Licentiate Thesis in Combustion of Biofuels

Knocking Combustion in a Heavy-Duty Spark-Ignited Engine Fueled by Methanol

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Abstract

Challenges regarding greenhouse gas emissions in general, and especially emissions of carbon dioxide, highlight the need to reduce the use of fossil fuels, which requires more efficient combustion engines and a transition to renewable fuels, such as e-methanol. As knocking combustion limits the efficiency of a spark-ignited engine, thereby increasing fuel consumption and the emissions, it is a very relevant research topic of today.

The research literature has proposed several explanations for knocking combustion. A generally accepted hypothesis is that knock is predominantly initiated from so-called hot spots, i.e. exothermic centers with a deviation in temperature. Nevertheless, the scientific literature suggests that hot spots may not be present in all engine-fuel configurations. Moreover, some studies indicate that other reactivity spots within the engine, such as fuel-rich spots and oil spots, can contribute to knock as well.

The standard approach to mitigating knock is to retard spark timing when knock is detected in earlier cycles. Therefore, this approach penalizes the cycles that would have experienced normal combustion at optimal spark timing, thereby reducing overall combustion efficiency. Hence, a preferred solution for controlling knock is to predict in-cycle if knocking will occur and adjust spark timing accordingly. However, the research literature presents conflicting results regarding the possibility of predicting knock before spark timing.

This thesis evaluates the potential for predicting the conditions that lead to in-cycle knocking combustion in a heavy-duty spark-ignition engine running on methanol, as well as assessing strategies for mitigating knock and enhancing engine efficiency.

The thesis also investigates other potential root causes of auto-ignition in the engine-fuel configuration, including whether lubricant oil entering the combustion chamber can be a contributing factor.

The results indicate that it is not possible to accurately predict prior to spark timing whether a cycle will knock. Knock control after spark timing is unlikely to be effective due to the significant overlap in combustion characteristics between normal and knocking cycles. Lubricant oil, rather than hot spots or fuel-rich spots, was demonstrated to be the most likely cause of knock in the current engine-fuel configuration.

Sammanfattning

Utmaningar kopplade till utsläpp av växthusgaser i allmänhet och koldioxid i synnerhet understryker behovet av att minska användningen av fossila bränslen. Detta kräver mer effektiva förbränningsmotorer och en övergång till förnybara bränslen, såsom e-metanol. Eftersom knackande förbränning begränsar verkningsgraden hos en gnisttänd motor och därmed ökar både bränsleförbrukningen och utsläppen är det ett högaktuellt forskningsområde.

Den vetenskapliga litteraturen har föreslagit flera förklaringar till knack. En allmänt accepterad hypotes är att knack främst initieras av så kallade "hot spots", det vill säga exotermiska centra med temperaturavvikelser. Samtidigt visar litteraturen att hot spots inte alltid förekommer i alla motorbränslekombinationer. Dessutom finns studier som pekar på andra reaktiva områden, såsom bränslerika zoner och oljefläckar, som möjliga orsaker till knack.

Standardmetoden för att motverka knack är att senarelägga tändtidpunkten när knack upptäckts i tidigare cykler. Denna metod bestraffar dock även de cykler som skulle ha haft en normal förbränning vid optimal tändning, vilket därmed minskar den totala förbränningseffektiviteten. En önskvärd lösning för att reglera knack är därför att kunna förutsäga inom en förbränningscykel om knack kommer att inträffa och justera tändtidpunkten utifrån denna information. Tidigare forskning har dock visat motstridiga resultat vad gäller möjligheten att förutsäga knack före tändning.

Denna avhandling syftar specifikt till att klargöra, för en tung gnisttänd motor som drivs med metanol, potentialen att inom en förbränningscykel förutsäga om knackande förbränning kommer att inträffa, samt om den kan mildras inom samma cykel.

Avhandlingen har även undersökt andra möjliga grundorsaker till självantändning i motorbränslesystemet, däribland huruvida smörjolja som tränger in i förbränningskammaren kan vara en bidragande faktor.

Resultaten visar att det inte är möjligt att med hög noggrannhet förutsäga före tändtidpunkten om en cykel kommer att knacka eller inte. Reglering av knack efter tändning bedöms inte som fördelaktigt, på grund av stort överlapp i förbränningskaraktäristik mellan normala och knackande cykler. Smörjolja, snarare än hot spots eller bränslerika zoner, visade sig vara den mest sannolika orsaken till knack i den aktuella motorbränsleuppsättningen.

Acknowledgement

This thesis would not have been achievable without the support of my supervisors Associate Professor Ola Stenlåås and Associate Professor Andreas Cronhjort. They have given me terrific support and guidance throughout the entire thesis period. I would not have any experimental data without Andreas Lius and Ludvig Adlercreutz, who configured and ran the test engine. I am also thankful to all my great colleagues who shared knowledge, inspiration, and laughter, making the journey possible. Andrew Huberman's podcast has both provided valuable tips for working more efficiently and inspired me to contribute to research in general. Last, but not least, I want to thank my family (the cat included) and friends who have encouraged me to continue when times were challenging.

Nomenclature

Abbreviations

ATDC	After top dead center
BTDC	Before top dead center
CA10/50/90	Crank angle at 10/50/90% burned
CAD	Crank angle degree
CFR	Cooperative fuel Research
CI	Compression ignition
CR	Compression ratio
DI	Direct injected
DWI	Direct water injection
EOC	End of combustion
EVO	Exhaust valve open
EVC	Exhaust valve close
GHG	Green-house gases
HD	Heavy-duty
$IMEP_g$	Gross indicated mean effective pressure
$IMEP_n$	Net indicated mean effective pressure

ITE	Indicated thermal efficiency
IVO	Intake valve open
IVC	Intake valve close
KI	Knock intensity
KO	Knock onset
KLSA	Knock limited spark advance
LTHR	Low temperature heat release
LW	Livengood-Wu
MAPO	Maximum amplitude of filtered pressure oscillations
MBT	Maximum brake torque
MFB	Mass fraction burned
MON	Motor octane number
N	Engine speed
NIMEP	Net indicated mean pressure
NTC	Negative temperature coefficient
Op.Cond.	Operating condition
OI	Octane index
P_{cyl}	In-cylinder pressure

PFI	Port fuel injected
RCEM	Rapid compression and expansion machine
RON	Research octane number
SCR	Single cylinder research
ST	Spark timing
SI	Spark-ignition
SOC	Start of combustion
TDC	Top Dead Center
T_{im}	Temperature in intake manifold
T_{exh}	Temperature in exhaust manifold
T_u	Temperature of the unburned gas

Definitions

Fuel-rich spot	Spot with increased reactivity due to local fuel-enrichment
Hot spot	Spot with increased reactivity due to deviation in temperature
Oil spot	Spot with increased reactivity due to induced oil droplets

List of publications

The thesis are based on the following published research papers.

I **In-cycle predictability and control of knock in a PFI HD SI engine fueled with methanol**
Ainouz, F., Lius, A., Cronhjort, A., and Stenlaas, O
Submitted to SAE, ICE2025: 17th International Conference on Engines and Vehicles

II **Correlating Particle Number Emissions to the Rotation of the Piston Ring**
Adlercreutz, L., Lius, A., Ainouz, F., Cronhjort, A. et al.
SAE Int. J. Fuels Lubr. 16(3):2023

III **Correlation of Oil Originating Particle Emissions and Knock in a PFI HD SI Engine Fueled with Methanol**
Ainouz, F., Adlercreutz, L., Cronhjort, A., and Stenlaas, O
SAE Technical Paper 2023-24-0036, 2023

Content

Introduction

The Otto engine was invented in the 1800s and has been widely used in the transportation sector ever since [1]. Knocking is an anomalous combustion phenomenon that limits engine efficiency [2]. Consequently, it has been studied for decades. When the spark-induced flame travels through the combustion cylinder, it compresses the unburned gas (end-gas), resulting in increased temperature, pressure, and density of the end-gas. The related chemical reactions can cause part of the mixture to auto-ignite, subsequently releasing a large amount of its chemical energy. The close to instantaneous release of energy results in high local pressures and shock waves propagating through the engine [1]. These shock waves result in a pinging sound, hence the term “knocking”. Since knocking combustion can damage the engine, most operations at high load are run at sub-optimal conditions to suppress it [3].

Motivation

Challenges regarding CO_2 emissions and greenhouse gases, along with the need to reduce fossil fuel usage require more efficient combustion engines and a transition to renewable fuels, such as methanol [4].

Since mitigating of knock prevents spark-ignited (SI) engines from operating at optimal conditions with the cost of increased fuel consumption and emissions, knock is a very relevant area of research today [5].

A challenge with SI engines is to ignite the fuel-air mixture at the optimal time within a combustion cycle. If the spark timing is set too early, the high combustion temperatures may lead to knocking combustion and potential damage to the engine. However, igniting too late results in lower combustion temperatures and slower combustion, leading to greater heat losses and reduced combustion efficiency.

The possibility of estimating if a combustion cycle will knock or not, in advance prior to spark timing, has shown inconsistent results in the literature [6–12].

In [6], Kalghatgi et al. computed ignition delays at different pressures and temperatures for a range of gasoline surrogates in a direct-injected (DI) SI engine, using chemical kinetics. The obtained ignition delays were then used to parameterize the Arrhenius function, which was subsequently applied to calculate the Livengood-Wu (LW) integral, thereby predicting if, and when, a cycle would knock. The calculated knock onsets agreed well with the experimental knock onsets. The above approach was verified in another engine by Kalghatgi et al. [7] using five fuels with different chemical compositions. Hot spots were assumed to be the root cause of knocking in both engines.

However, the results above contradicted the experimental observations by Lius et al. [8,9] on a heavy-duty (HD) SI engine fueled with methanol. The concluding results of these two papers were that knocking combustion could not be predicted prior to spark timing and that hot spots were likely not the root cause of auto-ignition. Königsson [13] reached the same conclusion about hot spots when investigating auto-ignition in a compression ignition context, after experimental work on the same engine, but with a diesel dual-fuel configuration and primarily fueled by methane.

The primary motivation for this thesis has been to determine whether the truth regarding knock predictability in a HD SI engine, fueled by methanol, aligns more closely with the results by Kalghatgi et al. or those by Lius et al. and Königsson.

The secondary motivation for this thesis work has been to investigate the relationship between oil-originating particles and knocking combustion. When running the engine on high-octane fuels, such as methanol, factors other than the fuel itself may influence combustion. Oil droplets with a low octane number (ON) can enter the combustion chamber, potentially impacting both temperature and chemical composition. This may lead to local spots with increased reactivity and reduced ON, thereby increasing the engine's tendency to knock.

Research questions

The research questions are divided into two parts. The first part investigates whether hot spots are the root cause of knock in the current engine-fuel setup and explores the potential for in-cycle control to mitigate knock:

- Using auto-ignition modelling from Livengood-Wu, is it possible to predict in advance, before spark timing, whether a cycle will knock or not?
- If so, can an adaptive prediction method based on the modelled temperature in hot spots improve the knock predictability?
- After spark timing, how does the detection certainty of knock prediction vary with crank angle degree (CAD) and mass fraction burned (MFB)?

The above questions were examined in Paper I.

The second part explores the role lubricant oils play in knocking combustion:

- How is the particle number (PN), measured in the exhaust, affected by changing the piston rings' relative rotational position (i.e., ring gap offset) and by using different lubricant oils? This question was studied in Paper II through experiments with low-sooting combustion, where the PN could be attributed to lubricant oil entering the combustion chamber.

- Does a positive correlation between PN originating from the oil, and engine knock tendency exist? This question was investigated in Paper III.

Outline and contributions

Paper I aimed to clarify, specifically for a heavy-duty (HD) spark-ignited (SI) engine running on methanol, the in-cycle predictability of knocking combustion, both pre- and post-spark timing. The paper also discussed the potential for in-cycle knock control.

Paper II and Paper III explored the impact of lubricant oil on auto-ignition in the same engine-fuel setup. First, Paper II examined whether the amount of lubricant oil, entering the combustion chamber, could be altered by modifying the piston ring gap offset and by using oils with different properties. Next, Paper III investigated whether there is a correlation between PN, originating from the oil, and the engine's tendency to knock.

The author was the primary contributor to Paper I and Paper III. In these papers, the author took responsibility for defining the research questions, selecting appropriate methods, designing the experimental plans, conducting the modeling, and evaluating the data. Both papers were written collaboratively with the co-authors.

In Paper II, the author contributed as a co-author with analysis and documentation of a sub-set of the experimental results.

Supervisors Ola Stenlåås and Andreas Cronhjort provided continuous support throughout the thesis period, assisting with everything from defining research questions and analyzing experimental results to paper writing.

The main contributions of this thesis are as follows:

- Establishing that knocking cycles cannot, with a statistical certainty, be distinguished from normal cycles before spark timing in a port fuel injected (PFI) HD SI engine fueled by methanol. This supports the evidence that hot spots are not the root cause of auto-ignition in the current engine-fuel setup

- Concluding that any adaptation before spark timing, based on a hypothesized hot spot temperature, would be useless for mitigating knock

- The results concerning post-spark timing showed large overlaps between normal and knocking cycles, in terms of LW build up and combustion duration, even at 10CAD after top dead center (ATDC) and 50% MFB. This demonstrates that post-spark timing knock cycle control is unlikely to be beneficial. That means water injection to mitigate knock could penalize normal cycles more than a plain spark retardation to 1% knocking cycles (as done by a standard knock controller).

- Confirming previous research findings that a decreased ring gap offset increases the oil-originating PN. It was also revealed that a high volatility oil increases PN, whereas a high viscosity oil decreases it. These results indicate that PN can, at least to some extent, be controlled through engine configuration and oil properties.

- By altering the amount of oil entering the combustion chamber during knock-limited operation, expanding the knowledge base regarding the correlation between oil-originating PN and knock tendency. It was revealed that an increase in oil-originating PN correlates with an increased engine knock tendency.

Knocking combustion

As knocking combustion prevents an SI engine from running at optimal conditions, leading to reduced engine efficiency, increased fuel consumption, and higher emissions, it makes a relevant research topic of today.

The nature of knock

Multiple researchers, such as Kalghatgi [2], Reitz and Wang [14] refer to Heywood [1] for the definition of engine knock. Heywood describes knock as the pinging noise that propagates through the engine, when auto-ignition of fuel-air mixture in the end-gas (unburned gas) of an SI engine occurs ahead of the advancing flame front [1]. During this abnormal combustion, a significant amount of chemical energy is released in the end-gas. This energy release causes high local pressures which can result in high-amplitude pressure waves. These waves propagate through the combustion chamber, inducing engine block vibrations and, consequently, the characteristic knocking sound [1,2].

What causes knock?

As the spark-induced flame propagates through the combustion chamber, along with the volume changes from the piston movement, the end-gas is compressed. As a consequence, its pressure, temperature, and density increase. Finally, some portions of the fuel auto-ignite, releasing a significant amount of chemical energy in a cascade reaction [1]. As discussed by Pöschl and Sattelmayer [15], this causes high local pressures, leading to shock waves propagating through the engine. During this abnormal combustion, the end-gas burns significantly faster (5 to 25 times) than during normal combustion [1]. Results in [16] by Bradley et al. indicate that up to 40% of the fuel can be consumed in auto-ignition reactions.

As illustrated by Wang and Reitz [4], auto-ignition is related to both engine design, operating conditions and fuel quality, as all of these factors affect the pressure and temperature history within the cylinder.

Auto-ignition chemistry

Auto-ignition is strongly linked to the combustion of hydrocarbons under various conditions, such as i.e. temperature, pressure, equivalence ratio, etc. [4]. Westbrook demonstrated through analysis in [17] that auto-ignition in combustion engines is governed by a single fundamental reaction, i.e., the chain branching of hydrogen peroxide (H_2O_2). H_2O_2 accumulates during the compression at relatively low temperatures. However, when a specific temperature range (900-1000K) is reached it decomposes rapidly into OH radicals, which subsequently ignite the remaining fuel:

$$\mathbf{H_2O_2 + M \rightarrow OH + OH + M} \qquad (1)$$

In [17] Westbrook emphasizes that the time required to reach this critical decomposition temperature is the most dominant factor in determining when ignition will occur. Hence, any factor that decreases time to reach at this temperature will advance the ignition. Moreover, since the reaction involves a third body *M*, a higher pressure increases the probability of collisions, which reduces the critical temperature, and subsequently the time to ignition.

Negative temperature coefficient (NTC)

As Pöschl and Sattelmayer highlight in [15], the chemical reactions occurring within the cylinder are complex functions of pressure and temperature. In general, the auto-ignition time is decreasing with both increasing temperature and pressure. However, as discussed by Lindström [18], for long and paraffinic hydrocarbon chains, for a given pressure, the ignition delay can increase with rising temperature. This behavior is defined as the negative temperature coefficient (NTC), as described by Ji et al. [19]. As some important chemical reactions occur early in the compression process, when the temperature is low, this results in a first-stage heat release known as *low temperature heat release (LTHR)* or *cool flames*, as highlighted by Risberg et al. [20]. At a given pressure the induction time of a cool flame decreases with increasing temperature. However, formation of peroxy-chemistry radicals necessary for low-temperature oxidation ceases, resulting in a decrease in the cool flame's intensity, as detailed by Pekalski et al. [21]. Figure 1 displays auto-ignition time for n-heptane as a function of temperature at different pressures. Within specific temperature ranges, depending on pressure, ignition delay is increasing with rising temperature.

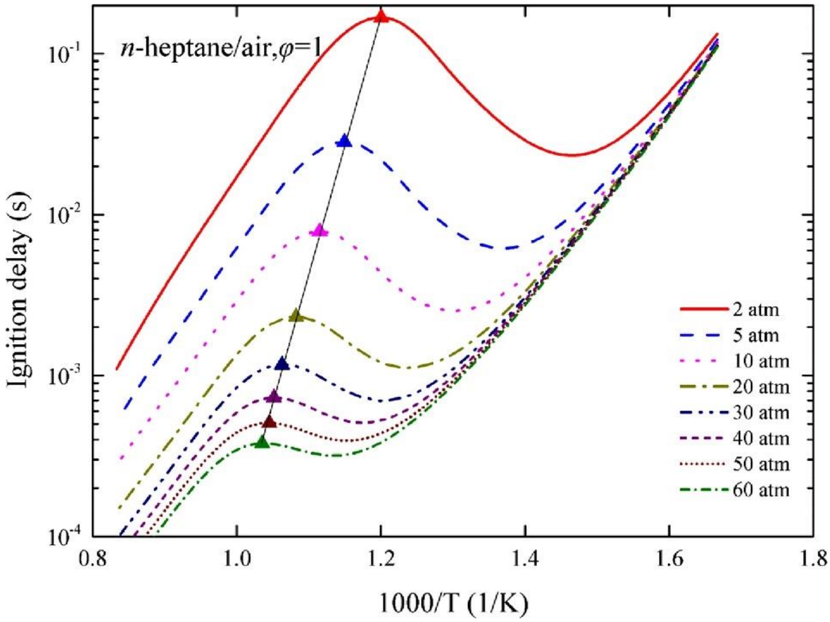

Figure 1. The plot shows that auto-ignition time is decreasing with increasing pressure. Except for a brief region, the auto-ignition time is decreasing significantly with increasing temperature. The negative temperature coefficient (NTC) region exists because different chemical reactions dominate at different temperatures. Reprinted with permission from Ji et al. [19].

Fuel properties

Since hydrocarbons vary in molecular size and structure, they exhibit significant differences in their ability of resisting auto-ignition [1]. As practical fuels are blends of a wide range of hydrocarbons, e.g. alkanes, cyclanes, alkenes, etc., there is a need to have a reliable measure of a fuel's anti-knock properties. This need has led to the development of the octane number (ON).

Octane number

A fuel's anti-knock property is defined by the ON. ON determines if knock will occur for the fuel in a specific engine during specific operating conditions. A higher ON, means a greater resistance to knock.

The octane number scale is based on two hydrocarbons, n-heptane (C_7H_{16}) and isooctane (C_8H_{18}). These fuels are also referred to as the primary reference fuels (PRF). By definition, n-heptane has a value of 0, and isooctane a value of 100. A mixture of 10% n-heptane and 90% isooctane is defined to have an ON of 90. The ON of a fuel is referring to the mixture of the two PRFs that would mimic the fuel's knock resistance [1]. Two standardized methods for computing a fuel's ON exist: research octane number (RON) and motor octane number (MON) [22,23]. RON tests are performed on a Cooperative Fuel Research (CFR) engine with a four stroke, standardized single cylinder with variable compression ratio (CR). The CFR engine is operated under standardized operating conditions, where CR and fuel-air ratio are adjusted to induce knock.

In the MON tests, more severe operating conditions are used to enhance the likelihood of knock [4]. For example, the intake temperature is significantly higher, and the spark timing is more advanced. The standardized operating conditions for the RON and MON tests are summarized below [1]:

Table 1. Operating conditions for the RON and MON tests in [1].

	RON	MON
Inlet temperature	52°C	149°C
Inlet pressure	Atmospheric	
Humidity	0.0036-0.0072 kg/kg dry air	
Coolant temperature	100°C	
Engine speed	600 rpm	900 rpm
Spark advance	13° BTDC (constant)	19-26° BTDC (varies w. compression ratio)
Air/fuel ratio	Configured for maximum knock	

The higher inlet temperature and the advanced spark timing (ST) make the MON test the more severe of the two, and as a consequence most fuels have a greater RON than MON. Nonetheless, it has long been known that RON or MON values alone are not sufficient to model the knocking behavior of practical fuels [1,24–27]. For example, fuel composition affects knock intensity. As discussed by Kalghatgi in [28], paraffinic fuels knock with higher intensity than aromatic fuels at the same engine load, speed and spark timing, despite having the same MON. To more accurately assess the anti-knock properties of a fuel, Kalghatgi [27] introduced an advanced metric known as the octane index (OI):

$$\mathbf{OI = RON - KS} \qquad (2)$$

Here, K is a constant depending on engine operating conditions, and S is the sensitivity of the fuel, defined as:

$$\mathbf{S = RON - MON} \qquad (3)$$

Higher OI indicates better anti-knock quality of the fuel. K can be negative, which implies that for a given RON, higher sensitivity (i.e. lower MON) correlates with greater resistance to knock. Results by Kalghatgi [29], from tests on twenty-three modern European and Japanese cars, displayed that in the majority of cases K is negative. Teodosio et al. [30] demonstrated through extensive empirical tests that fuel/air mixtures with two different fuels, but equal OI, have identical auto-ignition conditions if the pressure and temperature histories are equivalent.

Hot spots

Several studies, including those by Bäurle and Warnatz [31], Oppenheim [32], Hajireza et al. [33], and König et al. [34], have confirmed that the gas mixture is seldom homogeneous in terms of temperature and species concentration, resulting in local centers with increased reactivity. In this thesis, the term “hot spot” is used to refer specifically to centers with increased reactivity due to local variations in temperature.

As hot spots generally form the regions where auto-ignition occurs [35,36], they have been extensively studied in the literature. In [37], Schießl and Maas employed laser-induced fluorescence, together with computations of chemical kinetics, to investigate the temperature fluctuations in the end-gas. Their results indicate that the temperature in hot spots may exceed the average unburned gas temperature by more than 20K, over a geometric range of approximately 1mm to 1cm. Furthermore, simulations by Goyal et al. in [38] on a one-dimensional geometry, with chemical kinetics for methane, indicate that temperature fluctuations of around 10K are sufficient to create self-sustaining pressure oscillations. In [36], Hajireza et al. modeled the temperature in a hot spot as a sine wave with amplitude of 5-20K for a mixture of n-heptane and iso-octane. Their simulations suggest that both low- and high temperature reactions are present, and that the flame front, arisen from a hot-spot, increases with amplified temperature stratification. In experiments by Pöschl and Sattelmayer [15] on a rapid compression and expansion machine (RCEM), a temperature difference of around 20K between upper and lower parts of the cylinder was induced. Photographs showed that auto-ignition results in a fast-propagating flame in the direction of the temperature gradient, which in turn generates pressure waves. When these pressure waves were powerful enough and the mixture was sufficiently reactive, a bidirectional coupling between pressure waves and heat release was produced, which had the potential to lead to knocking combustion.

Fuel-rich spots

As highlighted by Glassman et al. [39], the minimum ignition energy is always found on the fuel-rich side of stoichiometric. In addition, Veloo et al. [40] demonstrated in simulations that methanol-air has the highest laminar flame speed at slightly fuel-rich mixtures. On the contrary, computations by Seki et al. [41] on a DISI engine displayed that ignition first occurs in the zone with the lowest equivalence ratio and the highest initial temperature. In [42], Negoroa et al. explored the inhomogeneities of air-to-fuel ratio of pre-ignition in a DISI engine. Three factors influencing auto-ignition were identified: latent heat of vaporization (LHV), specific heat ratio, and LTHR. As the equivalence ratio is increased, temperature within the cylinder is dropping more due to LHV which results in a lower temperature at intake valve closing (IVC). The temperature increase during adiabatic compression is dependent on the specific heat ratio of the mixture, γ_{mix}. A lower equivalence ratio increases γ_{mix}, which provides a larger temperature raise during the compression. Nevertheless, simulation results in [42] propose that if a fuel exhibits cool flames characteristics, leading to LTHR, a larger equivalence ratio can still result in a greater overall temperature increase, and consequently, an earlier ignition timing.

Figure 2, reprinted from Lius et al. [9], displays ignition delay contours in milliseconds (ms) for a lambda sweep of methanol and air, with the mixture calculated using Chemkin-Pro with mechanism from Mehl et al. [22]. The identical engine used in this thesis was used. Two lambda sweeps of the compression up to TDC are included in the plot. It is illustrated that despite the increase in air, the unburned gas temperature does not approach within approximately 90K away of entering a region of reactivity (measured horizontally from TDC to the 40ms isolines).

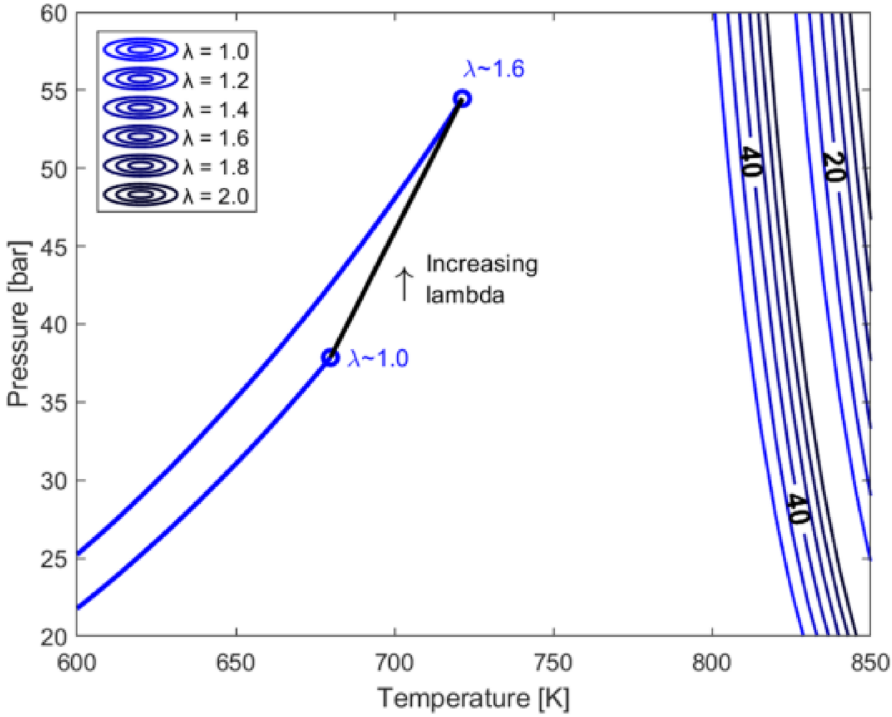

Figure 2. Ignition delay contours (in ms) for a lambda sweep without EGR, were calculated using Chemkin-Pro with the mechanism from Mehl et al. [43]. Compression traces for $\lambda = 1.6\ and\ \lambda = 1$ up to TDC are included in the plot. Reprinted with permission from Lius et al. [9].

Lubricant oils and oil spots

As mentioned by Pieter in [44], standard lubrication oils primarily consist of paraffinic and naphthenic compounds of 22-70 carbon atoms. Glassman highlights in [45] that these long-chain hydrocarbons have a high propensity to knock, presumed due to the low-temperature reactions in the early phase of the combustion. Therefore, as demonstrated by Ryan in [46], these oils generally have a lower ON than the fuel. Thus, if oil droplets enter the combustion chamber they can decrease the local ON and raise the engine's propensity to knock, as proved by Inoue et al. [47], Zaccardi and Escudié [48], Takeuchi et al. [49], Kalghatgi and Bradley [50], and Amann and Alger [51]. Hence, an oil spot acts as a rich spot but with higher reactivity compared to a fuel-rich spot. This is particularly true if the corresponding fuel has a high ON, as is the case for e.g. methanol.

Knock detection and quantification

Knock is one of the major constraints in an SI engine, since it limits the value of the maximum engine compression and hence the maximum performance and optimal efficiency. Subsequently, detection of knock onset (KO), with its corresponding crank angle θ_{ko}, and quantification of knock intensity (KI) have been studied for decades, and several methods have been proposed as mentioned by Heywood [1] and by Millo and Ferraro [52]. Knock can be detected both within the time domain and within the frequency domain. The main methods can be categorized into the following categories [52]:
1. Methods based on cylinder pressure analysis
2. Methods based on engine block vibration analysis
3. Methods based on gas ionization analysis

Cylinder pressure methods

This category likely includes the majority of methods used in laboratory tests for development of fuels and engines [1,11,52–54]. Since these methods capture pressure oscillations arising from knock, they support detailed investigations on abnormal combustion behaviors [6]. However, the shortcomings are the requirement of one pressure sensor per cylinder and the high cost per sensor, which would become very expensive in mass-production of engines.
As the pressure oscillations arising from knock typically fall within a specific frequency range, as discussed by Brunt et al. [55], it is common to apply high- or band-pass filters to the pressure signal in order to distinguish the knock-induced pressure oscillations from noise [11,56]. Cylinder pressure methods include:

Maximum Amplitude of Pressure Oscillations (MAPO)

As discussed by Shahlari and Ghandhi in [57] and by Siano and D'Agostino in [58], MAPO is likely the most common used time-based method to measure knock intensity. It refers to the maximum amplitude of the high- or band-pass filtered pressure signal P_{filt} within a crank angle window around KO:

$$\boldsymbol{MAPO} = \max_{\boldsymbol{\theta_0 \leq \theta \leq \theta_0 + \varphi}} \left| \boldsymbol{P_{filt}} \right| \tag{4}$$

Here, θ_0 is the crank angle marking the start of the computation window and φ the length of the window. In work by Leppard [11], $\theta_0 = 30$CAD BTDC and $\varphi = 100$CAD were used with the motivation that this is the interval where knock is expected. As highlighted by Cavina et al. in [59], the only criterion for the window is that it must be large enough to contain the filtered pressure oscillations arising from knock. If MAPO exceeds a specific knock threshold, KO is said to occur (see Figure 3) at the corresponding crank angle, θ_{ko}.

Determining an appropriate threshold value is, as Kalghatgi states in [2]: “a dilemma faced in all knock studies”. If the threshold value is set too high, the method will not detect low knock events. On the other side, if the threshold is set too low even normal combustion cycles may be classified as knocking.

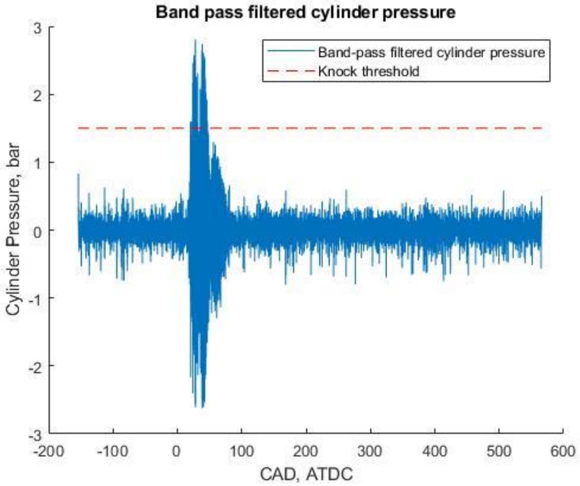

Figure 3. Band-pass filtered cylinder pressure and knock threshold. Knock onset is defined as when the amplitude of the pressure signal exceeds the set threshold.

Normalized MAPO (MAPONORM)

Despite the usefulness of MAPO as a knock detection method in laboratory tests, it has a couple of disadvantages. Interfering harmonic pressure waves may result in a peak value, which does not reflect the sum of the waves’ amplitudes, as noted by Shahlari and Ghandhi [57]. Moreover, if engine speed increases, the amplitude of the pressure signal’s spectrum rises [56,59,60], regardless of whether knock is present. As a consequence it is difficult to set a constant threshold applicable for a wide range of engine speeds. In [56], Siano et al. managed this issue by normalizing MAPO as:

$$MAPO_{NORM} = \frac{MAPO}{MAPO_{REF}} \tag{5}$$

Here $MAPO_{REF}$ is the maximum pressure oscillation computed from a cranking window before the combustion process for the same engine cycle. This normalization makes it possible to keep the same threshold for knock at different engine speeds.

Integral of Modulus of Pressure Oscillation (IMPO)

IMPO is a measure of the energy content of the high frequency pressure oscillations (including noise), Zhen et al. [61]:

$$\boldsymbol{IMPO = \frac{1}{N}\sum\nolimits_{1}^{N}\int_{\theta_0}^{\theta_0+\varphi}\left|P_{filt}\right| d\theta} \tag{6}$$

Integral of Modulus of Pressure Gradient (IMPG)

IMPG refers to the modulus of the pressure derivative [62]:

$$\boldsymbol{IMPG = \frac{1}{N}\sum\nolimits_{1}^{N}\int_{\theta_0}^{\theta_0+\varphi}\left|\frac{dP_{filt}}{d\theta}\right| d\theta} \tag{7}$$

Signal Energy of Pressure Oscillation (SEPO)

As highlighted by Eng et al. [63], the total wave intensity is proportional to the square of the pressure oscillations. Therefore, SEPO [64], computed by integrating the square of P_{filt} over a crank angle window starting from θ_{ko}, is a practical method for quantifying knock intensity. Generally a $\Delta\theta$ in the range of 5-20CAD is used [53,65,66].

$$\boldsymbol{SEPO = \int_{\theta_{ko}}^{\theta_{ko}+\Delta\theta} {P_{filt}}^2\, d\theta} \tag{8}$$

Heat release rate methods based upon in-cylinder pressure

The pressure oscillations and chemical reactions during knocking combustion also affect the heat transfers to the cylinder walls. Results by Wang et al. [67] estimate that during heavy knock nearly 40% of the total fuel energy is lost through heat transfer to cylinder walls. This is almost four times the heat transfer during normal combustion. Another finding in [67] was that the local pressures within the cylinder are extremely uneven during knocking combustion. Heat release rate, $\frac{dQ}{d\theta}$, is calculated according to the 1st law of thermodynamics [1]:

$$\boldsymbol{\frac{dQ}{d\theta} = \frac{\gamma}{\gamma-1}P\frac{dV}{d\theta} + \frac{1}{\gamma-1}V\frac{dP}{d\theta}} \tag{9}$$

Here, γ is the ratio of specific heats, P is the pressure, and V is the volume. A drawback of this method is that it assumes a thermodynamic equilibrium within the cylinder, i.e., uniform pressure [57], which, as mentioned above, is not the case during knocking combustion.

Engine block analysis

Knock detectors used in mass-production are generally based on engine block vibration analysis [58,68]. The high-pressure oscillations, induced by the end-gas auto-ignition, propagates through the combustion chamber, causing vibrations on the entire engine block. These vibrations can be detected by an accelerometer connected to the engine block. The accelerometer typically contains a piezoelectric element which transforms the mechanical vibrations into electrical signals, Dues et al. [69]. Thus, one low-cost sensor can detect knock from all the cylinders. However, the signal-to-noise-ratio (SNR) is lower and as it takes some time for the vibrations to reach the engine block, KO detection is delayed compared to cylinder pressure methods. The delayed KO is illustrated in Figure 4, as pointed out by Millo and Ferraro [52].

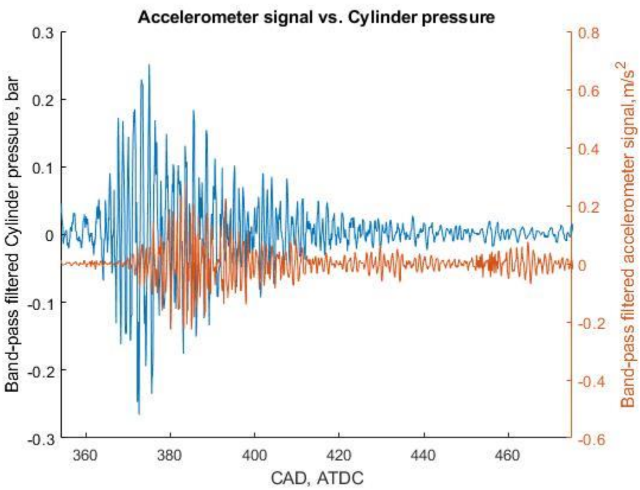

Figure 4. Band-pass filtered cylinder pressure (blue) vs. band-pass filtered accelerometer signal (red) for a knocking cycle. It is evident that the knocking oscillations are delayed in the accelerometer signal, and therefore it detects KO later. A band-pass filter of 4-25kHz was applied to both the cylinder pressure and the accelerometer signal.

The standard method to detect knock is to integrate the band-pass filtered accelerometer signal over the crank angles where knock is likely to occur. This method is known as the Integral of Modulus of Accelerometer Oscillations (IMAO) [70]:

$$\boldsymbol{IMAO} = \frac{\mathbf{1}}{\boldsymbol{N}}\sum\nolimits_{\mathbf{1}}^{\boldsymbol{N}}\int_{\boldsymbol{\theta_0}}^{\boldsymbol{\theta_0+\varphi}}\left|\boldsymbol{\alpha_{filt}}\right|\boldsymbol{d\theta} \tag{10}$$

Here, α_{filt} is the filtered accelerometer signal. Typically, the crank angle window is set from TDC to 40CAD ATDC, as discussed by Eriksson and Nielsen [71]. In analogy with IMPO, IMAO is a measure of the energy content of the high-pressure oscillations.

As pointed out in [52], several of the pressure based methods can also be applied to vibrational methods. For instance, MAPO can be substituted with the maximum amplitude of the band-pass filtered accelerometer signal. The energy content of the pressure oscillations can be captured in both the time and frequency domain, using the equal approach as for the cylinder pressure. In analysis by Siana et al. on experimental data [70], both the Discrete Wavelet Transform (DWT) and Auto-Regressive Moving Average (ARMA) model were applied to the accelerometer signal. The results showed good agreement with MAPO from cylinder pressure, but at the cost of a high computational expense.

Several studies have been conducted to determine the optimal location for mounting the accelerometers [69,72–74]. Dues et al. [69] established some general guidelines:

- Stiff locations centrally positioned on the lower part of the engine block
- Distanced from noise creating parts, such as the valve train and accessory drive.
- Between two cylinders, as it gives better stiffness compared to at a cylinder center line

Nevertheless, mechanical vibrations occur during normal combustions, and vibrations induced by knock needs to be separated from these. The main mechanical vibrations, as highlighted by Millo and Ferraro [52], include:

- Intake valve closing
- Exhaust valve closing
- Piston slap

Wagner et al. [75] listed some of the limitations of using an accelerometer as a knock sensor:

- Small knock events generally have low SNR
- Knock oscillations may not propagate through the engine block to the sensor

- Interfering noise, such as valve motion and piston lap, can be interpreted as knock
- The accelerometer does not capture knock resonances outside its bandwidth.
- The sensitivity to detect knock varies from cylinder to cylinder

Gas ionization methods

During the combustion process within an engine cylinder, ions are produced. Through applying a small direct current (DC) voltage over the spark gap an ion current is created. This current is directly proportional to the amount of combustion ions in the spark gap area and later, as combustion occurs, around the cylinder [76]. Hence, if the ionization current is present it implies that combustion is ongoing, and if current is not existing means no combustion [77]. In [76], this methods showed promise in detecting both misfire and pre-ignition, controlling knock, and obtaining cam phasing. Two drawbacks with this method are its additional cost and the computational complexity [78].

Combustion modeling

As it is well known that knock is related to temperature and pressure within the model [1,4,7], it is required to obtain these, through measurements or estimates, to predict if, and when, knock will occur.

Two-zone combustion model

In this thesis, a 2-zone combustion model consisting of one unburned zone and one burned zone, with uniformed pressure over both zones, was used to estimate the instant state within the cylinder. The details of the modelling work are described in Paper I. By using the ideal gas law together with a residual gas model from Eriksson and Nielsen [71], temperature at IVC could be obtained. By assuming adiabatic compression from IVC to start of combustion (SOC), the ratio of specific heats, γ, can be computed. γ together with the measured in-cylinder pressure, P_{cyl}, is then used to estimate both MFB and the unburned gas temperature, T_u. See the section *Methodology* in Paper I for details of the computations.

Modelling of ignition delay

The ignition delay within a combustion cycle can be predicted by using the Livengood-Wu (LW) integral introduced by Livengood and Wu [79], together with an Arrhenius function developed by Arrhenius [80].

Livengood-Wu

If one presumes two things during the induction chemistry period:

- the total production of critical species is solely related to the gas state
- the quantity of critical species required for auto-ignition is constant

Then, it can be assumed that auto-ignition takes place when the LW integral attains unity, as in Equation 1:

$$\int_{t=0}^{t_i} \frac{dt}{\tau} = 1 \qquad (11)$$

Here, t is the time passed since the start of end-gas compression (t=0), τ is the ignition delay at the instant pressure and temperature, and t_i is the time of auto-ignition [1,79]. τ can be modelled as in Equation 2:

$$\frac{\tau}{\tau_0} = f(T)\left(\frac{P}{P_0}\right)^{-n} \qquad (12)$$

Where τ_0 is the ignition delay observed at pressure P_0 at a set temperature T and n is a constant [79].

Arrhenius function

A common approach to model τ is by using an Arrhenius function [1], which was also adopted in this thesis.

$$\tau = Ae^{\frac{B}{T}}P^{-n} \qquad (13)$$

In the thesis, the constants in eq. (13) were optimized using multiple least square regression, as done by Kalghatgi [6], over a wide range of operating conditions. $1/T$ and *ln(P)* were set as independent variables, and *ln(τ)* as the dependent variable. The overall unburned gas temperature was estimated using the 2-zone combustion model. The hypothesized hot spot temperature was assumed to be fixed at $T_{HS} = T_u + 20K$. Pressure was given by the measured in-cylinder pressure. Since KO from MAPO, $\theta_{ko,exp}$, and engine speed *N* were known, the ignition delay at every CAD could be calculated.

Wiebe modeling

As Lindström et al. point out in [81], the combustion progression in a 2-zone combustion model can be modeled through the Wiebe function:

$$\boldsymbol{X_b = 1 - exp\left[-a\left(\frac{\theta - \theta_0}{\Delta\theta}\right)^{m+1}\right]} \tag{14}$$

Here, θ_0 is the start of combustion, and $\Delta\theta$ is the combustion duration. The combustion mode parameter m describes the shape of the combustion. A greater accelerating flame speed gives a higher m. The parameter a is dependent on the percentage of end of combustion (EOC) is set to. For instance, a is computed as followed with EOC=98%:

$$\begin{aligned} \boldsymbol{a} &= \boldsymbol{-ln(1 - X_{b,EOC})} \\ &= \boldsymbol{-\,ln(0.02)} \\ &= \boldsymbol{3.91} \end{aligned} \tag{15}$$

Knock control

As pointed out by Lezius et al. in [82] knock is usually mitigated by retarding the ignition timing. However, this approach also decreases the efficiency of the engine. To achieve an adequate trade-off between efficiency and not damaging the engine, production car engines of today are normally equipped with a knock sensor (accelerometer) together with a knock controller, Ängeby et al. [83]. Beneath, this method together with other common knock control methods are described.

Spark retardation

As discussed by Heywood in [1] and by Grandin et al. in [84] a common approach to mitigate knock is to retard the spark timing. Thus the high combustion temperatures and peak pressures, which elsewise may lead to knock, are reduced and knock can be mitigated, as shown by Lavoie et al. [85]. Vice versa, experimental results from Thomasson et al. in [86], on a 5-cylinder gasoline Saab Variable Compression (SVC) engine, indicated an increase from 1% to 20-40% (dependent on cylinder) of cycles knocking, when spark timing was advanced 4CAD from borderline condition. Another finding in [86] was that advancing the ST resulted in a larger fraction of cycles of high knock intensity.

However, retarded ignition negatively impacts normal combustion cycles by lowering combustion temperatures and slowing the combustion process. This leads to reduced combustion efficiency and increased heat losses. [1].
Lius et al. [9] demonstrated the loss in efficiency resulting from retarded ST in experiments on the same engine fuel-setup as used in this thesis. Their

results showed a relative drop in indicated thermal efficiency (ITE) of approximately 10% when ST was retarded 10CAD from knock limited spark advance (KLSA) at 1200rpm and 15bar $IMEP_g$. In experiments by Ayala et al. [87] on a DISI engine fueled with toluene and PRF120 showed similar characteristics. For example, a spark retardation of 20CAD from the maximum brake torque (MBT) resulted in a drop in net indicated mean effective pressure ($IMEP_n$) of about 20% at engine speed 1500rpm and load 3.5bar $IMEP_n$.

In-cycle suppression of knock

Mitigate knock in-cycle can be achieved by fuel-enrichment, as detailed by Singh and Dibble [88], or by water injection, as demonstrated by both Lius et al. [89] and Saharin [90].

Fuel injection

Experiments on a single cylinder research (SCR) engine [88], using PFI gasoline, examined the effects on knock intensity from direct injecting fuel into the combustion chamber after ST. Their results revealed that knock intensity consistently decreased with increasing amounts of excess fuel injected; for example, a 1.6kg/hr fuel injection resulted in a reduction from 0.7bar to 0.2bar KI. Since earlier fuel injection was correlated with both lower knock intensity and a prolonged SOC, it was hypothesized that the fuel quenched the flame propagating from the spark plug. Therefore, disturbing a small flame is likely to have a greater impact than disturbing a larger one. However, as fuel injection increased, combustion duration decreased rapidly while cycle-to-cycle variations increased, thereby increasing the potential risk of misfires. Another drawback of using fuel injection to suppress knock is of course the rise in fuel consumption and increased emissions.

Water injection

Saharin [90] explored the effects of a stoichiometric blend of ethanol and water on ignition delay on a rapid compression machine (RCM). At temperatures in the range of 750-860K and compression pressure 30bar, i.e. which resemble engine-like conditions, ignition delay decreased in all cases at 30% volume fraction water compared to neat ethanol. At most the ignition delay reduced from 9ms to 4.5ms. The reduced ignition delay was attributed to the chain branching reaction between hydrogen peroxide (H_2O_2) and hydroxyl (OH) using water as a third body:

$$\mathbf{H_2O_2(+H_2O) \leftrightarrow OH + OH(+H_2O)} \qquad (16)$$

However, simulated ignition delay times using models from Frassoldati et al. [91] and an unpublished version of the Aramco mechanism yielded inconsistent results, as reported in [90]. The Aramco model predicted increased reactivity and shorter ignition delays with added water at compression temperatures above 830K, but reduced reactivity and longer ignition delays at lower temperatures. The model from Frassoldati et al. predicted reduced reactivity and longer ignition delays at all temperatures.

In experimental work on the identical engine-fuel setup as in this thesis [89], Lius et al. examined the effects of direct injected water (DIW) on knock and nitric oxide (NO_x). Their results, at 10bar $IMEP_g$ and 1200rpm showed that a 5ms water injection resulted in knocking cycles dropping from 3% to none. However, this reduction came at the price of a reduction in combustion efficiency from 95% to 88%. Another finding in [89] was that the injected water lowered the exhaust temperature, which in turn resulted in a lower IVC temperature. Subsequently, combustion phasing could be advanced with DWI.

Methodology

The thesis consisted of three experimental studies aimed at addressing the research questions presented in the introduction section.

Knock predictability study

This research analyzed through experiments and modeling, whether it is possible to distinguish knocking cycles from normal cycles before spark timing (see methodology flowchart in Figure 5). The study also revealed how the knock predictability varied with CAD and MFB post-spark timing. Additionally, a Wiebe model was parameterized continuously in-cycle to predict the progress of each combustion cycle. Sweeps of load, engine speed, and intake manifold temperature were run. Spark timing was advanced to either MBT or KLSA for each operating condition.

Measured in-cylinder pressure was used to experimentally detect knock and knock onset using MAPO, as explained in the section *Maximum Amplitude of Pressure Oscillations (MAPO)*.

A residual gas model from Eriksson and Nielsen [71], in combination with a 2-zone combustion model detailed in Paper I, was used to estimate the instant state of the unburned gas within the cylinder. Knock was then predicted through LW, as described in the section *Combustion modeling*. This process was applied to all combustion cycles for each operating condition tested. Normal distributions of measured in-cylinder pressure, estimated unburned gas temperature, and the LW integral were computed to assess the confidence level at which knocking and normal cycles could be distinguished before spark timing.

Post-spark timing, a statistical analysis of the in-cylinder state and combustion characteristics was performed for both normal and knocking cycles. This was done to assess, at what confidence level and for every CAD and percent of MFB, whether a cycle would knock or not.

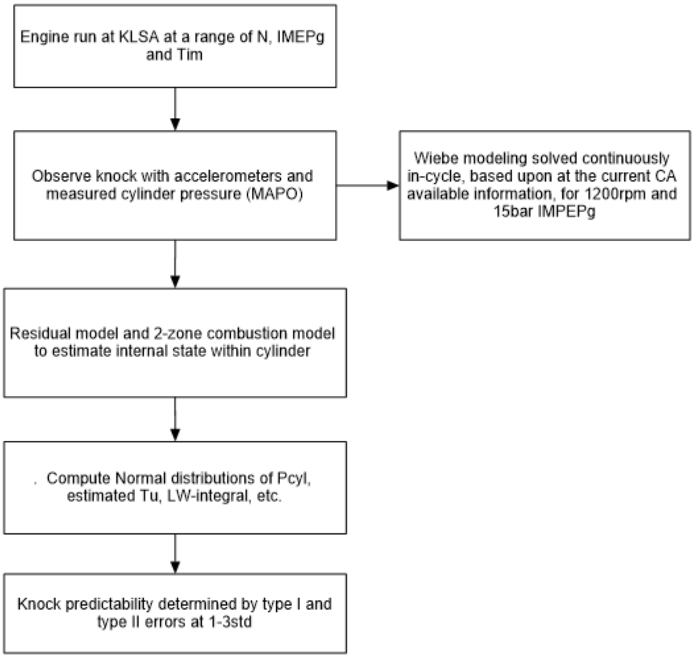

Figure 5. Flowchart of the methodology used in the knock predictability study.

Oil entrainment study

The second experimental study investigated how oil entering the combustion chamber could be altered by changing the piston ring gap and using lubricant oils with different viscosities and volatilities (see methodology flowchart in Figure 6). The engine was run on methanol at stoichiometric conditions, i.e., a low-sooting fuel. Hence, the measured PN in the exhaust could be assumed to originate from the lubricant oil. Three different oil compositions were used in the experiment. The piston rings' rotational offset was locked into three different positions, along with free rotating rings. The engine was run at operating conditions selected from the World Harmonized Stationary Cycle (WHSC) operating points of a full-size engine. Start of fuel injection was altered to change lambda. Fuel timing was configured to accomplish full vaporization of the liquid fuel, and the end of injection was hold constant through all the experiments. No EGR was added to the engine. Particle measurements were conducted with a TSI EEPS 3090 Engine Exhaust Particle Sizer Spectrometer measuring particle size distributions in 32 bins, ranging from 5.6nm to 560nm in size.

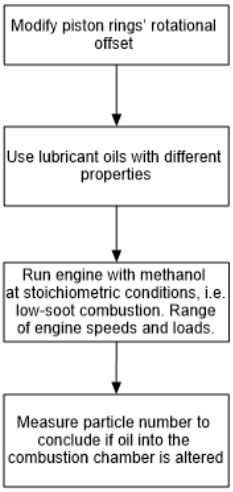

Figure 6. Flowchart of the methodology used in the oil entrainment study.

Oil entrainment influence on knock

This experiment investigated the influence of lubricant oil on auto-ignition by examining the correlation between PN and the engine's tendency to knock (see methodology flowchart in Figure 7). As in the previous study, different oils and varying piston ring offsets were used to alter the amount of oil into the engine. As the engine was run on methanol at stoichiometric conditions, i.e., a low-sooting fuel, measured PN was a marker of the amount of oil entering the cylinder. Sweeps of load and engine speed were run. Spark timing was, for each operating condition and oil-ring configuration, advanced to either MBT or the engine control's knock limit.

The increase in oil entering the engine was expected to result in an extension of oil-rich spots, leading to higher reactivity (see section *Lubricant oils and oil spots*). Thus, if knock tendency increased with higher PN, under identical spark timing and thermodynamic conditions, it would be interpreted as higher reactivity due to the induced oil. Knock was detected using MAPO.

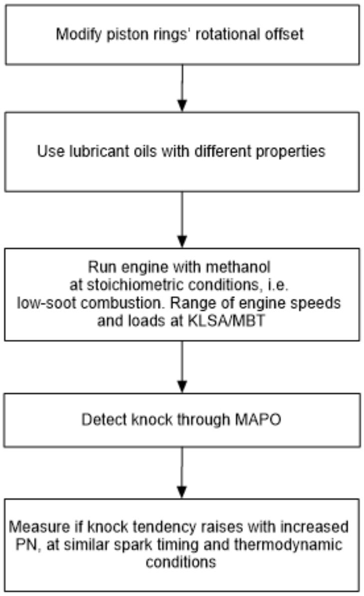

Figure 7. Flowchart of the methodology used when examining the oil entrainment influence on knock.

Experimental engine

Experiments were performed on a Scania HD PFI single-cylinder engine. The engine is based on a HD CI engine with one separate runner per inlet port. This concept may result in a stratified charge, which can influence the local equivalence ratio close to the spark plug [92]. A flash-mounted piezoelectric transducer was used to measure the in-cylinder pressure. The in-cylinder pressure was band-pass filtered in the range of 4-10kHz to obtain pressure oscillations used for MAPO analysis. Two accelerometers were positioned on the engine block and sampled at a minimum of 75kHz and filtered with the equivalent band-pass filter as the cylinder pressure. Pressure in the intake manifold, in-cylinder and exhaust, together with CAD, were all continuously sampled at each 0.1CAD. Engine specifications are listed in Table 2:

Table 2. Engine specifications.

Displaced volume	1.950l
Stroke	154mm
Bore	127mm
Connecting Rod	255mm
Compression ratio	14:1
Number of Valves	4
Intake Valve Open (IVO)	-14CAD ATDC
Intake Valve Close (IVC)	-154CAD ATDC
Exhaust Valve Open (EVO)	145CAD ATDC
Exhaust Valve Close (EVC)	355CAD ATDC

Fuel

In all three experimental studies, the engine was fueled with methanol at stoichiometric conditions. This procedure ensured low-sooting combustion and that the PN could be traced to lubricant oil entering the combustion chamber.

Results

The results connected to the thesis' research questions are summarized below.

Knock detection pre-spark timing

As highlighted in the introduction, knock is associated with high in-cylinder temperature, pressure and LW build-up. Therefore, to assess knock predictability, it was required to explore if these were higher for knocking cycles compared to normal cycles. Figure 8 shows normal distributions over LW build-up for both normal and knocking cycles. In this case, engine speed was 1200rpm and the $IMEP_g$ was 15bar. However, the same pattern, with similar distributions of pressure, temperature, and LW build-up between normal and knocking cycles appeared for all other operating conditions as well, which is laid out in detail in Paper I. Hence, for the given engine-fuel setup, hot spots are likely not the root cause of auto-ignition, and knock can therefore not be predicted before spark timing. Consequently, any in-cycle regulation, based on a hypothesized hot spot temperature, would not be effective.

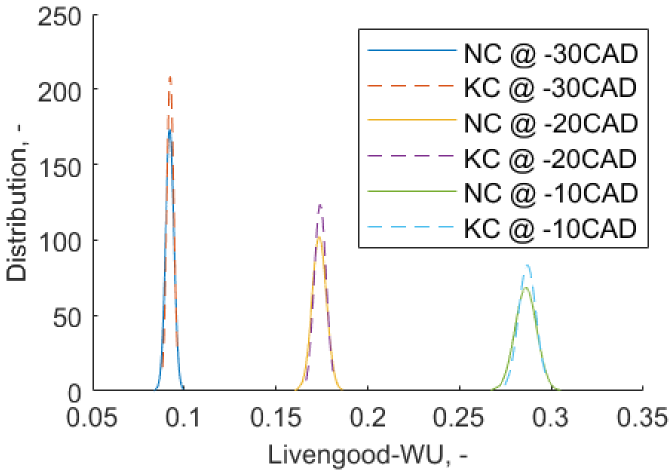

Figure 8. Normal distributions of LW build-up at -30, -20, and -10CAD ATDC. Normal cycles (NC) and knocking cycles (KC) have very similar distributions. The engine speed was 1200rpm and the $IMEP_g$ was 15bar.

Knock detection post-spark timing

The spark timing distributions shown in Figure 9 for an engine speed of 1200rpm and $IMEP_g$ of 15bar were similar across all other operating conditions. As illustrated in the figure, the distributions are close to identical for knocking and normal cycles. Nevertheless, when spark timing is slightly retarded (in this case to about -8.3CAD ATDC) knock disappears.

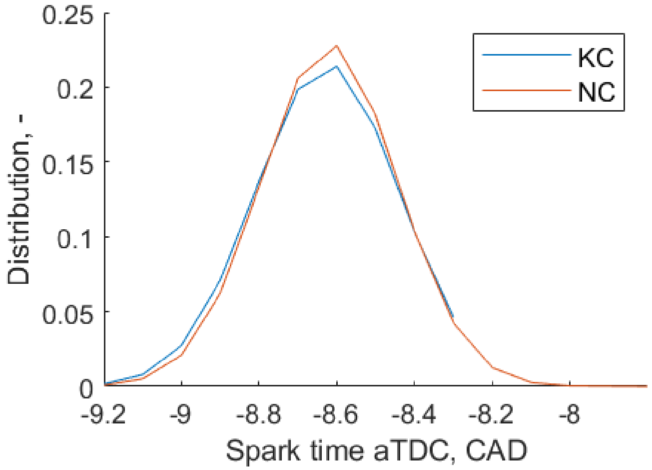

Figure 9. Normal distributions of spark timing for knocking and normal cycles. The engine speed was 1200rpm and the $IMEP_g$ was 15bar. The distributions are nearly identical.

In Figure 10, distributions of start of combustion (SOC) and combustion duration are displayed for both normal and knocking cycles at an engine speed of 1200rpm and an $IMEP_g$ of 15bar. Overall, knocking cycles have an earlier SOC and burn faster than normal cycles. Still both metrics exhibit significant overlaps. For instance, 74% of normal cycles are misinterpreted as knocking cycles within 3 standard deviations (σ) when we choose to capture knocking cycles based on crank angle at 10% fuel mass burnt (CA10). This pattern of overlap was similar across all analyzed operating conditions.

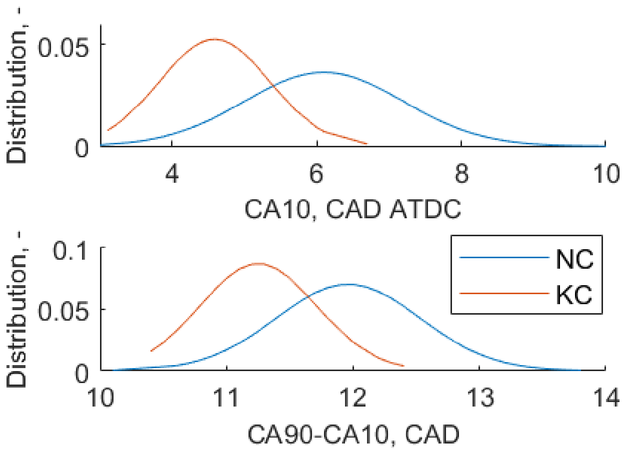

Figure 10. Normal distributions of start of combustion (upper plot) and combustion duration (lower plot) for knocking and normal cycles. The engine speed was 1200rpm and $IMEP_g$ was 15bar. It is clear that knocking cycles both start to burn earlier and burn faster compared to normal cycles. However, both metrics show significant overlaps.

Knock control post-spark timing

Figure 11 illustrates how type I and type II errors in knock detection certainty, based on capturing knock within 1-3σ of MFB, vary with MFB. As shown, both type I and type II errors decrease until MFB is around 40-50%, at which point at least about 15% type I errors and 20% type II errors persist.

Liu et al. [93] demonstrated through engine experiments on an SCR engine, equipped with DI, that direct water injection (DWI) is an efficient method to mitigate knock. However, Lius et al. [89] showed through experiments on the same engine-fuel configuration as in this thesis, that DWI to suppress knock may reduce the indicated thermal efficiency (ITE). For example, the earliest tested post-spark timing DWI resulted in an absolute drop in ITE of about 0.8%. In contrast, the drop in ITE from retardation of spark timing was only 0.4% per CAD. As displayed in Figure 9, most knock occurs when spark timing is around -8.6CAD ATDC but disappears when spark timing is approximately -8.3CAD ATDC. Hence, retarding spark timing by just 0.3CAD reduces ITE by only 0.12%.

Given the large type I and type II errors, along with the potentially greater drop in ITE from DWI compared to spark retardation, DWI may not be a practicable method to mitigate knock in the current engine-fuel configuration.

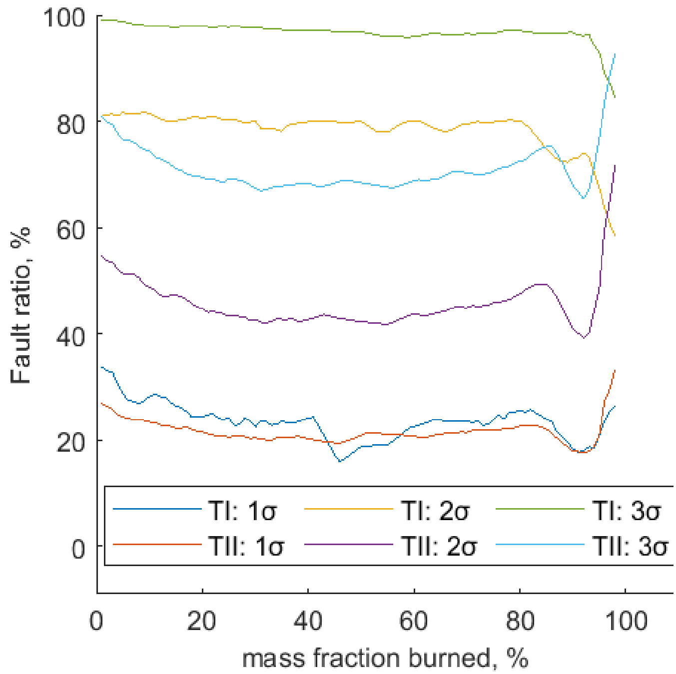

Figure 11. Type I (T1) and Type II (T2) errors vs. MFB at engine speed of 1200rpm and $IMEP_g$ of 15bar, averaged over five data points. It shows that, in most cases, the proportion of both type I and type II errors decreases until MFB is about 40-50%.

Oil composition's and engine configuration's influence on PN

It was demonstrated that both oil composition and piston ring offset could alter PN, as shown in Figure 12. High-volatility oil increased PN, while high-viscosity oil reduced it. All locked ring configurations resulted in lower PN compared to free-floating rings. Among the locked configurations, decreasing the ring gap offset resulted in increased PN.

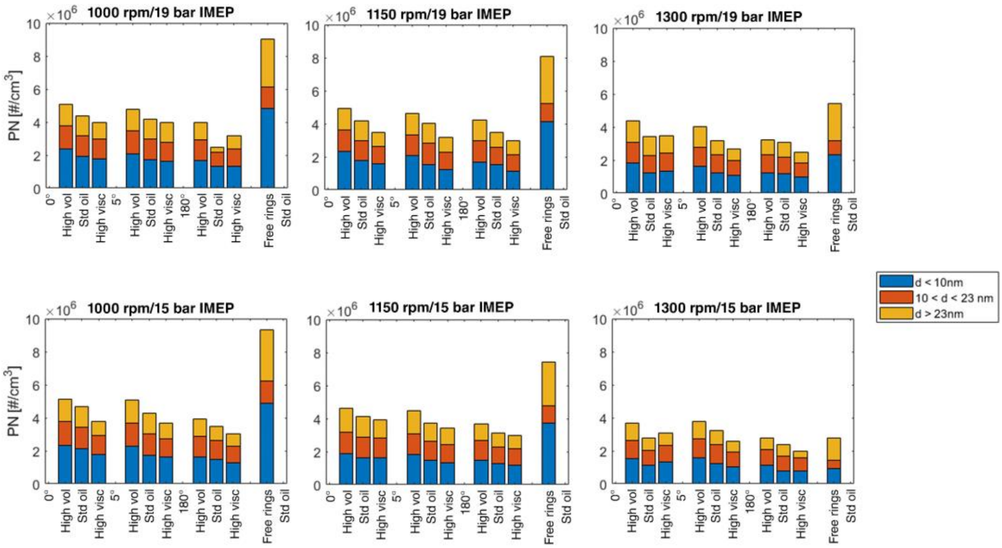

Figure 12. PN variation for different oils, piston ring configurations, and operating conditions. Reprinted with permission from Adlercreutz et al. [94].

Correlation between PN and knock

Only two operating conditions (low engine speed, medium load: N=1000rpm, $IMEP_G$=1.5MPa; and low engine speed, high load: N=1000rpm, $IMEP_G$=1.9MPa) exhibited a significant degree of knock tendency. Therefore, focus was placed on these conditions. To validate the hypothesis that an increase in oil-originating PN is associated with an increased knock tendency, it was required that the engine was operated under comparable thermodynamic conditions for all PN levels at each operating condition. Therefore, ignition delay (ST to CA10) and combustion duration (CA10 to CA90) were computed for each particle number case (PNC), as shown in Figure 13.

Regarding the high-load point, it is clear that both the start of combustion and combustion duration are similar across all PNCs. This indicates that the thermodynamic requirements were fulfilled.

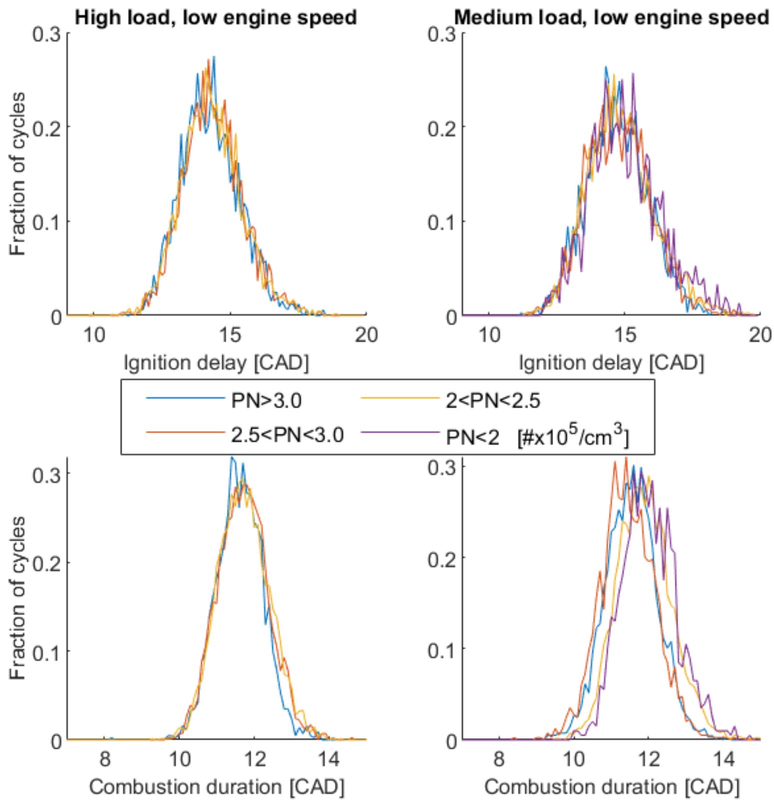

Figure 13. Ignition delay (upper plots) and combustion duration (lower plots) of different PNCs at low engine speed, and at both high and medium loads are shown. For the high-load point, both ignition delay and combustion duration display nearly identical distributions across all PNCs. On the other hand, at medium load, the combustion durations are split into two groups, one with shorter duration and one with longer.

To examine the impact of lubricant oil on auto-ignition, the ratio of knocking cycles was plotted versus the latest spark timing for all PNCs. As illustrated in Figure 14, this hypothesis holds true for the low-speed, high-load operating condition. Moreover, as anticipated, the advance of spark timing is more limited for the higher PNCs.

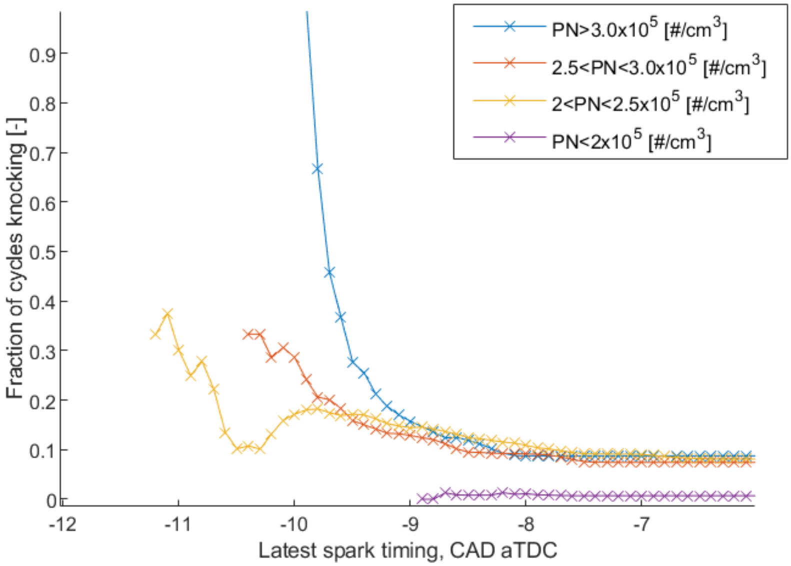

Figure 14. Fraction of cycles knocking compared to latest spark timing for different PN. Operating conditions were N=1000rpm and $IMEP_G$=1.9MPa. As oil-originating PN increases, the fraction of knocking cycles rises. In addition, the engine control system limits the spark timing advance more restrictively as PN is increased.

At medium load and low speed, the different PNCs were split into two groups: one with longer combustion duration and one with shorter, as shown in Figure 13. For both combustion durations, an increased knock tendency at higher PN levels was observed. Moreover, an increase of about 20% in PN had less effect on knock tendency than a decrease in burn duration of 0.35CAD. These results are discussed in more detail in Paper III.

Discussions

The experimental findings by Lius et al. in [8,9] and by Königsson in [13], as discussed in the *Introduction* section, along with the results presented in Paper I in this thesis, support the conclusion that hot spots are unlikely to be the root cause of auto-ignition in the current engine-fuel configuration. Therefore, an explanation must be found elsewhere. Increased local reactivity, with the potential to cause knock, from fuel-rich spots and oil spots is discussed below.

Fuel-rich spot trigger to auto-ignition

As demonstrated in Figure 2 in the section *Fuel-rich spots*, the unburned gas temperature is at least 90K below what is required to enter a region of reactivity at TDC for the given engine-fuel setup. Furthermore, since spark timing is around 10-15CAD BTDC for the operating conditions run in this thesis, this implies that the gas is even further away from a reactive region. In addition, as pointed out by Zhu et al. [95], methanol does not exhibit cool flame characteristics. As a result, no temperature increase due to LTHR would be added to a fuel-rich spot. Despite the fact, as discussed by Fernandez-Tarrazo et al. [96], that methanol-air has its lowest minimum ignition energy at a slightly fuel-rich mixture, this ignition energy is, as shown by Metzler [97], at most 25% lower compared to stoichiometric conditions. Taken together, potential inhomogeneities in the air-to-fuel mixture are unlikely to cause a highly reactive spot in the engine, and fuel-rich spots are most likely not the root cause of auto-ignition in the engine-fuel configuration used in this thesis.

Lubricant oils and oil spots

The experimental results from Paper III suggest that lubricant oil entering the combustion chamber can be a plausible source of auto-ignition. The oil consists of long carbon chains, and when they break, they form hydrocarbon radicals, which are highly reactive, as detailed by Glassman [45]. Hence, oil droplets can change the local composition of a mixture, thus creating reactive spots with a lower octane number and subsequently making the engine more prone to knocking. Moreover, the oil droplets increase the richness of the local mixture, which leads to even greater reactivity. When summarizing the results from previous research [47–51] along with the outcomes from this thesis, oil droplets are considered to be a more plausible cause of knock in the current engine-fuel configuration than both hot spots and fuel-rich spots.

Conclusions

This thesis has enhanced the knowledge regarding knocking combustion in a heavy-duty spark-ignited engine fueled by methanol. The key findings are summarized in bullets below.

- Knock cannot be accurately predicted before spark timing for the given engine and fuel
- Hot spots are unlikely to be the root cause of auto-ignition, and adaptive knock prediction based on a hypothesized hot spot temperature would likely be ineffective
- Knocking cycles start to burn earlier and burn faster than normal cycles. However, the overlap between normal and knocking cycles, in terms of combustion and LW build-up, may be too large to make post-spark timing knock control beneficial. For example, water injection can penalize normal combustion cycles more than simply retarding the spark timing to 1% knock occurrence (i.e., standard knock control).

- The amount of oil entering the cylinder through the piston-rings, and consequently the prevalence of oil-spots, can be altered by modifying the ring gap offset and by using oils of different properties.
    - Both a decreased offset and a high volatility oil increase oil-originating PN
    - A high viscosity oil decreases it
- PN is an indicator of the amount of oil entering the cylinder
- A higher PN has been shown to correspond to an engine more prone to knocking
- Oil spots acting as rich spots, i.e. increasing the reactivity within the engine, are believed to be the root cause of knock in the current engine-fuel configuration

Future work

The correlation between knock and oil should be investigated further under additional operating conditions and with other ring-oil configurations. Moreover, an interesting study would be to repeat the experiments in Paper I using some of the fuels employed in the experiments by Kalghatgi et al. [6,7]. This would help to explore whether there exists a fuel on which the engine can operate that would make knock predictable. Additionally, running the engine at knock-limited conditions with a fuel-rich mixture using an NTC fuel, would provide insights into whether the engine can be sensitive to fuel-rich spots.

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