The effects of prolonged ignition delay due to charge air temperature reduction on combustion in a diesel engine

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THE EFFECTS OF PROLONGED IGNITION DELAY DUE TO CHARGE AIR TEMPERATURE REDUCTION ON COMBUSTION IN A DIESEL ENGINE

A dissertation submitted to
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2013
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For my family

*Entia non sunt multiplicanda praeter necessitatem*

*Ockham’s razor*
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Panagiotis Kyrtatos
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Abstract

The present thesis concentrates on the effectiveness of $NO_x$ reduction in large four stroke diesel engines through cooling of the charge via the implementation of advanced Miller valve timing. In advanced Miller valve timing the inlet valve closure point is advanced to before the bottom dead centre, so as to expand the inlet charge before the compression, lowering the charge air temperature. Testing at extreme Miller degrees has shown a reversal of the expected trend of diminishing $NO_x$ emissions due to the reducing reactant temperature, with extreme Miller degrees leading to an increase of $NO_x$ emissions. The thesis thus aims to provide a clear understanding of the effects responsible for this $NO_x$ trend reversal at low charge temperatures. With this goal in mind various studies were performed. Through specialized experiments on a 6-cylinder medium speed marine diesel engine with a prototype 2-stage turbocharging system, and on a single-cylinder heavy duty engine, as well as 3D-CFD investigations for a more detailed insight into the related fuel spray and combustion phenomena a clearer understanding was achieved. The engine experiments employed in-cylinder (soot) luminosity measurements through optical probes in order to obtain soot evolution and temperature information, cycle-resolved exhaust $NO_x$ measurements, as well as commonplace measurements of in-cylinder pressure, heat release rate and averaged emission concentration.

The results show that $NO_x$ formation has a strong dependency on ignition delay (ID) and that increasing ID leads to a series of phenomena which are responsible for the increased $NO_x$ emissions.

In particular, the measurements and simulations showed that:

- The mixing rate of fuel with air increased with prolonged ID. This, in turn has been attributed to a combination of various factors:
  - Increased ID results in longer spray penetration enhancing fuel pre-mixing and air entrainment. Longer spray penetration leads
to higher diffusion combustion speed as the result of the elevated spray air entrainment and the better utilization of the available oxygen.

○ Increased cycle-to-cycle variation of peak pressure, soot cloud density and NO concentration, resulting from increased diffusion combustion rate during some cycles with long ID conditions. The increased diffusion combustion rate was shown to occur as a result of in-cylinder pressure fluctuations formed at random due to the large energy release rate during premixed combustion, the quantity of which scales with ID. The pressure fluctuations appear as superimposed pressure waves in the indicator diagram, and correspond to the excitation of the cylinder charge at its first radial mode. The speed of diffusion combustion was shown to scale with the intensity of the pressure fluctuations.

• There exist changes in soot temperature and oxidation rate at cycles where pressure oscillations were present. Soot temperature and oxidation rate increased with increasing pressure fluctuation intensity.

These results have a profound impact on the $NO_x$ produced in-cylinder and can be used to provide an explanation for the increase of $NO_x$ emissions observed with long ID. In particular they demonstrate:

• An increased temperature and oxygen availability due to mixing as the result of longer spray penetration and in-cylinder pressure fluctuations.

• An increased flame and post-flame gas temperature due to compression heating of the charge from the faster combustion.

• An increased flame temperature due to decreased radiation heat losses, as the result of faster soot oxidation rate under pressure fluctuations.

• A possibility of NO production in the premixed flame, which has more time to mix and thus is leaner.

• An increased NO formation rate due to pressure fluctuations which cause isentropic compressions. Such compressions lead to higher-
than-the-average reaction rates due to the exponential dependency of reaction rates on temperature.

- An increased probability of NO formation through prompt NO which becomes important at leaner premixed flame conditions.

The above observations and results provide a clear understanding of the effects responsible for the $NO_x$ trend reversal while they demonstrate the importance of single-cycle combustion characteristics with prolonged ID. As a result, they have a profound influence on the measurement and simulation approaches used currently for diesel engine research purposes.
Zusammenfassung


Für die Untersuchung der Verbrennungsvorgänge im Zylinder wurde einerseits die Standard-Instrumentierung für die Druck-Indizierung des Zylinders zur Berechnung des Brennverlaufs und für die Analyse der mittleren Abgasemissionen eingesetzt. Zusätzlich wurden auch neu entwickelte Systeme zur Zyklus-aufgelösten Untersuchung der Russ-Formation und Temperatur mittels einer optischen Sonde, sowie ein schnelles Entnahmeventil welches, gekoppelt mit einem schnellen Massenspektrometer, die Messung der NOx-Emissionen zyklusaufgelöst ermöglichte.

Die Resultate zeigen, dass die NOx-Bildung stark vom Zündverzug (ZV) abhängig ist. Weiter hat ein erhöhter ZV Einfluss auf zahlreiche weitere Phänomene, welche wiederum die NOx-Emissionen beeinflussen. Die Messungen und Simulationen zeigten:

- Durch den langeren und strker variierenden Zündverzug wurde, durch das Zusammenwirken der folgenden Faktoren, die Vermischung von
Luft und Kraftstoff erhöht, was folgende Einflüsse auf die Verbrennung zeitigte:


- Russtemperatur und Russoxidationsrate erhöhen sich mit zunehmenden Druckfluktuationen.

Diese Resultate haben einen fundamentalen Einfluss auf die NOx-Bildung und können, den Anstieg der NOx-Emissionen bei langen ZV zu erklären. Sie zeigen:

- Erhöhte Temperatur und Sauerstoffverfügbarkeit infolge der erhöhten Mischung von Luft und Kraftstoff als Folge der hohen Spray-Penetrationslänge und der Zylinderdruckfluktuationen.

- Erhöhte Flammm- und Rauchgastemperatur durch die Erwärmung der Ladung infolge der durch die schnellere Verbrennung verursachten Kompression.

- Erhöhte Flammtemperatur durch geringere Strahlungsverluste als Folge der schnelleren Russoxidation bei Zylinderdruckfluktuationen.

- Die Möglichkeit von NO-Bildung während der Vormischverbrennung, welche bei sehr langem ZV magerer wird.
• Erhöhte NO-Bildungsrate durch Zylinderdruckfluktuationen während der Diffusionsverbrennung, welche zu isentropen Kompressionen und Expansionen und damit zu Erwärmungen und Auskühlungen führen. Die durchschnittliche Reaktionsrate erhöht sich, da diese exponentiell von der Temperatur abhängt.

• Erhöhte Wahrscheinlichkeit von NO-Bildung über den prompt NO Mechanismus, welcher bei mageren Vormischverbrennungen an Gewichtung gewinnt.

Die zuvor genannten Beobachtungen und Resultate bieten ein klares Verständnis der Effekte, welche verantwortlich sind, dass sich der anfangs beschriebene NOx-Trend umkehrt. Weiter demonstrieren die Resultate die wichtige Stellung der einzelnen Verbrennungszyklen mit langerem ZV. Diese Erkenntnisse beeinflussen die Herangehensweise an Messungen und Simulationen in der Dieselmotorenforschung.
Chapter 1

Introduction

In recent years the main goal of diesel engine research and development has been the reduction of gaseous and particulate emissions, in combination with the improvement of engine efficiency. In the marine diesel engine sector in particular there has been a push for reduced exhaust nitrous oxide ($NO_x$) emissions, while maintaining or even improving engine efficiency and correspondingly fuel consumption and $CO_2$ emissions. Recent and future IMO legislations call for radical reductions (up to 80%) of engine-out $NO_x$ emissions from sea-going vessels by 2016 [1]. To achieve this, engine manufacturers are compelled to develop novel systems, which will allow future vessels to comply with the emission limits imposed by legislation. The aim of such novel systems should be the reduction of $NO_x$ while maintaining or improving the current levels of Specific Fuel Consumption (SFC). There exist two distinct technological directions which could be followed individually or in combination:

- **In-cylinder $NO_x$ reduction**, by reducing the amount of $NO_x$ formed during combustion

- **Using $NO_x$ reduction after-treatment technologies**, to reduce $NO_x$ in the exhaust stream

Past research has shown that both above approaches have benefits.

Motivation

This dissertation focuses on in-cylinder $NO_x$ reduction techniques in Direct Injection (DI) diesel engines, and in particular the potential and limitations of $NO_x$ reduction through the lowering of charge air temperature via
early inlet valve closure (Miller valve timing). Engine experimentation has shown that the potential for $NO_x$ reduction through this route is limited, albeit the reasoning behind the limitations is not well documented. This dissertation aims to provide a comprehensive overview of the sub-processes which lead to these limitations through experimental and numerical investigations.

To this end, the initial focus in this thesis is placed on in-cylinder emission formation, with specific highlighting of relevant NO formation mechanisms. The focus is then directed towards proposed and employed in-cylinder emission reduction technologies with specific insights on their respective limitations. Research results from investigations of relevant phenomena from different applications are also provided, presenting the effects of pressure fluctuations on combustion, soot and $NO_x$ emissions from premixed and diffusion combustion investigations.

The primary focal point of this dissertation is the application of Miller valve timing for $NO_x$ reduction purposes in large 4-stroke Diesels. The observed limitations in its application on conventional DI diesels, and specifically the effects of cylinder pressure fluctuations due to increased Ignition Delay (ID) on combustion and emission formation are studied through experimental investigations on two experimental facilities.

The experimental facilities used to conduct these experiments, as well as the instrumentation and methodology for obtaining and post-processing the measured results are presented in Chapter 2.

Additional insight into the processes which lead to these limitations in applications of Miller valve timing are also studied through the use of 3-D Computational Fluid Dynamics (CFD) simulations. The methodology and models employed in the CFD investigations are presented in Chapter 3.

Chapter 4 presents the experimental results, including the potential of Miller valve timing for $NO_x$ reduction and observed effects of increased ignition delay on cycle-to-cycle variation, air/fuel mixing, Heat Release Rate (HRR) and in-cylinder and exhaust emissions. These are followed by the Discussion in Chapter 5, where the findings of the experimental and simulation work are used to provide an understanding of $NO_x$ formation trends with decreasing charge temperatures. Finally, Chapter 6: Conclusions and Outlook presents a summary of the results, some proposals for the improvement of the $NO_x$ reduction potential of Miller valve timing and some suggestions for future investigations.
1.1 Emission Formation in Diesel Engines

Direct Injection diesel engine combustion is a complex process and is dependent on a number of parameters, which affect the fuel oxidation and emission formation. Of these parameters, the ones most relevant to \( NO_x \) and soot emission formation will be briefly discussed here. These parameters can be conveniently grouped into three categories, namely those related to fuel-air mixing, to oxygen availability and to temperature. These parameters can be controlled by the engine designers through changes in the fuel (fuel injection parameters/conditions) and air-paths (swirl, boost pressure, Exhaust Gas Recirculation (EGR), charge air temperature) of the engine.

It is commonly accepted that \( NO_x \) formation is dependent on temperature, oxygen availability and residence time [2]. On the other hand, soot production is mainly dependent on fuel-air stoichiometry and temperature, and soot oxidation is dependent mainly on temperature, oxygen availability and residence time [3].

Traditionally, diesel engine combustion produces high levels of \( NO_x \) and soot. During the mixing-controlled (diffusion) part of diesel engine combustion, very high flame temperatures and local oxygen availability promote \( NO_x \) formation in the near-stoichiometric regions. On the other hand, soot is formed in the rich core of the fuel spray, when the fuel droplets approach the hot burned gases [4]. Part of the soot then oxidises in the flame zone, where oxygen is available. The soot which is not oxidised escapes to the environment as particulate emissions. A graphical representation of how the local air-fuel ratio and temperature affect soot and \( NO_x \) formation is shown in the \( \phi - T \) map (Figure 1.1, [5]).

By examining the aforementioned simple approach to emission formation, it is clear that there exists a trade-off between soot formation and oxidation on the one hand, and \( NO_x \) formation on the other; high-temperature lean combustion will promote \( NO_x \), whereas locally richer combustion will promote soot emissions.

1.1.1 \( NO_x \) Formation Pathways

It is generally accepted that the three main \( NO_x \) formation mechanisms are the thermal, the prompt and the fuel \( NO_x \) [2, 6–8]. Fuel \( NO_x \) is formed through the oxidation of nitrogen present in the fuel. Distillate fuels con-
tain very low concentrations of nitrogen [2,6], and thus fuel NO\textsubscript{x} formation is not significant in the context of diesel engine combustion. Thermal NO production, represented by equations first introduced by Zeldovich and now widely known as the extended Zeldovich mechanism, is considered to take place in the very hot burned gas region. At high temperature NO is formed mainly through the dissociation of molecular nitrogen and oxygen. Thermal NO formation rates are very temperature dependent, and appreciable amounts of NO are only formed above 2000K [6]. This is due to the high activation energy (38000K) for the production of nitrogen atoms from the dissociation of molecular nitrogen.

Although the thermal NO production is understood to be the main source of NO in engines [2,6,9], the so called prompt NO is increasingly considered as an important contributor. Prompt NO is formed within the reaction zone, through the reaction of the CH radical with molecular nitrogen to produce a nitrogen atom. This nitrogen atom then produces NO in the same way as in the extended Zeldovich mechanism. The activation energy for the CH-N reaction is 11060K, which compared to the activation energy for the dissociation of molecular nitrogen (38000K) is significantly lower.
This results in this particular NO formation pathway being more significant at low temperatures.

1.1.2 \( NO_x \) Formation in Diesel Engines

The process of \( NO_x \) formation in diesel engines has been studied experimentally through optical and direct sampling or dumping methods. Temporal information on the average \( NO_x \) concentration within the cylinder during diesel engine combustion have been obtained through cylinder dumping methods, where the cylinder contents during combustion are extracted from the cylinder, expanded/cooled rapidly in order to freeze any ongoing reactions and then analysed [10]. These investigations showed that the bulk of \( NO_x \) is produced during diffusion combustion, with very small influence of premixed combustion on the process. Nonetheless, the data produced in these investigations do not provide any spatial information about \( NO_x \) production, and the temporal accuracy has been called to question due to the uncertainty of the speed of cooling to freeze the composition reactions.

Local \( NO_x \) concentration information has been obtained through direct sampling [11, 12] and optical investigations in optically accessible engines [13–15]. Results from direct sampling from within the flame region showed similar results with the cylinder dumping experiments, with a rapid increase of concentration during diffusion combustion [11]. The temporal evolution of NO and other species at the sampling point are shown in Figure 1.2 [11].

More recently, results of NO evolution in optically accessible engines have been obtained using Planar Laser-Induced Fluorescence (PLIF) imaging. Work from Dec and Canaan [14] on NO formation in a single-cylinder optically accessible engine under conventional diesel engine conditions showed that NO forms at a near-constant rate during combustion, with the formation beginning just after the start of diffusion combustion around the fuel jet periphery, where high temperatures exist and excess oxygen is available. The end of NO formation was found to be well after the end of combustion, with significant formation occurring in the hot post-combustion gases prior to their gradual cooling due to mixing with fresh gases and expansion. The NO production rate as estimated from the measurements in [14] is shown along with the measured HRR in Figure 1.3.
Figure 1.2: Measured NO and other species evolution during combustion within the flame of a DI diesel engine using direct sampling [11].

Figure 1.3: HRR and estimated NO production rate using PLIF imaging under conventional diesel engine conditions [14].

In [14] it is argued that premixed combustion is too fuel rich to lead to the creation of significant amount of thermal NO, and this argument is supported by the optical measurements. Nonetheless the fact that premixed combustion affects $NO_x$ emissions is acknowledged, with two explanations offered:
• The rapid in-cylinder pressure rise due to premixed combustion creates higher temperatures during diffusion combustion, leading to higher $NO_x$ production rates during the latter.

• With high premixed combustion percentage, more of the combustion is likely to occur near Top Dead Centre (TDC), leading to high fuel-specific $NO_x$ emissions due to higher local and average temperatures.

Finally, contrary to conventional diesel engine conditions where NO formation takes place near the flame tip during diffusion combustion, optical diagnostics in early-injection, low-temperature, long ignition delay combustion have shown that reactions occur throughout the cross-section of the spray, provided enough premixing of the spray occurs prior to ignition [15]. This gives an indication that NO formation could occur throughout the spray at these conditions.

### 1.2 In-Cylinder $NO_x$ Reduction

#### 1.2.1 Techniques

For the specific application of combustion in diesel engines, there exists a widely reported [2,9] correlation between adiabatic flame temperature and resulting $NO_x$ emissions. This is supported by the nature of the NO formation kinetics presented previously, which are very temperature dependent. Following this observation, diesel engine manufacturers have introduced technologies which aim to reduce the adiabatic flame temperature, with considerable success. Since the adiabatic flame temperature is dependent on the temperature and composition of the reactants, the following possibilities exist to alter the $NO_x$ formation rate:

• Change in cylinder charge composition (eg. EGR, nitrogen or other inert gas addition, inlet air humidification) to increase the specific heat of the reactants and/or reduce the oxygen availability through dilution

• Direct cooling of the flame through water evaporation (direct water injection, fuel water emulsion etc.)
• Reduction in the reactant temperature (e.g. charge cooling, Miller valve timing, reduced compression ratio)

or a combination of the above have shown to be effective in-cylinder measures to reduce engine-out NO\textsubscript{x} emissions from diesel engines.

In modern high-speed diesel engines, the combination of high boost pressures, high injection pressures, cooled EGR and multiple injections have led to a reduction of both soot and NO\textsubscript{x} emissions. Smaller droplet sizes and enhanced air-fuel mixing reduce soot production and promote oxidation, while high EGR rates reduce flame temperatures lowering NO\textsubscript{x} production. More recently, it has been shown that further lowering combustion temperatures, using very high EGR rates and/or low end-of-compression temperatures can further reduce or even completely eliminate soot production, while also reducing NO\textsubscript{x} production [4,5,16–18].

### 1.2.2 Limitations

There exist reported cases where the correlation between adiabatic flame temperature and NO\textsubscript{x} falls through [19–22]. In the cases cited, changes in a multitude of engine operating conditions and factors are observed to either cause the NO\textsubscript{x} emissions to increase following a decrease in the adiabatic flame temperature, or result to the NO\textsubscript{x} emissions remaining unchanged despite significant variations in the adiabatic flame temperature. In [19] Musculus presents an extensive study on the effects of increased proportion of premixed combustion on NO\textsubscript{x}, with experimental results, showing that a significant increase of the former results to an increase of the latter. Additionally, there exist studies on the limitation of reaching very low NO\textsubscript{x} levels through the reduction of adiabatic flame temperature. Flynn et al [23] argue that there is a flammability limit for sustaining a flame which is above the temperature limit for very low NO\textsubscript{x} emissions and thus flames will inevitably produce NO\textsubscript{x}. A flame temperature below this limit will result in excessive amounts of unburned hydrocarbon emissions, and thus a significant reduction in efficiency.

### 1.3 Miller Valve Timing

As mentioned previously, a promising technology which allows the attainment of low end-of-compression temperatures is Miller valve timing. In the
Chapter 1 Introduction

Figure 1.4: Standard and Miller valve timing cycle in-cylinder pressure and average temperature [25].

Miller process, the Inlet Valve Closure (IVC) point is moved significantly earlier in the cycle compared to traditional systems, normally taking place well before Bottom Dead Centre (BDC) [24]. This allows the expansion of the charge air before it is compressed, leading to lower temperatures at the end of compression. Figure 1.4 shows the expected changes in cycle pressure and average cylinder temperature due to Miller valve timing [25]. The Miller cycle has been shown to lead to significant reductions of $NO_x$ emissions, while also achieving lower maximum cylinder pressures and reduced thermal loading of components [17, 25–30]. Also, from a thermodynamic point of view, since the average cycle temperature is reduced, the heat losses are reduced, giving the possibility for improved efficiency. In typical applications, the efficiency change due to lower heat losses can be up to 5%, which compensates for the loss of efficiency due to the loss of positive work (assuming positive scavenge pressure) from the earlier inlet valve closure, which is of the order of 1.5% [26]. This commonly known as ”Miller loss” is shown graphically in the $p – V$ diagram in Figure 1.5 [26]. Since the inlet valves remain open for a reduced amount of time, to achieve the same specific output from the engine, higher boost pressures (of up to 10 bar [25]) and higher turbocharger efficiencies are required. The pressure ratio limit for current radial compressor stages is about 4.5, thus the need for multiple stages arises, increasing complexity and cost, and introducing control difficulties [26]. Furthermore, the reduced inlet valve opening duration introduces prob-
problems at part- and low-load operation. At low loads smoke emissions are significantly higher and load acceptance deteriorates, since the turbochargers cannot produce the boost required. In some cases [25] it is reported that auxiliary aids to the turbocharger are essential to allow start-up and low-load operation of the engine, when extreme Miller timing is used.

An additional disadvantage of the use of Miller timing is the increase of ignition delay due to lower end-of-compression temperatures. This leads to increased proportion of premixed combustion resulting in very rapid pressure rise which causes, among other things, increased stressing of the piston rings and noise. Such drawbacks are intensified when using low cetane number fuels such as Heavy Fuel Oil (HFO) [17]. These issues can be partially alleviated through the use of injection rate shaping, where the initial injection rate during ID is lowered to reduce the amount of premixed combustion, or multiple injections, where a pilot injection is introduced to reduce the main injection ID.

These problems could be overcome by using fully Variable Valve Trains (VVT). VVT systems allow the engine to work with a late IVC at low loads, while switching to Miller timing at higher loads. However, VVT systems are complex, costly and, often, unreliable.

Instead of VVT systems, several turbocharger assist or intake air conditioning designs have been proposed to aid the operation of the engine at low loads, with inconsistent success. In [27], a heated intake system was used, to raise the temperature of intake gases to ensure acceptable combus-
tion. In [25], an electrically driven blower was used to provide extra boost at part load, which reduced the soot in the exhaust gases significantly, but increased $NO_x$ emissions. Finally, in [27] and [28], several systems of power input and extraction from the turbocharger have been studied, showing good results in terms of efficiency increase.

1.4 Effects of Long Ignition Delay

As mentioned previously, one of the effects of Miller timing is the reduction of end-of-compression temperature, which results in a prolonged ignition delay. The prolonged ignition delay in turn gives rise to large proportions of premixed combustion and thus high pressure rise rates. The resulting effects of the prolonged ignition delay and high pressure rise rates in diesel engines - namely in-cylinder pressure fluctuations and high cycle-to-cycle variation - are discussed in the following subsections.

1.4.1 Pressure Fluctuations in Diesel Engines

Pressure oscillations in combustors and combustion systems have been studied extensively with respect to their source, their effects on combustion and emission formation, their possible effects on the structural integrity of the combustion system and their effective control.

In internal combustion engines, research has focused on determining the source of pressure oscillations within the combustion chamber and trying to control and reduce them primarily for noise pollution and structural integrity purposes [2, 31–41]. The pressure oscillations, also commonly referred to as “knock”, are identifiable in the engine indicated diagram as a superimposed pressure wave on the in-cylinder pressure trace, which typically persists for the vast proportion on the engine expansion stroke. A sample cycle where pressure oscillations are present is shown in Figure 1.6 [2].

Typical pressure oscillation frequencies for internal combustion engines range from 5 to 10 kHz in automotive applications [2], and below 5 kHz in larger engines, which allows the differentiation of pressure oscillations from higher frequency noise in the cylinder pressure signal. Limiting noise pollution is especially important in modern automotive diesel engine applications, where high injection pressures induce high pres-
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Figure 1.6: Indicated diagram showing normal (a), slightly knocking (b) and intensely knocking (c) cycles [2].

sure rise rates. Numerous numerical [31,32] and experimental [33,34] investigations concerning the effects of combustion chamber shape on knocking frequency and intensity, with focus on noise emissions have been conducted. With respect to engine structural integrity, the main concern has been piston surface, piston ring, cylinder head and liner damage due to induced high local gas velocities, which result in increased heat transfer to the walls, creating potential for overheating and increased wear [2,33]. Additionally, fatigue and erosion issues arise due to the cyclic loading from the pressure fluctuations and high pressure pulses [2].

Source of pressure oscillations

The source of pressure fluctuations has been extensively researched in Spark Ignition (SI) and more recently in diesel Compression Ignition (CI) and Homogeneous Charge Compression Ignition (HCCI) engines. As early as the 1930s Draper [42] showed that sudden increases of the local pressure in the cylinder due to high local heat release rates, create pressure oscillations in the charge air which persist for a large proportion of the cycle.

In SI engines, knock occurs from the spontaneous auto-ignition of a portion of end gas which is compressed and heated during combustion, leading to high local pressure rise rates and resulting in pressure oscillations [2].

In diesel and HCCI combustion, pressure oscillations arise from very high pressure rise rates which drive the combustion chamber into an acoustic
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13

resonance [31–33, 35, 36, 39–43]. The high pressure rise rates are caused from the rapid heat release rate during premixed combustion, typically caused after a prolonged ignition delay. These high pressure derivatives excite the combustion chamber gas cavity to vibrate at its natural frequencies. In HCCI applications especially, but also in Premixed Combustion Compression Ignition (PCCI), the inhomogeneity of the ignition inside the combustion chamber either due to hot spots, the inhomogeneity of the mixture/sprays or random effects, intensifies these pressure oscillations [33,41]. In order to distinguish between the two types of pressure oscillations, those appearing in compression ignition systems are commonly referred to as “ringing” [35–38]. It is understood that CI engines generally have higher amplitude pressure oscillations due to the higher pressure rise rates and higher compression ratios, but ringing rarely results in engine damage and is generally avoided for reasons of noise emission [35].

Modes of vibration

As mentioned previously, during rapid heat release rate, the combustion chamber gasses will be excited at their natural frequencies of oscillation. The modes of the resulting oscillations can be found by using the proposed acoustic pressure wave formula [33]:

$$f_{m,n} = \frac{C * \rho_{m,n}}{\pi * B}$$

(1.1)

Where $f_{m,n}$ is the specific vibration frequency for mode $(m, n)$ (in Hz), $C$ is the local speed of sound (in m/s), $\rho_{m,n}$ is the vibration mode number and $B$ is the cylinder bore (in m). According to [33], the combustion chamber gases show the highest oscillation intensities in the first vibration mode, where the propagation of the pressure waves is in the radial direction. This observation was validated in [33] through measurement of the pressure at different points in the combustion chamber simultaneously, which allowed an accurate measurement of the temporal and spatial evolution of the induced waves.

Figure 1.7 shows the shape of the different modes of vibration for a cylindrical combustion chamber, as well as their respective $\rho_{m,n}$ values [33]. The $\rho_{1,0}$ value for the first radial mode is 1.84, which results in a main mode of vibration occurring at a frequency of around 6 kHz for a cylinder bore of 80 mm (typical automotive), assuming an average gas temperature of
Figure 1.7: Shape of the different modes of vibration for a cylindrical combustion chamber and the respective $\rho_{m,n}$ value [33].

1800K.

Effects of pressure rise rate on pressure fluctuation intensity

As mentioned previously, past research has shown a very strong influence of rapid pressure rise on ringing in CI engines. In [40], Griffiths and Whitaker showed that ringing intensity is reduced when the pressure rise rate due to heat release was reduced. Similar results were shown in [31], where a CFD investigation of combustion chamber resonances within the engine bowl of a DI diesel engine indicated strong pressure oscillations can be caused by localised rapid increases in pressure. Finally, Shiga et al. [41] showed an exponential dependency of ringing intensity on maximum rate of pressure rise, by varying the amount of EGR and thus varying the reactivity of the premixed combustion. Figure 1.8 shows the results from [41] on the relationship between maximum rate of pressure rise and knock intensity.

Methods to reduce pressure oscillations

The direct relation between pressure rise rate and pressure fluctuation intensity presented above leads to a straightforward conclusion that to reduce pressure oscillations one should reduce the pressure rise rate. In traditional DI diesel engines, this can be done in three ways:

- Reduction of the amount of premixed combustion through the reduction of ID, either though charge air temperature increase, use of fuel with improved ignitibility (higher cetane number) [12], the use of a
pilot injection to increase temperature and provide ignition precursors to the main injection [38] or the use of a combustion chamber heating device (glow plug).

- Reduction of amount of premixed combustion through reduced fuel injection during ID, either through reduced injection pressure or injection rate shaping

- Reduction in the premixed combustion rate, through reduced air-fuel mixing or change in composition (EGR) to reduce the reaction rate [41]

Alternatively in HCCI or PCCI engine operation, where ID is long by design and the pressure oscillations result from inhomogeneous reactivity due to inhomogeneity of the charge or local hot spots, a reduction of pressure oscillations can be achieved through increased homogeneity of the mixture, alleviation of hot spots or reduced reactivity of the mixture through a change in composition (lean combustion, high EGR rates). Finally, changes in the frequency of pressure oscillation in order to reduce noise emissions to the environment can be achieved through combustion chamber and piston bowl redesign [31,34].

Figure 1.8: Measured effects of maximum rate of pressure rise on knock intensity [41].
1.4.2 Cycle-to-Cycle Variation

Cycle-to-cycle variation, where the in-cylinder pressure varies significantly on a cyclic basis, is a very commonly observed phenomenon in SI engines. These variations in pressure are caused by changes in the burn rate for each successive cycle, which can have numerous root causes; cyclic variation in the cylinder gas motion, cyclic variation in the amount of fuel, air and exhaust gases present in the cylinder, or cyclic variation of the mixture composition near the spark plug [2].

Significant cycle-to-cycle variations are less common in conventional CI diesel engines. This is due to the nature of CI combustion, which is directly controlled by the fuel injection. Fuel injection primarily governs air-fuel mixing and thus combustion. Any cyclic variation in background turbulence (swirl, etc.) is minimal, and will not affect the combustion rate significantly.

Nonetheless, there exist cases where CI combustion also exhibits cyclic variability; the root cause of this variability has been connected to instabilities in the fuel injection system or to prolonged ignition delay. Koizumi et al. [44] showed that the cyclic variation observed in the indicated mean effective pressure of a indirect injection diesel engine was caused by variations in the injected mass. Similarly, Wing [45] found that cyclic variations observed in a rotary fuel-pump injected diesel engine were due to variations in the injection timing between cycles.

Apart from variations observed due instabilities of injection systems, studies have also shown an increase of cyclic variation with prolonged ignition delay. In [46], studies of cold start in CI engines showed that colder in-cylinder conditions led to increased ID, which resulted in heavy cycle-to-cycle variations in in-cylinder pressure. Furthermore, in [37], [47] and [48] high cycle-to-cycle variations were observed in DI diesel engines when changing the intake temperature and injection timing parameters in order to create conditions of prolonged ignition delay. Studies concerning the variation of in-cylinder pressure with various fuels have shown a dependency of cyclic variation on the ignition characteristics of the fuels tested [49–51]. In [51] there is a reported correlation between ignition delay due to changes in Cetane Number (CN) and cyclic variation, with decreased ignitibility of the fuel leading to increased fluctuations in in-cylinder pressure.

HCCI engine operation also exhibits cyclic variations, mainly due to ran-
dom changes in local gas composition from cycle to cycle [33, 35]. Finally few publications have focused on the cyclic variability exhibited in the in-cylinder pressure in conventional diesel engines [45, 49], with the main focus being on the pressure increase rate rather than peak pressure.

Figure 1.9 shows a typical pressure trace from multiple cycles during cold start, which exhibit cycle-to-cycle variations [46].

Cycle-to-cycle variation in emissions

Studies of the cycle-to-cycle variations in emissions from diesel engines have been limited. This can be attributed to the limited cyclic variation of in-cylinder pressure which is encountered under conventional diesel conditions, which leads to the assumption that limited variation in emissions will be present. Nonetheless, some publications have hinted on the possibility of significant cyclic variations arising due to various reasons.

Wing [45] used NO emission modeling to predict the effect of cyclic variation in injection timing on $NO_x$ emissions. The study showed an increase of the order of 5% in average $NO_x$ emissions when a point with fluctuating injection timing was compared to an average, stable point due to the higher contribution of $NO_x$ of the advanced injection cycles.

Under conditions where the injection is assumed to be stable, investigations have also showed significant fluctuations in emissions. In [52], fast NO measurements in a heavy duty diesel engine showed significant variations
in the NO concentration in the exhaust at constant operating conditions. Ultra-fast crank angle-resolved NO measurements in the exhaust stream of a marine two-stroke and a marine four-stroke engine showed variations of 20-25% and 15-20% respectively from cycle-to-cycle, at constant running conditions [53,54].

Significant cyclic variations in NO production rate which were not coupled to changes in HRR were also observed in complete cylinder dumping experiments during combustion in a DI diesel engine in [10]. Finally, Wagner [55] showed that under conventional diesel and constant injection conditions, NO concentrations measured through sapling of the exhaust showed cyclic variations of the order of 10%, while in-cylinder pressure, ID and HRR showed only very slight cyclic variation. Nonetheless, there was no clear correlation between variations in HRR and NO observed in this study, leading to the conclusion that variations in NO emissions were caused by random effects, possibly not coupled to HRR.

In terms of cyclic variation of in cylinder soot mass in DI diesel engines, there have been numerous studies which show significant cycle-to-cycle variation [51,55–57]. Zhao and Ladomatos [56] argue that the large cycle-to-cycle variations in the time-resolved in-cylinder soot radiation measured using an optical probe are due to the random movement of the soot cloud, or random changes in location of the soot cloud in different cycles. On the other hand, Jakob et al. [51] argue that the observed cyclic variation in soot luminosity measured in an optical single-cylinder diesel engine are caused by combustion instabilities, since they were amplified when using fuels with lower CN, and thus longer resulting ignition delay. Finally, investigations of soot location and intensity using soot luminosity and soot-LII (Laser Induced Incandescence) in an optically accessible engine showed high soot luminosity variations with split injection, while the measured HRR remained relatively constant [57]. Figure 1.10 shows the measured in-cylinder pressure, apparent HRR and combustion luminosity for 20 different cycles [57]. The first injection burns in purely premixed fashion, thus showing very limited luminosity. The second injection has a significant proportion of diffusion combustion during which there is soot production, and the peak luminosity exhibits variations of the order of 30% of the average peak luminosity.
1.5 Effects of Pressure Oscillations on Combustion

The effects of acoustic oscillations on combustion have been studied extensively in a wide variety of combustion systems. The studies have generally shown an increase in evaporation and air-fuel mixing rates under acoustic excitation, leading to increased combustion rates.

Single fuel droplet combustion

Research in evaporation and combustion of single fuel droplets at atmospheric conditions within acoustic fields has shown that pressure oscillations increase both evaporation and combustion rates [58–61]. Blaszczyk [58] showed that high frequency (200Hz-5kHz), high energy pressure oscillations consistently increased the combustion rate of single diesel fuel droplets by 2-10%, when compared to non-oscillating cases. This increase was attributed to increased air-fuel mixing due to the relative movement of gas molecules caused by the vibrating air field. At air excitation frequencies below 100Hz, results showed very unstable combustion of the
Figure 1.11: Experimental results showing the effects of pressure oscillation of different amplitudes (□, 90 dB; +, 100 dB; ◊, 110 dB; Δ, 115 dB) and frequencies on single diesel droplet combustion rate ($k_{rel}=1$ for non-oscillating combustion) [58].

Fuel droplets due to flame quenching from the very high air motion caused by the air oscillation. Results from these experiments showing the effects of pressure oscillation of different amplitudes and frequencies on combustion rate ($k_{rel}=1$ for non-oscillating combustion) are shown in Figure 1.11 [58]. Additionally, through non-reacting and reacting experiments, Saito et al. [59, 60] showed that forced acoustic oscillation enhanced the evaporation and combustion rate of single kerosene and diesel fuel droplets. Finally, Kumagai and Isoda [61] showed similar results, and argue that effects of pressure fluctuation observed in single droplet combustion should also apply to spray combustion. The argumentation behind this states that since the droplet motion due to the spray velocity will rapidly decline, this will lead to combustion of the single droplets at similar rates as in still-air conditions.

**Spray combustion**

In continuous combustors, acoustic pressure oscillations are frequently studied in order to understand their interaction with air-fuel mixing and chemical reaction rates, which strongly affect combustion and emission formation. In such combustors, the acoustic excitation is either externally forced
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Figure 1.12: Flame length of a coaxial natural gas diffusion flame with and without acoustic excitation, as a function of pressure fluctuation amplitude [66].

(via a loudspeaker), produced due to excitation of natural modes of the system or generated by the chemical reactions within the system [62]. For this last source of acoustic excitation to take place, the Rayleigh criterion must be met. The Rayleigh criterion [63] states that if the heat addition (in this case heat release) is positively correlated with pressure, then the pressure oscillation will be sustained.

Studies have shown that the structure of premixed, partially premixed and diffusion flames can change significantly when they are excited acoustically. In general, acoustic excitation of flames has shown to increase turbulent intensity, enhance the transition from laminar to turbulent flow, increase the burn rate, increase homogeneity of the mixture and affect emission formation [64–73].

Yoshida et al. [64] showed that turbulence in turbulent jet diffusion flames is increased when they are externally subjected to acoustic excitation, significantly enhancing combustion rate, while shortening and broadening the flame. Additionally, these non-reactive and reactive experiments showed that under resonant conditions the transition from laminar to turbulent flow is enhanced.

A shortening and broadening of the flame was also observed under oscillating conditions in [65], where spray combustion investigations were conducted in a Rijke-tube combustor, and [66], where diffusion flames were externally excited using a loudspeaker. These experiments also showed that the individual droplet lifetime was significantly reduced when oscillations were present, and created flames which had premixed flame characteristics.
Figure 1.13: Oxygen concentration and temperature distribution across the cross-section of a coaxial natural gas diffusion flame with and without pressure fluctuations of 21 mbar at 181 Hz, for three different nozzle sizes (50 mm, 150 mm, 250 mm) [66].

(more blue color rather than yellow, as a result of less soot in the flame). Figure 1.12, taken from [66], shows the flame length of a coaxial natural gas diffusion flame with and without acoustic excitation, as a function of pressure fluctuation amplitude.

Finally, in [66], pressure oscillations were shown to increase oxygen concentration in the flame region, leading to a more evenly distributed temperature profile, with higher temperatures near the normally rich flame core. Figure 1.13 shows the oxygen concentration and temperature distribution across the cross-section of a coaxial natural gas diffusion flame with and without pressure fluctuations, for three different nozzle sizes.

1.5.1 Effects of Pressure Fluctuations on Emissions

In terms of emissions from acoustically excited flames, most research has focused on soot, CO and NO\textsubscript{x} emissions. It is generally accepted that through the increase of air-fuel mixing caused by acoustic excitation, there follows a reduction in soot formation and an enhancement of soot and CO oxidation [66, 69–71].

Soot emissions

In experimental investigations of soot presence in the flame and soot emissions, pressure oscillations have been shown to influence both soot formation and soot oxidation. As mentioned previously, results from experiments
with a coaxial natural gas diffusion flame showed a complete absence of soot from the flame when large amplitude pressure fluctuations were present, which changed the coloring of the flame from yellow to blue [66]. Photographs of the two flames, with and without acoustic excitation are shown in Figure 1.14.

The argumentation for the absence of soot from the flame is multifaceted. On the one hand, Ferreira et al. [70] argue that large oxygen concentrations in the flame due to increased mixing lead to decreased soot production, through the conversion of the hydrocarbon radical (RH) directly to carbon monoxide and not to $C_2H_2$, which is a main precursor for soot. On the other, increased flame temperature and oxygen concentration due to enhanced mixing, as described in the previous section, also lead to increased oxidation of soot in acoustically excited flames [66,70–72].

In all, both soot formation and oxidation are effected by pressure oscilla-
Figure 1.15: LPG burner soot signal at different positions inside the flame (3 cm, 6 cm and 10 cm from the burner orifice), as a function of external acoustic excitation intensity at 500 Hz [72]

...tions, indicating improved air-fuel mixing and increasing homogeneity of the air-fuel mixture, resulting in lower soot emissions from diffusion flames. Figure 1.15 shows the soot signal at different positions inside the flame (3 cm, 6 cm and 10 cm from the burner orifice), as a function of external acoustic excitation intensity, for a LPG burner, indicating significantly lowered soot presence for increasing oscillation intensity [72].

**CO emissions**

Measurements of CO concentration and emissions from various spray combustion configurations have shown similar results to soot concentration measurements [66, 69, 70]. Under oscillating conditions, observed higher mixing of fuel and air results in higher O₂ concentrations within the flame, as shown in Figure 1.13, which lead to a more complete oxidation of CO. The CO concentration across the flame cross-section for the same flames as in Figure 1.13 is shown in Figure 1.16 [66].
Figure 1.16: CO concentration across the cross-section of a coaxial natural gas diffusion flame with and without pressure fluctuations of 21 mbar at 181 Hz, for three different nozzle sizes (50 mm, 150 mm, 250 mm) [66].

**NO\textsubscript{x} emissions**

Contrary to soot and CO oxidation, where increased mixing of fuel and air is univocally favorable, the effects of pressure fluctuations on NO\textsubscript{x} formation and emissions are not so clear-cut. For NO\textsubscript{x} formation there seems to be a stronger dependency on the air/fuel mixing degree of the flame. There have been reported cases in the literature where acoustic excitation of flames resulted in increased [67,69,70] and decreased [66,70,73] NO\textsubscript{x} emissions.

As mentioned previously, there is a strong dependency of NO\textsubscript{x} formation on temperature, oxygen availability and residence time. Thus, the effects of pressure oscillations on these parameters are of importance to NO\textsubscript{x} emissions.

In [66] and [70] it was shown that pressure oscillations lead to increased homogeneity of the combustion, due to enhanced mixing. This, in the case of lean premixed combustion leads to lower equivalence ratios and thus lower peak temperatures, leading to lower NO\textsubscript{x} formation rates. Furthermore, faster mixing of hot burned gases under acoustically excited conditions results in lower residence times, also promoting less NO\textsubscript{x} production. The
spatial distribution of $NO_x$ concentration across the cross-section of a coaxial natural gas diffusion flame from [66] is shown in Figure 1.17. As can be seen, the $NO_x$ concentration, especially for the smallest nozzle size case, is dramatically reduced, due to the higher degree of mixing, which results in a partially premixed flame with excess air and reduced temperature. Conversely, in rich diffusion combustion flames, where reactions occur close to the stoichiometric equivalence ratio, pulsed combustion leads to an increase in $NO_x$ emissions due to local increases in temperature (due to faster combustion) and oxygen availability in the flame region [67, 69, 70]. In addition, Ferreira et al. [70] argue that the reduction in soot presence in the flame reduces radiation heat transfer from the flame, which can result in higher flame temperatures, promoting $NO_x$ formation. Finally, Oran and Gradner [62] state that there can also be an effect of pressure oscillations directly on $NO_x$ formation: the pressure oscillations are essentially near-isentropic compressions and expansions which result in a corresponding temporal fluctuation in temperature. Chemical reaction rates such as $NO_x$ production rate, which are generally known to be of Arrhenius type, are exponentially dependent on temperature. Thus, reactions will be accelerated more by the positive temperature cycle of the oscillation than
Due to the abovementioned mechanisms, the results in [70] showed an up to threefold increase in $NO_x$ emissions from a LPG burner, when subjected to pressure oscillations of various frequencies (0 to 800 Hz) and intensities (10 to 30 mbar). The $NO_x$, $CO$, $CO_2$ and $O_2$ concentrations with increasing oscillation frequency can be seen in Figure 1.18 [70].

Overall, due to the abovementioned reasons, the effect of pressure oscillations on $NO_x$ emissions depends strongly on the air to fuel ratio of the flame. In fact, Lyons [74] showed that increased air/fuel uniformity, similar to what was observed in acoustically excited flames, resulted in an increase in $NO_x$ emissions only when the average equivalence ratio was above 0.7. In leaner cases, increased uniformity resulted in a reduction of $NO_x$ emissions.
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1.5.2 Effects of Pressure Fluctuations on Diesel Engine Combustion

Even though the source and control of CI ringing combustion has been extensively researched in the literature, the research on effects of the pressure oscillations on combustion and emission formation in internal combustion engines has, to the author’s knowledge, been minimal.

Recent results from Rusly et al. [37, 38] and Martin et al. [39] in optically accessible DI diesel engines have shown effects of pressure fluctuations on the soot cloud. More specifically, under long ignition delay conditions, where premixed combustion-induced pressure fluctuations are present in individual cycles, there exists visible oscillation of the soot cloud at the same frequency as the pressure fluctuations, indicating mass transfer due to the local gas velocities induced from the pressure waves.

In [37, 38] pressure oscillations caused fluctuations in the flame location, similar to the movement of the flame caused by engine swirl, but in a cyclical rather than circumferential manner. The flame movement, as illustrated by the sequence of flame boundaries plotted in Figure 1.19, is completely decoupled from the swirl motion, and in fact the flame moves against the swirl direction in some cases.

Figure 1.19: Temporal sequence of flame boundaries locations within the combustion chamber of a optically accessible DI diesel engine. The arrows show the temporal evolution of the flame centroid location [37].
In [39], similar oscillations were observed in pool fires towards the end of HRR. These pool fires, created due to long spray penetration as a result of prolonged ignition delay, which resulted in spray impingement on the piston surface, showed lateral movement because of the pressure oscillations. In addition to the movement of the pool fires, a correlation between peak in-cylinder soot luminosity and in-cylinder pressure oscillations for individual cycles at constant inlet and injection conditions was observed. At cycles with increased pressure oscillation intensities, higher Spatially Integrated Natural Luminosity (SINL) was detected (Figure 1.20). This observation can be explained by increased mixing near the cylinder surface due to pressure oscillations, which results in higher soot formation and oxidation in the remaining fuel present. It should be noted that these experiments were conducted at conditions where only premixed combustion was present, thus any soot luminosity will be due to pool fires as a result of wall impingement. It can be reasonably assumed that when the increased mixing due to pressure fluctuations is not present, any remaining fuel will not be oxidised, and will be emitted in the form of unburned hydrocarbons.

Figure 1.20: Maximum Spatially Integrated Natural Luminosity (SINL) plotted against pressure oscillation intensity for individual cycles at constant inlet and injection conditions [39].
Chapter 2

Experimental Procedure

This chapter gives a description of the experimental procedure which was followed to obtain insight into the potential and limitations of NO\textsubscript{x} reduction through Miller valve timing, as well as to better understand the effects of prolonged ignition delay and in-cylinder pressure fluctuations on combustion and emissions.

The two engine test benches which were built up and used to perform all the experiments are presented in the first section. This is followed by a description of the measurement equipment which was used, including sensors for in-cylinder pressure and soot measurements, analysers for steady-state and transient exhaust gas measurement, and specialized equipment for cycle-to-cycle measurement of exhaust NO concentrations.

2.1 Engine Testbeds

The experimental investigations were conducted on two medium-speed, heavy duty, Common-Rail, direct injection, 4-stroke diesel engines, albeit with very different characteristics and capabilities. A six-cylinder near-production engine, fitted with a prototype two-stage turbocharging system and run with different valve cams was used to study the NO\textsubscript{x} reduction potential of Miller valve timing. A single cylinder experimental test engine which allows the independent setting of inlet and exhaust parameters was used for detailed investigations of combustion and emissions under long ignition delay conditions. These two engines are presented in the sections below.
Table 2.1: Wärtsilä 6L20 engine specification.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Number of Cylinders</td>
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<td>6</td>
</tr>
<tr>
<td>Bore</td>
<td>mm</td>
<td>200</td>
</tr>
<tr>
<td>Stroke</td>
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<td>280</td>
</tr>
<tr>
<td>Compression Ratio</td>
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</tr>
<tr>
<td>Nominal Speed</td>
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</tr>
<tr>
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<td>Number of valves/cylinder</td>
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<tr>
<td>Maximum injection pressure</td>
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</tr>
<tr>
<td>Maximum in-cylinder pressure</td>
<td>bar</td>
<td>200</td>
</tr>
<tr>
<td>Number of injections/cycle</td>
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</tr>
<tr>
<td>Number of injector orifices</td>
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<td>9</td>
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<tr>
<td>Turbocharging</td>
<td></td>
<td>ABB 1 and 2-stage</td>
</tr>
</tbody>
</table>

2.1.1 Large Engine Research Facility (LERF)

The Large Engine Research Facility (LERF) is part of the Competence Centre for Energy and Mobility (CCEM) in the Paul Scherrer Institut (PSI), located in Villigen, Switzerland. The facility was built to be used for research into new turbocharging and combustion concepts on marine diesel engines with flexible air and fuel delivery systems and was used within the HERCULES-B project for investigations into the NO\textsubscript{x} reduction potential of Miller valve timing.

The test engine housed in the research facility and used for the present measurements is a Wärtsilä 6L20 Common Rail, 4-stroke, medium speed marine Diesel engine. The engine uses different configurations of single and 2-stage turbocharging systems, developed by ABB Turbo Systems. The engine specifications and important engine characteristics are listed in Table 2.1. An external and internal view of the LERF test facility can be seen in Figure 2.1.

Throughout the course of the experiments, the engine configuration was changed from single to two-stage turbocharging, and different Miller valve timing cams were used to change Top Dead Centre (TDC) temperature. The TDC temperatures tested ranged from \(~740\text{K}\) (extreme Miller) to \(~900\text{K}\) (standard baseline valve timing).
Figure 2.1: External and internal view of the LERF test facility in PSI.

### Table 2.2: Wärtsilä 6L20 engine TDC temperatures for different valve timings.

<table>
<thead>
<tr>
<th>Name</th>
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<th>Turbocharger Setup</th>
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</thead>
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<tr>
<td>Baseline</td>
<td>900K</td>
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</tr>
<tr>
<td>Miller 1</td>
<td>800K</td>
<td>2-stage</td>
</tr>
<tr>
<td>Miller 2</td>
<td>760K</td>
<td>2-stage</td>
</tr>
<tr>
<td>Miller 3</td>
<td>740K</td>
<td>2-stage</td>
</tr>
</tbody>
</table>

In addition to the valve timing changes, the after-cooler water flow can be controlled to vary the inlet charge temperature, which allowed a further TDC temperature control range of 25K for any given valve setting.

Table 2.2 contains the approximate TDC temperature for each different valve timing configuration tested, with the after-cooler temperature set at its default setting of 56°C.

Parallel to the changes in valve timing, the turbocharger setup was altered to achieve different charge air pressures. Different compressor and turbine sizes and nozzles were used in both the low and high pressure stages, as required, so as to achieve similar cylinder air densities, in order to keep the air/fuel ratio approximately constant, irrespective of valve timing.

The engine fuel injection system is a Common-Rail type system, capable
Table 2.3: LERF diesel fuel analysis.

<table>
<thead>
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<th>Parameter</th>
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<tbody>
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<td>Viscosity at 40°C</td>
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<tr>
<td>Cetane Number</td>
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<td>51</td>
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<tr>
<td>Distillation analysis:</td>
<td></td>
<td></td>
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<tr>
<td>at 180°C</td>
<td>Vol. %</td>
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</tr>
<tr>
<td>at 250°C</td>
<td>Vol. %</td>
<td>37.8</td>
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<tr>
<td>at 340°C</td>
<td>Vol. %</td>
<td>95.4</td>
</tr>
<tr>
<td>at 350°C</td>
<td>Vol. %</td>
<td>98.4</td>
</tr>
<tr>
<td>distillation start</td>
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</tr>
<tr>
<td>10% temperature</td>
<td>°C</td>
<td>208</td>
</tr>
<tr>
<td>50% temperature</td>
<td>°C</td>
<td>266</td>
</tr>
<tr>
<td>90% temperature</td>
<td>°C</td>
<td>323</td>
</tr>
<tr>
<td>95% temperature</td>
<td>°C</td>
<td>338</td>
</tr>
</tbody>
</table>

of a single injection, with freely adjustable Start of Injection (SOI) and rail pressure up to 1500bar. The injection rate is trapezoid-like, with maximum fuel injection rates occurring very soon after the injector valve lift.

Additional information about the LERF facility, the engine and the research work conducted on it can be found in [75, 76].

Fuel used during experiments

A single type of conventional diesel fuel was used throughout the experimental procedure on the LERF. Data for the fuel are shown in Table 2.3.

2.1.2 MTU-396 Single Cylinder Engine

This single-cylinder experimental engine is located in ETH Zurich and is used for detailed investigations into combustion and emission formation under controlled inlet and fuel injection conditions. The experimental engine is based on a MTU 396 series engine, which has been fitted with a Ganser Common Rail fuel injection system. The engine is supplied with pressurized air (up to 5bar), and the intake air can be conditioned through heating and cooling to a range of temperatures from 17 to 100°C. The
Table 2.4: MTU-396 single cylinder engine specification.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Cylinders</td>
<td></td>
<td>1</td>
</tr>
<tr>
<td>Bore</td>
<td>mm</td>
<td>165</td>
</tr>
<tr>
<td>Stroke</td>
<td>mm</td>
<td>185</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td></td>
<td>13.7</td>
</tr>
<tr>
<td>Speed Range</td>
<td>rpm</td>
<td>800-2100</td>
</tr>
<tr>
<td>Number of valves/cylinder</td>
<td></td>
<td>4 (3 with extra access)</td>
</tr>
<tr>
<td>Maximum injection pressure</td>
<td>bar</td>
<td>1600</td>
</tr>
<tr>
<td>Maximum in-cylinder pressure</td>
<td>bar</td>
<td>155</td>
</tr>
<tr>
<td>Number of injections/cycle</td>
<td></td>
<td>3</td>
</tr>
<tr>
<td>Number of injector orifices</td>
<td></td>
<td>8</td>
</tr>
<tr>
<td>Inlet pressure</td>
<td>bar</td>
<td>1-5</td>
</tr>
<tr>
<td>Inlet temperature</td>
<td>°C</td>
<td>17-100</td>
</tr>
</tbody>
</table>

exhaust gas back pressure can be independently set using an exhaust gas throttle. The engine specifications and important engine characteristics are listed in Table 2.4.

The original cylinder head configuration is a 4-valve design. For the purpose of the experiments, one of the two exhaust valves was replaced with a water-cooled sensor adaptor, which allows the placement of additional pressure or optical sensors, as well as gas-sampling devices. This allowed additional access to within the cylinder bowl area. The independent setting of inlet and exhaust parameters allowed this change without significant deterioration of the cylinder scavenging.

A view of the test engine can be seen in Figure 2.2.

For the purpose of this investigation, the MTU single-cylinder engine was run in two different conditions, to obtain short and long ID results. The conditions chosen for the comparison are presented in Table 2.5.

Table 2.5: Conditions for short and long ID measurements on the MTU engine.

<table>
<thead>
<tr>
<th>Name</th>
<th>Inlet Temp.</th>
<th>TDC Temp.</th>
<th>Inlet Press.</th>
<th>TDC Press.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Short ID</td>
<td>79°C</td>
<td>920K</td>
<td>2bar</td>
<td>65bar</td>
</tr>
<tr>
<td>Long ID</td>
<td>19°C</td>
<td>810K</td>
<td>1.3bar</td>
<td>42bar</td>
</tr>
</tbody>
</table>
Chapter 2  Experimental Procedure

2.2 In-Cylinder Measurements

This section contains information about the in-cylinder measurements conducted throughout the experiments in both experimental facilities. The first two sub-sections present the available in-cylinder accesses for placement of the various sensors in each of the experimental test-benches. Then the two final sub-sections explain the principles of in-cylinder pressure indication and in-cylinder soot measurement through three-color pyrometry. It should be noted that in-cylinder measurements in both facilities were conducted at a sampling rate of 5 samples/°CA (0.2°CA resolution).
2.2.1 In-Cylinder Measurements on the LERF

For the purposes of the experiments, three bores in total were drilled on the cylinder head of cylinder 6 (the cylinder closest to the free end of the engine) of the 6L20 engine. Two of the three bores were drilled at an angle from the top of the cylinder, in order to allow the placement of two pressure sensors or combinations of pressure and optical sensors. In these apertures one M8 and a second M10 size sensors can be placed with direct, flush-mounted access to within the piston bowl. The M10 access is placed between the two exhaust valves, whereas the M8 is situated between one of the inlet and one of the exhaust valves. The third access is from the side of the cylinder, which allows the mounting of a pressure sensor used for in-cylinder pressure pegging, with access to the cylinder near the M8 mounting point through a narrow bore.

A view of the cylinder head as seen from within the cylinder, which reveals the exact location of the bores is shown in Figure 2.3. Further drawings and 3D-CAD models designed by Kistler, which show cross-sections of the cylinder head are shown in Figures 2.4 and 2.5.

2.2.2 In-Cylinder Measurements on the MTU

The in-cylinder pressure measurements on the MTU-396 single cylinder engine are performed through a cylinder head side-access, which allows pressure measurements from within the piston bowl. The pressure measurement location is between the inlet end exhaust valves. A view of the MTU-396 cylinder head which shows the location of the pressure indication bore is shown in Figure 2.6.

In order to gain additional access into the cylinder, since the available space was not adequate for further bores, one of the exhaust valves was replaced with a fixed dummy-valve. Different configurations of this dummy valve allow the placement of various different sensors, ranging from pressure sensors, optical sensors and fast sampling valves for direct sampling of cylinder gases during the high pressure cycle. During the current experiments a new, water-cooled dummy valve was manufactured and used, in order to be able to place a second, high accuracy pressure sensor. This gives the possibility, along with the main pressure sensor, to characterise the pressure waves present under long ignition delay conditions. A drawing of the MTU dummy valve access is shown in Figure 2.7.
Figure 2.3: Drawing of the Wärtsilä 6L20 engine cylinder head, showing the location of the bores for in-cylinder measurements.

Figure 2.4: Drawings of the cross-section of the Wärtsilä 6L20 engine cylinder head, showing the bores for direct access to within the piston bowl.

2.2.3 In-Cylinder Pressure Measurement

In-cylinder pressure indication was performed using Kistler piezoelectric sensors. As mentioned previously, at least two bores in each of the cylinder heads allowed the simultaneous measurement of two pressure traces, from two different locations within the piston bowl. Two simultaneous measurements were taken in order to allow the determination of the shape
Figure 2.5: 3D-CAD drawings of the cross-section of the Wärtsilä 6L20 engine cylinder head, showing the bores for direct access to within the piston bowl.

Figure 2.6: Drawing of the MTU in-cylinder pressure indication access.

and direction of pressure waves, when those arose under long ignition delay conditions.

In the LERF test-bench, the in-cylinder piezoelectric sensors were pegged using a piezoresistive sensor through the side access within the cylinder. This allowed accurate pressure pegging during the expansion of the Miller valve timing. In the MTU engine, pressure pegging was performed using a piezoresistive sensor in the inlet, and pressure was pegged during the inlet valve opening time near the BDC.
2.2.4 In-Cylinder Soot Measurement

For the measurement of the in-cylinder soot concentration, the principle of three-color pyrometry was used. The calculated soot concentration, also known as the $KL$ factor, is measured using a miniaturized Optical Light Probe (OLP), which has been developed through a collaboration between ETH Zurich, Kistler AG and Sensoptic AG [77].

The OLP is an optical fiber which allows light radiation to travel from the cylinder, through an amplifier, to a light sensor. It features a sapphire lens at its tip, which through an externally controlled heating system is maintained at 600°C during engine operation. This allows minimal contamination of the lens from particulate matter, in order to achieve a constant soot radiation signal. The optical signal obtained from the probe is spatially...
integrated through a $140^\circ$ viewing angle, as shown in Figure 2.8. Before the light enters the amplifier, the light is filtered at three different wavelengths (680nm, 790nm, 903nm), with the intensity of each wavelength being recorded at each time step.

**In-cylinder soot concentration calculation**

The $KL$ factor is used as a measure of the in-cylinder soot mass concentration. This is proportional to $K$, which is the absorption coefficient per unit of soot cloud thickness and is proportional of soot mass concentration [79, 80], and $L$, which is the flame thickness.

In order to calculate $KL$ from the light intensities measured using the OLP, the two-color method, developed in 1932 by Hottel and Broughton [81], is employed. This is based on the fact that the emissivity of a luminous flame is numerically equal to its absorptivity, and uses the light intensity at two different frequencies to deduce the soot mass concentration.

According to [81], the wavelength-dependent emissivity of a soot-containing flame is a function of $KL$ as follows:

$$
\epsilon (\lambda, T) = 1 - e^{-\frac{KL}{x^2}}
$$

(2.1)
Where:

$K$: Absorption coefficient per unit of soot cloud thickness along the line of sight, and is a function of particle concentration per m

$L$: Geometrical flame thickness along the optical axis

$\alpha$: Experimentally derived exponent which describes the influence of the wavelength on the emission potential and takes values of 1 to 1.4 [82]. In diesel engine soot measurements, values of 1.39 [81] and 1.38 [82] have been quoted.

As a first step in the determination of the in-cylinder soot concentration, the three light intensities are calibrated in order to derive a wavelength-specific black body temperature ($T_{BB}$), using Planck’s law of radiation. The calibration is performed using a Tungsten-Lamp and an integrating sphere, as shown in [79,83,84]. Plank’s law states:

$$i(\lambda, T) = \frac{2C_1}{\lambda^5 \left(e^{\left(\frac{C_2}{\lambda T}\right)}-1\right)}$$ \hspace{1cm} (2.2)

The apparent black body temperature ($T_{BB}$) is the temperature of a black body which emits the same amount of radiation as any diffuse body:

$$i(\lambda, T_{BB}) = i(\lambda, T)$$ \hspace{1cm} (2.3)

The emissivity of a diffuse body is defined as:

$$\epsilon(\lambda, T) = \frac{i(\lambda, T_{BB})}{i(\lambda, T)} = \frac{\lambda^5 \left(e^{\left(\frac{C_2}{\lambda T_{BB}}\right)}-1\right)}{\lambda^5 \left(e^{\left(\frac{C_2}{\lambda T_{BB}}\right)}-1\right)}$$ \hspace{1cm} (2.4)

Following equation 2.4, and since the emissivity of a non-black body is below 1, the apparent black body temperature needs to be lower than the soot cloud temperature.

Combining equations 2.1 and 2.4 and solving for $KL$, one obtains:

$$KL = -\lambda^\alpha ln \left(1 - \frac{\left(e^{\left(\frac{C_2}{\lambda T}\right)}-1\right)}{\left(e^{\left(\frac{C_2}{\lambda T_{BB}}\right)}-1\right)}\right)$$ \hspace{1cm} (2.5)

After solving equation 2.2 for $T$ (apparent black body temperature), equation 2.6 balances equation 2.1 for two different wavelengths, which makes
the apparent soot cloud radiation-temperature $T$ the only unknown. $KL$ can be derived by introducing $T$ in equation 2.5.

\[
\left(1 - \frac{\left(e^{\frac{C_2}{\lambda T}} - 1\right)}{\left(e^{\frac{C_2}{\lambda_1 T_{BB}}} - 1\right)}\right)^{\lambda_1} = \left(1 - \frac{\left(e^{\frac{C_2}{\lambda_2 T}} - 1\right)}{\left(e^{\frac{C_2}{\lambda_2 T_{BB}}} - 1\right)}\right)^{\lambda_2}
\] (2.6)

For the calculation presented above to be applicable in diesel engine in-cylinder soot concentration measurements, the following assumptions have to be made [56, 79, 81–84]:

- The soot mass concentration and soot cloud temperature are uniform in the field of view.
- Soot radiation is isotropic
- The scattering of radiation due to soot particles is equal to zero. This introduces only a relatively small error [82] due to the fact that particle sizes in diesel engines range from 30 to 500nm [85], and the shortest wavelength measured is 680nm.
- Any contamination of the lens due to non-organic deposits does not effect the light intensity, or effects all wavelengths uniformly.

The abovementioned calculation is used to calculate the soot cloud temperature and a value of $KL$ for a pair of measured wavelength intensities. In the case of 3-color pyrometry, the measurement of three different wavelengths allows the calculation of three temperatures and corresponding $KL$ values by combining each pair of intensities, the values of which should match when the calibration is correct. This allows a further check of validity for each measurement.

**In-cylinder soot evolution**

This section aims to present a typical in-cylinder soot evolution with the corresponding points of interest for the separate study of the soot formation and oxidation processes. Figure 2.9 shows a typical measured injection rate, HRR and $KL$ factor, averaged for 150 consecutive cycles.
Chapter 2  Experimental Procedure

Figure 2.9: Typical shape of multiple cycle-averaged measured injection rate, heat release rate and $KL$ factor for a DI diesel engine.

The shape of the $KL$ factor depicts the typical progress of soot concentration in the combustion chamber during combustion. At the start of the diffusion combustion phase, soot production increases the concentration of soot in the cylinder. Towards the end of injection, soot oxidation becomes significant, resulting in a limitation of the rate of increase of soot concentration. At the point where soot production and oxidation are equal the maximum of the $KL$ signal can be found. Finally, from this point onwards soot oxidation dominates until temperatures and/or oxygen availability in the soot cloud are too low to allow further oxidation. The former happens due to the expansion of the gases as the piston moves downwards. The latter can result either from the dissipation of injection or intake induced turbulence, which will reduce the amount of mixing between soot and fresh charge air, or due to the limitation of oxygen availability at rich conditions. The calculation of $KL$ factor needs to be stopped at a certain black body temperature, since the signal to noise ratio of the optical signal from this point onwards is close to 1. In the investigations presented here the calculation was stopped when the calculated black body temperature falls below 1300K.

The important characteristics of soot concentration relevant for this study are early soot formation, late soot formation/early soot oxidation and late
soot oxidation. The characteristics of each part of the soot cycle were studied using individual cycle $KL$ values in the following way:

- **Early soot formation**: Early soot formation is characterised by the initial slope of the $KL$ signal. The slope of the $KL$ signal was calculated using of the value of the $KL$ factor 5°CA after the initial positive $KL$ value.

- **Late soot formation/early soot oxidation**: The result of the interaction between soot formation and oxidation is depicted in the value of cycle peak $KL$. Even though it is impossible to determine the exact contributions of formation and oxidation on this value, past experience has shown that the maximum value of $KL$ is mainly affected by oxidation, since formation is assumed to be relatively constant.

- **Late soot oxidation**: The latter parts of soot oxidation rate are characterized by the slope of the $KL$ factor after the peak. Since there is a continuous interaction between soot formation and oxidation, a characteristic oxidation rate was defined to be depicted by the slope of the $KL$ trace from the maximum negative slope of $KL$ (minimum of the derivative of $KL$) to a point 5°CA later in the cycle. Since the oxidation rate is also a function of soot concentration, the relative oxidation rate between different operating conditions or different individual cycles at constant conditions is better depicted in the maximum negative slope of $KL$, normalized by the peak cycle $KL$.

Figure 2.10 shows schematically the different phases on a typical $KL$ trace.

**In-cylinder soot measurements in the LERF**

In the present experiments the OLP was placed in the M8 access of the cylinder head. A M8 adaptor was constructed so that the tip of the OLP protrudes 1mm into the cylinder. The 50° angle of the bore to the horizontal resulted in a direct view of 3 of the injector 9 sprays through the optical sensor. Even though not all the combustion chamber is optically accessible through this aperture, the soot evolution in each spray is assumed to be approximately constant, and thus the shape of the $KL$ factor calculated
Figure 2.10: Typical KL factor evolution, showing the different parts of the in-cylinder soot evolution (formation-dominated, mixture of formation and oxidation, oxidation-dominated sections) and the characteristic values used to quantify each section.

from the light intensities measured is representative for the entire cylinder. A drawing of the bore with the sensor placement and viewing angle is shown in Figure 2.11.

Limitations

Despite the significant advantages that the OLP provides for obtaining insight into in-cylinder soot evolution, especially on how the soot formation and oxidation processes are affected by engine and environmental parameters, there are exist some limitations in its application and information acquired. Due to the design of the sensor, the field of view is restricted to only part of the combustion chamber. This allows only qualitative measurements to be conducted, since the only a portion of the flame regions is viewed. Additionally, the necessary simplification that the soot cloud is uniform is obviously false, increasing the uncertainty of the measurements. Nevertheless, the OLP has been used in the past for various investigations with considerable success. [83,84,86–90].
Chapter 2 Experimental Procedure

2.3 Exhaust Gas Measurements

The exhaust gas measurement procedures and equipment used in both experimental test-benches are described in this section. Initially the equipment used for the steady-state measurements is presented, followed by a brief description of the fast sampling valve and high speed exhaust gas analysis system used for the cycle-resolved exhaust gas analysis.

2.3.1 Steady-State Exhaust Gas Measurements on the LERF

The exhaust gas analysis in the LERF was performed using an AVL SESAM FTIR spectrometer. This has the capability of 1 Hz broad spectrum exhaust gas analysis, allowing the simultaneous measurement of multiple species.

For the exhaust gas soot measurement, an AVL 439 partial flow opacimeter was used for all experiments. The opacimeter continuously measures the light absorption and scattering of part of the exhaust flow, giving an indication of the amount of soot particles it contains per unit volume. This device also has a speed of 1 Hz. Both aforementioned devices can be used for steady state and transient measurements.

Figure 2.11: Drawing of the LERF M8 in-cylinder access used for the OLP. The OLP is shown at its mounting position, with the viewing angle shown superimposed.
For specific steady-state points where increased accuracy of soot emissions was deemed necessary, an AVL Smoke Meter device was used.

### 2.3.2 Steady-State Exhaust Gas Measurements on the MTU

Time-averaged exhaust gas $NO_x$ measurements were taken continuously using a chemiluminescence $NO_x$ analyzer. The exhaust gas analysis also included $CO$ and $CO_2$ analysers, as well as a FID (Flame Ionization Detector) for Unburned Hydrocarbons (UHC) measurement.

### 2.3.3 Cycle-to-Cycle Exhaust Gas Measurements on the MTU

For the determination of how individual cycle combustion characteristics affect exhaust gas emissions, the exhaust gas concentration of $NO$ was measured for individual cycles at specific engine running conditions exhibiting high cycle-to-cycle variations. To achieve this, part of the exhaust gas was sampled near the exhaust valve during the exhaust valve opening, and the $NO$ concentration of the sampled gas was measured using a fast V&F AirSense mass spectrometer. The gas sampling was performed using a fast-sampling valve, which was designed and built in-house.

**Fast-sampling valve**

The fast-sampling valve was developed and constructed within LAV to be used as a high speed actuated sampling valve for in-cylinder and exhaust gas and particle sampling. The valve is actuated using a hybrid electromagnetic-hydraulic system with driving pressures of 600 to 1000 bar, which allow controlled valve opening times down to 1ms duration. More information about the fast sampling valve design and operation can be found in [91]. The valve tip and needle were designed to be able to withstand the high pressures and temperatures present in the combustion chamber and the exhaust stream of modern diesel engines. The valve system includes a dilution/purge system, which ensures sufficient cooling, dilution of the sample volume, freezing of the chemical composition or purging of the valve depending on the application used.
Measurement procedure

In the present measurements, the fast-sampling valve was used exclusively in the exhaust stream of the engine. The valve was opened 15ms after the exhaust valve opening time, and was closed before the opening of the exhaust valve of the next cycle. This was done to ensure that only gases from the specific cycle were sampled. The representative NO value for the cycle was taken as the maximum value of the NO concentration measurement. The simultaneous logging of the in-cylinder pressure, the fast-sampling valve opening and the NO concentration measurement, allowed the correlation of the NO concentration to an individual cycle. After a single cycle measurement the valve was purged with air before the next measurement was started.

A sample graph showing the measured in-cylinder pressure, the sampling valve opening and the measured NO trace is shown in Figure 2.12.

2.4 Heat Release Rate analysis

In internal combustion engine research the calculation of the apparent Heat Release Rate (HRR) from the in-cylinder pressure measurements is a very valuable tool to determine effects of different parameters on combustion.
In this investigation, a detailed analysis of the pressure trace to deduce the HRR for each individual cycle is required. This was done using the cylinder measurement post-processing software WEG [92], which has been developed in-house. For the calculation of apparent HRR, the assumption that the cylinder volume has a constant spatial distribution of pressure must be made. In the cases with extensive pressure fluctuations, where pressure changes extensively depending on location within the cylinder, the pressure trace must be smoothed significantly, in order to obtain an inferred, spatially-averaged pressure. To achieve the required accuracy for the calculation of the premixed combustion and to avoid excessive HRR fluctuation due to artificial effects from the pressure oscillations, each cycle was individually smoothed using a polynomial fit. This is especially important for single-cycle measurements, where cycle averaging cannot be used to reduce the pressure signal noise levels. Polynomials of different length were used at different points in the cycle, in order to achieve variable smoothing for compression, premixed combustion and diffusion combustion/expansion.

2.4.1 Apparent Mixing Rate

In order to study the effects of in-cylinder conditions to the diffusion combustion, it is useful to introduce the apparent characteristic mixing time, which is deduced from the HRR. The apparent characteristic mixing time ($\tau_{mix}$) is a combustion parameter which can be used as a measure of the apparent mixing during diffusion combustion. Given that during the diffusion phase of combustion, the reaction rate is limited by the mixing of fuel with air, the evaporated fuel can be related to the burned fuel using the characteristic mixing time as a measure of the fuel/air mixing:

$$\frac{dQ_{diff}}{d\theta} = \frac{1}{\tau_{mix}} \times Q_{available}$$  \hspace{1cm} (2.7)

$$\tau_{mix} = \frac{Q_{available}}{dQ_{diffusion}/d\theta} = \frac{m_{fuel Evaporated} - m_{fuel Burned}}{dm_{fuel Diffusion}/d\theta}$$  \hspace{1cm} (2.8)

In the calculation of the characteristic mixing time, the mass of the evaporated fuel which is available at any given point is approximated using the $d^2$ law, which states that:

$$d_{drop}^2 = d_{0,drop}^2 - \beta \times t$$  \hspace{1cm} (2.9)
where $d_{\text{drop}}$ is the instantaneous droplet diameter, $d_{0,\text{drop}}$ is the initial droplet diameter, assumed to be equal to the Sauter mean diameter and calculated using the Kamimoto correlation [93], and $\beta$ is the evaporation coefficient. During the present analysis $\beta$ was kept constant for cycles with constant in-cylinder and injection conditions.

As mentioned previously, $\tau_{\text{mix}}$ is a spatially global measure of air-fuel mixing during diffusion combustion. It is mainly influenced by the level of turbulence in the spray and flame region, and by the rate of air entrainment into the spray plume not induced by turbulence. The former is mainly influenced by turbulence-enhancing parameters (injection pressure, background turbulence etc.), whereas the latter is mainly affected by alterations in the spray form. At constant charge and injection conditions, changes in $\tau_{\text{mix}}$ are expected to be mainly due to increases in turbulence levels near the flame region since only minor alterations in the spray itself are expected.
Chapter 3

3-D CRFD Simulation Procedure

In the context of this thesis, 3-D CRFD simulations were used to improve the understanding of observed phenomena on spray combustion and emission formation. On the one hand, simulations of the LERF engine were used in order to study in increased detail the effects of reduced charge air temperature on spray formation and combustion, as well as NO\textsubscript{x} emission formation. Simulations of a sector of the engine cylinder were conducted using the commercial CFD software package Star-CD, version 4.14. On the other hand, simulations of a single spray within a constant volume combustion chamber at diesel-like conditions were used to investigate the effects of cylinder pressure fluctuations on air-fuel mixing. Additional information about these investigations can be found in [94] and [95] respectively. This chapter aims to present the grid and the relevant spray and combustion models used throughout the engine and spray simulation investigations. The results of the investigations are presented in Chapter 4, along with the results from the experimental investigations.

3.1 LERF Engine Simulations

3.1.1 LERF Engine Grid

The simulations were performed on a grid representing a 1/9th sector of the LERF engine cylinder, corresponding to the area occupied by one injector spray plume. The grid, kindly provided by Wärtsilä, is one used by the company for engine development purposes. Although the grid was created for the 20 series engine, some modifications were required in order to match the parameters of the test engine. The grid used in the following investigations was an axisymmetric model.
Chapter 3  3-D CRFD Simulation Procedure

Figure 3.1: Side view of the 1/9th sector grid of the W20 LERF engine at BDC (left) and TDC (right).

of 1/9th of the cylinder, so the asymmetrical design in the cylinder head around the intake and exhaust valves had to be approximated by a cylindrically extruded feature (see Figure 3.1). The small differences in the flow field caused by these elements were deemed unimportant in this investigation. Most of the grid consists of hexahedral cells, arranged in the azimuthal direction around the cylinder axis. The crevice volumes are modelled by an extra volume at the junction of the cylinder head and the wall. Cylindrical boundary conditions are used on the azimuthal faces, with wall boundaries on the top, bottom and side faces to represent the head, piston and wall respectively. To control the movement of the piston, a mesh moving code was used. Since inlet conditions are of minimal importance in the investigations, rather than modelling the entire intake flow process, the simulation was started from BDC before combustion in order to keep the computational expense at a reasonable level. The initial fluid conditions were set to the corresponding experimental measured pressure and estimated temperature, with no initialized swirl motion. The grid contains 185 665 cells at BDC and 36 670 cells at TDC, with a typical grid spacing around 1.5 mm.

3.1.2 Models Used

Due to the complexity of phenomena occurring during an IC engine combustion process, it is necessary to use models for computation of the main processes. The models used to model spray formation, break-up, evapora-
tion are described briefly in this section.

**Spray models**

The mass flow rate of fuel through the injector nozzle was obtained through injection rate measurements from an injection rate analyser. The injector nozzle parameters were taken from the specifications given by the manufacturer. Droplet diameter was modelled with a Rosin-Rammler distribution. The properties of the droplets were represented using dodecane fuel. Secondary droplet breakup was modelled with the Reitz-Diwakar model [96], which models the bag and stripping breakup regimes. The researchers experimentally determined the following breakup criteria for bag and stripping breakup regimes:

- **Bag Breakup:**
  
  \[
  W_e > 6
  \]  
  \[(3.1)\]

- **Stripping Breakup:**
  
  \[
  \frac{W_e}{Re^{1/2}} > 0.5
  \]  
  \[(3.2)\]

Where \( W_e \) is the Weber number (the ratio between aerodynamic forces to surface tension forces on a droplet) and \( Re \) is the droplet Reynolds number (the ratio of inertial forces to viscous forces). The model assumes that the droplet will break up when the breakup conditions are satisfied for longer than the characteristic breakup time \( t_{bag} \) or \( t_{strip} \):

\[
t_{bag} = C_1 \sqrt{\frac{\rho_l r_d^3}{\sigma}}
\]  
\[(3.3)\]

\[
t_{strip} = C_2 \frac{r_d}{v_{rel}} \sqrt{\frac{\rho_l}{\rho_g}}
\]  
\[(3.4)\]

Where \( C_1 \) and \( C_2 \) are empirical constants, \( \rho_l \) is the density of the liquid, \( r_d \) is the radius of the droplet, \( \sigma \) is the surface tension, \( v_{rel} \) is the relative velocity between the droplet and the gas, and \( \rho_g \) is the density of the gas. At breakup, the droplet will separate into a number \( N_{d,child} \) of just stable child droplets (i.e. the breakup criterion is exactly satisfied), calculated by mass conservation:
\[ N_{d,child} * r_{d,child}^3 = N_{d,\text{parent}} * r_{d,\text{parent}}^3 \] (3.5)

Droplet-wall interaction was modelled using the Bai model [97], which models the stick, spread, rebound, splash and breakup regimes. The model reflects the stochastic nature of the impingement by using a random procedure to determine some of the quantities relating to post-impingement status. Therefore, secondary droplets from a splash event have a distribution of sizes and velocities.

**Chemistry models**

The chemical reaction models used were chosen primarily for simplicity purposes. Nonetheless, all models used are very commonplace in this types of studies.

**Ignition:**

The time scale of the autoignition in diesel engines is relatively long compared to the fluid dynamic time scale, therefore a model is required that takes into account the effects of diffusive and convective species transport [6]. For this study, the Shell Ignition model was used [98], which was originally developed to model knock in spark-ignition engines and was later adapted to model the autoignition of diesel fuels [99, 100]. The Shell ignition model simulates the ignition mechanism with eight reaction steps between five generic species. The individual species concentrations are solved by numerically integrating the differential equations for their change rates. To reflect the ignition behaviour of a certain fuel, a total of 26 parameters need to be adjusted. Various studies have shown that the Shell model is able to predict, under engine conditions, the negative temperature coefficient observed in experiments [6], and is arguably the most widely used autoignition model.

**Fuel composition:**

Real-world diesel fuels consist of a range of different molecules, including different chain length hydrocarbons and traces of pollutants such as sulphur. Since it is computationally expensive to calculate the combustion of such multi-component fuels and due to the difficulties in characterising their behaviour, surrogate fuels are often used in combustion simulation.
The fuel used for this study is $C_{16}H_{20}$, with the global one step combustion reaction shown below:

$$C_{16}H_{20} + 13O_2 = 16CO_2 \ast 10H_2O$$  \hspace{1cm} (3.6)

Surrogate fuels are merely a representation of the real fuel, giving an average molecule size and the ratio of carbon to hydrogen.

**Combustion:**

Simulating the combustion in a transient simulation with a large grid requires a model. In this study, the Laminar And Turbulent Characteristic Time scale Eddy BreakUp model (EBU LATCT), provided in the Star-CD package, was used. Although without any physical substance, this model is widely used in IC engine development because it gives good correlation with measurements, without the large computational expense associated with physically accurate models.

The fundamental concept of the EBU model is that the rate of combustion is determined by the rate at which parcels of unburned mixture within the turbulent flame brush are broken down into smaller ones, such that the area between the unburned mixture and the hot gases is sufficient to allow a reaction to take place [6]. The LATCT model has been developed by Patterson et al. [101] specifically for modelling combustion in DI diesel engines. It was recognised that, in diesel engines, the initiation of combustion is limited by the laminar time scale, since the turbulent time scale can be very low due to the high injection velocities. Therefore the turbulent characteristic time model proposed by Magnussen [102] was further developed to take into account the laminar characteristic time scale.

In the model, the fuel consumption rate $R_f$ is expressed based on a single step reaction:

$$R_f = \frac{\rho \ast A_{EBU} \ast \min \left( Y_f, \frac{Y_{O_2}}{r_f}, B_{EBU} \frac{Y_p}{1+r_f} \right)}{\tau_c}$$  \hspace{1cm} (3.7)

Where $r_f$ is the stoichiometric air-to-fuel ratio, the subscripts $f, O_2$ and $p$ denote fuel, oxygen and products respectively and the constants $A_{EBU}$ and $B_{EBU}$ are empirical parameters that may be tuned for different situations. In the current investigations $A_{EBU}$ and $B_{EBU}$ were tuned using engine measurements for relevant in-cylinder conditions.
The characteristic combustion time scale \( \tau_c \) is related to the laminar time scale \( \tau_l \) and the turbulent time scale \( \tau_t \) by a delay coefficient \( f \).

\[
\tau_c = \tau_l + f \tau_t \tag{3.8}
\]

The laminar time scale \( \tau_l \) is derived from Arrhenius reaction rate:

\[
\tau_l = A^{-1} \exp \left( \frac{E}{RT} \right) \tag{3.9}
\]

where \( A \) is a pre-exponential constant. The turbulent time scale \( \tau_t \) is directly proportional to the eddy turnover time (the ratio between the turbulent kinetic energy \( k \) and its dissipation rate \( \epsilon \)):

\[
\tau_t \propto \frac{k}{\epsilon} \tag{3.10}
\]

The parameter \( f \) describes the transition from the laminar to the turbulent regime and ranges in value from zero to one.

NO formation:

Formation of NO was calculated using the extended Zeldovich mechanism, which models the thermal NO formation. In this study, \( NO_x \) formed through the prompt and fuel routes was not taken into account, since the thermal model typically accounts for at least 80% of all NO formed in Diesel engines.

The accuracy of predictions of exhaust \( NO_x \) concentrations using the extended Zeldovich model depend strongly on the accuracy of the local temperature and composition predictions. For typical diesel engine simulations, an accuracy of 20% can be expected [6].

### 3.2 Spray Simulations

The spray combustion simulations are based on a high-pressure and temperature constant volume combustion chamber setup at the Sandia National Laboratories [103]. The model of the constant volume setup used here has been validated using experimental data available on the Engine Combustion Network Libraries [104]. The validation of the simulation setup, as well as additional information about the simulation work conducted can be found in [95,105].
The following sections aim to provide a description of the experimental setup, the numerical grid and models which were used, as well as the boundary conditions employed for the investigations of the effects of pressure fluctuations on spray development and air/fuel mixing.

### 3.2.1 Sandia Bomb

The Sandia high temperature and pressure constant volume combustion chamber is a cube-shaped volume of characteristic dimension \( l_{\text{char}} = 108\, \text{mm} \), which can be setup to emulate diesel-like conditions during the fuel injection period. Fuel is introduced in the camber using a Common Rail fuel injector, to which different single-hole fuel injector tips of variable nozzle hole diameter can be fitted. In the present investigations the nozzle diameter studied was 0.1mm. A schematic of the Sandia Bomb is shown in Figure 3.2.

**Figure 3.2:** Schematic of the Sandia bomb experimental setup.

**Sandia bomb grid**

The 3D mesh used for the Sandia bomb calculations consists of cubic cells with sides of 2mm, with a refined section in the centre of the cube, along the spray length. The refined section was chosen to have 1mm cube cells for the reactive simulations, and 0.5mm cube cells for the non-reactive
calculations. The grid size was chosen based on a compromise between precision and computational cost.

Figure 3.3 shows a section of the Sandia bomb mesh along the spray axis, with the refined part of the mesh in the middle of the cube.

### 3.2.2 Models Used

**Spray models**

For the modeling of the spray primary and secondary break-up, the same models as described in section 3.1.2 were used.

**Chemistry models**

In this work a 2-Dimensional Conditional Moment Closure Model (2D CMC) was chosen for the modeling of the fuel-air reactions and the flame structure. Despite its increased computational effort requirements, this model was chosen in place of the the simpler EBU model due to its more accurate representation of the flame structure and combustion turbulence interaction, which was deemed necessary for this study. In-depth information on 2D CMC and its application for spray combustion can be found in [105,106].
The CMC model approach solves transport equations for conditional means for a certain species $\alpha$. The conditional mean for each species $\alpha$, $Q_\alpha(\eta, x, t)$, is given by the expression for conditional mean:

$$Q_\alpha(\eta, x, t) = (Y_\alpha(x, t)|\xi(x, t) = \eta) \quad (3.11)$$

where $\eta$ is the mixture fraction variable for the conserved scalar and $\xi(x, t)$ is the mixture fraction evaluated at point $x$ in time $t$. As presented in [106] and [105], mean values of species $\alpha$ are used as the non fluctuating part of the mass concentration of $\alpha$:

$$Y_\alpha(x, t) = Q_\alpha(\eta, x, t) + Y''_\alpha(x, t) \quad (3.12)$$

Then, transport equations for species are obtained by introducing the total derivative of 3.12 in the RANS Favre Averaged Species Equations:

$$\frac{\partial Q_\alpha}{\partial t} + \langle u_i|\eta \rangle \frac{\partial Q_\alpha}{\partial x_i} = \langle N|\eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \langle \omega_\alpha|\eta \rangle + e_Y + e_Q \quad (3.13)$$

where

$$e_Y = -\langle \rho \frac{\partial Y''_\alpha}{\partial t} + \rho u_i \frac{\partial Y''_\alpha}{\partial x_i} - \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Y''_\alpha}{\partial \eta} \right) |\xi(x, t) = \eta \rangle \quad (3.14)$$

and

$$e_Q = \left\langle \frac{\partial}{\partial x_i} \left( \rho D \frac{\partial Q_\alpha}{\partial x_i} \right) + \rho D \frac{\partial \xi}{\partial x_i} \left( \frac{\partial}{\partial x_i} \frac{\partial Q_\alpha}{\partial \eta} \right) |\xi(x, t) = \eta \right\rangle \quad (3.15)$$

The above terms are not closed, and thus the following assumptions are made:

- All terms contained in $e_Q$ are inversely dependent on Reynolds number, which in this work is very high near the combustion zone, and thus $e_Q$ can be neglected.

- Fluctuations in density and diffusivity are neglected.

- The unknown term $e_Y$ is closed since:

$$e_Y \tilde{P}(\eta) = \frac{\partial}{\partial x_i} \left( \langle \rho u_i Y''|\eta \rangle \tilde{P}(\eta) \right) \quad (3.16)$$
Following these assumptions the conditional transport for species can be written as:

\[
\frac{\partial Q_\alpha}{\partial t} + \langle u_i | \eta \rangle \frac{\partial Q_\alpha}{\partial x_i} - \langle N | \eta \rangle \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \frac{1}{\bar{\rho} \hat{P}(\eta)} \frac{\partial}{\partial x_i} \left[ \langle \rho u''_i Y'' | \eta \rangle \hat{P}(\eta) \right] = \langle w_\alpha | \eta \rangle
\]  

(3.17)

Similarly, the conditional transport equation for the temperature can be derived:

\[
\langle N | \eta \rangle \frac{\partial^2 Q_T}{\partial \eta^2} + \langle N | \eta \rangle \left[ \frac{1}{\langle c_P | \eta \rangle} \left( \frac{\partial \langle c_P | \eta \rangle}{\partial \eta} + \sum^{N}_{\alpha=1} c_{P,\alpha} \frac{\partial Q_\alpha}{\partial \eta} \right) \right] \frac{\partial Q_T}{\partial \eta} + \langle w_H | \eta \rangle + \frac{1}{\langle c_P | \eta \rangle} \frac{1}{\rho} \frac{\partial}{\partial t} \hat{P}(\eta) - \frac{1}{\hat{P}(\eta)} \frac{\partial}{\partial x_i} \left[ \langle u''_i T'' | \eta \rangle \bar{\rho} \hat{P}(\eta) \right]
\]  

(3.18)

Solutions to equations 3.17 and 3.18 provide temperature and species concentration at each location in the domain considered. To complete the CMC model, sub-models for Conditional Turbulent fluxes, Conditional Velocities and Conditional Density and Pressure rate of change together with the chemical sources have to be provided.

Conditional turbulent fluxes

The conditional turbulent fluxes for any quantity \( \Phi \) are modelled with gradient fluxes:

\[
\langle u'_j \Phi'' | \eta \rangle = -D_t \frac{\partial Q_\Phi}{\partial x_j}
\]  

(3.19)

where the turbulent diffusivity is deduced from the mean flow field quantities as:

\[
D_t = \frac{\mu_i}{S_{Ct}}
\]  

(3.20)

Conditional velocities

The conditional velocities are modelled based on a linear relationship:

\[
\langle u_i | \eta \rangle = \bar{u}_i - \frac{D_t}{\xi^{m2} \partial x_i} \left( \eta - \tilde{\xi} \right)
\]  

(3.21)
Conditional density and pressure rate of change

The pressure is assumed constant in the conserved scalar space, therefore the rate of change of pressure can be written as:

\[
\left\langle \frac{1}{\rho} \frac{\partial P}{\partial t} \right\rangle = \frac{1}{\langle \rho \rangle} \frac{\partial P}{\partial t}
\]

(3.22)

and the conditional density is calculated with the law of perfect gasses:

\[
\langle \rho | \eta \rangle = \frac{PW_\eta}{RQ_T}
\]

(3.23)

The pressure rate of change term must be retained in the conditional temperature equation, as it is important for engine calculations.

Conditional chemical sources and heat release rate

Closure of the chemical source terms is performed at first-order; this means that the conditional expectation for the chemical source terms depend only on the conditional mean of the reactive scalars, temperature and pressure and not on their fluctuations.

For the chemical sources and the heat release rate we obtain:

\[
\langle w_\alpha | \eta \rangle = \dot{\omega}_\alpha (Q_\alpha, Q_T, P)
\]

(3.24)

\[
\langle w_\mathcal{H} | \eta \rangle = - \sum_{\alpha=1}^{N} h_\alpha \langle w_\alpha | \eta \rangle
\]

(3.25)

3.2.3 Boundary Conditions

For the study of the effects of in-cylinder pressure fluctuations on spray development and fuel-air mixing, spray simulations with externally forced pressure fluctuations were performed. The pressure fluctuations were introduced as sinusoidal pressure fluctuations on the side wall boundary in place of the solid wall boundary, which resulted in a pressure wave vertical to the pray direction. The two wall boundary conditions used for the non-excited and acoustically excited cases are presented below:

- Non-acoustic cases:

  In the non-acoustic cases the boundary conditions at the walls were chosen as solid wall boundary conditions. These boundary conditions
do not allow mass exchange over the boundaries, and constrain the flow to within the domain. Furthermore, the boundary was chosen to be adiabatic, to not allow heat exchange with the walls.

- **Acoustic cases:**

  In the acoustically excited cases, the side walls were set to transient wave boundary conditions. These boundary conditions allow the pressure waves existing in the analysed volume to be "absorbed" by setting the pressure gradient on the wall to zero, and thus do not allow the pressure wave to be reflected. This types of boundaries were also used to force the pressure fluctuations on the one side of the volume and thus introduce an acoustic field in the volume. This was done by forcing the wall pressure to sinusoidally fluctuate, as shown in equation 3.26:

\[
p_{\text{wall}}(t) = p_0 + p' \sin(2\pi ft) \quad (3.26)
\]

Where \(p_0\) is the averaged pressure of the domain, \(p'\) is the pressure fluctuation intensity, and \(f\) is the required frequency of the resulting acoustic field.

### 3.2.4 Simulation Initial Conditions

The initial gas conditions chosen for the spray simulations were chosen to represent diesel engine-like conditions. Constant gas temperature of 1000K and a pressure of 43.3 bar for the non-reactive and 42.1 bar for the reactive cases were chosen. Different gas compositions and were chosen to simulate the effects of EGR on the flame. The injected fuel quantity of 17.8 mg and injection duration of 6.8 ms were kept constant throughout. The simulation conditions are presented in Table 3.1.

In terms of the acoustic excitation, various variations in excitation frequency and intensity were studied in order to observed the effects on spray formation, fuel-air mixing and combustion. For the non-reactive simulations, the studies concentrated on excitation frequency variations at 2 bar excitation intensity, as well as excitation intensity variations at 2.5kHz excitation frequency. Tables 3.2 and 3.3 list the excitation frequency and intensity combinations studied for the non-reactive and reactive cases respectively.
Table 3.1: Sandia bomb simulation parameters.

<table>
<thead>
<tr>
<th>$X_{O_2}$</th>
<th>$T_{init}$</th>
<th>$P_{init}$</th>
<th>$\rho_{init}$</th>
<th>$m_{fuel}$</th>
<th>$t_{inj}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>%</td>
<td>K</td>
<td>bar</td>
<td>kg/m$^3$</td>
<td>mg</td>
<td>ms</td>
</tr>
<tr>
<td>Non-reactive</td>
<td>0</td>
<td>1000</td>
<td>43.3</td>
<td>14.8</td>
<td>17.8</td>
</tr>
<tr>
<td>Reactive 21%</td>
<td>21</td>
<td>1000</td>
<td>42.1</td>
<td>14.8</td>
<td>17.8</td>
</tr>
<tr>
<td>Reactive 15%</td>
<td>15</td>
<td>1000</td>
<td>42.1</td>
<td>14.8</td>
<td>17.8</td>
</tr>
<tr>
<td>Reactive 10%</td>
<td>10</td>
<td>1000</td>
<td>42.1</td>
<td>14.8</td>
<td>17.8</td>
</tr>
</tbody>
</table>

Table 3.2: Parameter variation for non-reactive simulation cases.

<table>
<thead>
<tr>
<th>Frequency kHz</th>
<th>Fluctuation Intensity bar</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 2, 2.5, 3, 4, 5, 6, 7, 8, 9, 10, 11, 18</td>
<td>2</td>
</tr>
<tr>
<td>2.5</td>
<td>1, 2, 3, 4, 5</td>
</tr>
</tbody>
</table>

Table 3.3: Parameter variation for reactive simulation cases.

<table>
<thead>
<tr>
<th>Frequency kHz</th>
<th>Fluctuation Intensity bar</th>
<th>$X_{O_2}$ %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1, 2.5, 6, 10, 18</td>
<td>2</td>
<td>21</td>
</tr>
<tr>
<td>2.5</td>
<td>1, 2, 3, 5</td>
<td>21</td>
</tr>
<tr>
<td>2.5</td>
<td>2</td>
<td>21, 15, 10</td>
</tr>
</tbody>
</table>
Chapter 4

Experimental and Simulation Results

As discussed in Chapter 1 of this work, the application of Miller valve timing and other similar techniques which are based on the reduction of reactant temperature so as to lower the adiabatic flame temperature and thus reduce $NO_x$ formation, have been shown to have significant limitations. The present chapter presents the experimental observations and simulation results, in order to provide a comprehensive insight into the $NO_x$ emission reduction potential of Miller valve timing and the inherent problems that limit its application for near-zero $NO_x$ emissions. To this end, the chapter begins with the presentation of the improvement in the $NO_x$-SFC tradeoff achieved on the LERF engine testbed through the application of successively increasing Miller degrees and corresponding adjustments in two-stage turbocharger setups to achieve near-constant air-fuel ratios. This first section also includes observed limitations in the $NO_x$-SFC tradeoff at high Miller degrees.

Subsequent sections focus on the effects of long ID on air-fuel mixing, spray penetration and $NO_x$ formation in premixed combustion. These were studied through experimental and 3D CFD investigations on the LERF engine with increasing Miller degree and ID.

Lastly, the final two subsections of this chapter focus on the observed increase of cycle-to-cycle variation of pressure and emissions in both test-benches, and on the characteristics and effects of premixed combustion-induced pressure fluctuations on combustion and emissions observed when reactant temperature is reduced. In addition to the experimental investigations, the study is supported by 3D CFD investigations of the effects of pressure fluctuations on fuel-air mixing and chemical reactions of non-reactive and reactive sprays in a constant volume combustion chamber.
4.1 Effects of Miller Valve Timing on $NO_x$ emissions

As mentioned in previous sections, the main aim of engine manufacturers is to improve the $NO_x$-SFC tradeoff. In the present experiments the improvement in the $NO_x$-SFC tradeoff, as an important attribute of engine design, has been acquired for the LERF 6-cylinder engine testbench by reducing the cycle temperature through the use of Miller valve timing. In order to achieve similar air-fuel ratio values while advancing the IVC point, the boost pressure was increased for increasing Miller degree. Through changes in the injection system (SOI, rail pressure) the $NO_x$-SFC tradeoff for different loads and different Miller degrees was obtained. In the first step of advancing the IVC, the benefit in the $NO_x$-SFC tradeoff is substantial. Figure 4.1 shows the change in the $NO_x$-SFC tradeoff when going from Baseline (temperature at TDC = 900K) to Miller 1 (temperature at TDC = 800K) for a medium and a high load point.

In the plot it is clear that by advancing the IVC, a $NO_x$ reduction of around 55% and 40% was possible for high and for medium load respectively, while maintaining constant SFC. This result is in line with the results available in the literature [17,25–30], since the lower reactant temperature results in lower adiabatic flame temperature, and thus lower thermal $NO_x$ formation rates.
Figure 4.2: NO$_x$-SFC tradeoffs for medium and high load, for the baseline ($T_{TDC}=900K$), the Miller 1 ($T_{TDC}=800K$), the Miller 2 ($T_{TDC}=760K$) and the Miller 3 ($T_{TDC}=740K$) cases.

4.1.1 Miller Valve Timing Limitations

The relationship between the reduction in the calculated adiabatic flame temperature through the reduction of reactant temperature and NO$_x$ emissions has been proven not to be valid in many cases [19–22]. In the present experiments a further advancement of the IVC point, which results in temperatures at TDC lower than 800K, leads to changes in the NO$_x$ reduction trends. The NO$_x$-SFC tradeoffs for increasing Miller degree (baseline, Miller 1-3) are shown in Figure 4.2, for the same medium and a high load at the LERF engine.

As evident in the graphs, a further decrease of TDC temperature from 800K to below 750K does not further increase the NO$_x$-SFC tradeoff benefit. At high load, the higher Miller degree cases show no improvement over Miller 1. At lower loads the trend reverses completely, leading to an increase of NO$_x$ emissions for constant SFC when moving from Miller 1 to Miller 3.

It should be noted at this point that there is a significant difference between the medium and high loads in the in-cylinder pressure at the point of SOI, due to the different boost pressures provided by the turbocharger. Indicatively, the in-cylinder pressure at SOI for the medium load is around 40% lower than the high load with the Miller 3 configuration, and 30% lower with the baseline configuration. This difference in cylinder pressure results in large differences in ignition delay between the medium and high loads, due to the near-linear dependency of ignition delay to charge pressure (in [2] the referenced empirical exponent for the pressure in the ID calculation...
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Figure 4.3: NOx emissions plotted versus ID for medium and high loads at constant injection (pressure and timing) and approximately constant charge air density conditions.

ranges from 0.7 to 2, depending on the data fit chosen).

To study this reversal in NOx trend in greater detail, one can look at ID plotted versus NOx emissions, for different loads. By changing the charge air temperature, while maintaining approximately constant charge air density and constant injection pressure, duration and timing, the trend of NOx can be deduced. Figure 4.3 shows the NOx emissions plotted versus ignition delay for different Miller degrees and effective cycle temperatures, for the same medium and high load.

At both loads a clear minimum at around 0.8ms ID can be observed in the NOx emissions for the specific combination of injection pressure, injection duration and engine characteristics. For cycle temperatures that result in ID shorter than 0.8ms, the NOx follows the expected trend of lower emissions when the adiabatic flame temperature is lower. Beyond this value of ID (at colder charge conditions) the NOx emissions increase significantly to a value up to 2g/kWh higher than the minimum for the current measurements. For the high load, the same inlet temperatures result in lower ID, since the charge pressure from the turbocharging system is higher. The observations from Figure 4.3 are in line with the previous observations from Figure 4.2, indicating reversal in NOx emission trends with decreasing cycle temperature and a correlation between NOx emissions and ID.
4.2 Effects of Long Ignition Delay

In the following sections a deeper understanding of the possible causes of this \( NO_x \) trend reversal with increasing ID will be attempted through the detailed analysis of relevant observed phenomena. As will be shown, most of the observed phenomena which result in the \( NO_x \) emission increase at low charge temperatures, are connected to the prolonged ignition delay. Due to the complexity and interconnection of the phenomena studied, the study is divided into three distinct sub-sections:

- Effects directly connected to ignition delay and the corresponding spray formation; namely increase of \( NO_x \) emissions due to increased spray penetration and air engulfment due to longer ignition delay

- Effects connected directly with the proportion of premixed combustion which changes with ID; namely increase of \( NO_x \) emissions due to \( NO_x \) formed in premixed combustion or \( NO_x \) formed from the high temperature premixed combustion products during diffusion combustion

- Effects connected to observed pressure fluctuations and cycle-to-cycle variability due to the long ignition delay and stochastic phenomena; namely increase of \( NO_x \) emissions due to higher \( NO_x \) emission arising from individual cycles

4.2.1 Observed Mixing Effects

When studying the HRR for different Miller degrees, an increase in the diffusion combustion rate can be observed; namely, for increasing Miller degree and ID, at similar TDC charge air density but reduced TDC temperature, the apparent mixing rate is increased. Figure 4.4 shows the HRR, integrated HRR and characteristic mixing rate for the three different Miller degrees at the same load, SOI and rail pressure. The calculated values were plotted using an average of 150 consecutive cycles for each Miller point. This was done due to the degree of cycle to cycle variability, which forces the need to capture the average characteristics of all cycles.

It is interesting to note that the measured heat release rates and related calculated parameters show an increase in combustion speed with increas-
ing Miller degree. The results show that the integrated HRR for Miller 3 surpasses the Miller 1 and Miller 2 cases immediately from the premixed combustion phase. This can be attributed to a higher degree of premixing due to the longer ignition delay. This point will be further discussed later in this thesis.

Another characteristic is that the diffusion combustion speed is increased with decreasing charge temperature. This is faintly observable in the plotted HRR, and more clearly in the characteristic mixing rate plot. Whereas the explanation of the increased premixed combustion is clear, the understanding of the increased diffusion combustion speed multi-faceted. This can be attributed to:

- increased flame area due to the longer penetration of the spray prior to ignition, leading to better utilisation of the charge air oxygen and faster air-fuel mixing during diffusion combustion

- increased air/fuel mixing rate due to other effects, which lead to increased turbulence around the flame and faster diffusion combustion. Such effects have been observed in combustion research in partially premixed and diffusion combustion flames under the presence of pressure fluctuations, as was presented in section 1.5.

A more detailed study of the possible reasons for the increased characteristic mixing rate will also be presented later in this work.

**Spray penetration before ignition**

As discussed in the previous section, one of the explanations for the increased HRR observed with increasing ID is the longer spray penetration
prior to ignition. This effectively leads to better pre-mixing and utilisation of the available oxygen, since the spray reaches deeper into the combustion chamber.

The effects of longer spray penetration on fuel-air mixing due to prolonged ID were investigated using the 3-D CFD simulation of the LERF cylinder sector. In order determine the effects of ID on mixing and HRR without the temperature interference, the Miller 3 case was simulated and then the simulation was repeated with artificially delayed ID (the calculation of the ID integral was started with a delay). The resulting calculated HRRs and integral HRRs are presented in Figure 4.5, along with the characteristic mixing rate. Similarly to what was observed in the experimental results shown in Figure 4.4, the simulations show a significant increase in the overall speed of combustion with the increased ID. Despite the long ID, the premixed combustion part with the late ID overtakes the integral HRR of the early ignition case. Furthermore, the speed of diffusion combustion, as seen in the characteristic mixing rate, is significantly increased with the longer ID.

The reason behind the faster combustion lies precisely in the mixing of the fuel with air throughout the combustion period. As expected, up to the point of ignition the two sprays are identical. After the ignition of the short ID case, the local temperature and pressure increase, leading to a reduction in the momentum of the spray. The difference in spray penetration at the point of ignition for the two sprays can be seen in Figure 4.6, where the mixture fraction distribution is shown at the respective point of ignition. The reduction in momentum in the short ID case results in a reduction in the penetration of the spray, reducing the mixing of fuel with air and diminishing the overall utilization of the available oxygen. Figure 4.7 shows
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Figure 4.6: Simulated mixture fraction distribution at the respective point of ignition for the short ID (left) and the long ID (right) cases.

Figure 4.7: Simulated mixture fraction distribution at the 373°C point for the short ID (left) and the long ID (right) cases.

the mixture fraction distribution for the two cases at the 373°C point. It is clear that in the long ID case the spray has penetrated longer into the cylinder, resulting in better utilization of the available oxygen. Overall, this results in an enhancement of combustion speed, with an increased premixed portion and a simultaneous speeding-up of the diffusion combustion portion.

Although not physically consistent, the investigation presented above gives an indication of the effects of prolonged ignition delay of air-fuel mixing, ceteris paribus.
4.2.2 \( NO_x \) Formation due to Premixed Combustion

As discussed in Chapter 1.1.2, experiments in conventional DI diesel engine combustion have shown that \( NO_x \) formation occurs near the spray tip during diffusion combustion [10–15]. The argument against \( NO_x \) formation during premixed combustion is that at conventional diesel conditions premixed combustion is too fuel rich to attain the temperature and oxygen concentrations which would lead to significant formation of thermal \( NO_x \) [13–15]. Nonetheless, it has been proposed that a contributing factor for the observed \( NO_x \) trend reversal with increasing ID could be the increase of \( NO_x \) production due to the increased premixed combustion proportion [15,19]. This can happen in two ways:

- During the prolonged ignition delay period, the fuel spray mixes with charge air, leading to leaner premixed combustion. This could lead to conditions where during the premixed flame the temperatures and oxygen concentrations reached are enough to increase the overall \( NO_x \) emissions. This is partially supported by data from the optical experiments in [15] and [19], which show increased air-fuel mixing and OH chemiluminescence across the spray cross-section when ignition delay was prolonged. Nonetheless, this data does not provide any indication that the increase in \( NO_x \) emissions at lower charge temperatures is related to \( NO_x \) formed during premixed combustion.

- The hot combustion products of premixed combustion are compressed further and simultaneously mixed with available oxygen during diffusion combustion. This could lead to increased \( NO_x \) emissions, provided the premixed combustion products are not diluted fast enough to freeze \( NO_x \) formation.

Due to the present inability to test these theories experimentally, arising from the lack of optical access, which leads to a lack of temporal and spatial information of \( NO_x \) formation, a simple investigation of the plausibility of NO formation arising from thermal NO was performed using the CFD setup.

The computational investigation focused on the simulated LERF Miller 3 case and the Miller 3 case with artificially prolonged ID. The NO reactions were computed using the extended Zeldovich mechanisms, as outlined in
section 3.1.2. The NO formation rate for both cases is presented along with the HRR and the in-cylinder NO mass progress in Figure 4.8. The presented simulation results clearly show NO formation in the premixed phase of the long ID case, which equates to about 20% of the total NO produced in this cycle. Although in this simulation the ignition delay was artificially prolonged, it shows that very long ignition delays could result in NO produced in the premixed phase, provided the premixed combustion is very high in magnitude (around 50% of total burned fuel in this case) and very fast. Although this result was expected, its accuracy is questionable, considering the inaccuracy of prediction of the reaction rate of the premixed combustion from the EBU model.

4.2.3 Cycle-to-Cycle Variations

As discussed in section 1.4.2, conventional diesel engine combustion is characterised by limited cyclic variation in pressure and resulting HRR. Any observed variations have often been attributed to fuel injection system instabilities [44,45]. Nevertheless, some authors have recognised an increased cycle-to-cycle variation in diesel engines at conditions which promote prolonged ignition delay or fuels with low cetane numbers [37,46–48,51].

Occurrence of cycle-to-cycle variation

In the present experiments on the LERF engine testbed, using the measurement results from the various Miller configurations, a similar trend as
reported in the literature was observed. Increased ignition delay resulted in increased cycle-to-cycle variations of the pressure, with clear fluctuations in pressure rise rate and peak pressure value and location, albeit with minimal cycle-to-cycle changes in ignition delay, even at extreme Miller conditions. This indicates that the differences in the cycle pressure arise from changes in combustion rate and not ID.

Figure 4.9 shows the pressure of 150 measured cycles plotted on a single graph, for short (Baseline, $T_{TDC} = 900K$) and long (Miller 3, $T_{TDC} = 740K$) ID conditions, for medium load. The averaged pressure is overlaid in each case in bold black.

To quantify the cyclic variability of the pressure trace, the standard deviation of peak pressure value and location for 150 consecutive cycles for the different valve timings is shown in Table 4.1. Prior to the calculation the pressure traces were smoothed to avoid any interference of noise and in-cylinder pressure fluctuations on the result. The standard deviation is shown in bar and crank angle (CA) for the peak pressure and location respectively, and also given as a percentage. The percentage standard deviation of the location is calculated in CA referenced to gas exchange TDC.

Table 4.1 shows significant increase in the standard deviation of the location and the value of the maximum pressure with increasing Miller degree. At medium load the standard deviation of peak pressure is below 1% in the baseline case, and increases monotonically to 3.6% for Miller 3. At high load the increase is less pronounced, changing from 0.7% to 1.7%.
Table 4.1: In-cylinder pressure statistics for different engine configurations of the LERF testbed.

<table>
<thead>
<tr>
<th>Load</th>
<th>Std. Deviation</th>
<th>Peak P. Location</th>
<th>Peak P. Location</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline</td>
<td>bar/CA</td>
<td>0.81</td>
<td>0.29</td>
</tr>
<tr>
<td>%</td>
<td></td>
<td>0.71</td>
<td>0.078</td>
</tr>
<tr>
<td>Miller 1</td>
<td>bar/CA</td>
<td>1.34</td>
<td>0.57</td>
</tr>
<tr>
<td>%</td>
<td></td>
<td>1.33</td>
<td>0.15</td>
</tr>
<tr>
<td>Miller 2</td>
<td>bar/CA</td>
<td>2.37</td>
<td>0.77</td>
</tr>
<tr>
<td>%</td>
<td></td>
<td>2.31</td>
<td>0.2</td>
</tr>
<tr>
<td>Miller 3</td>
<td>bar/CA</td>
<td>3.58</td>
<td>0.53</td>
</tr>
<tr>
<td>%</td>
<td></td>
<td>3.6</td>
<td>0.14</td>
</tr>
</tbody>
</table>

The difference between medium and high pressure can be attributed to the ignition delay, which is longer in the medium load point due to lower in-cylinder pressure at TDC.

The increase of the standard deviation of peak pressure with increasing ignition delay can also be shown schematically. Figure 4.10 shows the standard deviation of peak pressure against ignition delay for many different combinations of Miller cams, inlet temperature settings (through changes in the intercooler) and turbocharger configurations, for medium load and for constant injection conditions (injection pressure and timing). The plot clearly shows that there exists a relationship between cycle-to-cycle variation and ignition delay, with longer ignition delay leading to increased cycle-to-cycle variation.

### 4.2.4 Cycle-to-Cycle Variations of Emissions

Experiments to establish the effects of ignition delay on cycle-to-cycle variations of emissions were conducted on both testbenches. The LERF testbench was used to determine the cyclic variability of the in-cylinder soot cloud using the OLP at various inlet conditions, as outlined in section 2.2.4. The single-cylinder MTU testbench was used to determine the cyclic variability in exhaust gas NO emissions under short and long ignition delay conditions. The MTU testbench was chosen for this investigation due to the ability to perform tests at more controlled conditions (constant injection) and the fact that the single-cylinder arrangement suits these single-cycle
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Figure 4.10: Variation of the standard deviation of peak pressure with ignition delay, achieved through different combinations of valve timing, inlet temperature and boost pressure settings at medium load and constant injection pressure and timing.

exhaust gas measurements, in order to avoid measurement interference from other cylinders.

Cycle-to-cycle variation of in-cylinder soot

To determine the cycle-to-cycle variation of in-cylinder soot depending on ignition delay, the LERF engine was run at a medium load for Miller 3 and Baseline valve timings, while simultaneously using the OLP to measure the soot luminosity in-cylinder. Figure 4.11 shows the $KL$ factor of 150 consecutive cycles along with the average $KL$ factor and the average HRR of all cycles for each condition. Note that the average $KL$ factor is calculated using the cycle average of the single signal luminosities to calculate the average $KL$, in order to reduce the error associated with averaging the individual cycle $KL$ factors [56].

The results show significantly increased cycle-to-cycle fluctuation of $KL$ factor for the Miller 3 conditions when compared to the Baseline. This is of course expected, considering the cycle-to-cycle variation which was observed in the pressure (as shown in section 4.2.3) and the corresponding HRR (as will be shown later in section 4.2.7) for the Miller 3 conditions.
Cycle-to-cycle variation of exhaust gas NO

The cycle-to-cycle variation of exhaust gas NO was measured on the MTU single-cylinder engine, using the fast sampling valve as outlined in section 2.3.3. The conditions for short and long ID chosen for the comparison are presented in Table 2.5.

Similarly to the measurements from the LERF engine, the cycle-to-cycle variation of in-cylinder pressure was significantly increased for the long ignition delay case when compared to the short ignition delay case. The calculated standard deviation of the cycle peak pressure was measured to be 0.94bar for the long ID case, which was about 1.2%, compared to 0.51bar for the short ID case, or about 0.5%. This cycle-to-cycle variation was also reflected in the cycle NO measurements in the exhaust. The measured standard deviation of cycle NO relative to the average was almost doubled, from 2.4% to 4.6% when changing the inlet conditions to achieve longer ignition delay. Furthermore, the range which the cycle NO varied in individual cycles was also increased from around 8% of the average NO to around 12% for the long ID case. These results are summarized in Table 4.2.

The measured cyclic variation of NO gives an indication of the possible effects of single-cycle emissions on the overall average engine emissions, which has been reported seldom. Wagner [55] used a similar technique of exhaust gas sampling to measure cyclic variation in DI diesel engines, with
Table 4.2: Standard deviation of peak pressure (in bar and % of maximum) and cycle NO concentration (in ppm and % of maximum), as well as the peak to peak range of single cycle NO measurements relative to the average cycle NO concentration (in %) for short and long ID cases measured on the MTU single-cylinder engine.

<table>
<thead>
<tr>
<th></th>
<th>Standard Deviation</th>
<th>Peak To Peak</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Peak Pressure</td>
<td>Cycle NO</td>
</tr>
<tr>
<td></td>
<td>bar</td>
<td>%</td>
</tr>
<tr>
<td>Short ID</td>
<td>0.51</td>
<td>0.5</td>
</tr>
<tr>
<td>Long ID</td>
<td>0.94</td>
<td>1.2</td>
</tr>
</tbody>
</table>

reported measured variations of the order of 10%, thus quite similar to the current case. Nonetheless there has been no correlation of cyclic variation in NO emissions arising from longer ID thus far.

4.2.5 Pressure Fluctuations

As described in section 1.4.1, pressure oscillations in cylindrical combustion chambers of internal combustion engines have been studied extensively in the past. In compression ignition engines, pressure oscillations have been shown to arise from high pressure rise rates, which drive the combustion chamber into acoustic resonance. In this section, the pressure fluctuations which arise under prolonged ignition delay conditions will be studied in terms of their morphology, their source and the observed effects on combustion and emission formation.

Pressure fluctuation repeatability

As was mentioned before, in the current study reductions in the charge air temperature through changes in the IVC point allowed the significant increase of ignition delay. The long ignition delay coupled with high rates of injection prior to ignition by using high injection pressures and fast opening of the injector valve resulted in very high rates of heat release during premixed combustion. This in turn resulted in pressure oscillations when ID was sufficiently long. Figure 4.12 shows the 150 cycle-average pressure traces for the two cases with the same injection conditions and duration, but different TDC temperature.

Note that the SOI is at 350°CA and injection pressure is 1000bar for both
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Figure 4.12: In-cylinder pressure average of 150 consecutive cycles for Baseline ($T_{TDC}=900K$) and Miller 3 ($T_{TDC}=740K$) configurations at constant injection conditions and duration., showing at high pressure fluctuations for the Miller 3 case.

cases. Also note that there is a difference in pressure since the density was kept approximately constant. The pressure plot shows a very significant difference between short ID and long ID cases. The colder case exhibits a twofold increase in ID, while also showing a clear overlaid pressure oscillation which persists until late in the cycle. The fact that the pressure oscillation is apparent in the pressure trace which has been averaged over 150 consecutive cycles, indicates that the pressure oscillations are in phase between different cycles.

**Pressure fluctuation frequency**

As outlined in section 1.4.1, the modes of the resulting oscillations can be found by using the proposed acoustic pressure wave formula [33]:

\[
f_{m,n} = \frac{C \cdot \rho_{m,n}}{\pi \cdot B}
\]

(4.1)

Where $f_{m,n}$ is the specific vibration frequency for mode $(m, n)$ (in Hz), $C$ is the local speed of sound (in m/s), $\rho_{m,n}$ is the vibration mode number and $B$ is the cylinder bore (in m).
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Figure 4.13: Spectral Power Density of the in-cylinder pressure of 150 consecutive cycles for Baseline (left) and Miller 3 (right) cases of the LERF engine.

According to [33], the $\rho_{1,0}$ value for the first radial mode is 1.84. For the LERF engine dimensions and conditions, the first mode corresponds to around 2.5kHz, assuming a temperature in the burned gases of around 1800K. The second ($\rho_{2,0}=3.054$) and third ($\rho_{0,1}=3.832$) modes have frequencies of around 4 and 5kHz respectively.

For the MTU single-cylinder engine, where the bore is 165mm, the corresponding frequencies are 3kHz, 5kHz and 6.2kHz for the first and second and third modes respectively.

The Fast Fourier Transforms (FFT) of all 150 cycles for the Baseline and the Miller 3 cases of the LERF engine are shown in Figure 4.13.

The figure shows that the first mode (2.5kHz) is prominent in both cases, whereas the second and third modes are less so. This is in line with the literature [33, 42], which states that the combustion chamber gases show the highest oscillation intensities in the first vibration mode, where the propagation of the pressure waves are in the radial direction.

In addition, the Miller 3 case shows a 10-fold increase in intensity of oscillation for the first mode of vibration when compared with the Baseline case. This indicates that there is a relationship between ID, or alternatively the amount of heat release during premixed combustion, with the intensity of oscillations.
Pressure fluctuation intensity

Past research has shown a very strong influence of rapid pressure rise on ringing in CI engines. In the current experiments, a broad variation of TDC temperature resulted in a range of ID from 0.3ms to 1ms, with constant injection conditions. This allowed the investigation of the effects of the amount of premixed combustion on ringing intensity.

Figure 4.14 shows the peak intensity of oscillation for the first mode of vibration averaged for 150 consecutive cycles plotted against the ID with constant injection conditions. Similar to [41], there seems to be an exponential dependency of pressure oscillation intensity with ID, and as a result with the amount of premixed combustion.

The results presented in Figures 4.10 and 4.14 are also in line with past research which has shown a connecting between the occurrence of pressure fluctuations and cycle-to-cycle variations in compression ignition engines. Vessner et al. [33] showed that large cycle-to-cycle variations in pressure exist at conditions which result in ringing combustion. Eng [35] showed that the cyclic variability of pressure increases with increasing ringing intensity.
Measurement and characterization of pressure waves

Although the underlying cause of pressure fluctuations, namely the high pressure rise rate during premixed combustion when ID is increased, is well established in the literature, to this author’s knowledge the exact source of the fluctuations is less well understood. Previous studies of ringing CI combustion led to the assumption that autoignition is initiated at certain hot spots in the engine. Bradley and Kalghatgi [107] argue that slight inhomogeneities of the temperature or mixture will result in slight differences in ID at different locations.

As ID is increased, the exponential dependency of ID on temperature will result in higher differences in local reaction rate, leading to significant differences in local ID. This, if taken to the limit in a case where long ID exists in a DI diesel engine with a certain number of sprays, can result in conditions where the earlier autoignition of one spray due to temperature or mixture inhomogeneities leads to the successive ignition of adjacent sprays. This would essentially constitute the internal combustion engine equivalent of the Rayleigh criterion, where pressure is positively correlated to HRR, leading to successive increases in the pressure rise front during premixed combustion and finally to very high fluctuation rates. After ignition, the pressure waves dissipate due to the lack of further enhancement. The dissipation rate is expected to be engine-dependent.

To test this assumption in the current experiments, considering the limited access available for in-cylinder measurements, it was deemed necessary to study the shape of the pressure fluctuations, as well as try to infer the approximate point of initiation of the fluctuations for the cycles where ringing was observed.

To determine the shape of the fluctuations two pressure sensors were used simultaneously, mounted at different locations in the chamber of the LERF engine. As shown in Figures 2.3 and 2.4, one sensor was mounted between the two exhaust valves, whereas the other was mounted between an exhaust valve and an inlet valve, thus forming a 90° arc between them.

As expected, at short ID conditions, the pressure measurements were very similar between the sensors, baring the expected pressure signal noise. On the contrary, at high ID conditions there were significant differences between the two sensor readings. In all, 5 different types of relationship between the two pressure sensor outputs were observed. Pressure traces from all different types of fluctuations are shown in Figure 4.15, along with
a design of the expected fluctuation shape and the location of the fluctuation node in relation to the pressure sensor positions. Note that all data shown is taken a single measurement of 150 cycles at constant inlet and injection conditions. Also note that the red line corresponds to the sensor placed between the exhaust valves whereas the blue line corresponds to the sensor placed between an inlet and an exhaust valve.

Figure 4.15a shows a cycle where there is no pressure fluctuation within the cylinder (apart from signal noise). Figure 4.15b and 4.15c show cycles where fluctuations are significantly stronger at one of the sensor locations. Since it has been previously established that the main excited mode is the first radial mode, this leads to the assumption that the first ignition point which gives rise to the fluctuations is close to either sensor respectively, or around 180° away from the each measurement point. In cases 4.15b and 4.15c the sensor that is showing less fluctuation can be assumed to be near or at the fluctuation node point.

Figure 4.15d shows both pressure signals fluctuating in phase. This can be assumed to arise when the ignition point is located within the 90° arc formed between the two sensors. Finally, Figure 4.15e shows the pressure traces fluctuating exactly 180° out of phase. Here the ignition point location needs to be such that the node line sits between the two measurement points.

A statistical analysis of the fluctuation data at different conditions can be used to obtain a better understanding of the ignition source. Figure 4.16 shows the distribution of occurrences of cycles with each of the types of fluctuation observed above. Out of the ringing cycles, around half are fluctuating in phase. In below 10% of the cycles the pressures are fluctuating out of phase and in around 40% one of the two sensors is recording significantly higher fluctuations. The cycles where the red pressure trace is fluctuating significantly more than the blue trace are roughly double in number when compared to the blue trace fluctuation being more pronounced.

From the statistical analysis we can deduce the following conclusions:

- In more than 75% of the ringing cycles, the ignition location is either between the two sensors, or near the red sensor. This means that in the vast majority of the cycles the initial ignition point is near the exhaust valves. This can be expected since the exhaust valve surfaces are expected to be significantly hotter than the inlet valve
Figure 4.15: Comparison of the recorded pressure traces for 5 different pressure fluctuation types and the assumed fluctuation shape and node line.
side, leading to higher charge air temperatures around these and higher probability of hot spots.

- In the cases where the sensors are ringing out of phase, the blue trace is shifted by $180^\circ$, whereas the red trace is in phase with the rest of the cases. This indicates that the ignition point is again near the red sensor, again supporting the conclusion above.

- The cases where the blue sensor exhibits a clearly higher fluctuation than the red are less than 10\% of the total, and could be caused by local hot spots due to existence of lube oil mist which spontaneously oxidises, or inhomogeneity of burned gas from the previous cycle. Alternatively they can be caused by random turbulent effects of the particular spray cone which result in mixture formations which promote autoignition.

Overall, the results show that the pressure fluctuations are most probably caused by differences in autoignition points, enhanced by temperature gradients in the combustion chamber.

### 4.2.6 Effects of Pressure Fluctuations on a Spray

Past research has shown increased fuel-air mixing as a result of acoustic excitation of sprays, resulting in a shorter and broader flame and increasing
Figure 4.17: Effects of acoustic excitation of 2bar at 1000Hz on temperature, mass fraction of fuel vapor and turbulent kinetic energy distribution at 3ms after SOI.

HRR [64–73]. In the present study, numerical simulations of a single spray within a constant volume combustion chamber have been used to study the effects of pressure fluctuations on spray formation and fuel-air mixing. As described in section 3.2.4, the study was focused first on the effects of pressure fluctuations on non-reactive sprays, in order to determine the effects on spray formation and fuel-air mixing under imposed pressure fluctuations. This is followed by reactive spray simulations, where the effects on combustion rate and flame shape are investigated. Both simulation setups were initially validated against experimental data under non-acoustic conditions. More information about the simulation validation can be found in [95].

**Effects of pressure fluctuations on non-reactive sprays**

The main focus in the non-reactive spray simulations was to determine the effect of pressure fluctuations on the physical parameters which influence the flow-spray interaction, turbulence and fuel-air mixing.

**Effects of pressure fluctuations on the spray shape**

Figure 4.17 shows the temperature, mass fraction of fuel and turbulent kinetic energy distribution of the non-reactive spray under acoustic excita-
Figure 4.18: Turbulent kinetic energy for non-acoustically and acoustically excited (2bar at 1000Hz) sprays at 3ms after SOI.

tion of 2 bar intensity and 1000Hz frequency. As expected, the addition of an acoustic excitation vertical to the direction of the spray causes a lateral movement of the spray corresponding to the frequency of the excitation.

The alternating pressure gradient introduced results in a velocity component vertical to the direction of the spray, which varies in magnitude with time, while alternating from positive to negative. This results in the characteristic shape that is shown in Figure 4.17, where, depending on the time of introduction into the cylinder, the fuel droplets are diverted from the spray axis towards the walls. This vertical velocity component results in a shorter and wider spray, as was previously observed in [64].

The imposed pressure fluctuations also result in a significantly higher turbulent kinetic energy dissipation rate, as can be seen in Figure 4.18, which compares the turbulent kinetic energy distribution for a non-excited and an excited case 3ms after start of injection. Note that the maximum turbulent kinetic energy in the non-excited case is about 9 times higher than the excited case ($662.2 \text{m}^2/\text{s}^2$ compared to $75.8 \text{m}^2/\text{s}^2$) at this point. This results in higher fuel-air mixing and air entrainment in the spray.
Effects of pressure fluctuation frequency

The effects of the pressure fluctuation frequency on the spray formation and fuel-air mixing were studied by varying the excitation frequency while keeping injection and charge air parameters and fluctuation intensity constant. In order to quantify the degree of mixing of fuel and air for each case, the two following quantities were calculated:

- the area of the iso-surface at stoichiometric conditions
- the total mass of fuel near to stoichiometric conditions

Figure 4.19 shows the variations of the two parameters introduced above with changing excitation frequency for different times after start of injection, normalised by the values for the non-acoustically excited case. Both quantities increase rapidly and show a peak between 2 and 4kHz for this setup, and then decrease gradually towards the non-acoustically excited values. In both cases, the maximum value is around 60% higher than the corresponding value without the pressure fluctuations, indicating a significantly faster mixing under these excitation conditions.

A deeper understanding of the results presented above, as well as the trends observed, can be obtained by studying the cause of increased mixing under conditions with induced pressure oscillations. As mentioned previously and shown in Figure 4.18, the introduction of the acoustic field results in a more even distribution of the turbulent kinetic energy in space, with
lower resulting maximum values of kinetic energy. This distribution of kinetic energy results from the spatial pressure gradient introduced by the pressure fluctuations, which results in a motion of the flow vertical to the spray direction, resulting in the transport of the kinetic energy.

The pressure gradient between two positions due to the pressure oscillations also results in a lateral transport of fuel. The combination of the lateral transport of turbulent kinetic energy and fuel results in a increased mixing observed; if either turbulent kinetic energy or fuel was transported individually, no increase in mixing would be observed. A transport of turbulent kinetic energy without fuel would result in a dissipation of kinetic energy without increased mixing of fuel with air, whereas a transport of fuel only would result in a lateral motion of fuel, which will be subsequently brought back to its original position. The combination of the two results in increased mixing, with only part of the fuel returning to the original position.

In order to comprehend the effect of pressure fluctuation frequency on the abovementioned source of increased mixing, the understanding of the connection between frequency and wavelength is important. It is commonly known that the frequency of the oscillation, which represents the number of changes in flow direction at a single point in space per unit time, is inversely proportional to the wavelength, which is a measure of the gradient of the pressure:

\[
\lambda = \frac{\alpha_{\text{air}}}{f}
\]  

(4.2)

where \(\lambda\) is the wavelength, \(\alpha_{\text{air}}\) is the speed of sound of air and \(f\) is the frequency of oscillation.

Thus, higher frequency of oscillation results in increased changes in direction per unit time, while also resulting in increased pressure gradients due to the lower wavelength. On the one hand a high rate of changes in direction results in limited lateral movement away from the spray core, resulting in reduced mixing. On the other hand, increased pressure gradients result in increased lateral velocity components in the flow, resulting in increased mixing. The combination of the two effects results in the existence of an optimum frequency, where the changes in direction per unit time and the induced lateral velocity resulting from the pressure gradient result in a maximum of transport of turbulence and fuel away from the spray axis.

The result of the above description can be seen graphically in Figure
4.20, where the turbulent kinetic energy distribution of the same spray at non-acoustically excited (left) and acoustically excited at 2500Hz (centre) and 18000Hz (right) is shown at 4ms after SOI. The figures show an increased distribution of the turbulent kinetic energy at 2500Hz compared to 18000Hz, resulting from the increased lateral movement due to more time for the transport of fuel and turbulence at these conditions, as was shown previously in Figure 4.19.

Effects of pressure fluctuation intensity

The effects of the pressure fluctuation intensity on fuel air-mixing in a spray have been studied in this section by varying the intensity of the forced acoustic excitation at a constant frequency of 2500Hz. Figure 4.21 shows the increase in surface area and fuel mass of the mixture at stoichiometric conditions for different times after SOI as a function of pressure fluctuation intensity, normalized by the area and mass respectively of the spray at non-excited conditions.

Both plots show an increase in the area and mass respectively, with increasing intensity. The mass of fuel at near stoichiometric conditions increases monotonically with increased pressure fluctuations, as expected. This is caused by the increased pressure gradient arising from increased intensity, which results in higher induced velocity vertical to the spray direction. The stoichiometric surface area initially increases and then decreases for
Figure 4.21: Spray stoichiometric surface area and fuel mass available around stoichiometric conditions for varying acoustic excitation intensities at different times after SOI and at constant 2500Hz excitation frequency, normalized by the non-acoustically excited values.

Figure 4.22: Mixture fraction distribution for acoustically excited sprays at 2 bar (left) and 5 bar (right) intensity and 2500Hz, 4ms after SOI.

these conditions at intensities above 3 bar. The reason for the observed decrease in area is the excessive wrinkling of the spray arising at very high fluctuation intensities, which results in fragmentation of the stoichiometric iso-surface, thus resulting in a smaller nominal area, even though air-fuel mixing is increased. This can be clearly seen in Figure 4.22, where the mixture fraction distribution is shown for two acoustically excited sprays at 2500Hz frequency, the one with 2 bar (left) and the other with 5 bar fluctuation intensity.
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Figure 4.23: Temperature distribution for non-acoustically excited, reactive (left), acoustically excited non-reactive (centre) and reactive (right) at 2 bar intensity and 1000Hz fluctuation frequency, 3ms after SOI.

Effects of pressure fluctuations on reactive sprays

In the following section, the influence of pressure fluctuations on fuel sprays which are allowed to chemically interact with their surroundings are studied for various fluctuation frequencies and intensities. The analysis presented in the previous section on non-reactive sprays showed that pressure fluctuations increased air-fuel mixing, with increasing mixing at increasing fluctuation intensity, and a maximum increase in stoichiometric mass of 60% at 2500Hz excitation frequency and 2bar excitation intensity. In this section the main focus has been placed on the effects of pressure fluctuations on flame shape and length, as well as the rate of heat release.

Effects of pressure fluctuations on the flame shape

Figures 4.23, 4.24 and 4.25 show the temperature, mixture fraction and turbulent kinetic energy distributions respectively, for non-acoustically excited reactive (left), acoustically excited non-reactive (centre) and reactive (right) at 2 bar intensity and 1000Hz fluctuation frequency, 3ms after SOI. The three figures show that the increase in fuel-air mixing resulting from the imposed pressure fluctuations result in a shortening and broadening of the flame, as was also observed in the experiments in [64]. The fuel which
is carried away of the spray core and is mixed with the surrounding air is oxidized faster, resulting in the observed shorter flame and the increase in
peak temperature shown in Figure 4.23.

The effects of the turbulence-combustion interaction are shown in Figure 4.25 where the maximum turbulent kinetic energy at the acoustic reactive spray (shown in dark red) is higher than in the non-acoustically excited case. This leads to the conclusion that there is an interaction between the chemical reactions and the acoustic field, as will be discussed further in the following section.

Effects of pressure fluctuations on the heat release rate

To study the effects of pressure fluctuations on HRR, the oxygen consumption with time was studied for different cases. This was chosen in place of the release of energy due to the inability to calculate the HRR from the pressure using the first law of thermodynamics approach as is customary because of the error induced from the forced pressure fluctuations.

Figure 4.26 shows the total mass of oxygen consumed with time for non-acoustically excited and acoustically excited flames. The plot shows a significant increase in the rate of oxygen consumption for the acoustic case, both for what is perceived to be the premixed and the diffusion phases of combustion, indicating an influence on chemistry as well as the physical mixing. In the acoustically excited case, the ignition delay is slightly shorter, indicating an increase in the chemical reaction speed in addition to the faster mixture preparation. The increased chemical reaction speed can be attributed to the exponential dependency of the chemical reactions to temperature, and thus to local pressure fluctuations which could be approximated as local adiabatic compressions/expansions. Chemical-acoustic interactions are discussed further in section 5.1.3 as well as in [62].

A faster chemical reaction speed is also observed during the premixed combustion phase, where the slope of the oxygen consumption is steeper for the acoustically excited case. Furthermore, an equal proportion of fuel is consumed during premixed combustion in the acoustically excited case, despite the earlier ignition. This can be explained by the increased mixing during the ID period for this case, which results in more fuel being available for combustion earlier in time.

Finally, during the diffusion combustion phase, again the acoustically excited case shows a steeper slope when compared to the non-acoustic case. This observation can be attributed mainly to the increased air-fuel mixing caused by the pressure fluctuations, as was observed in the non-reactive
Cases, which results in higher HRR.

In addition to the increased mixing caused by the fluctuations, there is a positive correlation between HRR and pressure, which can be seen as a superimposed fluctuation in the oxygen consumption graph. This serves as a further indication of the influence of the pressure fluctuations on the chemical reaction speed.

Effects of pressure fluctuation frequency

The effects of changes in the pressure fluctuation frequency on the oxygen consumption rate, and thus the HRR, at different times after start of injection can be seen in Figure 4.27. The figure shows the variation of consumed oxygen at 2, 3 and 4ms after SOI for different pressure fluctuation frequencies and 2 bar pressure fluctuation intensity, normalised by the consumed oxygen without pressure fluctuations at the same points in time after SOI.

Contrary to the observations of the non-reactive cases, the influence of the fluctuation frequency is limited on the HRR. The plot shows a relatively
constant increase in the HRR, ranging from about 10% to 18%, irrespective of the excitation frequency. This is possibly contrary to what was expected, since the influence of the frequency on the mixing was expected to have a similar effect on the observed HRR.

Based on the observations above and the findings of the study of the non-reactive sprays, one can conclude the following:

- The increase in HRR due to pressure fluctuations is partially caused by the increased pre-mixing of the spray before ignition, as was observed in the non-reactive cases, which increases the amount of premixed combustion.

- During both premixed and diffusion combustion, the influence of pressure fluctuations on chemistry is significant. The higher frequency of pressure oscillations result in faster compressions/expansions, which result in higher local temperature fluctuations due to the limited time for heat losses, thus increasing the effect on HRR. This counter-balances the effect of reduced mixing at higher oscillation

\textbf{Figure 4.27:} Total mass of consumed oxygen for different fluctuation frequencies and 2 bar pressure fluctuation intensity, normalised by the mass of consumed oxygen for the non-acoustically excited case, at 2, 3 and 4ms after SOI.
• There exists an interaction between the combustion and the local turbulent kinetic energy, as was shown in Figure 4.25, which is independent of excitation frequency and results in increased diffusion combustion rate.

Effects of pressure fluctuation intensity

The variation of oxygen consumption with increasing pressure fluctuation intensity is shown in Figure 4.28. The figure shows the mass of consumed oxygen for different pressure fluctuation intensities and 2500Hz fluctuation frequency, normalized by the oxygen consumption of the non-acoustic case, at 2, 3 and 4ms after SOI.

The results show a monotonic increase in HRR with Pressure fluctuation intensity, as expected. This result can be attributed to the fact that increases in the pressure fluctuation intensity result in increases in both the mixing and the chemical reactivity, thus leading to higher HRR.
4.2.7 Effects of Pressure Fluctuations on HRR

As discussed in the introduction and was shown in the previous section through 3D CFD investigations on a constant volume combustion chamber, the presence of pressure oscillations in various combustion systems has been shown to increase heat release rate due to increased mixing of fuel and air and chemical reactivity. To this author’s knowledge, to this point there has been no mention of such effects in internal combustion engines.

In order to determine any such effects, a detailed analysis of the pressure trace to deduce the apparent HRR for each individual cycle is required. Throughout the following analysis, 150 consecutive cycles at constant charge air and injection conditions were used. This was done in order to ensure that the observed effects were due to cycle-to-cycle variations and not due to other charge air or injection effects.

To study the effects of pressure fluctuations on apparent HRR in detail, two individual cycles from Miller 3 configurations at medium load are used. Figure 4.29 shows the unfiltered and the resulting filtered pressure traces for two cycles at constant injection and charge air conditions, with and without ringing.

It is interesting to note that the cycles shown in Figure 4.29 are consecutive cycles on the same cylinder, which leads to the assumption that conditions (temperature, pressure, spray formation etc.) are constant. The observed difference in resulting peak pressure between the two cycles is shown to be larger than 10bar.
Figure 4.30: Injection rate and resulting HRR (left) and integrated HRR (right) of two consecutive cycles showing ringing and not ringing combustion, at a medium load with the Miller 3 valve timing configuration.

The HRR analysis of the two pressure traces shows clear differences in the burn rate between them. Figure 4.30 shows the HRR and integrated HRR for the two cycles. From these plots it is clear that even though the ID and the premixed combustion phase are similar in both cycles, the diffusion combustion in the high ringing cycle is much faster.

Effects of pressure fluctuations on the apparent mixing rate

To study the effects of pressure fluctuations on HRR in depth, it is helpful to use the apparent characteristic mixing time ($\tau_{mix}$) which is deduced from the HRR and was introduced in section 2.4. As mentioned previously, $\tau_{mix}$ is a spatially global measure of air-fuel mixing during diffusion combustion. Figure 4.31 shows the calculated inverse characteristic mixing time plotted against crank angle for the same high and low ringing cycles. The plot suggests a connection between the occurrence of pressure oscillations and the speed of diffusion HRR. Since the pressure oscillations arise during the premixed combustion phase, the spray to this point and the premixed combustion are expected to remain generally unaffected. The effects are seen during the mixing controlled diffusion combustion phase, where the apparent heat release rate and the deduced apparent mixing rate are significantly increased for the cycle which exhibits ringing. It is interesting to see that the calculated mixing rate is significantly increased for most of the cycle, until well after the end of injection (see Figure 4.30 for injection rate). Nonetheless, the mixing rate during the injection duration is mostly
Figure 4.31: Calculated inverse characteristic mixing time of two consecutive cycles showing ringing and not ringing combustion, at a medium load with the Miller 3 valve timing configuration.

Figure 4.32: Maximum value of calculated inverse characteristic mixing time of 150 consecutive cycles at a medium load with the Miller 3 valve timing configuration, plotted against the individual cycle pressure fluctuation intensity.
affected by the pressure fluctuations. The calculation of the peak apparent mixing rate for multiple cycles can be used to establish a trend connecting the intensity of pressure fluctuations and diffusion HRR for a cycle. Figure 4.32 shows the maximum of the calculated inverse characteristic mixing time plotted against the intensity of the pressure oscillation for each of the 150 consecutive cycles at constant, long ID conditions. The results show a clear increase of cycle mixing rate, resulting from higher diffusion combustion rate at cycles with higher pressure oscillation intensity.

4.2.8 Effects of Pressure Fluctuations on Emissions

In section 4.2.4 a thorough investigation of the cyclic variability of emissions under long ignition delay conditions was presented. This investigation showed an increase of cyclic variability in both observed in-cylinder soot cloud density and single-cycle NO concentration in the exhaust when ignition delay was increased. These investigations also showed that these cyclic variations could be partially connected to the observed pressure oscillations induced at random by the premixed combustion. In the following subsections the observed effects of pressure fluctuations on single cycle in-cylinder soot evolution and NO emissions will be presented.

Effects of pressure fluctuations on in-cylinder soot

As described in section 2.2.4, the study of the soot evolution during individual cycles at long ignition delay conditions were conducted on the LERF engine testbench using the OLP sensor. In order to determine any effects of pressure oscillations on soot evolution the same two cycles at the Miller 3 engine configuration are used also in this investigation. These two characteristic cycles are used here to establish a first understanding of observed effects. This is followed by a study of the full range of 150 cycles, where characteristic points in the $KL$ evolution are used to deduce more generalised trends.

The $KL$ factor traces for the two previously described high and low ringing cycles are shown in Figure 4.33. The stark differences observed in the mixing rates are also depicted in the measured $KL$ factors.

The soot formation rates are similar for both cases. However, the oxidation rate in the high ringing cycle is shown to be significantly higher than the
low ringing cycle. Initially, the high oxidation rate leads to a very fast drop in the increase of the $KL$ value, leading to a significantly lower $KL$ peak. This is followed by a negative slope in the $KL$ trace which seems to be similar in both cases. However, if one considers the amount of soot present in either case, the resulting oxidation rate, normalized by the soot concentration in each case, is considerably higher for the high ringing cycle. It is interesting to note that the difference in $KL$ value between the two cycles starts being clearly visible around $370^\circ$CA, which corresponds approximately to the end of fuel injection (Figure 4.30), even though the apparent mixing rate is higher earlier in the cycle (Figure 4.31). Prior research has shown that towards the end of injection, soot oxidation starts being dominant. This, coupled to the fact that $KL$ is very similar for both cycles before $370^\circ$CA, gives a further indication that pressure oscillations affect mainly soot oxidation rather than soot formation.

Figure 4.34 presents the measured 2-colour soot temperature results. These are to be expected, considering the previously presented results from the HRR and mixing rate analysis for the two cycles. The measured soot temperature for the cycle that exhibits high ringing is around 50K higher than the low ringing cycle for the initial part of diffusion combustion.
This is the direct result of the significantly higher HRR during this time, which results in higher flame temperatures. As has been observed in the $KL$ factor trace, following the 380°CA point the calculation of the soot temperature for the high ringing cycle is stopped, since the black body temperature is reduced to below the threshold value of 1300K.

The characteristic points on the $KL$ trace which indicate a faster oxidation rate with increasing ringing intensity can be studied for all 150 cycles at constant conditions (Figure 4.35).

Figure 4.35a shows how the initial slope of the $KL$ factor, representing the soot formation rate, varies with the pressure oscillation intensity. Even though there is a slight variation in formation rate between individual cycles, no direct connection between pressure oscillation intensity and soot formation can be observed. This leads to the conclusion that the pressure oscillations do not in this case cause a clear reduction in soot formation. This observation is opposing what was reported in [70], where higher oxygen presence in the flame due to pressure oscillations reduced soot production. However, one should stress that premixed flames were studied in [70], where the enhanced mixing increased the oxygen content in the regions before the flame location, essentially leading to combustion in leaner
Figure 4.35: Calculated characteristic cycle soot formation rate (a), maximum value of KL factor (b) and characteristic soot oxidation rate (c) of 150 consecutive cycles at a medium load with the Miller 3 valve timing configuration, plotted against the individual cycle pressure fluctuation intensity.
conditions. During diffusion combustion in the DI diesel case, one should expect increased air-fuel mixing to lead to a shift of the location of the flame regions towards the direction of the rich spray core, but the flame regions are still expected to be at near-stoichiometric locations. This is expected to lead to similar levels of soot formation, irrespective of air-fuel mixing rates.

On the contrary, the value of the peak of $KL$ during the cycle clearly shows a strong dependency on pressure oscillation intensity (Figure 4.35b). Even considering the dependency of peak $KL$ on both soot formation and soot oxidation, the clear relation between peak $KL$ and the intensity of oscillation observed can be attributed to significantly increased early soot oxidation caused by the oscillations, since the soot formation was found to be relatively constant irrespective of oscillation intensity. This result is consistent with previous research on spray combustion [66,70–72], which showed increased oxidation rate in the presence of pressure oscillations. This observation however contradicts results from [39], where the maximum soot concentration during a single cycle was observed to be positively correlated with pressure oscillation intensity. This is understood to be caused by the fact that in [39], very limited diffusion combustion was present due to the low loads studied (short injection duration), and measured soot luminosity was from pool fires resulting from fuel impinged on the piston surface.

The results of the study of the slope of $KL$ during what is assumed to be pure soot oxidation showed that the late stages of soot oxidation are only faintly affected by pressure oscillations. Figure 4.35c shows the variation of the slope of the $KL$ trace, normalised by the maximum value of $KL$ for each individual cycle, with pressure oscillation intensity. As mentioned previously, the normalisation of the slope is done in order to have a comparative measure of oxidation rate, which is clearly dependent on initial soot concentration in the cylinder. The wide spread of the points does not allow any concrete conclusions to be derived from the plot, other than a weak dependency of soot oxidation on pressure oscillation intensity, similar to the previous conclusion (Figure 4.35b).

Finally, Figure 4.36 shows the variation of maximum soot temperature measured using the OLP plotted against the in-cylinder pressure fluctuation intensity. The plot shows a significant increase in soot temperature of the order of up to 100K with increasing pressure fluctuation intensity. This can be understood to be a result of increased mixing in the flame, leading
to increased temperatures of the flame. In addition, the reduced presence of soot in the highly fluctuating cycles, as shown in Figures 4.34 and 4.35b, is expected to result in reduced radiation cooling of the flame, further increasing flame temperature, as was shown in [70]. The measured increased soot temperature can also be used, in combination with the measured increased mixing, to explain the increase in soot oxidation, since the reaction rate of soot oxidation is exponentially dependent on temperature [108,109]. The effects of the increased flame temperature on emissions are analysed further in Chapter 5: Discussion.

Effects of pressure fluctuations on exhaust gas NO emissions

Similarly to the investigations of the observed effects of pressure fluctuations on soot cloud density evolution, the effects on single cycle NO concentration in the exhaust has been studied using the MTU single-cylinder testbench. The conditions used for this investigation are the same short ID (‘stable’) and long ID (‘unstable’) conditions described in section 2.1.2. Naturally, due to the imposed charge air conditions, which were chosen to be vastly different in terms of temperature and pressure in order to
achieve large differences in ID, the absolute levels of NO emissions from the two cases cannot be compared directly. Nonetheless, relative values of NO emissions, normalised by the average NO concentration measured for all cycles can be used.

Figure 4.37 shows the the normalised individual cycle measurements of NO concentration using exhaust gas sampling above the exhaust valve plotted against the cycle pressure fluctuation intensity, for 25 short ID cycles and 40 long ID cycles. The long ID cycles have been displaced by 2% to higher values, in order to create an estimated ”fit” of the two measurements.

The results show a clear increase in cyclic variation for the long ID case, as was reported in section 4.2.4. The NO concentration in the short ID case fluctuates by ±4% around the mean, whereas in the long ID case the peak-to-peak value is almost 12%.

Furthermore, as expected, an increase in pressure fluctuation intensity can be observed for the long ID case, with the value of the maximum FFT of a single cycle at 4000Hz doubling from 0.04 to 0.08. This has come as the result of a ID increase from about 0.3ms in the short ID case to about 0.85ms in the long ID case.

Nonetheless, the maximum fluctuation intensity achieved in the long ID
case is significantly lower than the one measured in the LERF engine with the Miller 3 configuration (see Figures 4.32, 4.35). This can be attributed to two factors:

- The maximum ignition delay achievable in the MTU engine is significantly lower than the Miller 3 configuration of the LERF engine, due to higher end-of-compression temperatures (810K compared to 740K for Miller 3). Thus the energy released during premixed HRR is lower in the MTU engine long ID case compared to Miller 3 at medium load, resulting in lower fluctuation intensity. According to the results presented in Figure 4.14 for various Miller valve timings on the LERF engine, the average cycle fluctuation intensity for 0.85ms ignition delay is 0.06, which is only slightly higher than the value measured in the MTU engine under long ID conditions (0.05).

- In addition to the above, the in-cylinder pressure chosen for the MTU engine (around 40bar at SOI) was significantly lower than the Miller 3 medium load point in the LERF engine (around 65bar at SOI). This difference was necessary in order to increase the ID in the MTU engine to achieve increased proportion of premixed combustion, considering the lowest achievable TDC temperature with the testbed configuration was 810K. The reduced in-cylinder pressure and air density leads to increased spray penetration, with the spray hitting the piston bowl prior to ignition, leading to piston wetting in the case of the MTU engine. Using the empirical correlation for spray penetration as a function of time, charge air density and temperature, fuel injection pressure and nozzle geometry from [110], as well as the relevant piston geometries, it was calculated that at the long ID conditions in the MTU it takes 0.6ms for the spray to reach the piston surface. Thus at the start of combustion (ID=0.85ms), part of the spray will be impinged on the piston. This is expected to reduce the amount of fuel available during premixed combustion, leading to reduced pressure rise rates which result in reduced pressure oscillation intensities. In contrast, in the LERF engine at Miller 3 conditions, the spray was calculated to have travelled 0.71mm in 1.1ms, well below the piston bowl distance which is at 0.78mm.

Despite the abovementioned limitations, Figure 4.37 shows a slight trend of increased cycle NO with increased pressure oscillation intensity. At
high pressure fluctuation intensity (>0.05), all measured cycles showed above-average exhaust NO concentration values. These results lead to the assumption that the increased air-fuel mixing observed for cycles with increased pressure fluctuations, which was shown to lead to increased diffusion HRR and soot oxidation rate, also leads to increased thermal NO formation. This conclusion can be further supported by the higher soot temperatures measured for fluctuating cycles in Figure 4.36, indicating higher flame temperature in combination to the the presence of excess oxygen during combustion and in the post-combustion gases.

These results are in line with similar investigations from acoustically excited non-premixed spray combustion, albeit in atmospheric conditions [67,69,70]. The understanding is that increased mixing due to the pressure fluctuations leads to increased temperature and oxygen availability to the flame, leading to an increased volume near stoichiometry in rich diffusion flames.
Chapter 5

Discussion

In the previous chapter, various distinct but possibly correlated characteristics of combustion with increasing Miller degree were presented. In this chapter an understanding of the effects with respect to $NO_x$ emissions of these observations is offered.

The primary observation of the experimental investigations has been the existence of a $NO_x$ minimum when attempting to reduce $NO_x$ emissions through successive charge air temperature reduction. As shown in section 4.1.1, beyond the temperature point where $NO_x$ reaches a minimum, further temperature reduction results in increased $NO_x$ emissions and eventual deterioration of the $NO_x$-SFC tradeoff. This goes contrary to theory and expectations, which state that a reduction in reactant temperature will lead to a reduction in adiabatic flame temperature, and thus to lower $NO_x$ levels.

As mentioned in the Introduction, numerous studies on the understanding of this reversal in $NO_x$ trends can be found in the literature. In various experimental investigations a relation between the proportion of premixed combustion and $NO_x$ has been observed. At constant injection conditions, the proportion of premixed combustion is directly proportional to ID, and thus lower temperature leads to greater proportion of premixed combustion. It has been argued that beyond a threshold, the increase of $NO_x$ due to the higher proportion of premixed combustion surpasses the reduction of $NO_x$ as a result of colder reactants, thus justifying the observed reversal in trends.

Contrary to what is commonly expected, it has been proven that a single variable such as the adiabatic flame temperature is unable to capture all $NO_x$ trends, since $NO_x$ production is a very complex process, likely to be a function of more than a single global parameter. Therefore, a more
in-depth understanding of the causes of this trend reversal is important. This chapter serves to aggregate the information presented in Chapter 4 and formulate an understanding of the individual effects of long ignition delay on \( NO_x \) emissions; in particular the observed \( NO_x \) trend reversal. Mirroring the \( NO_x \) production process, the presentation of effects is split into three categories:

- Effects which increase local temperature and thus increase \( NO_x \) production rate

- Effects which increase oxygen availability to the flame and surrounding regions, increasing \( NO_x \) production rate

- Increases in \( NO_x \) production rate through means not connected to local temperature or oxygen concentration

This aims to provide a more detailed insight into the interconnection of the individual observations and effects.

### 5.1 Effects Leading to Increased Temperature

It is well understood that high local temperatures created during combustion are the main driving force behind \( NO_x \) production in DI diesel engines. As mentioned in section 1.1, the reactions that lead to \( NO_x \) formation are exponentially dependent on temperature. In particular the thermal NO pathway, which is understood to account for around 80% of the total NO formed in diesel engines \([2, 6]\), is only significant at temperatures above 2000K. Thus, changes in the local temperature can result in significant changes in the exhaust \( NO_x \). This section looks into characteristics of combustion under extreme Miller valve timing and with long ID which can result in an increased local temperature promoting \( NO_x \) production mainly through the thermal NO route.
5.1.1 HRR Effects Leading to Increased Temperature

The main source of heat which results in in-cylinder $NO_x$ formation is the oxidation of injected fuel with air. Increases in the HRR are expected to result in increased local temperature in and around the flame regions, and as a result enhanced $NO_x$ formation. The experimental and simulation results presented in Chapter 4 showed increased average and single cycle HRR under longer ID arising from lower charge temperatures. These increases are expected to contribute to the $NO_x$ trend reversal in the following ways:

**Increased mixing due to spray penetration**

The computational investigation presented in section 4.2.1 showed that prolonged ID results in increased spray penetration. The spray penetration is directly related to air engulfment and ultimately oxygen usage, since the oxygen at the regions of the cylinder at the squish region and near the walls are reached by the fuel spray. Increasing the spray penetration thus leads to increased combustion rate which results in higher local temperatures. This increase in local temperature is expected to lead to higher $NO_x$ production rates, leading to higher exhaust gas $NO_x$ emissions.

**Increased mixing due to pressure fluctuations in single cycles**

The experiments conducted in the present study, presented in sections 4.2.3 and 4.2.5, showed increased cycle-to-cycle variation and increased individual cycle pressure fluctuation intensity arising from premixed combustion. The increased Miller degree was shown to result in an exponential increase in the average fluctuation intensity of all cycles with longer ID, as shown in Figure 4.14.

The individual cycle HRR analysis performed in section 4.2.7 showed that cycles with high pressure fluctuation intensity have significantly increased diffusion HRR. In addition to this, the simulation results of a single spray under forced acoustic excitation presented in section 4.2.6 showed increased HRR with increasing pressure fluctuation intensity, leading to higher peak temperatures. As presented in Chapter 1, such coupling of pressure fluctuation intensity and HRR has been previously observed in droplet combus-
tion [58–61] and spray combustion [64–73], but, to this author’s knowledge, never before in internal combustion engines.

The cycles which present increased HRR are expected to contribute more \( NO_x \) emissions than the average cycle, due to the higher local temperatures present. The findings presented in section 4.2.8, where measured soot and consequently flame temperatures were shown to increase with increasing pressure fluctuation intensity, support this train of thought.

This was also the case in rich diffusion flames [67, 69, 70], where increased mixing caused from pressure fluctuations resulted in higher flame temperatures and thus \( NO_x \) formation. In fact, due to the exponential dependency of \( NO_x \) production rate on temperature, the ringing cycles are expected to increase the average \( NO_x \) emissions significantly. This assumption is further supported by the findings in section 4.2.8, where single-cycle NO concentration in the exhaust of the MTU engine were shown to increase with higher pressure fluctuation intensity.

In addition to the effects which lead to increases in local temperature presented above, higher combustion rates additionally result in increased cylinder pressure earlier in the cycle, leading to further increases in the local and global temperature, as is argued in [19]. On the one hand the reactants which enter the diffusion flame are hotter, resulting in higher combustion temperature. On the other hand, the reactants produced early in the cycle are further compressed, increasing their temperature and thus \( NO_x \) production in the burned gases. Furthermore, the reduced duration of combustion results in less time for heat transfer to occur, resulting in higher temperatures in the burned gases, similarly to what has been previously reported in [111].

Overall, the effects presented in the discussion above are expected to result in higher average \( NO_x \) formation. Nonetheless, it should be noted that since the above effects improve the efficiency and thus the SFC of the engine due to faster combustion, their combined effect on the \( NO_x \)-SFC tradeoff is not necessarily unfavorable (being equivalent to increasing injection pressure).
5.1.2 Radiation Heat Transfer Effects Leading to Increased Temperature

Previous experimental and computational research has shown that increased ID and proportion of premixed combustion are expected to produce less soot, leading to reduced radiative heat transfer from the flame [112–114]. It is argued that this reduction in heat transfer could lead to increased NO\textsubscript{x} emissions due to higher flame temperatures.

In [113] the influence of soot radiation on in-cylinder temperature and NO\textsubscript{x} formation is studied at various engine conditions. Cases with increased ID showed less soot radiation, which is normally expected to reduce flame temperature by 25-50K. This temperature reduction is expected to result in a NO\textsubscript{x} reduction of above 10%. Thus, the reduced presence of soot during combustion can result in reduced radiation cooling of the flame, increasing flame temperature and as a result NO\textsubscript{x} formation. Similar effects can be expected in the present experiments, where long ignition delays lead to increased premixed combustion proportions. Furthermore, as outlined in section 1.5.1, spray combustion in the presence of pressure fluctuations is believed to lead to reduced soot production [70] and increased soot oxidation [66,70–72].

In the present DI diesel engine experiments, the in-cylinder optical measurements of cycles showing increased pressure fluctuation intensity presented with decreased peak KL values and slightly increased late soot oxidation rates (Figures 4.35a-c). While no clear reduction of soot formation was observed, the increased soot oxidation is believed to arise from increased dilution, which also led to increased diffusion HRR as presented previously. This conclusion is in line with experimental results from [37,38] obtained from an optically accessible DI diesel engine, which showed movement of the soot cloud similar to that caused by swirl, due to pressure oscillations induced by the premixed combustion. Furthermore, soot temperature was measured to scale with pressure fluctuation intensity (Figure 4.34), supporting this theory.

Overall, the observed reduction of soot cloud density due to prolonged ID and pressure fluctuations are expected to lead to a reduction in the radiation heat losses from the flame. This in turn leads to increased flame temperature, thus resulting in enhanced thermal NO\textsubscript{x} production rate.
5.1.3 Increased Local Reactivity due to Pressure Fluctuations in Single Cycles

The presence of pressure fluctuations in reactive flows has been extensively studied in gas turbine reactors, where acoustic excitations are commonplace. In relation to the present experiments, there is limited potential for parallelization of acoustic effects between gas turbine reactors and diesel engines, due to the different natures of the source of excitation. Nonetheless, according to [62], the presence of pressure oscillations can influence chemical reaction rates due to local temperature and pressure effects. Chemical reaction rates, which are generally known to be of Arrhenius type, are exponentially dependent on temperature. These reactions include the exothermal reaction of hydrocarbon oxidation, as well as the nitrogen oxidation to form NO. A pressure fluctuation will cause a local temperature fluctuation, which will have an average temperature equal to the mean of the two temperature peaks. However, due to their exponential dependency on temperature, reactions will be accelerated more by the positive temperature cycle of the oscillation than the negative one. This will result in a net reaction rate in the presence of fluctuations which will be higher than the reaction rate if the temperature was constant and equal to the mean. Thus, in the presence of pressure fluctuations, the HC reaction and $NO_x$ production rates will be higher, resulting in higher flame temperatures and enhanced $NO_x$ production. The effects of pressure fluctuations on chemical reaction rate were seen in the computational investigation in section 4.2.6, where the HRR of a spray under acoustically excited conditions was shown to fluctuate as a result of the fluctuations.

Naturally the experimental validation of this theory is very complicated, due to the incapabilities to run controlled experiments in such environments, to measure time- and spatially-resolved NO concentrations and to decouple the effects of pressure fluctuations on chemical kinetics from other effects. Nonetheless, assuming the pressure fluctuations are fast enough to be considered isentropic compressions and expansions, one can calculate a 3.2% increase in the NO production rate for a cycle with $60\pm5\text{bar}$ compared to the average cycle, assuming an average temperature of $2200\text{K}$ and the reduced Zeldovich mechanism. For a cycle with $60\pm10\text{bar}$ fluctuations, the in NO production rate is increased to around 13% compared with the a constant pressure cycle.
5.2 Mixing Effects Leading to Increased Oxygen

As mentioned previously, the $NO_x$ production rate is a function of temperature and oxygen availability. Thus, any effects leading to increased oxygen in the flame and the high temperature post-flame gases will lead to higher NO formation. In this section the effects of observed combustion characteristics under extreme Miller timing are studied with respect to their consequences on oxygen availability at the high temperature regions in-cylinder.

5.2.1 Increased Mixing due to Spray Penetration

As shown in section 4.2.1, prolonged ID leads to increased spray penetration, resulting in increased air entrapment and improved oxygen utilization. Albeit important for CO and HC emission reduction as well as soot oxidation, the increased oxygen availability in the flame and in the hot burned gas regions is expected to result in increased $NO_x$ production.

5.2.2 Increased Mixing due to Pressure Fluctuations in Single Cycles

The increase of air-fuel mixing observed in single cycles due to pressure oscillations, as presented in sections 4.2.6, 4.2.7 and 4.2.8, should also lead to increased oxygen availability. This is further supported by the fact that faster soot oxidation was observed in the fluctuating cycles, as shown in Figures 4.33 and 4.35b,c. The increased mixing in the flame due to the pressure fluctuations is expected to contribute to the increase of $NO_x$ emissions, as was observed in [67,69,70].

5.3 Increased $NO_x$ Formation due to Other Effects

Apart from the increase in $NO_x$ formation expected from increased flame temperature and oxygen availability, due to mixing and reduced radiation
heat transfer effects, there are two further suggested reasons for increased $NO_x$ emissions when ID is increased. These are discussed briefly below:

### 5.3.1 NO Production in Premixed Flame

The increase in ID due to charge air temperature reduction was shown in chapter 4 to lead to increased premixed combustion proportion. In addition to this, the increased time until ignition and penetration of the spray are expected to lead to parts of the spray to be well mixed during premixed combustion, as was shown in [15].

Even though in-cylinder sampling and optical measurements have suggested there is no appreciable $NO_x$ production during premixed combustion due to the limited oxygen availability [10–15], the increased mixing expected with long ID could lead to significant thermal NO production in the premixed phase.

Results from the numerical investigation with artificially prolonged ID (section 4.2.2) showed that it is possible for thermal NO (Zeldovich mechanism was used) to be produced during premixed combustion. The simulation results (Figure 4.8) showed 20% of the total NO production was formed during premixed combustion in the prolonged ID case. Thus, it is conceivable that increases in the amount of NO formed in premixed combustion could contribute to the observed $NO_x$ trend reversal with prolonged ID. Nonetheless, [19] argues that even provided that the mixture which burns in premixed combustion is sufficiently lean to produce $NO_x$, NO chemistry is too slow for sufficient amounts to be formed in premixed combustion.

### 5.3.2 NO Production due to Prompt NO

According to the literature [2, 6], prompt NO in normal diesel conditions has a limited contribution to the overall $NO_x$ production. However, with reducing temperature, the contribution of prompt NO relative to thermal NO could increase, leading to an underestimation of NO when only considering the thermal part.

Even though there is no specific indication in the current experimental or simulation results that this could be a contributing factor, the authors of [8] argue that, in lean mixtures, the relative contribution of prompt NO is greater. Furthermore, the lower temperature dependency of prompt NO when compared to thermal NO could result in higher proportion of prompt
NO at cold conditions. Thus, considering that the premixed combustion is in fact leaner, and there is no change in the diffusion combustion equivalence ratio, the overall prompt NO levels could increase in extreme Miller conditions. Nonetheless, the increase in prompt NO proportion is unlikely to single-handedly cause the observed NO trend reversal. Given that charge air temperatures are lower, leading to reductions in thermal NO production, also the chemical reaction rates for prompt NO will decrease, leading to higher proportions of prompt NO but lower total NO formation.
Chapter 6

Conclusions and Outlook

Previous research on DI diesel engines has shown potential for in-cylinder NO\textsubscript{x} reduction through advanced Miller valve timing, whereby the cylinder charge is expanded before compression to reduce charge air temperature and thus adiabatic flame temperature. In this work, tests conducted with extreme Miller valve timing coupled with two-stage turbocharging on a direct injection medium speed diesel engine showed a reduced potential of NO\textsubscript{x} reduction, with the trend of NO\textsubscript{x} reduction reversing with decreasing adiabatic flame temperature.

The experimental and numerical investigations presented in this work aimed to provide further insight into the potential and limitations of the use of extreme Miller valve timing as a means of NO\textsubscript{x}-SFC tradeoff improvement. In the literature, reports of a positive relationship between adiabatic flame temperature and NO\textsubscript{x} emissions are commonplace. However, as shown in the present experimental work amongst others, the NO\textsubscript{x}-SFC tradeoff benefits obtained through the reduction of cycle temperature are restricted.

In the following sections the observations from the experimental and simulation work are listed, followed by an interpretation of the results. Then, a proposal of possible ways to improve the NO\textsubscript{x} reduction capabilities of extreme Miller valve timing based on the findings of this work is presented. Finally, the chapter is closed with the outlook of how the findings of this work can be used to improve the understanding of the observed combustion and emission phenomena using detailed experimental investigations and modern simulation tools.
6.1 Experimental and Simulation Observations

The experiments with increasing Miller valve timing and simulations with increasing ID showed:

- A limit in the $NO_x$-SFC tradeoff benefit offered by increasing Miller degree at high load, and an eventual deterioration of the tradeoff at lower loads

- A correlation between ID obtained through changing cycle temperature and $NO_x$ emissions for constant charge density and injection conditions, with a clear $NO_x$ minimum at a certain level of ID

- Increasing cycle-to-cycle variability of in-cylinder pressure, soot cloud density and single cycle exhaust NO concentration with prolonged ID

- Presence of in-cylinder pressure fluctuations corresponding to the main radial excitation frequency of the cylinder gases arising at random at long ignition delay conditions. These pressure fluctuations were found to arise from the increased amount of premixed combustion due to the long ID, and persisted well into the expansion phase of the cycle

- Exponentially increasing average and single cycle in-cylinder pressure fluctuation intensity with prolonged ID

- Increasing occurrence of cycles with pressure fluctuations with increasing ID

- An increase of the speed of combustion due to longer spray penetration caused by the prolonged ID. The increased spray penetration resulted in increased pre-mixing and air entrainment, ultimately improving the available oxygen utilization

- An increase in air-fuel mixing of a spray under acoustic excitation. The degree of air-fuel mixing was found to be dependent on the frequency of oscillation, and increased monotonically with fluctuation intensity. This, coupled to observed increases in the chemical reaction rates under pressure fluctuations, resulted in higher HRR of the spray under pressure oscillating conditions
• Increased measured apparent mixing levels of diffusion combustion in cycles where pressure fluctuations appeared. The apparent air-fuel mixing levels were shown to scale with pressure fluctuation intensity.

• Increased soot temperature and oxidation rate as a result of increased mixing in the cycles with pressure fluctuations. Both soot temperature and oxidation rate were shown to scale with pressure fluctuation intensity.

• Increased single-cycle $NO_x$ concentration in the exhaust with increasing cycle in-cylinder pressure fluctuation intensity.

6.2 Interpretation of Results

The experimental and simulation observations presented above, coupled to literature review on similar phenomena from different spray combustion applications, can be used to explain the $NO_x$ emission increase with long ID. The individual and combined effects of the observed phenomena on $NO_x$ emissions are provided here:

• Increased temperature and oxygen availability due to mixing, as a result of longer spray penetration and in-cylinder pressure fluctuations.

• Increased flame and post-flame gas temperature due to compression heating of the charge from the faster combustion rate.

• Increased flame temperature due to decreased radiation heat losses, resulting from of faster soot oxidation rate under the presence of pressure fluctuations.

• Possibility of NO production in the premixed flame, which has more time to mix and thus is leaner.

• Increased NO formation rate because of pressure fluctuations which cause isentropic compressions. These lead to higher-than-the-average reaction rates due to the exponential dependency of reaction rates on temperature.
• Increased probability of NO formation through prompt NO becoming important at leaner premixed flame conditions.

Overall, the observed results and conclusions provide an understanding of the $NO_x$ trend reversal observed, and show the importance of single-cycle combustion characteristics at these conditions. The findings of this work can be used for the improvement of the $NO_x$ reduction potential using Miller valve timing. Furthermore, the establishment of the influence of single cycle characteristics on overall emission trends should result in an revision of the ”averaged” measurement procedures and simulation approaches used currently for diesel engine research purposes.

### 6.3 Possibilities for Reduced $NO_x$ Emissions through Miller Valve Timing

The analysis presented above showed that the main cause of the $NO_x$ trend reversal with increased ID due to charge temperature reduction is the increased amount of fast premixed combustion. The findings lead to the conclusion that an effective way to diminish or eliminate this reversal is to reduce the amount or the reactivity of the premixed combustion. An brief analysis of possible ways to achieve this is presented below.

#### 6.3.1 Pre-Injections

Pre-injections, whereby a small amount of fuel is injected before the main injection, have been widely used for the purpose of reduction of premixed combustion. The main goal of pre-injections in most modern high-speed diesel engine applications is to reduce the combustion noise [12, 115, 116], which is correlated with the rate of change of pressure; this in turn is directly proportional to the amount and speed of premixed combustion. In past research, pre-injections have been shown to lead to reduced $NO_x$ emissions [17, 22, 38, 117–119]. Specifically for medium speed applications with Miller valve timing, a clear improvement in the $NO_x$-SFC tradeoff has been reported with the employment of pre-injections. In the context of the present research, pre-injections could be used to reduce the ignition delay in combination with extreme Miller valve timing, in order
to reduce the $NO_x$ trend reversal and achieve higher $NO_x$ reduction. An additional advantage will be the ability to reduce mechanical wear of the engine parts and noise through the reduction of the main injection ID.

6.3.2 Injection Rate Shaping

Injection rate shaping is similar in concept to the utilization of pre-injections, but is preferred due to injection stability and injector needle lifetime issues with increased number of needle closures per cycle. The idea is to reduce the amount of premixed combustion by reducing the injection rate prior to ignition. This has been shown to result in reduced $NO_x$ emissions when used in combination with extreme Miller timing [17,119].

6.3.3 Exhaust Gas Recirculation

In isolation, the $NO_x$ reduction potential of EGR is well established [17,119]. EGR reduces the flame temperature by reducing the amount of available oxygen and increasing the heat capacity of the reactants, thus reducing thermal $NO_x$ formation.

In the context of reducing the observed $NO_x$ trend reversal with increasing Miller degree, the use of high EGR values leads to a reduction of the reaction rates. Even under long ID conditions, EGR can lead to a reduction in the premixed combustion rate, which would reduce pressure fluctuation intensity, as has been shown previously in [41]. Thus, the combination of extreme Miller valve timing with EGR can lead to a reduction in the observed pressure fluctuations.

6.3.4 Fuel Characteristics

Finally, a method to reduce the ID is the use of higher cetane number (CN) fuels. The use of high CN fuels in diesel engines has been shown to result in reduced ID and, as a consequence, reduced premixed combustion energy. Higher cetane number fuels have also been shown to affect emissions in previous research [12,111].
6.4 Outlook

The experimental and numerical investigations presented in this work have provided an improved understanding of the effects of prolonged ignition delay on HRR, $NO_x$ and other emissions. Nonetheless, there is still potential for extending the understanding in this field, in the direction of the application and basic understanding of the phenomena.

In the direction of the application of Miller valve timing for further $NO_x$ emission reduction, there exists significant potential for the reduction or elimination of the $NO_x$ trend reversal through different technologies, as was shown in section 6.3. The different technologies presented should be tested in combination with extreme Miller valve timings, and considering the specific application limitations.

For the improvement of understanding of the phenomena, different combinations of experimental and simulation work can be performed. The extension and improvement of cycle-to-cycle measurements of NO concentration in the exhaust gas stream in extreme Miller conditions is essential for the improvement in understanding of the effects of single cycles on the $NO_x$ trend observed, compared to average cycle effects such as spray penetration. This will allow a de-coupling of the observed effects of single and averaged cycles which was not possible in the experiments performed in this work.

Further understanding can be obtained by cycle-resolved exhaust gas soot measurements which can be used to correlate the single-cycle soot luminosity measurements with an exhaust soot mass value. As with $NO_x$ measurements, there is a potential to determine how single cycle characteristics effect the averaged exhaust soot emissions.

One of the limitations faced in this work was the inability to determine the effects of individual observations of combustion characteristics on the overall process of combustion and emission formation. This is in general an inherent limitation of engine measurements, since limited accessibility on measurement and control of individual phenomena is present. A particular example is the effects of pressure fluctuations on spray formation, spray combustion and emissions at high pressure environments, which was only studied through simulation in this work. These limitations can be partially overcome by more controlled, idealised experiments. A possibility would be to study the effects of pressure oscillations in a constant volume combus-
tion chamber, where optical measurements in addition to the simulations can aid in the validation of the simulation results and ultimately in the understanding of the relevant phenomena. These phenomena can also be studied in simulations of sprays in transient (moving piston/engine) environments. The advantage of the simulations in this case is the ability to de-couple the pressure fluctuations from other phenomena by forcing them as boundary conditions.

In terms of other observations, engine simulations can provide an estimate of the amount of radiation heat transfer as a result of the soot presence in the flame. The latest combustion and soot models have shown very good agreement with experiments in terms of soot cloud location and density [105], thus they can be used to estimate the amount of flame cooling or loss thereof, when changes in the soot cloud density occur.
# Appendix A

## Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$B$</td>
<td>Cylinder bore</td>
</tr>
<tr>
<td>$BDC$</td>
<td>Bottom Dead Centre</td>
</tr>
<tr>
<td>$C$</td>
<td>Local speed of sound</td>
</tr>
<tr>
<td>$CA$</td>
<td>Crank Angle</td>
</tr>
<tr>
<td>$CAD$</td>
<td>Computer Aided Design</td>
</tr>
<tr>
<td>$CCEM$</td>
<td>Competence Centre for Energy and Mobility</td>
</tr>
<tr>
<td>$CFD$</td>
<td>Computational Fluid Dynamics</td>
</tr>
<tr>
<td>$CI$</td>
<td>Compression Ignition</td>
</tr>
<tr>
<td>$CMC$</td>
<td>Conditional Moment Closure</td>
</tr>
<tr>
<td>$CN$</td>
<td>Cetane Number</td>
</tr>
<tr>
<td>$d_{drop}$</td>
<td>Droplet diameter</td>
</tr>
<tr>
<td>$d_{0,drop}$</td>
<td>Droplet Sauter mean diameter</td>
</tr>
<tr>
<td>$DI$</td>
<td>Direct Injection</td>
</tr>
<tr>
<td>$dQ/d\theta$</td>
<td>Heat release rate</td>
</tr>
<tr>
<td>$E$</td>
<td>Activation energy</td>
</tr>
<tr>
<td>$EBU$</td>
<td>Eddy BreakUp</td>
</tr>
<tr>
<td>$EGR$</td>
<td>Exhaust Gas Recirculation</td>
</tr>
<tr>
<td>$f$</td>
<td>Delay coefficient for transition from laminar to turbulent regime</td>
</tr>
<tr>
<td>$f_{m,n}$</td>
<td>Specific vibration frequency for mode $(m,n)$</td>
</tr>
<tr>
<td>$FID$</td>
<td>Flame Ionization Detector</td>
</tr>
<tr>
<td>$FTIR$</td>
<td>Fourier Transform Infrared spectroscope</td>
</tr>
<tr>
<td>$HCCI$</td>
<td>Homogeneous Charge Compression Ignition</td>
</tr>
<tr>
<td>$HFO$</td>
<td>Heavy-Fuel Oil</td>
</tr>
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# Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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<td>HRR</td>
<td>Heat Release Rate</td>
</tr>
<tr>
<td>IC</td>
<td>Internal Combustion</td>
</tr>
<tr>
<td>ID</td>
<td>Ignition Delay</td>
</tr>
<tr>
<td>IMO</td>
<td>International Maritime Organization</td>
</tr>
<tr>
<td>IVC</td>
<td>Inlet Valve Closure point</td>
</tr>
<tr>
<td>$k$</td>
<td>Turbulent kinetic energy</td>
</tr>
<tr>
<td>$k_{rel}$</td>
<td>Combustion rate under acoustic excitation, relative to non-acoustically excited</td>
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<tr>
<td>$K$</td>
<td>Absorption coefficient per unit soot cloud thickness</td>
</tr>
<tr>
<td>KL</td>
<td>Measure of in-cylinder soot concentration</td>
</tr>
<tr>
<td>$L$</td>
<td>Flame thickness</td>
</tr>
<tr>
<td>LATCT</td>
<td>Laminar And Turbulent Characteristic Time scale</td>
</tr>
<tr>
<td>LERF</td>
<td>Large-Engine Research Facility</td>
</tr>
<tr>
<td>LII</td>
<td>Laser Induced Incandescence</td>
</tr>
<tr>
<td>LPG</td>
<td>Liquified Petroleum Gas</td>
</tr>
<tr>
<td>$N_d$</td>
<td>Number of droplets</td>
</tr>
<tr>
<td>$NO_x$</td>
<td>Nitrogen Oxides</td>
</tr>
<tr>
<td>OLP</td>
<td>Optical Light Probe</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure</td>
</tr>
<tr>
<td>PCCI</td>
<td>Premixed Combustion Compression Ignition</td>
</tr>
<tr>
<td>PLIF</td>
<td>Planar Laser-Induced Fluorescence</td>
</tr>
<tr>
<td>PSI</td>
<td>Paul Scherrer Institute</td>
</tr>
<tr>
<td>$R$</td>
<td>Universal gas constant</td>
</tr>
<tr>
<td>$R_f$</td>
<td>EBU fuel consumption rate</td>
</tr>
<tr>
<td>$r_f$</td>
<td>Stoichiometric air-to-fuel ratio</td>
</tr>
<tr>
<td>$r_d$</td>
<td>Radius of a droplet</td>
</tr>
<tr>
<td>$Re$</td>
<td>Reynolds Number</td>
</tr>
<tr>
<td>RH</td>
<td>Hydrocarbon Radical</td>
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<tr>
<td>SFC</td>
<td>Specific Fuel Consumption</td>
</tr>
<tr>
<td>SI</td>
<td>Spark Ignition</td>
</tr>
<tr>
<td>SINL</td>
<td>Spatially Integrated Natural Luminosity</td>
</tr>
<tr>
<td>SOI</td>
<td>Start of Injection</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
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## Nomenclature

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<th>Description</th>
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<tr>
<td>$t_{bag}$</td>
<td>Bag Breakup time</td>
</tr>
<tr>
<td>$t_{strip}$</td>
<td>Stripping Breakup time</td>
</tr>
<tr>
<td>$T_{BB}$</td>
<td>Black Body temperature</td>
</tr>
<tr>
<td>$TDC$</td>
<td>Top Dead Centre</td>
</tr>
<tr>
<td>$UHC$</td>
<td>Unburned Hydrocarbons</td>
</tr>
<tr>
<td>$V$</td>
<td>Volume</td>
</tr>
<tr>
<td>$v_{rel}$</td>
<td>Relative velocity between a droplet and the gas</td>
</tr>
<tr>
<td>$VVT$</td>
<td>Variable Valve Timing</td>
</tr>
<tr>
<td>$We$</td>
<td>Webber Number</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>Experimentally derived exponent which describes the influence of wavelength on the emission potential</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Droplet evaporation coefficient</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Turbulence dissipation rate</td>
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<tr>
<td>$\lambda$</td>
<td>Wavelength</td>
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<tr>
<td>$\rho$</td>
<td>Density</td>
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<tr>
<td>$\rho_{m,n}$</td>
<td>Vibration mode number</td>
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<tr>
<td>$\sigma$</td>
<td>Droplet surface tension</td>
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<tr>
<td>$\tau_c$</td>
<td>Characteristic combustion time</td>
</tr>
<tr>
<td>$\tau_l$</td>
<td>Laminar time scale</td>
</tr>
<tr>
<td>$\tau_{mix}$</td>
<td>Apparent characteristic mixing time</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Equivalence Ratio</td>
</tr>
</tbody>
</table>

### Subscripts

<table>
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<tr>
<th>Symbol</th>
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<tbody>
<tr>
<td>$d$ or $drop$</td>
<td>Droplet</td>
</tr>
<tr>
<td>$diff$</td>
<td>Diffusion</td>
</tr>
<tr>
<td>$f$</td>
<td>Fuel</td>
</tr>
<tr>
<td>$g$</td>
<td>Gas</td>
</tr>
<tr>
<td>$l$</td>
<td>Liquid</td>
</tr>
<tr>
<td>$O_2$</td>
<td>Oxygen</td>
</tr>
<tr>
<td>$p$</td>
<td>Products</td>
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Journal Publications


Conference Publications

• P. Kyrtatos, K. Hoyer, P. Obrecht, K. Boulouchos, Recent developments in the Understanding of the Potential of In-Cylinder NOx Reduction though Extreme Miller Valve Timing, accepted for *CIMAC Congress 2013*, Shanghai


• C. Wik, K. Hoyer, T. Matt, P. Schuermann, P. Kyrtatos, 2-Stage Turbo Charging on Medium Speed Engines Results from the LERF-Test Facility, *16th Supercharging Conference*, 2011, Dresden, Germany


• C. Wik, H. Salminen, K. Hoyer, C. Mathey, S. Voegelin, P. Kyrtatos, 2-Stage Turbocharging on Medium Speed Engines Future Su-
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