that of natural gas. As the flame develops it converges to the stretch
experienced by the natural gas flame. The values of stretch experienced by the blend fuels are in general between those experienced by the base fuels. The global flame stretch experienced by the base fuels in the current tested conditions is at the same order of magnitude as reported by other relevant experimental research studies [30], [34],[32].

In order to appreciate the effect of Markstein length on the flame velocity at engine like conditions, the same conceptual analysis as presented in section 5.2.4 has been performed for the base fuels at $\Phi = 0.8$. On the assumption of an infinitesimally thin flame, and negligible effect of the tangential turbulent straining such as flame stretch is continuously decreasing with flame radius, the model described by eq. 3.3, was used to derive the ratio of the stretched flame velocity to the unstretched flame velocity ($S_b/S_u^0\sigma$) of the base fuels. The unstretched flame velocity is defined as the burning velocity multiplied by the expansion factor. The combustion parameters at spark timing conditions as reported in Table 6.1 were used. To facilitate such conceptual analysis, the same methodology was followed as in chapter 5 whereas eq.3.4 was substituted to eq.3.3 and the model has been solved with respect to the stretched flame velocity using eq.3.5.

The flame radius has been iterated from 1 mm to 20 mm and the results are depicted in Figure 6.11. The crosses correspond to a flame stretch of 1250 1/s. Initially as the stretch rate experienced by the flame attains its highest value, $L_b$ has its maximum effect on the stretched flame velocity. The stretched flame velocity of natural gas can be as much as 30% higher as compared to its unstretched flame velocity, owning to the effect of a negative Markstein length. On the other hand, gasoline having relatively high positive values of Markstein length can experience a stretched flame velocity less than half of its unstretched velocity.

As the flame develops and the global stretch rate is reduced, the effect of Markstein length on the flame velocity is decaying. As mentioned earlier, wrinkling of the flame by the turbulence will maintain the global stretch rate to a value of $\sim$1250 1/s. In the context of turbulent flamelet regime, the turbulent flame front propagates with a rate equals to $S_b$. In order to approximate the velocity of the turbulent flame front of the base fuels, the values of $S_u^0$ and $\sigma$ are substituted in the relation $S_b/S_u^0\sigma$ at a stretch rate of 1250 1/s. The velocity of the turbulent flame front resulted to be 2 m/s for natural gas and 1.6 m/s for gasoline. The velocity of the turbulent flame front is 23% faster for natural gas than gasoline despite its lower burning velocity, owning to the value of Markstein length.
The conceptual analysis reflects the mechanism of an increase in burning rate with DF ratio in lean burn conditions, owning to the reduction in the value of Markstein length. Further discussions and correlations of the burning rate of the various DFs with their associate values of Markstein length will be presented in the next section.

At stoichiometry, DF50 and DF75 resulted to have faster burning rates compared to the base fuels. Natural gas was faster than DF25 and to larger extent gasoline. As already commended in the previous section, the faster flame evolution exists from the very initial stages of the flame establishment regime where the flame propagates with a near laminar velocity. The experimental findings of the DFs being faster than the base fuels at $\Phi = 1$ have been also observed in the laminar constant volume combustion experiments of chapter 4. As it has been reported, at a pressure of 5 bar, with 25% increase in the DF ratio there is 4% and 20% reduction in burning velocity and Markstein length respectively. However, DF50 resulted to be the fastest fuel in the initial stages of laminar combustion. That was attributed to a best balance between the two fundamental combustion parameters $S_u^0$ and $L_b$ that allowed for a faster flame evolution compared to the rest of the fuels. It is therefore concluded that in the current experimental conditions, the faster burning rate of DF50 and DF75 compared to the base fuels at $\Phi = 1$, is attributed to the same mechanism. Further experimental evidence of stoichiometric DF mixtures being faster than base fuel mixtures in an SI engine environment have been presented in the studies from the research group of Di Iorio et al. [36] [36].

Following the fundamental experimental study, it has to be noted that phenomena of thermo-diffusive flame instability that will increase the flame velocity and therefore the burning rate in the SI engine are expected to occur at $\Phi = 1$ and pressures above 5 bar. Mixtures with a
lower Markstein length are more prone to instabilities. As DF ratio increases flame is more likely to experience such phenomena. The effects of thermo-diffusive instability on the flame velocity of DF mixtures are out of the scope of the present study.

At rich conditions ($\Phi = 1.25$), with 25% increase in DF ratio the burning rate is decreased by 6% in the flame establishment regime. As it is clearly reported in the fundamental study, in comparison to the lean conditions, as the AFR becomes richer the stretch sensitivities of the test fuels are relatively converging to a single value, implying that $S_o$ has a higher influence on the combustion process. As the DF ratio decreases, rich flames at pressures above 5 bar are becoming inherently unstable from their nature. Flame instability is also a contributor to the faster burning rate experienced with a reduction of the DF ratio.

The average CoV of flame radius in the range of 10 to 25$^\circ$CA AIT has been defined as the flame variability. The flame variability of all DFs at all tested AFRs is presented in Figure 6.12. For the base fuels, and stoichiometric to lean mixtures, the CoV of the flame radius within the flame establishment regime has been reported by other relevant experimental studies to lie within the range of 20 to 35% [35], [34], [162].

![Figure 6.12. Flame Variability – AFR Sweep.](image)

Considering the flame variability at the lean mixtures ($\Phi = 0.8$, 0.83), there is an overall exponential decrease with DF ratio although gasoline at $\Phi = 0.8$ deviates from the overall trend. In contrast, at $\Phi = 1.25$ there is a clear exponential increase in flame variability with the DF ratio. At stoichiometric conditions, the flame variability remains relatively constant in comparison to the lean and rich conditions, with DF50 resulting in the most stable flame. For all tested AFRs, there is a tendency for the fuels having the fastest burning rates in the flame establishment regime, to give the lowest flame variabilities.
At $\Phi = 0.83$, the flame variability and subsequently the $\text{CoV}_{\text{IMEP}}$ presented in section 6.2.3 are exponentially decreased with the increase of DF ratio. There is a strong consistency between the flame variability and the $\text{CoV}_{\text{IMEP}}$ supporting the comments of Hamai et al. [151] that flame variability at the early stages of combustion is a strong indicator of $\text{CoV}_{\text{IMEP}}$.

### 6.3.4.2 Load Sweep

Following the prescribed analysis, it has been found that the effects of the fuel characteristics on the burning rate and flame variability as experienced in the flame establishment regime are still preserved in the initial as well as in the developed flame regime. The only noticeable exception corresponds to the stoichiometric natural gas mixture being faster than gasoline in the establishment and initial flame regime but not in the developed one. Only lean mixtures have been tested for the engine load and speed sweep. It is expected that the flame behaviour in the flame establishment regime will be consistent in the initial as well as in the developed flame regime.

As it has been already discussed, the effect of Markstein length dominates the flame propagation at lean burn conditions. Although an extensive analysis has been presented for the base fuels, there was no direct evidence as for the associate values of Markstein length of the DF blends and their effect on flame propagation. In an effort to correlate the burning rate of the different DFs with their associate values of Markstein length, an extensive analysis has been performed at $\Phi = 0.8$ and three different engine loads corresponding to a MAP = 0.44, 0.52, and 0.61 bar. The values of Markstein length for the different DFs as reported in the fundamental study at an absolute pressure of 5 bar have been used. The peak engine load was selected to give near 5 bar absolute pressure at the point of spark in order to be as consisted as possible to the test pressure in the fundamental study. Experiments at a medium load were also performed to reveal the trend in the response of flame behaviour with an increase of in-cylinder pressure manifested by a gradual increase in engine load. For a low to high engine load, the average absolute pressure at the point of spark corresponds to 4, 4.4, and 5.1 bar. The peak in-cylinder pressures derived with pure natural gas fuelling and corresponds to 10.5, 13, 18.7 bar. All experiments performed at an engine speed of 2000 RPM. The results are illustrated in Figure 6.13. At each MAP, the data are correlated with a suitable polynomial fit.

There is a strong linear correlation of the 5% MFB location and the associate value of $L_b$ of each fuel at all tested loads. The phenomenon implies that the stretch sensitivity of the DFs is conserved from constant volume to the engine combustion and the burning rate in the
flame establishment regime is governed by the value of $L_b$. The studies of Brequigny et al. [33],[34], under similar test conditions, reported a linear correlation of the 5% MFB with the value of Lewis number of the fuel-air mixture. The Markstein length is mainly depended on the Lewis number of the mixture implying that the phenomena experienced in the current study are consisted with the findings of Brequigny et al. [33],[34]. Evaluated at a MAP = 0.61 bar, with a 0.2 mm decrease in $L_b$ the burning rate is increased by 5%.

It can be also noted that there is a non-monotonic increase in burning rate with the increase of load. As DF ratio increases the effect of an increased burning rate with the engine load is decaying. From low (MAP = 0.41 bar) to high (MAP = 0.61 bar) engine load, the rate of increase of burning rate with the DF ratio evaluated by the slope of the fitted lines, is decreased by 36% at $\Phi=0.8$. The phenomena are attribute to the fact that as in-cylinder pressure increases, evident by an increase in load, the value of $L_b$ of the pure liquid fuel is approaching that of pure gas as reported by Gu et al. [50]. It is therefore expected that in the flame establishment regime, the effect of a faster burning rate with the increase of the DF ratio will continuously decay as engine load further increases as long as flames are not affected by instability.

As it was expected, the linear increase in burning rate with the DF ratio as experienced in the flame establishment regime is preserved in the initial as well as in the developed flame regime for all tested loads as it is illustrated in Figure 6.14.
The flame variability at all tested engine loads is presented in Figure 6.15. An exponential decrease in flame variability with the DF ratio is clearly illustrated. The response of flame variability with the DF ratio supports the discussion in the previous section verifying the critical influence of $L_b$ on the combustion stability under lean burn conditions. The flame variability seems to decrease with an increase in load for all DFs possible attributed to a reduction of $L_b$ with pressure.

While lean homogeneous operation in SI engines has previously demonstrated the ability to reduce fuel consumption and pollutant emissions [163], the degree of lean burn is limited by increasingly slow and unstable combustion. Following the discussions in the present study, the value of $L_b$ is a dominant parameter for extending the capabilities of lean burn combustion both from a flame stability and velocity prospective.
6.3.4.3 Speed Sweep

Having analysed the DF combustion process with respect to the AFR and engine load it is now time to present the flame behaviour of the base fuels as well as DF50 at a sweep of engine speed. During the engine speed sweep, the AFR was set to \( \Phi=0.8 \) and the engine load was targeted at an IMEP of 1.7 bar on natural gas fuelling. This implies a change in throttle position between the three test engine speeds. The upper plot of Figure 6.16 illustrates the 5% MFB location indicative of the overall burning rate in the flame establishment regime, versus the three test fuels. On the lower plot the flame variability is presented.

The burning rate of all tested fuels increases with engine speed. Natural gas is found to have the fastest burning rate in all three engine speeds and gasoline the slowest. The difference is reduced as engine speed increases. It is not clear from the current experimental method if the phenomena are attributed to the fuel characteristics, or to the shift of the combustion process in the distributed reaction zone, whereas the effect of flame stretch on the burning rate is expected to decay. Experiments in a constant volume vessel as well as in an SI engine environment under various levels of turbulence concluded that mixtures with a low Markstein length are able to attain higher levels of wrinkling for a set value of turbulence [34]. Methane, having a lower Markstein length than isooctane was found to have a faster flame evolution under increased turbulent levels [34] [53]. The difference was increased with higher turbulence levels. Understanding the limitations of the current analysis as mentioned at the start of the paragraph, further investigation on the effect of turbulence to the burning rate is undertaken in section 7.4.
As far as the flame variability is concerned, there is no obvious trend with respect to a change in engine speed. For gasoline and to a lower extent DF50 there is a clear separation of the flame variability at a speed of 2750 RPM compared to the other two engine speeds. Natural gas seems considerably less sensitive than the other two fuels for a change in engine speed. The above experimental phenomena can be explained by the findings of Aleiferis et al. [152] reporting that at a low flow velocity and/or turbulence in the cylinder, as expected at 1250 RPM, the flame stays close to the spark-plug gap and is prone to quenching effects due to increased heat losses with the electrodes. On the other hand, too high velocity and/or turbulence cause large portions of the flame to be convected rapidly from the electrodes and the flame to quench in the resulting stretch. Thus, a moderate flow velocity is of benefit, that will both convect the flame kernel away from the spark plug gap and will not quench the flame kernel in the bulk flow. It seems that in the present study, such beneficial conditions are experienced at 2000 RPM.
6.4 Chapter Summary

The current chapter presents the findings from an experimental campaign performed in an optically assessed SI engine. Optical diagnosis has been integrated with in-cylinder pressure analysis to investigate the mechanism of flame velocity and stability with the addition of natural gas to gasoline in a DF blend. Experiments are performed under a sweep of engine load (MAP = 0.44, 0.51, 0.61 Bar), speed (1250, 2000, 2750 RPM) and equivalence ratio (Φ = 0.8, 0.83, 1, 1.25). Natural gas was added to gasoline in three different energy ratios 25%, 50% and 75%. At lean burn conditions (Φ=0.8) the 5% Mass Fraction Burned (MFB) location derived through optical analysis is linearly related with the associate value of Markstein length of each fuel, at all test loads. For stoichiometric combustion, DF50 and DF75 exhibit a faster burning rate in comparison to the base fuels. Contrary to the lean mixtures, at Φ=1.25, the burning rate increases with a decrease of the DF ratio. For all test AFRs, there is a tendency for the fuels having the fastest mass burning rates to give the lowest flame variabilities. The same experimental phenomena are still preserved in the initial (0-10% MFB) as well as in the developed (10-90% MFB) flame regime. It has been concluded that within the flamelet combustion regime the effect of Markstein length is dominating the lean burn combustion process both from a stability and velocity prospective. The effect of the burning velocity on the combustion process gradually increases as the air fuel ratio shifts from stoichiometric to fuel rich values.
Chapter 7

7 On the Transition from Constant Volume to Engine Combustion

7.1 Introduction

The definition of the transition mechanism characterising the difference in burning rate from the constant volume to SI engine combustion has been documented in section 3.5.3. The response of the mass burning rate with the addition of gaseous to liquid fuel has been investigated in both experimental environments and reported in chapters 4 and 6. In the current chapter, the transition mechanism will be investigated for lean, stoichiometric and rich mixtures. The response of the transition mechanism with the DF ratio will be evaluated. The influential parameters involved at each AFR will be comprehensively discussed. For the base fuels, the sensitivity of the burning rate to the presence of turbulence will be assessed through a conceptual analysis of the burning rate definitions derived in section 3.5, and associate experimental data.

7.2 Burning Rate Comparison

The Mass Fraction Burned (MFB) durations derived from the engine experiments at MAP = 0.44 bar and 2000 RPM and those obtained at an absolute pressure of 5 bar from the constant volume combustion experiments are plotted in Figure 7.1 in two different axes. A
pressure of 5 bar absolute was selected as it was the closest to the average pressure (4 bar) at ignition timing during the SI engine experiments.

Consistent with our previous discussions, the duration of 0-10% and 10-90% MFB has been used as an indication of the overall burning rate in the development and developed flame regime respectively.

As shown in Figure 7.1, at lean mixtures (Φ = 0.8) the response of the burning rate with the addition of gaseous to the liquid fuel differs from the constant volume to the engine environment. On the other hand, the overall trends appear similar between the two experimental environments for stoichiometric and rich mixtures. It has to be noted that for rich mixtures the constant volume experiments performed at Φ = 1.2 whereas the engine experiments at Φ = 1.25.

Following the overall trends at Φ = 0.8, it can be stated that the burning rate in the engine environment is monotonically decreased with the DF ratio. In the constant volume environment all DFs are faster than the base fuels with the pure gaseous fuel being slower than the liquid fuel. Similar phenomena have been observed in the development and developed flame regime. In comparison to the constant volume combustion, as justified in section 6.2.1 the global stretch rate experienced by the flame is about 7 times higher for the engine combustion attributed to the effect of turbulence. From this prospective, it is expected that the stretch sensitivity of the flame will have a higher effect in the engine than in the constant volume environment. Indeed, as comprehensively discussed in the previous chapter the Markstein length dominates the engine combustion process at Φ = 0.8. In the constant volume combustion, only the flame establishment phase (R_f ≈ 2.5 mm) is found to be dominated by the Markstein length. As the flame develops and stretch rate is reduced the effect of laminar burning velocity dominates the constant volume combustion process. In chapter 4, all DFs are found to have a higher burning velocity than the base fuels at Φ = 0.8 and 5 bar. This is reflected in their overall burning rate characteristics with all DFs being faster than the base fuels. These findings are supporting the previous comments indicating that the overall burning rate in the constant volume environment is dominated by the laminar burning velocity. It is then concluded that at Φ = 0.8 the difference on the response of burning rate with the DF ratio between the two experimental environments is due to a different underlined combustion mechanism.
Figure 7.1. Superimposed MFB durations from constant volume and engine experiments for all tested fuels.
At rich conditions, the combustion process is found to be dominated by the laminar burning velocity in both combustion environments as documented in chapters 4 and 6. As discussed in section 5.3.1 there is an uncertainty with regards to the value of burning velocity for methane at $\Phi = 1.2$ and 5 bar. The measured burning velocity of methane in the current constant volume experiments is higher compared to the values presented in literature. Excluding the burning rate of methane from the overall trend, it can be stated that the burning rate is monotonically decreased with the DF ratio for both combustion environments. It can be then verified that at rich conditions the constant volume and the engine combustion have the same mechanism reflected in the response of burning rate with the DF ratio. The combustion mechanism is dominated by the laminar burning velocity of the combustible mixture.

At stoichiometric conditions, there is a degree of similarity in the response of the burning rate with the DF ratio between the two experimental environments. At stoichiometry, the combustion mechanism is not dominated by either the Markstein length or the laminar burning velocity. Both fundamental combustion parameters are contributing to the combustion mechanism in comparable proportions. Attributed to the higher stretch induced by the turbulence, the Markstein length is expected to be a stronger contributor to the engine combustion than to the constant volume. In the developing flame regime, DF75 and pure gaseous fuel is slower than the liquid fuel in the constant volume combustion. In contrast, in the engine combustion, DF75 and pure gaseous fuel are faster than the liquid fuel. The particular findings support the higher proportional contribution of Markstein length in the engine as compared to the constant volume combustion.

### 7.3 The effect of Transition Mechanism

The percentage variation of the burning rate with an increase of the DF ratio differs from the constant volume in comparison to the engine environment. In order to quantify the response of the transition mechanism to the DF ratio, the MFB durations corresponding to the pure liquid fuel (PRF95 for the CVCV and gasoline for the engine) has been used as a reference for comparison. The percentage difference from the MFB duration of the pure liquid fuel is derived for the rest of the fuels in the developing and developed flame regime. For both experimental environments, the percentage difference in burning rate is presented in Figure 7.2. A positive difference implies a slower burning rate than that of the liquid fuel and vice versa. As illustrated, for a particular fuel under consideration the change in the percentage
difference of burning rate from the CVCV to the engine experiments is attributed to the transition mechanism.

In the developing flame regime, at $\Phi = 0.8$, the transition mechanism resulted in an average reduction of 26% in the burning rate of all DFs relative to the pure liquid fuel. In contrast, the transition mechanism increases the burning rate of pure gaseous fuel by 30% relative to the liquid fuel. At $\Phi = 0.8$, the combustion mechanism in the engine environment is driven by the Markstein length and in the constant volume by the laminar burning velocity. Moving from the constant volume to the engine environment, all DFs having a higher burning velocity than that of the pure liquid fuel experienced a decrease in the percentage difference in burning rate relative to that of the liquid fuel. The higher burning velocities are not reflected in the engine combustion due to the dominance of the Markstein length. On the other hand, the pure gaseous fuel having the lowest Markstein length and also the lowest burning velocity showed an increase in burning rate relative to the liquid fuel. In the developed flame regime, for dual fuel ratios higher than about 50% the transition mechanism resulted in an exponential increase of the burning rate relative to the pure liquid fuel.

At $\Phi = 1$, in both the developing and developed flame regime, for dual fuel ratios higher than 25% the transition mechanism results in an exponential increase of burning rate relative to the liquid fuel. The largest effect of the transition mechanism corresponds to the pure gaseous fuel. As compared to the pure liquid fuel, the transition mechanism increases the burning rate of the gaseous fuel by 17% and 31% in the developing and developed flame regime respectively.

At rich conditions, the transition mechanism cannot be clearly analyzed due to the inconsistency of the tested equivalence ratios between the two experimental environments. As a general trend, the effect from the transition mechanism seems to increase with DF ratio. However, if the same equivalence ratio was tested the difference in burning rates in the constant volume environment is expected to approach those in the engine. Therefore, for rich mixtures sufficiently off-stoichiometry, the effect from the transition mechanism is expected to be relatively similar for all tested fuels. That is attributed to the fact that the combustion mechanism is dominated by the laminar burning velocity in both combustion environments.
Figure 7.2. Sensitivity of DF ratio on the burning rate at lean, stoichiometric and rich conditions.
7.4 Turbulence Sensitivity

The effect of turbulence is a main contributor to the transition mechanism. Considering the burning rate definitions as documented in section 3.5, the sensitivity of a particular fuelling mode to turbulence can be derived following the subsequent conceptual analysis. Throughout the analysis the combustible mixture is treated as spatially homogeneous with the same equivalence ratio and composition in both combustion environments. Hence, only experimental data at \( \Phi = 0.8 \), and \( \Phi = 1 \), have been considered. The ratio of the mass burning rate in the engine to the mass burning rate in the constant volume combustion vessel is given by,

\[
\frac{m_{b,\text{Eng}}}{m_{b,\text{CVCV}}} = \frac{\rho u_{\text{Eng}} S^0_{\text{Eng}} I_{0E} Y_T A_T}{\rho u_{\text{CVCV}} S^0_{\text{CVCV}} I_{0C} Y_L A_L}
\]  

(7.1)

In the above equation, the density ratio is not affected by the flow field. The ratio of burning velocities is depended on the temporal difference in pressure and temperature between the two experimental environments during a particular combustion process. In an engine environment, through the compression stroke and up to the point of ignition the in-cylinder thermodynamic conditions are governed by the piston compression. At the time of ignition, the ratio of burning velocities can be computed using chemical kinetics knowing the associate thermodynamic conditions. As discussed in section 5.3.1 there is currently no kinetic mechanism capable of reliably predicting the burning velocity of the blended fuels. It is therefore necessary to constrained the analysis to the base fuels.

From section 3.5, the ratio of stretch factors can be decomposed to,

\[
\frac{I_{0T}}{I_{0L}} = \frac{1 - \frac{L_{b,\text{Eng}} \sigma_{\text{Eng}}}{S^0_{u,\text{Eng}}} a_{\text{Eng}}}{1 - \frac{L_{b,\text{CVCV}} \sigma_{\text{CVCV}}}{S^0_{u,\text{CVCV}}} a_{\text{CVCV}}}
\]

(7.2)

As justified in experimental literature [50][47] and discussed in section 5.2.3, the effect of temperature and residual gasses on the Markstein length is relatively weak as compared to the effect of pressure. The Markstein length \( (L_b) \) can be reasonable treated as being explicitly depended on pressure, equivalence ratio, and composition. The difference in pressure at the point of spark between the constant volume (5 bar absolute) and the engine
environment is within 1.1 bar. As reported by Gu et al. [50] the Markstein length of methane and isoctane reduces exponential with pressure although after about 4 bar it starts to reach a plateau. On average, from 1 to 4 bar the Markstein length is reduced by more than 3 times for methane and isoctane air mixtures. However, from 4 to 5 bar the Markstein length is reduced by \( \approx 15\% \). Following the experimental findings of Gu et al. [50] the Markstein length at the point of ignition is expected to be comparable in the two experimental environments. It is then reasonable to assume that the Markstein length in the constant volume environment is similar to that in the engine environment \( (L_{bEng} \approx L_{bCVCV}) \). The validity of the current analysis is compromised as the difference in pressure between the two combustion environments increases. Thus, the analysis is applied only in the flame developing regime whereas the difference in pressure is kept to a minimum. The pressures experienced by the flame at \( \Phi = 0.8 \), and \( \Phi = 1 \) are shown in Figures 4.15 and 6.5 for the constant volume and the engine environment respectively. Recognizing the fact that,

\[
\frac{L_{bEng} \sigma_{Eng}}{S_{uEng}} \ll \frac{a_{Eng}}{a_{CVCV}} \quad (7.3)
\]

the ratio of the stretch factors can be then treated as having a dominant dependence on the ratio of stretch rates experienced by the flame in the engine to that in the constant volume environment such as,

\[
\frac{I_{0T}}{I_{0L}} \approx \frac{a_{Eng}}{a_{CVCV}} \quad (7.4)
\]

The ratio of stretch rates is dominated by the natural ability of turbulence in wrinkling the surface area of the flame. An increase in the flame surface area due to wrinkling will inherently increase the stretch experienced by the flame and subsequently the ratio of stretch factors.

The onset of flame instability is mainly depended on the Markstein length as well as on the stretch experienced by the flame. At the time of ignition, the Markstein length is similar for both experimental environments. A high enough stretch can stabilize the flame. As experimentally justified in section 6.1, in the very initial stages of engine combustion (MFB < 5\%) the flame will sense only the high frequency fraction of turbulent spectrum and the flame propagates with a rate equals to the laminar flame velocity. As the flame gradually
develops the turbulence will wrinkled and stretch the flame. In the context of the current analysis, a similar effect from flame instability is assumed between the two experimental environments. Thus, the effect of flame instability is not contributing to the difference in mass burning rate between the two experimental environments. Although this assumption is reasonable for the very initial stages of flame evolution, as the flame develops its validity may be compromised.

Following the previous discussion, it can be then concluded that the turbulence effect is given by,

\[
K_{Turb} = \frac{I_{0_T} A_T}{I_{0_L} A_L} = \frac{\dot{m}_{b,Eng}}{\dot{m}_{b,CVCV}} \frac{\rho_u \cdot S_{Eng}}{\rho_u \cdot S_{CVCV}}
\]  

(7.5)

To facilitate the derivation of the turbulence effect, the absolute values of the mass burning rate of the base fuels in the developing flame regime are derived at \( \Phi = 0.8 \), and \( \Phi = 1 \). The mass burning rate is calculated by multiplying the 10% MFB duration \( (T_{10\% MFB}) \) with the 10% of the total mass \( (M_{Tot}) \) as indicated in eq. 7.6. The resulted mass burning rates are shown in Figure 7.3.

\[
(T_{10\% MFB})(0.1M_{Tot})
\]  

(7.6)

From constant volume to engine combustion the burning rate is increased by 1.9 and 2.7 times for the liquid and gaseous fuel respectively at \( \Phi = 0.8 \), and 1.42 and 1.8 times at \( \Phi = 1 \). From constant volume to engine combustion the mass burning rate of pure gaseous fuel is increased by 31% and 23% more compared to that of the pure liquid fuel at \( \Phi = 0.8 \), and \( \Phi = 1 \) respectively.
The unburned gas density multiplied by the laminar burning velocity is commonly called the laminar burning flux. To compare the sensitivity of the base fuels to turbulence, the ratio of mass burning rate needs to be normalized by the ratio of burning fluxes as illustrated in eq. 7.5. The thermochemical values as used for the derivation of the turbulence effect are summarized in Table 7.1. The laminar burning fluxes in both combustion environments are computed and illustrated in Figure 7.4.
On the Transition from Constant Volume to Engine Combustion

<table>
<thead>
<tr>
<th>Fuel</th>
<th>$T_{\text{Spark}}$ (K)</th>
<th>Abs. $P_{\text{Spark}}$ (bar)</th>
<th>$M_{\text{Tot}}$ (g)</th>
<th>$\sigma$ (kg/m$^3$)</th>
<th>$\rho_u$ (m/s)</th>
<th>$S_u^0$ (mm)</th>
<th>$L_0$ (mm)</th>
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</thead>
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<tr>
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<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>DF100</td>
<td>548</td>
<td>4.1</td>
<td>1.549</td>
<td>3.99</td>
<td>1.90</td>
<td>0.494</td>
<td>-0.12</td>
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<tr>
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<td>3.89</td>
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<td>0.548</td>
<td>0.63</td>
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<tr>
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<td>DF100</td>
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<td>4.2</td>
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<td>4.39</td>
<td>1.93</td>
<td>0.658</td>
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<tr>
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<td>3.9</td>
<td>0.16</td>
<td>4.92</td>
<td>2.02</td>
<td>0.72</td>
<td>0.42</td>
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<tr>
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<tr>
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<td>10.5</td>
<td>5.37</td>
<td>4.49</td>
<td>0.166</td>
<td>-0.12</td>
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<td>6.59</td>
<td>4.89</td>
<td>0.33</td>
<td>0.42</td>
</tr>
</tbody>
</table>

Table 7.1. Thermochemical characteristics of the base fuels

The burning flux of the liquid fuel is higher than the gaseous fuel due to its higher density and burning velocity of the liquid fuel. However, the transition from constant volume to the engine combustion reduces the burning flux of the liquid fuel whereas at the same time and in contrast to the liquid fuel, the transition increases the burning flux of the gaseous fuel. That is mainly attributed to the effect of piston compression and the lower heat capacity of the gaseous fuel. As discussed in section 6.3.1, due to the piston compression and the lower heat capacity, the gaseous fuel resulted to have on average 21K higher temperature at the point of ignition as compared to the liquid fuel. In addition, as discussed in section 5.3.1 the burning velocity of the gaseous fuel is more sensitive to an increase in temperature than that of the liquid fuel. At the point of spark, the pressures are within 1.1 bar between the two combustion environments although the temperature is on average 165 K higher in the engine than in the constant volume combustion.
The effect of turbulence on increasing the mass burning rate is lumped into a non-dimensional constant \( K_{\text{Turb}} \) as derived in eq. 7.5. For the base fuels, the effect of turbulence is computed and presented in Figure 7.5. It is evident that the gaseous fuel is more sensitive to the presence of turbulence in comparison to the liquid fuel at both equivalence ratios. The effect of turbulence on increasing the mass burning rate is 12% and 14% higher for the gaseous compared to the liquid fuel at \( \Phi = 0.8 \) and \( \Phi = 0.1 \) respectively. In comparison to the liquid fuel, the higher turbulence sensitivity of the gaseous fuel is associated with its lower value of Markstein length.
The higher turbulent sensitivity of the gaseous fuel can be explained considering the discussion in section 2.3.3. In particular, as experimentally justified by Aleiferis et al. [35] and supported by the current study, fuels with a lower Lewis number and hence Markstein length are more easily wrinkled by turbulence due to their thermodiffusively unstable nature. On the other hand, flames correspond to positive Markstein length fuels tend to naturally stabilize under turbulence as the velocity at the flame crests will be reduced in contrast to the velocity of the cusps that will be increased. This phenomenon leads to an inherent smoothing of the flame wrinkles, and reduces the ability of turbulence to wrinkle the flame. Such experimental findings are also supported by further relevant experimental literature. The experimental studies of Lawes et al. [53] and Brequigny et al. [34] reported that mixtures with low Markstein length have a higher ability to be wrinkled by turbulence [53] [34] compared to mixtures with higher Markstein length.

**7.5 Chapter Summary**

In the current chapter, the transition from constant volume to engine combustion has been investigated. At $\Phi = 0.8$ the mass burning rate in the constant volume combustion is dominated by the laminar burning velocity whereas in the engine combustion by the Markstein length. The combustion mechanism is found to be different between the two experimental environments only for lean mixtures. The transition mechanism characterizes the difference in burning rate between the constant volume and the engine combustion. For
stoichiometric to lean mixtures, the transition mechanism has its largest effect on the pure gaseous fuel. At stoichiometry, for a dual fuel ratio higher than 25% the transition mechanism resulted in an exponential increase of the burning rate relative to the pure liquid fuel. The turbulence sensitivity of the base fuels has been also investigated at $\Phi = 0.8$ and $\Phi = 1$. The effect of turbulence on the increase of the mass burning rate is on average 13% higher for the gaseous as compared to the liquid fuel attributed to its lower Markstein length. On a phenomenological level, the experimental findings are consisted with relevant experimental literature.
Chapter 8

8 Concluding Remarks and Open Challenges

8.1 Conclusions

The current thesis aimed to establish a structured scientific understanding on the basis of fundamental combustion characteristics for the combustion mechanism of binary blends of natural gas and gasoline in SI engines. This has been achieved on both a fundamental and practical level. Numerical analysis aid the understanding on the contribution of the fundamental combustion parameters laminar burning velocity ($S_{u0}$) and Markstein length ($L_b$), on the velocity of a propagating stretched flame. The transition mechanism from laminar to engine combustion has been also investigated for the purposes of the current research. Consequently, the increase in mass burning rate due to the effect of turbulence has been conceptually evaluated for pure gaseous and liquid fuels.

8.1.1 Constant Volume Combustion

On a fundamental level, driven by the inadequate literature information, the effects of methane addition to PRF95 (95%volliq iso-octane and 5%volliq n-heptane) on the fundamental combustion parameters, $S_{u0}$ and $L_b$ were experimentally investigated in a cylindrical combustion vessel at $\Phi$=0.8,1,1.2, $P_{\text{initial}}$= 2.5,5,10 Bar and a constant $T_{\text{initial}}$=373 K. For $L_b$$<$$0$, the flame velocity increases under stretch and vice versa. Methane has been
used as a natural gas surrogate and PRF95 as a gasoline surrogate. Methane was added to PRF95 in three different energy ratios 25%, 50% and 75%. Spherically expanding flames visualised through schlieren photography were used to derive the flow corrected flame velocities, from which the corresponding $S_u^0$ and $L_b$ were obtained.

At $\Phi=0.8$, it has been found that the sensitivity of the flame to stretch for all Dual Fuels (DFs), characterised by $L_b$, is biased towards that of methane being the least sensitive fuel. The effect decays as pressure increases. In contrast, at $\Phi=1.2$ the value of $L_b$ for all DFs was lower than methane and comparable to that of PRF95. At $\Phi=1$, with a 25% increase in the DF ratio, the value of $L_b$ is reduced by 16%, 20%, 28% at a pressure of 2.5, 5 and 10 Bar respectively. At $\Phi=0.8$ and to less extend $\Phi=1$, methane attained negative values of $L_b$ at 5 and 10 bar. As the equivalence ratio shifts from lean to rich values, the value of $L_b$ is relatively converge for all fuels. As pressure increases, $L_b$ is reduced for all fuels with PRF95 being the most sensitive. As experimentally justified, mixtures with lower $L_b$ have a higher propensity to thermodiffusive flame instability. Flame instability is promoted with an increase in pressure.

As far as $S_u^0$ is concerned, at $\Phi=0.8$ all DFs are faster than PRF95 at 2.5 and 5 Bar. At 10 Bar the value of $S_u^0$ for all DFs is comparable to that of PRF95. In contrary, at $\Phi=1.2$ all DFs are slower even compared to methane. At $\Phi=1$, with a 25% increase in the DF ratio the value of $S_u^0$ is reduced by 2%, 4% and 5% at pressure of 2.5, 5 and 10 Bar respectively. As pressure increases, $S_u^0$ is reduced for all fuels with methane being the most sensitive.

The fuels’ mass burning rate is inferred from their Mass Fraction Burned (MFB) durations. The MFB duration has been derived through thermodynamic analysis of the acquired pressure traces in the combustion vessel. As a general trend, it has been found that the burning rate is driven by the burning velocity at 2.5 and 5 bar. Consequently, at $\Phi=0.8$ all DFs were on average 22% and 27% faster than PRF95 in the developing (0-10% MFB) and the developed (10-90% MFB) flame regime respectively. At $\Phi=1.2$, PRF95 is the fastest fuel whereas DF75 and DF50 are even slower than methane. However, at a pressure of 10 bar the burning rate of all fuels is critically affected by phenomena of flame instability. The effect of flame instability altered the trends in burning rate compared to the two lower pressures. It was concluded that the effect of flame instability on the burning rate is stronger than the effect of pressure.

For stoichiometric to lean mixtures, there is a positive synergy for blending methane to PRF95 due to the convergence of $L_b$ of the blended fuel towards that of pure gas and $S_u^0$. 

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Concluding Remarks and Open Challenges

towards that of pure liquid. These findings indicate a distinct synergy for the utilization of dual fuelling in energy efficient lean burn combustion applications.

8.1.2 Numerical Analysis

A numerical model has been put forward to predict the stretched laminar flame velocity whilst extending the understanding on the influential parameters involved.

Through current numerical contributions on the basis of Lewis number, an optimised Markstein length model has been reconstructed and validated with experimental results.

It has been found that the effect of Markstein length can critically change the velocity of a propagating flame especially at lean burn conditions. It was concluded that the effect of heat and mass transport dominate the Markstein length.

8.1.3 SI Engine Combustion

An experimental campaign has been undertaken in an optical SI engine to characterise and scientifically understand the mechanism of natural gas-gasoline DF combustion, and the importance of flame-stretch interactions under a sweep of engine load (MAP : 0.44, 0.51, 0.61 Bar), speed (1250, 2000, 2750 RPM) and equivalence ratio (Φ= 0.8, 0.83, 1, 1.25). Premixed mixtures have been used throughout the experimental investigation. Consistent with the constant volume combustion, natural gas was added to gasoline in three different energy ratios 25%, 50% and 75%. The fuels’ mass burning rate is inferred from their Mass Fraction Burned (MFB) durations.

For lean burn combustion,

It has been found that at Φ=0.83 the burning rate and the CoV_{IMEP} become less sensitive to the spark duration as the DF ratio increases (natural gas is added to gasoline). For the shortest spark duration, there is a strong exponential decrease in the CoV_{IMEP} with the DF ratio.

In the flame establishment regime (0-5% MFB), at Φ=0.8, with 25% increase in the DF ratio the burning rate is increased by 8%. The 5% MFB location is linearly scaled with the associate value of L_b of each fuel at all test loads, implying that the effect of L_b dominates the combustion process under lean burn conditions. The flame stretch sensitivity of the tested fuels characterised by L_b is maintained from constant volume to engine combustion.
Concluding Remarks and Open Challenges

With a 0.2 mm decrease in $L_b$ the burning rate is increased by 5% in the flame establishment regime.

The effects of the fuel characteristics on the burning rate as experienced in the flame establishment regime are still preserved in the initial (0-10% MFB) as well as in the developed (10-90% MFB) flame regime. At $\Phi=0.8$, with a 25% increase in DF ratio, the burning rate increases by 2% and 9% in the initial and developed flame regime respectively. As it has been concluded, even in developed turbulent flames propagating in the flamelet zone, flame stretch has a dominating effect on the mass burning rate under lean burn conditions.

For lean mixtures, the flame variability in the flame establishment regime that is found to be a strong indicator of $\text{CoV}_{\text{IMEP}}$, decreases exponentially with the increase of DF ratio. The response indicates a critical influence of $L_b$ on the combustion stability. It has been concluded that the value of $L_b$ is a dominant parameter for extending the capabilities of lean burn combustion both from a flame stability and velocity prospective.

From low (MAP = 0.41 bar) to high (MAP = 0.61 bar) engine load, the rate of increase of burning rate with the DF ratio in the flame establishment regime is decreased by 36% at $\Phi=0.8$. The phenomena are attributed to the fact that as in-cylinder pressure increases, evident by an increase in load, the Markstein length of gasoline is approaching that of natural gas.

Although in the flame establishment regime the burning rate of natural gas is always faster than that of gasoline and to a lower extend that of DF50, as engine speed increases the difference is reduced. It is not clear from the current experimental method if the phenomena are attributed to the effect of fuel characteristics, or to the shift of the combustion process in the distributed reaction zone, whereas the effect of $L_b$ on the burning rate is expected to decay.

For stoichiometric combustion,

In comparison to the base fuels, DF50 and DF75 exhibit a faster burning rate in the flame establishment regime attributed to a best balance between the two fundamental combustion parameters $S^0_u$ and $L_b$ that allowed for a faster burning rate to be attained. The phenomena are still preserved in the development and developed flame regime. Natural gas is faster than gasoline in the initial flame development phase although it becomes slower in the developed flame regime.

For fuel rich combustion,
Concluding Remarks and Open Challenges

Contrary to the lean mixtures, at $\Phi=1.25$ with 25% increase in DF ratio the burning rate is decreased by 6%, 5% and 9% in the establishment, development and developed flame regimes respectively. In comparison to the lean mixtures, the Markstein lengths of the test fuels are relatively converging to a single value at $\Phi=1.25$, implying that $S_u^0$ has a critical influence on the combustion process.

For all test AFRs, there is a tendency for the fuels having the fastest mass burning rates to give the lowest flame variability.

For evaluating the fuel’s performance for engine use, especially for lean burn combustion, $S_u^0$ is not sufficient. The value of $L_b$ has to be primarily considered.

8.1.4 Constant Volume to Engine Combustion

The transition mechanism characterises the difference in burning rate from the constant volume to the engine combustion. At lean conditions, the transition mechanism has its higher effect on pure gaseous fuelling. The mass burning rate of the gaseous fuel is increased by 31% more compared to that of the pure liquid fuel in the flame development regime (0-10% MFB). At stoichiometry, the transition mechanism favours the combustion of mixtures with a dual fuel ratio higher than about 25%. At fuel rich conditions sufficiently off-stoichiometry, the effect from the transition mechanism is expected to be relatively similar for all tested fuels.

For stoichiometric to lean mixtures, the effect of turbulence on the increase of the mass burning rate is on average 13% higher for natural gas as compared to gasoline. That is attributed to the lower Markstein length of the gaseous fuel.

8.1.5 Key Message

A comprehensive knowledge of the two fundamental mixture parameters $S_u^0$ and $L_b$ is essential for understanding and hence optimising the natural gas-gasoline dual fuel combustion in SI engines. The value of $L_b$ is a dominant parameter for extending the capabilities of lean burn combustion both from a flame stability and velocity prospective. The scientific knowledge and insides derived in the current research are based on the fundamental combustion characteristics of a combustible mixture. It is therefore expected that the derived scientific knowledge is globally applicable to any combustion application operating within the flamelet premixed combustion regime.
8.2 Open Challenges

Based on the key message of the current thesis, and considering the in-cylinder pressures of modern downsized engines that can well exceed 100 bar, the flame fundamentals at downsized like engine conditions needs to be further investigated. The mixtures in a downsized engine can be also excessively diluted with exhaust residuals. There is a general lack of fundamental combustion knowledge at such thermodynamic and chemical conditions. The open challenge is exacerbated if one considers binary fuel blends of natural gas and gasoline.

Themodiffusive flame instability that is promoted with higher pressure is proved to be a critical contributor to the turbulent flamelet combustion. However, there is no final quantitative agreement of the effects of flame instability on the mass burning rate. Consequently, solid well agreed models of such effect are currently missing from literature. The development of such models requires further insights on the response of nonequidiffusion flames, especially for binary fuel blends at downsized engine like conditions.

As the Markstein length is historically derived from stable flames, there exist an open challenge concerned with the sensitivity of a cellular flame to stretch and how such effects can be quantified. Is the Markstein length adequate to exclusively quantify the response of cellular flame to stretch? Considering the dominance of the Markstein length at lean burn combustion, that question is of exceptional practical importance and yet to be answered by the combustion community.

The effect of Markstein length on the mass burning rate is expected to decay as the combustion shifts from the flamelet to the distributed reaction zone regime. Further insights are needed in order to comprehensively understand how the effect of Markstein length is altered from such a transition.

As a first step, and before insights are given to the mentioned fundamental combustion challenges, it is important to determine whether the effect of Markstein length is still experienced when an SI downsized engine operates in optimal conditions to provide the highest thermal efficiency, with and without exhaust residuals.
Appendix

The targeted DF ratio (DF\text{Ratio}), equivalence ratio (\Phi), temperature (T) and pressure (P) in a particular test condition have to be given as inputs for the calculation of the partial pressures of the fuel-oxidizer, and their masses in the combustion vessel.

Fuel-air mixtures can be considered as,

\[ X_{CH_4} + (1 - X_{CH_4}) \left( x_{C_8H_{18}} C_8H_{18} + x_{C_7H_{16}} C_7H_{16} \right) + Z \left( O_2 + 4 N_2 \right) \] (A.1)

Where \( X_{CH_4} \) is the methane mole fraction in the blended fuel, and \( x_{C_8H_{18}} \) and \( x_{C_7H_{16}} \) is the iso-octane and n-heptane mole fraction in the base PRF95 fuel corresponds to 0.943 and 0.057 respectively. The number of oxygen moles per mole of the blended fuel is indicated with the letter \( Z \).

Considering the Lower Heating Value of methane (LHV\text{CH}_4 = 50 \text{ kJ/Kg}) and PRF95 (LHV\text{PRF95} = 50 \text{ kJ/Kg}), and given the energy fraction of methane (\( E_{CH_4} \)) and PRF95 (\( E_{PRF95} \)) in the DF blend, the partial pressures of the base fuels and the partial pressure of air can be evaluated following the analysis below,

\[ E_{PRF95} = 1 - E_{CH_4} \] (A.2)
\[ E_{DF} = E_{CH_4} \text{LHV}_{CH_4} + E_{PRF95} \text{LHV}_{PRF95} \] (A.3)

where \( E_{DF} \) is the total fuel energy in the DF blend. The mass fraction of methane (\( Y_{CH_4} \)) and PRF95 (\( Y_{PRF95} \)) in the DF blend can be defined as,

\[ Y_{CH_4} = \frac{E_{CH_4} E_{DF}}{\text{LHV}_{CH_4}} \] (A.4)
\[ Y_{PRF95} = 1 - Y_{CH_4} \] (A.5)

The mean molecular mass (\( \bar{W} \)) of the blended fuel is calculated through,

\[ \bar{W}_{\text{Fuel}} = \frac{1}{\frac{Y_{CH_4}}{\bar{W}_{CH_4}} + \frac{Y_{PRF95}}{\bar{W}_{PRF95}}} \] (A.6)
Appendix

Where \((W_{CH4})\) and \((W_{PRF95})\), are the molecular masses of methane and PRF95 respectively.
The molecular mass of PRF95 \((W_{PRF95})\) is given by,

\[
W_{PRF95} = x_{C_8H_{18}} W_{C_8H_{18}} + x_{C_7H_{16}} W_{C_7H_{16}}
\]  
(A.7)

The mole fraction of methane \((X_{CH4})\) and PRF95 \((X_{PRF95})\) is calculated as,

\[
X_{CH4} = Y_{CH4} \frac{\overline{W}_{Fuel}/W_{CH4}}
\]  
(A.8)

\[
X_{PRF95} = 1 - X_{CH4}
\]  
(A.9)

The gravimetric Air to Fuel Ratio (AFR) of the DF-air mixture assuming products of complete combustion and an oxidizer concentration \([O_2/(O_2+N_2)]\) of 0.2 is defined as,

\[
AFR = [(1/\Phi) (a + b/4) 5W_{Air}]/ \overline{W}_{Fuel}
\]  
(A.10)

Where \(a\) and \(b\) is the carbon and hydrogen atoms in the DF blend,

\[
a = 7.94X_{PRF95} + X_{CH4}
\]  
(A.11)

\[
b = 17.89X_{PRF95} + 4X_{CH4}
\]  
(A.12)

The mass fraction of the fuel \((Y_{Fuel})\) and air \((Y_{Air})\) in the multicomponent fuel and air mixture is calculated as,

\[
Y_{Fuel} = 1/(AFR + 1)
\]  
(A.13)

\[
Y_{Air} = AFR/(AFR + 1)
\]  
(A.14)

The mole fraction of the fuel \((X_{Fuel})\) and air \((X_{Air})\) in the multicomponent fuel and air mixture is obtained as,

\[
X_{Fuel} = Y_{Fuel} \overline{W}_{Mix}/ \overline{W}_{Fuel}
\]  
(A.15)

\[
X_{Air} = Y_{Air} \overline{W}_{Mix}/ \overline{W}_{Air}
\]  
(A.16)

Where \(\overline{W}_{Air}\) the molecular mass of pure air, \(\overline{W}_{Tot}\) is the molecular mass of multicomponent fuel and air mixture,
\[ \bar{W}_{\text{Air}} = 0.2W_{O_2} + 0.8W_{N_2} \quad (A.17) \]
\[ \bar{W}_{\text{Tot}} = \frac{1}{Y_{\text{Fuel}} + Y_{\text{Air}}} \quad (A.18) \]

The mole fraction of the base fuels in the multicomponent fuel and air mixture is calculated as,

\[ X_{PRF95_{\text{Mix}}} = X_{PRF95_{\text{Fuel}}} \quad (A.19) \]
\[ X_{CH4_{\text{Mix}}} = X_{CH4_{\text{Fuel}}} \quad (A.20) \]

Finally, the partial pressure of the base fuels and the partial pressure of air are given by,

\[ P_{PRF95} = X_{PRF95_{\text{Mix}}} P \quad (A.21) \]
\[ P_{CH4} = X_{CH4_{\text{Mix}}} P \quad (A.22) \]
\[ P_{\text{Air}} = X_{\text{Air}} P \quad (A.23) \]

Using the ideal gas law, the total mass \( M_{\text{Tot}} \) in the combustion vessel can be described as,

\[ M_{\text{Tot}} = \bar{W}_{\text{Mix}} PV_{\text{CVCV}} / RT \quad (A.24) \]

The mass of base fuels and the mass of air in the combustion vessel is given by,

\[ M_{\text{PRF95}} = M_{\text{Mix}} Y_{\text{Fuel}} Y_{PRF95} \quad (A.25) \]
\[ M_{\text{CH4}} = M_{\text{Mix}} Y_{\text{Fuel}} Y_{\text{CH4}} \quad (A.26) \]
\[ M_{\text{Air}} = M_{\text{Mix}} Y_{\text{Air}} \quad (A.27) \]
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