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Assessing single-fuel solutions enabling compression ignition of renewable methanol

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DOCTORAL DISSERTATION

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Abstract: In today's world, the transportation of goods via trucks and ships plays a pivotal role, and this trend is expected to persist in the foreseeable future, owing to its critical importance to society. However, the most common propulsion system for these vehicles, the compression ignition (CI) engine, commonly known as the diesel engine, relies heavily on fossil diesel fuel, resulting in significant emissions that need to be mitigated to achieve the climate goals. Transitioning to electric power for heavy-duty transport vehicles is challenging due to the need for large battery packs, which consume valuable cargo space and reduce load capability. For some applications, such as shipping, electrification simply cannot deliver the required autonomy. Instead renewable fuels present a more promising solution with hydrogen, ammonia, and alcohols as alternatives. Among those methanol has emerged as a particularly promising option, especially in the marine sector. Methanol's use in the chemical industry, coupled with its liquid state under normal conditions, makes it an intriguing alternative. While methanol production is currently predominantly based on natural gas, there is a growing emphasis on renewable production methods enabling bio-methanol and e-methanol, which could potentially make methanol a renewable fuel. In compression ignition engines, methanol exhibits unique combustion characteristics. Its higher heat of vaporization, coupled with the higher mass that must be injected, creates a significant cooling effect in the combustion chamber. While this effect reduces temperatures and mitigates nitrogen oxide (NOx) generation, it also poses challenges for ignition, particularly during start-up and colder conditions. The objective of this doctoral thesis was to investigate techniques that could facilitate single-fuel methanol CI ignition and provide recommendations for which concepts to further develop. To identify which concepts to investigate a literature review was conducted to identify the most promising single-fuel neat methanol CI concepts. Among these, the use of ignition improver, increased compression ratio and a pilot injection strategy were further investigated. However, other potentially beneficial concepts were also identified. The use of ignition improver, which has undergone extensive development and testing, involves blending it with methanol to enhance methanol's autoignition properties. This approach was tested by the EU FASTWATER project, where an engine was adapted to run on a fuel blend consisting of methanol with 3% ignition improver. Installed in a pilot boat in Sweden, this engine exhibited robust performance year-round, even in cold winter conditions, meeting stringent marine legislation limits without the need for aftertreatment. Analysis of the engine in combination of laboratory tests confirmed the significantly improved combustion characteristics with the addition of the ignition improver, but also highlighted lower emissions of carbon monoxide (CO) and NOx compared to diesel. However, blending an ignition improver additive with methanol necessitates a blending process, adding complexity to fuel production and increasing costs compared to pure methanol. This prompted further exploration into neat methanol concepts. As part of the pilot boat conversion, the piston was upgraded to a higher compression piston, to add more compression heat and partially counteract the cooling effect of methanol injection. While this helped in achieving stable combustion, the need for an ignition improver persisted, prompting investigation into whether increased compression ratio alone could enable stable combustion of neat methanol. Our tests confirmed that a sufficiently high compression ratio could indeed maintain stable methanol combustion, on its own, albeit with a potential limitation of the engine operating range and high load efficiency due to increased pressure levels. During this testing, we also tested a pilot injection strategy with promising results. With pilot injection, a small portion of fuel is injected early in the combustion process, causing less excessive cooling and thus igniting more easily. This early combustion provides heat to ignite the larger quantity of fuel injected later, improving the combustibility of neat methanol. Our research demonstrated that pilot injection significantly reduces the temperature requirement in the engine, enhances efficiency, and decreases NOx emissions compared to a single injection of neat methanol. In summary, there are various partial solutions available to address the challenges of achieving stable neat methanol combustion in CI engines. To advance this research further, it is crucial to integrate and optimize these different partial solutions. By combining techniques such as glow plug utilization, increased compression ratio, EGR and pilot injection, it might be possible to enable stable combustion of neat methanol. This holds the potential to significantly accelerate the decarbonization of heavy transport and contribute to a more sustainable future.

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Table of Contents

Abstract 8
Populärvetenskaplig sammanfattning 10
List of Papers 12
Author's contribution to the papers 13
Peer-reviewed papers not included in this thesis 14
Abbreviations 15

1 Introduction 17
1.1 Heavy-duty transport 18
1.1.1 Conventional compression ignition engines 18
1.1.2 Conventional diesel emissions and regulations 19
1.2 Solutions 21
1.2.1 Electrification 21
1.2.2 Renewable fuels 22
1.3 FASTWATER 26

2 Research Scope and Objectives 27

3 Methanol single-fuel engine concepts 28
3.1 Spark ignition 28
3.2 Pre-chamber 29
3.3 Compression ignition 30
3.3.1 Dual-fuel 30
3.3.2 Blending with diesel 31
3.3.3 Adding Ignition improver 31
3.3.4 Glow Plug 32
3.3.5 Increased In-Cylinder Temperature 33
3.3.6 Advanced Injection Strategies 34
3.3.7 Conclusion 35

4 Research output 36
4.1 Experimental setup 36
4.1.1 Engine 36
4.1.2 Emission measurements 39

4.1.3 Post processing 40
4.1.4 Experimental Accuracy 40
4.2 MeOH97 41
4.2.1 Pilot boat.....41
4.2.2 Comparing to diesel and MeOH100 42
4.3 Improving low load methanol CI.....50
4.3.1 Increased compression ratio 50
4.3.2 Pilot injection.....51
5 Conclusion.....58
5.1 Summary.....58
5.2 Future work 59
5.3 Thesis contribution 60
6 Acknowledgements.....61
7 References 62
Appendix 71

Abstract

In today's world, the transportation of goods via trucks and ships plays a pivotal role, and this trend is expected to persist in the foreseeable future, owing to its critical importance to society. However, the most common propulsion system for these vehicles, the compression ignition (CI) engine, commonly known as the diesel engine, relies heavily on fossil diesel fuel, resulting in significant emissions that need to be mitigated to achieve the climate goals. Transitioning to electric power for heavy-duty transport vehicles is challenging due to the need for large battery packs, which consume valuable cargo space and reduce load capability. For some applications, such as shipping, electrification simply cannot deliver the required autonomy.

Instead renewable fuels present a more promising solution with hydrogen, ammonia, and alcohols as alternatives. Among those methanol has emerged as a particularly promising option, especially in the marine sector. Methanol's use in the chemical industry, coupled with its liquid state under normal conditions, makes it an intriguing alternative. While methanol production is currently predominantly based on natural gas, there is a growing emphasis on renewable production methods enabling bio-methanol and e-methanol, which could potentially make methanol a renewable fuel.

In compression ignition engines, methanol exhibits unique combustion characteristics. Its higher heat of vaporization, coupled with the higher mass that must be injected, creates a significant cooling effect in the combustion chamber. While this effect reduces temperatures and mitigates nitrogen oxide (NO_x) generation, it also poses challenges for ignition, particularly during start-up and colder conditions.

The objective of this doctoral thesis was to investigate techniques that could facilitate single-fuel methanol CI ignition and provide recommendations for which concepts to further develop.

To identify which concepts to investigate a literature review was conducted to identify the most promising single-fuel neat methanol CI concepts. Among these, the use of ignition improver, increased compression ratio and a pilot injection strategy were further investigated. However, other potentially beneficial concepts were also identified.

The use of ignition improver, which has undergone extensive development and testing, involves blending it with methanol to enhance methanol’s autoignition properties. This approach was tested by the EU FASTWATER project, where an engine was adapted to run on a fuel blend consisting of methanol with 3% ignition improver. Installed in a pilot boat in Sweden, this engine exhibited robust performance year-round, even in cold winter conditions, meeting stringent marine

legislation limits without the need for aftertreatment. Analysis of the engine in combination of laboratory tests confirmed the significantly improved combustion characteristics with the addition of the ignition improver, but also highlighted lower emissions of carbon monoxide (CO) and NO_x compared to diesel.

However, blending an ignition improver additive with methanol necessitates a blending process, adding complexity to fuel production and increasing costs compared to pure methanol. This prompted further exploration into neat methanol concepts.

As part of the pilot boat conversion, the piston was upgraded to a higher compression piston, to add more compression heat and partially counteract the cooling effect of methanol injection. While this helped in achieving stable combustion, the need for an ignition improver persisted, prompting investigation into whether increased compression ratio alone could enable stable combustion of neat methanol. Our tests confirmed that a sufficiently high compression ratio could indeed maintain stable methanol combustion, on its own, albeit with a potential limitation of the engine operating range and high load efficiency due to increased pressure levels. During this testing, we also tested a pilot injection strategy with promising results.

With pilot injection, a small portion of fuel is injected early in the combustion process, causing less excessive cooling and thus igniting more easily. This early combustion provides heat to ignite the larger quantity of fuel injected later, improving the combustibility of neat methanol. Our research demonstrated that pilot injection significantly reduces the temperature requirement in the engine, enhances efficiency, and decreases NO_x emissions compared to a single injection of neat methanol.

In summary, there are various partial solutions available to address the challenges of achieving stable neat methanol combustion in CI engines. To advance this research further, it is crucial to integrate and optimize these different partial solutions. By combining techniques such as glow plug utilization, increased compression ratio, EGR and pilot injection, it might be possible to enable stable combustion of neat methanol. This holds the potential to significantly accelerate the decarbonization of heavy transport and contribute to a more sustainable future.

Populärvetenskaplig sammanfattning

Idag transporteras stora mängder gods runt om i världen med lastbilar och fartyg, vilket förväntas fortsätta även i framtiden då det är avgörande för samhällets funktion. Det vanligaste framdrivningssystemet för dessa fordon är kompressionständningsmotorn, även känd som dieselmotorn, som då vanligtvis drivs av fossilt dieselbränsle. Detta resulterar i betydande utsläpp som måste minskas, för att uppnå klimatmålen och minska de hälsorisker som kommer med inandning av utsläppen.

Att elektrifiera tunga transportfordon är en utmaning då det kräver stora batteripaket för att upprätthålla räckvidden, vilket i sin tur tar upp värdefull lastplats och vikt. Dessutom är batterimaterialen begränsade och bör användas där de kan ge mest nytta per enhet material, vilket inte nödvändigtvis är fallet här. Istället bör alternativa förnybara bränslen övervägas. Bland de alterantiva bränslena återfinns ammoniak, vätgas och alkoholer. Ammoniak har fått intresse eftersom det inte ger upphov till koldioxidutsläpp, dock har det visat sig sig leda till utsläpp av lustgas, en mycket potent växthusgas med en global uppvärmningspotential över 200 gånger värre än koldioxid. Dessutom är den svår att antända, har låg energidensitet och är svår att hantera. Vätgas är mer lovande för att minska koldioxidutsläppen eftersom förbränningen, teoretiskt, genererar endast vattenånga. Men det som hindrar vätgas är dess naturliga form som gas, tillsammans med dess låga energidensitet, cirka 10 gånger lägre än diesel vid 700 bar tryck, vilket komplicerar användning, transport och lagring. Alkoholer däremot är flytande vid normala förhållanden och används redan idag som bränsle i bensinmotorer. Användningen är dock ännu inte särskilt utbredd bland dieselmotorer. Mellan metanol och etanol har metanol fått mer intresse, särskilt inom marina transporter, vilket beror på att metanol är mer tillgängligt och har lägre tillverkningskostnad. Metanolproduktionen idag är huvudsakligen baserad på naturgas, dock finns det en ökande betoning på förnybar tillverkning som exempelvis bio-metanol och e-metanol, vilket gör metanol till ett förnybart bränsle.

I kompressionständningsmotorer uppvisar metanol unika förbränningsegenskaper. Dess högre ångbildningsvärme, dvs energin som krävs för förångning, tillsammans med den högre massa som måste injekteras, gör att det blir en kraftig kylningseffekt i förbränningskammaren. Detta minskar temperaturen och reducerar kväveoxid (NO_x) genereringen som annars inträffar vid högre temperaturer i förbränningskammaren. Det gör det dock svårare att antända metanol genom kompression samtidigt som metanol redan har ett högt antändningstemperaturkrav. Sammantaget försvåras särskilt uppstart och drift vid kallare förhållanden, och gör att man riskerar misständning.

Målet med denna doktorsavhandling är att undersöka vilka tekniker som kan användas för att underlätta antändningen av metanol och ge rekommendationer för vilka tekniker som ska fortsatt undersökas.

En lösning som har testats i en lotsbåt i Sverige, och som vi har analyserat och dokumenterat, är att blanda i några procent av en tändförbättrande tillsats i metanolen. Detta gör att blandningen får egenskaper som ger lättare antänding genom kompression. Motorn, som vi har analyserat, har visat väldigt bra resultat på driftsäkerhet och utsläppsmätningar, och har fungerat året runt trots kalla vinterdagar som annars lätt skapar problem. Bränsleblandningen som har 3% tändningsförstärkare testade vi sedan experimentellt i en forskningsmotor. Där påvisade vi de markant förbättrade förbränningsegenskaperna som metanol får med tändningsförstärkning. Vi såg också att det inte behövs lika mycket tändförstärkare när motorn körs hårt och är varm. Detta visar att det är mest vid kallare förhållanden som tillsatsen behövs. Vidare, visade studien att metanol har ansenligt lägre utsläpp av kolmonoxid och kväveoxider jämfört med diesel. Att blanda i en tändförbättrande tillsats kräver dock en blandningsprocess vilket lägger till en komplexitet till bränsle-tillverkningenvilket gör blandningen dyrare än ren metanol.

Ett annat lösning är att höja kompressionstalet i motorn, det vill säga hur mycket luften komprimeras innan bränslet injiceras för att antändas. Temperaturen på luften i motorn är nämligen direkt kopplad till hur mycket den komprimeras. Vi visade att ett tillräckligt högt kompressionstal kan upprätthålla en stabil förbränning av metanol. Dock måste man vara försiktig med att inte ha för högt kompressionstal då man riskerar att trycket i motorn blir större än vad den klarar.

En teknik som vi också undersökte är att injicera metanolen i omgångar vilket både kan sprida ut kylningseffekten och förvärma motorn. Detta genom att en liten andel metanol sprutas in först, med liten kylningseffekt, och antänds vilket kan ge tillräckligt med värme för antända den större andelen bränsle som sprutas in därefter. Detta koncept kallas pilotinsprutning och har genom vår forskning visat sig kunna ansenligt sänka kravet på temperaturen i motorn, öka effektivitet och sänka kväveoxidutsläppen.

Vidare gjorde jag en noggrann litteraturstudie för att kunna ge rekommendationer för vad fortsatt forskning ska fokusera på. Som sammanfattning kan man säga att det inte finns en lösning för stabil metanolförbränning i kompressionständningmotorer idag utan tändningsförstärkare. Dock finns det många dellösningar och för framtida forskning gäller det att kombinera de olika del lösningarna: glödstift, höjt kompressionstal, varm EGR och delad injektion för att hitta den bästa lösningen för att möjliggöra stabil förbränning av metanol. Sådana lösningar kan bidra till att kraftigt skynda på processen att defossilisera den tunga transporttrafiken och ta ett stort steg mot en mer miljövänlig framtid.

List of Papers

Paper I

Pu, Y.P., Dejaegere, Q., **Svensson, M.** and Verhelst, S., "Renewable methanol as a fuel for heavy-duty engines: a review on technologies enabling single-fuel solutions," Energies 2024, 17, 1719, doi:10.3390/en17071719.

Paper II

Svensson, M., Molander, P., Ramne, B., Tunér, M. and Verhelst, S., "The development and certification of a single fuel high speed marine CI engine on methanol," Proceedings of the 30th CIMAC World Congress, Busan, South Korea, Paper No. 535, 2023.

Paper III

Svensson, M., Tuner, M. and Verhelst, S., "Investigation of combustion characteristics of a fuel blend consisting of methanol and ignition improver, compared to diesel fuel and pure methanol," Proceedings of the SAE World Congress 2024, Detroit, USA, SAE Technical Paper 2024-01-2122, doi:10.4271/2024-01-2122.

Paper IV

Svensson, M., Tuner, M. and Verhelst, S., "Low Load Ignitability of Methanol in a Heavy-Duty Compression Ignition Engine," Proceedings of the SAE 2022 Powertrains, Fuels & Lubricants Conference & Exhibition (PF&L), Krakow, Poland, SAE Technical Paper 2022-01-1093, 2022, doi:10.4271/2022-01-1093.

Paper V

Svensson, M., Tuner, M. and Verhelst, S., "Experimental investigation of pilot injection strategies to aid low load compression ignition of neat methanol," Proceedings of the SAE World Congress 2024, Detroit, USA, SAE Technical Paper 2024-01-2119, 2024, doi:10.4271/2024-01-2119.

Author's contribution to the papers

Paper I

I participated in the planning and was solely responsible for the compression ignition part of the review, while spark ignition and pre-chamber was covered by the other authors. I also aided in the writing of the introduction and conclusion, but it was not my main responsibility. The peer-review responsibility was shared among the authors with everyone doing their respective parts but I also aided in the peer-review revision of the introduction, pre-chamber and conclusion sections. All author reviewed each other's parts and approved the full content of the paper.

Paper II

I participated in the experiments, interpretation and analyzing of the results, but the experiments were mainly carried out by the co-authors. I was, however, the main responsible for the information collection, writing and peer-review process with only some aid from the other authors through information and feedback.

Paper III

I was the main responsible for this paper, and so did most of the planning, experiments, analyzing, formulation of conclusion, manuscript writing and handling of the peer-review process. The co-authors aided by giving feedback and participating in discussions on the different parts of the experiment.

Paper IV

I was the main responsible for this paper, and so did most of the planning, experiments, analyzing, formulation of conclusion, manuscript writing and handling of the peer-review process. The co-authors aided by giving feedback and participating in discussions on the different parts of the experiment.

Paper V

I was the main responsible for this paper, and so did most of the planning, experiments, analyzing, formulation of conclusion, manuscript writing and handling of the peer-review process. The co-authors aided by giving feedback and participating in discussions on the different parts of the experiment.

Peer-reviewed papers not included in this thesis

Paper I

Hansson, J., **Svensson, M.**, Theorin, A., Tegling, E., Soltesz, K., Hägglund, T. and Åström, K.J., "Next Generation Relay Autotuners – Analysis and Implementation," IEEE Conference on Control Technology and Applications (CCTA), San Diego, CA, USA, 2021, pp. 1075-1082, doi:10.1109/CCTA48906.2021.9659234.

Paper II

Lundh, M., Theorin, A., Hägglund, T., Hansson, J., **Svensson, M.**, Åström, K.J. and Soltesz, K., "Model optimization for autotuners in industrial control systems," 26th IEEE International Conference on Emerging Technologies and Factory Automation (ETFA), Västeras, Sweden, 2021, pp. 1-4, doi:10.1109/ETFA45728.2021.9613187.

Abbreviations

aTDC	After Top Dead Center
bTDC	Before Top Dead Center
CA/CAD	Crank Angle Degree
CA50	Crank Angle at 50% burnt
CH_4	Methane
CI	Compression Ignition
CO	Carbon Monoxide
CO_2	Carbon Dioxide
COV	Coefficient of Variation
CR	Compression Ratio
DF	Dual-Fuel
DI	Direct Injection
ECA	Emission Control Areas
ECU	Engine Control Unit
EGR	Exhaust Gas Recirculation
FID	Flame Ionization Detector
FS	of Full Scale
FTIR	Fourier-Transform Infrared Spectroscopy
GHGs	Greenhouse gases
HC	Hydrocarbon
HCCI	Homogenous Charge Compression Ignition
HCHO	Formaldehyde
HD	Heavy-Duty
HVO	Hydrotreated Vegetable Oil
ICE	Internal Combustion Engine
IMEPg	Indicated Mean Effective Pressure gross
LNG	Liquid natural gas
MeOHXX	Methanol with 100-XXvol% ignition improver

MeOH100	Neat Methanol
MSS	Micro-Soot Sensor
N_2O	Nitrous Oxide
NO_x	Nitrogen Oxides
PC	Pre-Chamber
PFI	port Fuel Injection
PPC	Partially Premixed Combustion
PM	Particle Mass
PN	Particle Numbers
RoHR	Rate of Heat Release
SI	Spark Ignition
TDC	Top Dead Center
TRL	Technology readiness level

1 Introduction

Greenhouse gases (GHGs) are vital components of Earth's atmosphere, functioning as a natural heat trap to maintain the planet's temperature [1]. However, the excessive release of GHGs resulting from human activities has upset this equilibrium, leading to atmospheric warming, commonly referred to as global warming or climate change [2]. The primary GHGs include carbon dioxide (CO_2), methane (CH_4), nitrous oxide (N_2O), and fluorinated gases, where human activities contribute to emissions of all four gases, but most significantly to the emission of CO_2 [3]. Notably, a substantial portion of the CO_2 emissions stems from the combustion of fossil fuels [4].

In recent years, international efforts such as the IPCC's initiative to limit global warming and achieve "net zero" emissions by 2050, have gained significant attention [5]. Several countries, including the United States, Japan, and the EU, have committed to carbon neutrality by 2050 or earlier, setting specific targets to drastically reduce emissions [6, 7, 8]. For instance, the EU aims to decrease GHG emissions from cars and vans by 55% by 2030 compared to 1990 levels, while also targeting zero emissions from new vehicles by 2035, recognizing that road transport accounts for about 72% of transport-related GHG emissions within the EU, see Figure 1 [9, 10].

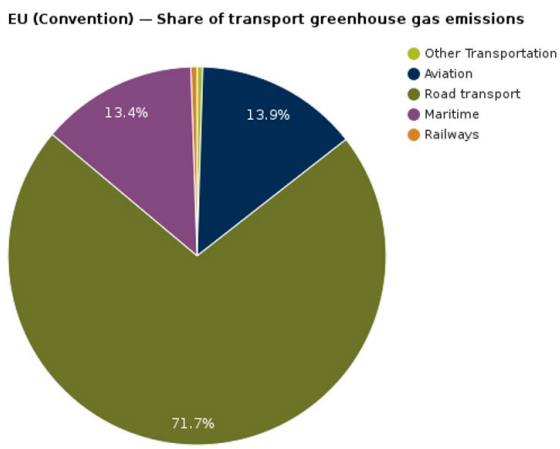

Figure 1 The share of transport greenhouse gas emissions in EU [10].

With transportation contributing approximately one-sixth of global GHG emissions, internal combustion engine (ICE) powered vehicles accounted for 74.5% of emissions in 2018, with heavy-duty trucks alone responsible for nearly 30% of global transportation emissions [11, 12]. In Europe, the transportation sector, encompassing road, rail, marine, and aviation, is accountable for 25% of GHG emissions, a figure targeted to be reduced by 90% by 2050 [13]. Consequently, there exists a pressing need for alternative power sources for heavy-duty transport.

While electrification remains a primary focus for reducing emissions in the transport sector, recent developments in EU policy have shifted towards the inclusion of carbon-neutral fuels as an alternative option [14, 10]. This policy shift has opened avenues for the use of renewable fuels like biofuels, based on biomass as a source for carbon and hydrogen, or e-fuels, using water electrolysis to get hydrogen and carbon capture to add carbon [15]. Renewable fuel, that are made from these sources, will be further explored in this thesis with the primary focus being usage in heavy-duty transport, specifically shipping, which is challenging to electrify.

1.1 Heavy-duty transport

1.1.1 Conventional compression ignition engines

The most common source of power today for heavy-duty transport is fossil diesel converted to motion through a compression ignition (CI) engine, which is the focus in this thesis. The conventional CI combustion process while running on diesel fuel works through these steps [16]:

Injection

The fuel is injected around top dead center (TDC) with a pressure of a few hundred bars or higher, atomizing the injected fuel into droplets.

Vaporization

Once in droplet form, the fuel absorbs heat from the surrounding air into which it is injected, causing it to vaporize and cool down the air.

Mixing

The vaporized fuel mixes with the air to create a fuel-air mixture, which ignites when the correct autoignition temperature and air-fuel ratio are achieved.

Premixed phase

Depending on the fuel type and in-cylinder conditions there is a delay from injection to ignition, called the ignition delay, that depends on how long it takes for the fuel-air mixture to reach ignitability conditions. Because of this the first part of the combustion, that is based on a premixed air-fuel mixture burns rapidly.

Mixing-controlled phase

Thanks to the heat generated in the premixed phase, subsequently injected fuel ignites more rapidly and burns as quickly as the injected fuel is mixed to achieve an ignitable air-fuel ratio. This phase is often referred to as the mixing-controlled or diffusion-controlled phase.

Late phase

The final phase occurs after fuel injection ceases, but some fuel remains that has yet to burn. As the piston descends, combustion continues at a slower rate, extending well into the expansion phase of the piston movement.

In comparison to a spark ignition (SI) engine, a CI engine typically operates in lean conditions to mitigate the risk of excessive soot emissions, resulting from rich combustion and because the combustion is mixing-controlled there is no need for throttling. Additionally, CI engines employ higher compression ratios (CR), as they do not face the issue of knock, which can occur in SI engines. These are some of the reasons why CI engines generally have higher efficiencies than SI engines.

1.1.2 Conventional diesel emissions and regulations

Due to the operational characteristics of conventional diesel engines and the properties of diesel fuel, engine-out emissions typically comprise elevated levels of nitrogen oxides (NO_x) and soot. NO_x forms primarily around stoichiometric air-fuel mixtures at high temperatures, a phenomenon normal in CI engines due in part to their high CR [17]. Additionally, soot originates from the long hydrocarbon (HC) chains present in diesel fuel, which are prone to forming particulate matter, especially because the combustion process occurs partly in locally very rich conditions.

To address the detrimental effects of these emissions, various regulations have been developed and implemented across different applications. In Europe, the Euro VI standard regulates on-road heavy-duty (HD) vehicles, while the Stage V standard governs other non-road HD applications [18, 19]. These standards are based on distinct steady-state and transient test cycles. For Euro VI, the prescribed cycles are the world harmonized stationary/transient cycles (WHSC/WHTC), whereas for Stage V, they are the non-road steady-state/transient test cycles (NRSC/NRTC). Detailed information on these standards, along with some non-road HD

applications, such as mobile machinery (NRE), generator sets (NRG), propulsion and auxiliary engines for inland waterway vessels (IWP/A), and railcars (RLR), is provided in Table 1.

While inland waterway vessels fall under Stage V regulations, ocean-going vessels navigating in Emission Control Areas (ECA) are subject to the IMO Tier III NO_x limit [20]. This limit is based upon the maximum engine speed, ranging from 3.4 g/kWh at engine speeds below 130 rpm to 1.96 g/kWh for engine speeds exceeding 2000 rpm; where testing procedures follow various ISO 8178 cycles depending on application, for various types of propulsion engines it is E3, for constant speed auxiliary engines it is D2, for variable speed and load auxiliary engines it is (C1) [21]. The E3 cycle is later used in this thesis as part of testing and can be seen in Table 2.

Table 1 European emissions standards for on-road HD vehicles and selected non-road HD applications [paper I].

Standard	**Euro VI**		**Stage V**			
Applications	Trucks/buses		NRE	NRG	IWP/A	RLR
Cycle	WHSC	WHTC	NRTC/NRSC	NRSC		
Engine Power [kW]	-	-	130-560	>560	≥300	-
CO [g/kWh]	1.5	4.0	3.5	3.5	3.5	3.5
HC [g/kWh]	0.13	0.16	0.19	0.19	0.19	0.19
NO_x [g/kWh]	0.40	0.46	3.5	0.67	1.8	2
PM [g/kWh]	0.01	0.01	0.045	0.035	0.015	0.015
PN [# /kWh]	8E11	6E11	-	-	1E12	1E12

Table 2 The ISO 8178 E3 cycle, based on the engine's rated power and speed [21].

Mode	1	2	3	4
Power (%)	100	75	50	25
Speed (%)	100	91	80	63
Emission weighting factors	0.2	0.5	0.15	0.15

With the tightening of regulations, engine developers have increasingly relied on advanced aftertreatment systems to mitigate the exhaust gases' harmful emissions. However, as regulatory requirements become more stringent, meeting them solely through aftertreatment systems becomes progressively challenging and costly. Consequently, engine manufacturers are now showing heightened interest in alternative power sources, driven not only by regulations concerning climate change but also by the potential of reduced cost if reliance on aftertreatment systems can be decreased.

1.2 Solutions

As it stands today the potential new sources of power for transport are electrification and transitioning to renewable fuels, with several proposed fuel alternatives. Below, these options will be summarized, compared, and evaluated using the "triple S" criteria proposed by Verhelst [22]. The three S criteria, stand for:

- Sustainable: It should be made from an endless energy source and have a closed cycle of resources, while causing negligible pollutant emissions upon usage.
- Scalable: The source needs to in abundance and at cheap cost, to make it possible to increase production without compromising its sustainability.
- Storable: It should be of relative high energy and power density, to ensure it does not compromise current applications' usability when the source of power is changed from the current standard.

And, if fulfilled, ensures the viability of the proposed power source solution.

1.2.1 Electrification

As a first option, the replacement of internal combustion engines with electrical power units driven by batteries is enticing due to its complete elimination of tailpipe emissions and direct utilization of electrical power for motion, as opposed to e-fuels, which necessitate the conversion of electricity into a fuel before generating motive power. However, the viability of this approach hinges on the availability of renewable electricity for battery charging and the implementation of emission-reducing practices in battery manufacturing to ensure sustainability. Failure to address these factors could undermine the environmental benefits of the transition.

Moreover, the scalability of materials utilized in batteries, such as cobalt and nickel in lithium-ion batteries, poses a significant concern due to their scarcity and high cost [23]. Hence, it is imperative to strategically allocate battery usage where it can yield maximal impact with minimal material consumption. Additionally, the lower energy density of batteries, in comparison to conventional liquid fuels see Figure 2, necessitates a larger vehicle space to achieve equivalent ranges between refuelings/recharging [24]. Consequently, battery electric vehicles are more suited for light-duty vehicles operating within urban environments, characterized by predominantly short driving distances. This approach optimizes battery material utilization while capitalizing on the absence of tailpipe emissions.

Conversely, for heavy-duty transport the constraints imposed by the substantial quantities of battery materials required limits the feasibility of battery electric

propulsion in this sector. Renewable fuels with higher energy density should be utilized instead [25, 26].

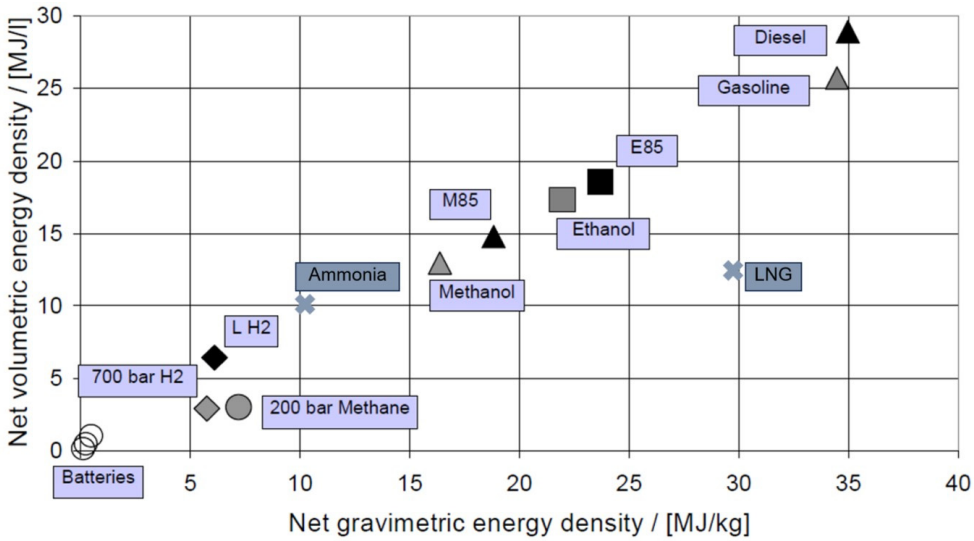

Figure 2 Volumetric and gravimetric energy density of various fuels [27, 24].

1.2.2 Renewable fuels

When considering renewable fuels, several alternatives with distinct advantages and disadvantages exist, each fulfilling the triple S criteria to varying degrees. In the following section, we will present and discuss these different alternatives, using the triple S criteria. Some of the renewable fuels that will be presented could be used in fuel cells which converts the fuel's chemical energy into electrical power and so utilizes an electrical powertrain. The downside with using fuel cells is they have a high production cost, use rare materials, and the durability is questionable with wear lowering the efficiency over time [28]. Considering this and that most heavy-duty vehicles use a CI engine, the fuels here presented will be discussed in terms of CI performance.

Hydrogen

To start, hydrogen serves as the fundamental element for all e-fuels, and so due to its higher simplicity in production and consequently more efficient power-to-fuel conversion than other e-fuels, thus rendering hydrogen scalable and sustainable. Notably, hydrogen lacks carbon atoms, thereby theoretically eliminating emissions such as CO, CO_2, and soot from combustion. In practice, experimental tests have

revealed trace levels of these emissions, attributed to lubrication oil slippage into the combustion chamber [29]. The emission of concern is instead NO_x, however, experimental research has shown that the emission level can be controlled through combustion techniques and aftertreatment systems [30].

Furthermore, hydrogen can achieve comparable efficiency to diesel fuel in engine operation despite its higher ignition difficulty, but for CI it requires a dual-fuel setup with a higher cetane fuel or a glow plug to create a hot spot with the required autoignition temperature [31]. However, the principal drawback of hydrogen lies in its storage and distribution challenges, primarily due to its gaseous state at ambient conditions and low energy density. Consequently, storage typically necessitates high-pressure gas containers ranging from 200 to 700 bar or liquefaction under cryogenic temperatures, -253C° [32]. Such complexities and associated costs render hydrogen storage and transportation problematic, thus compromising its viability in meeting the storage criteria. Additionally, even under 700 bar pressure, hydrogen exhibits a volumetric energy density approximately one-tenth that of diesel, aggravating the challenge of achieving equivalent driving ranges as conventional vehicles in a cost-effective manner [33].

Ammonia

Given the challenges associated with the storage and transportation of hydrogen, ammonia emerges as a potentially more viable carbon-free fuel alternative. While its production process is more complex and less efficient compared to hydrogen due to the requisite addition of nitrogen to form NH_3, ammonia is in liquid state at -33°C in ambient air pressure or at 20°C in a pressure vessel at 7.5 bar, which is better than hydrogen albeit still being less convenient than conventional fuels [34]. However, similar to hydrogen, ammonia exhibits a significantly lower energy density than conventional fuels, as depicted in Figure 2, necessitating larger fuel containers to achieve equivalent travel distances. Additionally, the toxicity of ammonia poses risks to human safety, necessitating stringent handling precautions [35].

When it comes to the use in CI engines, there are concerns regarding the use of ammonia due to its low cetane number and high autoignition temperature, rendering it challenging to ignite through compression alone. As a solution, ammonia is often utilized in dual-fuel mode with a secondary fuel to facilitate combustion [36]. Moreover, emissions from ammonia combustion, despite the absence of carbon molecules, remain a significant concern due to elevated levels of unburnt ammonia, NO_x, and N_2O, the latter exhibiting a 298 times higher global-warming potential per kg compared to CO_2 [37].

What distinguishes ammonia, beyond its lack of carbon atoms, is its potential for renewable production from renewable electricity, H_2, and N_2, rendering it scalable with power availability. While ammonia fulfils the criteria for storability, albeit not optimally, its viability as a future fuel is hindered by handling hazards and

suboptimal combustion properties. Nonetheless, in theory, ammonia holds promise as a sustainable and scalable fuel alternative.

Methane

Methane holds promise as a renewable fuel source, capable of being produced from renewable sources in the form of a biofuel, derived from waste, or as a e-fuel. While primarily sourced from fossil natural gas currently, its potential sustainability and scalability from renewable origins are noteworthy [38]. However, methane is in gaseous form under normal conditions and possesses a notably low energy density in that form. To address this limitation, it can either be pressurized to 200 bar or cooled to a liquid state. Liquefying methane by cooling it to -162°C, known as liquefied natural gas (LNG), offers a substantially higher energy density, see Figure 2, by shrinking the volume from gas by 600 times and, evidenced by the presence of LNG infrastructure and operational LNG-powered marine vessels, it becomes much more viable [39, 40]. Nonetheless, LNG faces challenges in storage and transportation because of the need for liquefaction, similar to hydrogen and ammonia, rendering it complex and thus more costly. Concerning CI of LNG, it is difficult to ignite through compression because of its high autoignition temperature and is so often used in combination with another fuel, of higher cetane number. While it is already utilized and boasts lower CO_2 and no sulfur oxide emissions, unburnt methane emissions pose significant environmental concerns, given methane's global warming potential CO_2 equivalent of 25, by mass [41, 37]. The storage complexity and global warming impact of methane slip, collectively, makes methane a complex fuel to use.

HVO

Hydrotreated vegetable oil (HVO) presents a promising renewable alternative to diesel, derived from waste lipids such as vegetable oil, tallow, or used cooking oil, primarily consisting of paraffinic hydrocarbons, yielding a low carbon fuel [42]. HVO shares similar properties with diesel, allowing it to serve as a drop-in fuel for diesel engines, which has led to the availability at some roadside filling stations already being available [43]. In terms of utilization in CI engines, HVO has demonstrated the ability to achieve lower unburnt HC and carbon monoxide (CO) emissions compared to diesel and burns with similar efficiency [44]. Consequently, HVO emerges as a sustainable and storable fuel option, however, its reliance on waste feedstocks for production imposes limitations on scalability.

Alcohols, methanol and ethanol

Alcohols have emerged as promising future fuel alternatives, with methanol and ethanol being the primary alcohols of interest. Among them, methanol has demonstrated superior potential due to its higher renewable production capacity and

reduced soot emissions resulting from the absence of a carbon-carbon bond [33, 45]. This had led to the focus in this work being methanol.

Methanol can be produced through various renewable methods, either as bio-methanol utilizing biomass as a carbon and hydrogen source, or as e-methanol employing carbon capture and water electrolysis [46, 47]. This renders methanol both sustainable and scalable, with the added benefit of being liquid at normal conditions, requiring less modifications to existing storage and transportation systems compared to ammonia and hydrogen. Thus, methanol fulfils all three criteria for a future renewable fuel. However, it is imperative to consider that methanol is corrosive, necessitating careful material selection and potentially requiring infrastructure modifications to enable safe storage [48]. Moreover, methanol can pose hazards to human health if ingested or in contact with the skin, although the chemical industry's extensive use of methanol together with the increased interest in the marine sector has provided established handling protocols [49].

Regarding the use of methanol in internal combustion engines, its lack of carbon-carbon bonds and the fact that each carbon atom is bonded to an oxygen atom makes it possible to completely eliminate soot emissions. It also has no sulfur atom, thereby avoiding sulfur oxide emissions as well. Methanol's properties as a fuel, see Table 3, include a high burning velocity, high autoignition temperature, and high heat of vaporization, contributing to excellent knock suppression, making it well-suited for SI engines [33]. However, the majority of heavy transport vehicles rely on conventional CI diesel engines. Retrofitting existing CI engines to operate on methanol presents an attractive alternative, particularly in the marine sector where vessels have long lifetimes and require the torque response associated with CI engines [50]. Furthermore, methanol's widespread use in the chemical industry facilitates its availability in ports, further incentivizing its adoption in the marine sector. Consequently, research and development efforts on methanol-powered marine vessels have intensified, with a significant number of vessels already in operation or in order, albeit predominantly utilizing dual-fuel concepts [39]. The reluctance to adopt neat methanol (MeOH100) engines stems mainly from methanol's poor CI properties, characterized by a high heat of vaporization, low cetane number, and higher fuel injection volumes, leading to significant cooling effects at injection, particularly affecting low-load and cold-start operation cases [51]. This makes further research into concepts that can use neat methanol in single-fuel CI engines of great interest.

Table 3 Fuel properties for methanol and diesel, from paper I.

Properties	Methanol	Diesel
Density at 0 C° and 1 bar [kg/m^3]	790	845
Lower heating value [MJ/kg]	20.09	43.2
Volumetric energy density [MJ/L]	15.87	36.5
Adiabatic flame temperature [K]	2143	~2200
Heat of vaporization [kJ/kg]	1100	225–280
Stoichiometric air–fuel ratio [kg/kg]	6.5	14.7
Flammability limit [vol%]	6.7–36	0.6–6.5
Autoignition temperature [K]	738	483~503
Laminar burning velocity at [m/s]	0.37	n.a.
Research/motor octane number	109/92	n.a.
(Derived) cetane number	3	>51

1.3 FASTWATER

This thesis was carried out as part of the EU-funded FASTWATER project, that has the goal of mitigating greenhouse gases and pollutant emissions of the shipping sector by utilizing methanol fuel. The FASTWATER project aims to do this through the development of retrofit kits and methanol engines, and showcasing it in a variety of vessels including a harbor tugboat, a pilot boat, and a coast guard vessel. Notably, the heavy-duty engine in the pilot boat was successfully converted to run on a single-fuel solution of methanol with 3% ignition improver (MeOH97). By blending in the ignition improver the cetane number is increased which decrease the requirement for autoignition. How this MeOH97 fuel blend works is further investigated in this thesis.

Additionally, FASTWATER encompasses the design of a methanol-powered river cruise vessel, logistical considerations for bunkering, revisions to rules and regulations, and crew training initiatives. Ultimately, FASTWATER will formulate comprehensive business plans, incorporating life cycle performance analyzes of costs, CO_2 emissions, and pollutant reductions, with the objective of commercializing the developed solutions.

2 Research Scope and Objectives

The scope of the research presented here is to explore single-fuel CI concepts capable of addressing the challenges associated with the use of neat methanol in CI engines. Building upon the concept utilized in FASTWATER, the specific objectives of this thesis are to:

- Investigate and analyzes different concepts for single-fuel methanol CI, and formulate recommendations on the most promising concepts for further development.
- Analyze the MeOH97 fuel blend, used in the pilot boat, and compare its combustion characteristics to diesel and MeOH100.
- Investigate and test different promising single-fuel methanol CI concepts, with the goal to go from MeOH97 to MeOH100.

The objectives were accomplished through a series of steps outlined below. Initially, an extensive literature review was conducted to identify all viable concepts with the potential to realize a single-fuel methanol engine as well as what gaps there are in knowledge. Subsequently, an analysis was done on the MeOH97 combustion characteristics and comparing it to MeOH100 and diesel, to assess their differences and the impact of the ignition improver. Based on these findings, the thesis delves into various concepts, identified in the review as potential solutions for MeOH100, needing further investigation. Finally, the study concludes with recommendations on which concepts should be prioritized for further development towards achieving stable CI of neat methanol.

3 Methanol single-fuel engine concepts

As mentioned before, methanol's high heat of vaporization, high autoignition temperature and large fuel injection volumes contribute to a significant cooling effect during injection that makes it hard to achieve autoignition conditions, which particularly affects low-load and cold-start compression ignition scenarios. Consequently, most research has been dedicated to addressing these ignition difficulties, leading to the proposal of several potential solutions.

As part of this thesis, I conducted a review study aimed at identifying the most promising concepts for methanol single-fuel engines, which resulted in Paper I included at the end of this thesis. The summary below outlines the various concepts identified in the review study and presents intriguing CI concepts with identified knowledge gaps. While the summary primarily focuses on compression ignition engines, which constituted the main research focus of this thesis, brief sections on SI and pre-chamber (PC) combustion of methanol are also included to highlight pros and cons of the different approaches.

3.1 Spark ignition

While methanol poses challenges for CI engines, its characteristics make it more suitable for employment in SI engines. Methanol SI engines were already tested back in the 1980s and 1990s through fleet trials [52, 53]. In SI engines, the fuel is injected either into the intake port (PFI) or directly into the cylinder (DI) during the intake stroke, leading to a premixed fuel/air mixture ignited by a spark, after which the homogeneous air-fuel mixture is combusted by a propagating flame front.

The predominant reason for the prevalence of CI engines in heavy-duty applications is the susceptibility of SI engines to knock, a phenomenon occurring when pockets of unburned mixture auto-ignite outside of the propagating flame front. This can result in damaging shockwaves within the engine. As engines increase in size, the likelihood of knock rises due to the longer propagation path of the flame, allowing more time for unburned pockets to autoignite.

Methanol's suitability for SI engines stems from its higher burning velocity and autoignition temperature compared to gasoline. These properties enable the propagating flame to reach unburned pockets more rapidly and the pockets require hotter conditions for autoignition, thus significantly reducing the risk of knock. Consequently, methanol SI engines can operate with higher CR and more advanced ignition timing, leading to improved performance and efficiency. Moreover, the enhanced knock resistance allows for the use of SI engines in larger applications than conventional gasoline engines, potentially rendering methanol SI engines a viable option for heavy-duty applications.

There are currently working HD truck engines running on neat methanol utilizing SI [54]. However, with larger engines for marine applications there are only simulation and laboratory-scale testing. These have shown promising results, with indications of efficiency and peak power comparable to diesel engines of similar size, however there is a notable absence of demonstrator engines in both industry and literature [55]. This could be attributed to the challenges associated with retrofitting existing diesel engines to this configuration, requiring the installation of both injectors and spark plugs, within the cylinder. Such re-tooling necessitates modifications to the cylinder head, making it more complex and costly.

3.2 Pre-chamber

The PC concept utilizes a small chamber connected to the main combustion chamber, where a fuel mixture is ignited by a spark. Subsequently, the mixture is expelled from the smaller chamber through one or more small holes, either as burning or as highly reactive jets that are quenched by the small holes. These burning or highly reactive jets then serve as a distributed ignition source, igniting the fuel-air mixture in the main combustion chamber [56]. This approach enables robust combustion even in conditions when other concepts like SI encounter knock or CI experience misfires.

Experimental research on methanol PC has shown potential of gross indicated efficiencies of around 45% with relatively low CO and HC emissions [57]. Furthermore, it has been observed that stable combustion can be achieved at leaner conditions compared to conventional SI engines, potentially reducing throttling and so pumping losses. While simulation studies have been conducted on larger engines, demonstrating potential for stable combustion as well, research is still lacking [58].

The combination of methanol, with its high octane number, and the knock-suppressing characteristics of PC technology has been proven to be a good match, facilitating stable methanol combustion. However, this is a relatively new concept with methanol and currently lacks extensive research and results. Additionally, implementing a PC requires adequate space, a spark system, and, depending on the

PC concept, a second fuel injection system, making it a more complex and costly system to use in retrofitting applications.

3.3 Compression ignition

This section provides an overview of various concepts, employed in CI engines, enabling stable methanol combustion. Starting with concepts utilizing other fuels or additives to achieve stable methanol combustion, and ending with single-fuel concepts on neat methanol.

3.3.1 Dual-fuel

The dual-fuel (DF) concept of combusting methanol is not a single-fuel solution, so not within the scope of this thesis, but is interesting as it is a technology that is available and used by many, especially in the hard to electrify sector of marine transport [59]. It works by injecting a small quantity of another fuel, that has better properties for CI than methanol, and as this other fuel combusts it creates enough heat to initiate the methanol combustion. This other fuel is today mainly diesel, but could be bio-diesel if available in enough quantities [60].

The positive aspect with DF is that the engine can be made to run solely on the second fuel when methanol is not available for refueling. This is likely why DF concepts with methanol are already available and used. The vessel owner using the engine does not need to worry about not being able to get methanol where the vessel is going and can thus continue the operations as usual and use methanol when available. This makes DF a great transition technology until methanol is readily available. The negative aspect is that with diesel being the common second fuel, because of its availability, it does not eliminate the use of fossil fuels.

The second fuel is especially important at colder conditions when methanol is the most difficult to ignite and only a minor part of the used fuel will be methanol [61]. However, there are operational conditions where over 90% of the total injected fuel energy, is from methanol, but this does not necessarily coincide with the vessel operating profile which could lead to a lot of diesel still being used [62, 63, 64]. This obviously offsets the benefits that methanol can deliver and also means the continued need to handle soot and NO_x emissions associated with diesel CI. Moreover, it requires two fuel systems which adds extra complexity and cost to the production of these engines and retrofitting.

There is no denying DF is a great concept to start the transition to neat methanol as it gives the engine users options, and so does not interrupt any use. However, society

must continue developing methanol engines as the DF concept does not utilize the full potential of methanol and also requires a second fuel.

3.3.2 Blending with diesel

Another transitional concept involves blending a second fuel with methanol to create a mixture with properties beneficial to compression ignition. Unlike the dual-fuel approach, this method eliminates the need for a second fuel system but introduces complexities associated with the blending process prior to refueling. One significant drawback is the inability to adjust the methanol-to-other-fuel ratio, resulting in a fixed blend that must be able to run in all conditions, which in turn will lower the methanol utilization.

Additionally, blending methanol with diesel requires the use of additives to facilitate mixing, as the difference in polarity between methanol and diesel prevent them from mixing, adding to the complexity and cost of the process [65]. Conversely, blending methanol with biodiesel presents a more favorable option, as these fuels can more easily blend, but this has only been tested with smaller fractions of up to around 15% methanol, as the blending fraction is still limited [66].

The challenges associated with blending a second fuel with methanol, including limited adjustability, the need for additives, limited methanol fraction and dependence on biodiesel availability, have hindered extensive research in this area. As a result, this concept has not gained significant interest compared to other methanol CI strategies.

3.3.3 Adding Ignition improver

Instead of blending with diesel, an ignition improving additive can be introduced to enhance the properties of methanol for CI. This additive aims to improve the ignition properties of methanol, particularly by elevating the cetane number compared to pure methanol. By employing this approach, the necessity for diesel fuel is eliminated and testing has demonstrated that even small concentrations of ignition improver, >3%, can be sufficient for stable CI combustion. However, ignition improver comes at a relatively higher cost compared to methanol, so minimizing the usage is desired to ensure cost-effectiveness and maintain the viability of this option.

Considerable research and testing has been conducted on the usage of ignition improver with methanol, particularly through projects like FASTWATER and its precursor, GreenPilot [67, 68]. In the GreenPilot project, a blend consisting of 95% methanol and 5% ignition improver was tested, yielding positive results that paved the way for further development in the FASTWATER project. As mentioned, a HD engine was successfully converted to run on methanol with 3% ignition improver, achieved certification to the NO_x Technical Code 2008 and meeting IMO Tier III

standards, all without the need for an aftertreatment system. That engine was later installed in a pilot boat and tested, with good real-world results proving the blend being a viable option with high technology readiness level (TRL) [69]. This makes the MeOH97 fuel blend interesting, as most existing publications only provide data on ignition improver percentages down to 5% and that is with the addition of intake heating to achieve stable combustion [70]. Further analysis on MeOH97 and why it is successful is therefore warranted, with additionally information on the difference the ignition improver makes compared to neat methanol and the improvements and downsides compared to diesel.

Nevertheless, this approach has demonstrated success through offering good efficiency and emission performance [71]. However, the use of an ignition improver adds to the overall cost of fuel production and requires an additional blending stage making neat methanol solutions preferable.

3.3.4 Glow Plug

Among the neat methanol concepts, the use of glow plugs has achieved the highest TRL and was developed and tested already in the 1970s, 1980s, and 1990s. This development was primarily motivated by U.S. concerns regarding petroleum imports, leading to a focus on neat methanol ignition by a glow plug or a hot spot. The concept operates by introducing methanol near a hot spot, which ignites and initiates combustion, the flame then jumps between injection jets around the injector until all jets are burning. Testing of this concept has demonstrated stable combustion during start-up and at low loads in both two-stroke and four-stroke engines [72, 73]. However, as engine temperature increases, the impact of the glow plug on combustion diminishes until it has no impact.

The ignition mechanism of a glow plug introduces unique characteristics to the combustion process. Since combustion initiates at a single point and spreads around the injector, it results in a prolonged heat release, consequently reducing efficiency [74]. Additionally, the integration of a glow plug requires space in the cylinder head, which may pose challenges, particularly in smaller engines. Retrofitting existing engines may necessitate changing parts if space for a glow plug is unavailable. Moreover, glow plug systems require additional maintenance, as they constitute an extra component with an unclear lifespan.

In summary, while glow plugs can offer stable combustion under cold conditions when used with neat methanol, they come with certain drawbacks that must be carefully considered when implementing this concept.

3.3.5 Increased In-Cylinder Temperature

The most common method employed by researchers to achieve stable methanol ignition is by heating the intake air making the in-cylinder conditions sufficiently hot to autoignite neat methanol. This approach has been utilized both independently and in conjunction with other concepts. However, it necessitates the installation of an intake heater, which presents certain drawbacks. Firstly, the additional heater consumes power, thereby reducing the overall efficiency of the engine system. Secondly, it leads to a decrease in air density, possibly compromising power density and efficiency. Lastly, the installation of a heater requires additional space and incurs additional costs. It would be more advantageous if the heat could be sourced from existing components within the engine system instead.

EGR

One potential system that could be utilized to introduce heat into the cylinder is exhaust gas recirculation (EGR), a method commonly employed in diesel engines to reduce NO_x emissions by recirculating exhaust gases back into the combustion chamber. The exhaust gases dilute the air-fuel mixture, which in turn lowers the combustion temperature and so decrease the generation of NO_x [75, 76]. With methanol CI engines, EGR can offer a dual benefit of reducing NO_x emissions while also providing additional initial heat to the combustion chamber. Unlike diesel engines, methanol engines do not exhibit a NO_x-soot trade-off, allowing for higher EGR levels without the risk of increased soot emissions and so a possibility of more NO_x reduction if needed.

Typically, EGR gases are cooled before being reintroduced into the cylinder. However, it could be possible to control the temperature of the EGR gases through a bypass regulator on the EGR-cooler and so control the in-cylinder temperature as needed. While EGR can lower NO_x emissions by almost 50%, it may lead to reduced efficiency due to prolonged heat release and a lowered air/fuel ratio, potentially resulting in increased CO emissions as a side effect [77].

Additionally, during start-up, the absence of exhaust gases means that EGR cannot be utilized, necessitating the implementation of an alternative start-up strategy in combination of the EGR concept.

Compression ratio

Increasing the CR is another approach to consistently introduce additional heat into the combustion chamber. This method was employed in the MeOH97 concept as part of the conversion process and is frequently utilized in other methanol engine designs. Unlike with diesel engines, methanol's cooling effect offsets the potential increase in heat from the elevated CR, preventing higher NO_x emissions.

Moreover, raising the CR can enhance thermodynamic efficiency. However, it also has the drawback of increasing unburnt emissions, as the higher crevice-to-volume

ratio leads to more fuel accumulating in areas close to colder walls and areas with reduced mixing [78]. Next to that, increased CR leads to higher pressure, which can become a problem at higher loads as the engine has a limited peak pressure causing limitations to operation range or reduces efficiency from retarded injection timing at the higher loads. The exact extent to which the CR affects methanol CI combustion and the maximum feasible CR has not been thoroughly investigated. However, it is evident that increasing the CR yields benefits for methanol CI combustion, but further research is warranted.

3.3.6 Advanced Injection Strategies

Given that the cooling effect from methanol injection significantly contributes to the challenges with methanol CI combustion, extensive research has been conducted on advanced injection strategies to mitigate this issue. Various methods involving early injections and injection splitting have been investigated, and these different concepts will be discussed below in the following sub-sections: Homogenous Charge Compression Ignition (HCCI), Partially premixed combustion (PPC) and pilot injection.

Homogenous Charge Compression Ignition

This injection strategy involves an early injection aimed at creating a homogeneous air/fuel mixture that combusts when conditions are right for autoignition. The concept behind this approach is twofold: firstly, the early injection mitigates the cooling effect by giving sufficient time for the surrounding heat to compensate for the temperature drop, as it occurs well before the ignition event; secondly, it promotes a more uniform mixture, reducing the likelihood of rich combustion and resulting in lower combustion temperatures, thereby lowering NO_x emissions. However, this concept presents challenges in terms of control, as there are fewer controllable parameters affecting ignition timing, leading to the possibility of ignition occurring either too early or too late, reducing efficiency. Additionally, the extended time available for mixing increases the likelihood of fuel accumulating in crevices, which in turn can elevate HC and CO emissions. Furthermore, research suggests that both gasoline and ethanol exhibit better performance with HCCI than methanol [79, 80].

Partially premixed combustion

PPC, or partially premixed combustion, is an intermediate concept between conventional CI and HCCI injection strategies. In PPC, an early injection, though not as early as in HCCI, is carried out during the compression stroke. This ensures that fuel and air are partially premixed before combustion occurs, thereby mitigating high temperatures and fuel concentrations. PPC still offers controllability through injection timing and prevents excessive fuel accumulation in crevices, unlike HCCI.

Research has shown significant potential for PPC, with diesel-like efficiencies and CO emissions, along with reduced NO_x and HC emissions [81]. Additionally, in PPC mode, particle mass (PM) and number (PN) emissions from methanol were found to be lower than Euro VI levels [82]. However, in many of the research papers on PPC, intake heating is used as only using PPC does not get the combustion started. Notably, it was observed that splitting the injection into two equally sized injections in PPC mode could increase efficiency, decrease the maximum pressure rise rate and lower the need for addition heating from other sources [83].

Pilot Injection

This strategy involves dividing the injection so that a smaller portion of the fuel is injected early as a pilot. Due to the reduced volume of the pilot injection, there is less cooling effect, thus increasing the likelihood of combustion. The heat generated from the pilot injection can then facilitate the ignition of the main injection, which occurs slightly later. Researchers have also explored this concept to some extent, indicating that the design of the pilot timing and size is crucial, as poor design choices can have adverse effects. A pilot injection that is too small may not effectively contribute to the combustion process, resulting in inadequate ignition and combustion. On the other hand, a pilot injection that is too large can lead to excessive heat release before TDC, which may cause engine damage due to increased pressure and temperature in the combustion chamber. Therefore, finding the optimal size for the pilot injection is crucial to ensuring efficient and controlled combustion in the engine [77].

3.3.7 Conclusion

As outlined in this chapter, there are several proposed concepts that could facilitate compression ignition of methanol, however, there are several knowledge gaps. To address some of these gaps, experimental testing and analysis were conducted as part of this thesis (as summarized in the next chapter), with a specific focus on the gaps regarding the MeOH97 fuel blend, increased compression ratio and pilot injection parameters, which were found to have high potential. Other concepts with high potential, but not tested here was the use of a glow plug, which was found to be the only technique addressing the start-up issue of neat methanol. However, it was found to have a non-optimal heat release and should so not be used more than necessary. Another concept of interest was exhaust gas recirculation (EGR), which can lower NO_x emissions and is especially interesting with methanol since there is no NO_x-soot trade-off.

4 Research output

In this section, a summary of the experiments and analyzes conducted in papers II to V will be presented. The section will start with an explanation of the experimental setup utilized, followed by an in-depth analysis of the MeOH97 fuel blend as investigated in papers II and III. Subsequently, the discussion will transition to the testing of MeOH100 concepts, identified in the review as promising but requiring further research. In the experiments, neat methanol possessed a chemical grade purity of 99.85% and in all cases using some methanol, the addition of 100-200 ppm of Infineum R655 was used for lubrication.

4.1 Experimental setup

As part of this thesis, experiments were conducted, as reported in papers III to V, on a heavy-duty research engine at the Department of Energy Sciences, Lund University. This engine served as the experimental platform for papers III to V, and the variations in engine configuration will be explained below. The only difference in measuring equipment was that paper IV utilized a Horiba MEXA-7000 emission analyzer, while papers III and V employed an AVL SESAM i60FT FTIR emission analyzer. Detailed descriptions of both instruments will be provided below, in conjunction with explanations of the main engine configuration and post-processing methodologies utilized.

4.1.1 Engine

The experiments were conducted using a customized Scania D13 in-line six-cylinder engine. To facilitate experimentation, the engine was adapted to operate on a single cylinder, see engine parameters in Table 4. This modification involved drilling holes in the pistons of the other five cylinders and disengaging their fuel and air systems. Engine speed was carefully controlled using an electric-motoring dyno, ensuring a consistent speed irrespective of engine load variations. A crank angle encoder was employed to accurately measure the engine's speed and position, sampling signals from all fast measuring devices at a rate of five signals per crank angle degree (CAD).

Table 4 Engine configuration.

Displaced volume	2124 cc
Stroke	160 mm
Bore	130 mm
Connecting Rod	255 mm
Number of Valves	4

Intake air was supplied using an air compressor. Precise control over air flow and pressure to the engine was achieved through a variable valve positioned between the compressor and the engine. Downstream of this valve, a heater and an airflow meter were installed, enabling adjustments to the intake air temperature and the measurement of air supply flow. For fuel supply, a low-pressure fuel pump transfers fuel from an external tank to a high-pressure fuel pump responsible for supplying the Scania XPI common rail injection system. To monitor fuel flow from the external tank, a precision gravity scale manufactured by Sartorius was employed. The different measuring instruments mentioned are presented in Table 5, with model number, measuring range and accuracy, and a layout of the engine with the equipment used can be seen in Figure 3.

Table 5 The different measuring instruments with what they measure, measuring range and accuracy.

Variable measured	**Model**	**Measuring range**	**Accuracy**
In-cylinder pressure	Kistler 7061B Kistler5011B10	0-250 bar	± 0.5% FS
Intake/exhaust pressure	Kistler 4075A10	0-10 bar	± 0.2% FS
Crank angle, engine speed	Kistler 2614CK	0-12000rpm	± 0.03 CA
Fuel injection pressure	Kistler 4067C	0-3000 bar	± 0.1% FS
Air flow Meter	Bronkhorst F-106bi	Max 125g/s	± 1% FS
Fuel scale Meter	Sartorius MSE12201S	0-12200 g	± 0.1 g

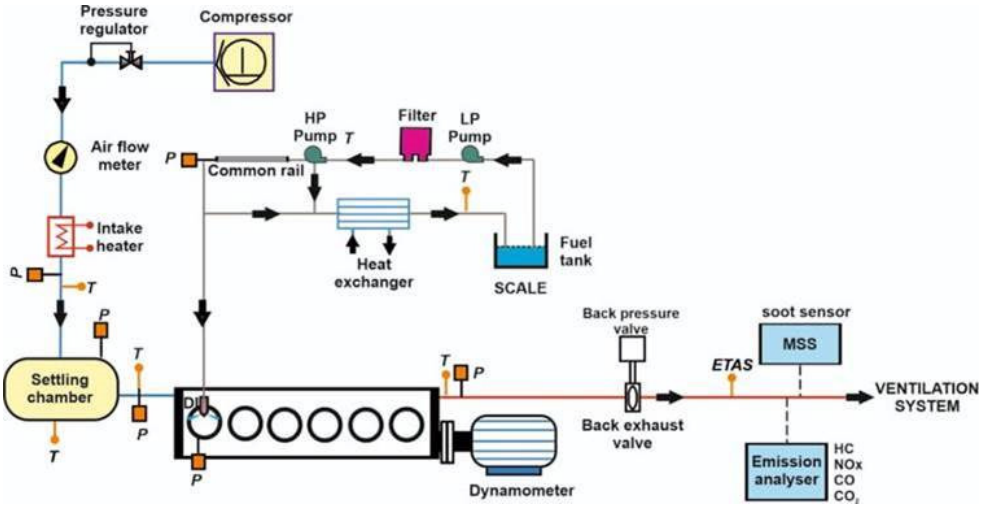

Figure 3 A schematic of the test set-up with the engine and measuring equipment [84].

In the conducted experiments, several modifications were made to the engine configuration, particularly when utilizing methanol as the primary fuel source, either as MeOH97 or MeOH100. To accommodate for the lower energy density of methanol, compared to diesel, a higher flow injector was employed, see Table 6. Additionally, different CR were utilized for methanol combustion across the various papers through the use of different pistons, as outlined in Table 7 (the reason for which will be explained later). It is noteworthy that the CR for diesel fuel remained consistent throughout all experiments.

Table 6 Injector parameters for diesel and methanol fuels respectively.

Parameter	**Diesel**	**Methanol**
Actuation type	Solenoid	Solenoid
Flow rate [pound per hour]	275	600
Number of Holes	9	12
Spray Angle [˚]	146	120

Table 7 CR used in the different papers, and the comparable diesel CR used throughout the thesis.

Usage	Paper II	Paper III	Paper IV	Paper V	Diesel
CR	24.3	26	17.3/40	26	17.3

4.1.2 Emission measurements

Two different emission analyzers were utilized throughout the conducted experiments, the Horiba MEXA-7000 emission analyzer in paper IV, and the AVL SESAM i60FT FTIR in papers III and V. These systems exhibit distinct differences, particularly in the measurement of HC emissions. The Horiba analyzer employs a flame ionization detector (FID), whereby the sample gas is introduced to a hydrogen flame that ionizes some of the HC [85]. This process generates a current proportional to the amount of HC, which can be measured. However, an FID has lower sensitivity to oxygenated HC, leading to underestimation of measurements from alcohols and aldehydes [86]. In contrast, the AVL SESAM utilizes the Fourier Transform Infrared Spectroscopy (FTIR) method, which exploits the fact that many compounds absorb infrared radiation at specific wavelengths. This method measures the infrared radiation absorbed by the emission sample, allowing for the identification of sample components based on the absorbed wavelengths, without suffering a loss of sensitivity to specific emissions [85]. This makes the AVL SESAM system advantageous for methanol combustion, and was therefore used in this thesis when possible. When the Horiba system with the FID was employed no correction factor was applied to the measurements, due to uncertainty surrounding the correction factor, neither in this thesis nor in the corresponding publication [87]. The accuracy of the both devises can be seen in Table 8.

For the measurement of soot emissions, an AVL Micro Soot Sensor (MSS) was employed, utilizing a photoacoustic method to quantify soot levels in a sample gas. The MSS emits modulated light with a wavelength of 808 nm towards the sample gas. As the radiation interacts with the soot particles, they undergo expansion and contraction due to heating and cooling, generating a sound wave. This sound wave is then detected, with the sound level correlating to the number of soot particulates present in the sample [84]. The accuracy of the MSS can be seen in Table 8.

Table 8 Emission analyzer used with measuring range and accuracy.

Analyzer	Emission	Range	Accuracy
Horiba MEXA-7000	CO/CO_2 NO_x TUHC O_2	0-1/16% 0-5000 ppm 0-10000 ppm 0-25%	± 1% FS ± 1% FS ± 1% FS ± 1% FS
AVL SESAM i60FT FTIR	All	0 up to 10000 ppm	≤ 2% of the measured value
AVL MSS	Soot	0.001-50 mg/m^3	± 0.001 mg/m^3

4.1.3 Post processing

Matlab was utilized for the post-processing of measurements, employing the equations detailed in Appendix which are based on Heywood [16]. These equations encompassed calculations for heat release, efficiency, and energy distribution. The efficiency and energy distribution calculations included gross indicated, thermodynamic, and combustion efficiencies.

Given the single-cylinder setup utilized, frictional and pumping losses were not experimentally determined and so not used in this thesis.

4.1.4 Experimental Accuracy

The experiments and measured data underwent several precautions to ensure the accuracy of the results presented in this work and in the associated papers. Prior to experiments, sensors were tested and, if necessary, calibrated, while emission analyzers were calibrated using reference gases. The accuracy of the measuring instruments and emission analyzers can be observed in Tables 5 and 8, respectively.

During engine operation, but before measurements, efforts were made to ensure a stable temperature was achieved, and motoring conditions were consistent with previous experiments, thereby ensuring coherence between experiments. The motored pressure trace was also utilized to calibrate the crank angle encoder TDC. Specifically, the peak pressure of the motored pressure trace was adjusted to be 0.4 CAD before TDC (bTDC), corresponding to an average thermodynamic loss angle [88].

During measurement, each test point was sampled over 300 or more cycles of steady combustion, with the ensemble average being utilized for calculations. Additionally, measured points were taken in a random order and repeated to detect any potential drift in measurements. Furthermore, in-cylinder pressure data underwent first-order Butterworth filtering before heat release calculations to remove high-frequency resonance, thus enhancing calculation accuracy. Additionally, standard deviation bars were added to selected figures of relevance to allow an assessment of the significance of the differences between results, and connecting lines between measured data point were added for easier comparison of trends.

An error analysis was also performed. Firstly, all data were analyzed to identify outliers, incorrect data, or any other anomalies. Secondly the cycle to cycle variations were measured within the same data point using the calculated standard deviation. Also, calculations were made of the measurement uncertainty based on the maximum measurement error of the equipment. In most cases were the standard deviations of the measured cycles larger than the measurement equipment error, which is why the bars in some of the plots show this standard deviation.

4.2 MeOH97

The addition of 3% ignition improver to methanol has been demonstrated to be effective in real-world conditions, as evidenced by the development, installation and testing of a heavy-duty MeOH97 adapted diesel engine [69]. However, despite this successful application, it was observed that there was a lack of research on the combustion characteristics of MeOH97, particularly concerning the impact of the comparably low percentage of ignition improver. Therefore, further investigation was conducted in this thesis to address this gap in knowledge. This was achieved through the analysis of the converted MeOH97 engine, in paper II, and by comparing the combustion characteristics of MeOH97 against diesel and MeOH100, in paper III. The findings from these two papers are summarized in this section with highlights from the publications.

4.2.1 Pilot boat

To analyze the MeOH97 engine, it is crucial to understand the modifications undertaken during the conversion process, which was mainly done by ScandiNAOS AB. The base engine utilized was a Scania DI16 V8 CI engine with a displacement volume of 16.4 liters, originally designed to run on the ED95 fuel, ethanol with 5% ignition improver, which in turn was developed based on a diesel engine version. During the conversion process, several key modifications were implemented. Firstly, the pistons were replaced to increase the compression ratio to 24.3, and higher capacity injectors were installed to compensate for the lower energy density of methanol. Additionally, material changes were necessary to address the corrosive nature of methanol, requiring compatible fuel filter containers, gaskets, and injectors. Furthermore, adjustments were made through the use of a new Engine Control Unit (ECU) to accommodate the specific requirements of MeOH97 fuel.

Following the modification, the determination of the optimal ignition improver percentage was crucial. This decision was based on testing by ScandiNAOS under challenging ignition conditions, including cold start-ups and load transients at 5°C ambient temperature. Through these tests, it was found that a minimum of 3% ignition improver was necessary to handle both scenarios effectively. Lowering the ignition improver percentage resulted in misfires during transients and unreliable cold starts. These results represent a significant advancement, particularly when compared to previous tests and development efforts, such as those in the GreenPilot project, which utilized 5% ignition improver.

Subsequently, the engine optimization process was undertaken with the objective of achieving the highest power output while meeting certification standards set by DNV for IMO NO_x Technical Code 2008. Testing was conducted on the ISO 8178 E3 cycle, see Table 2. As the engine was designated to operate at speeds exceeding

2000 rpm, the NO_x emission limit was set at 1.96 g/kWh (rounded to 2.0 g/kWh). The optimization process involved iterative steps, initially focusing on ensuring the engine's functionality across all operating conditions without specific efficiency or emission targets, except not having excessive CO and HC emissions which would indicative incomplete combustion. Subsequently, efforts were made to enhance efficiency at all load points, followed by optimization of emissions to achieve the NO_x target. These steps were iteratively repeated, with adjustments made to fuel pressure, injection timing, and pilot/post injections as deemed necessary.

The resulting optimized engine successfully met the certification goal and was rated for a power output of 415 kW at an engine speed of 2100 rpm. The final emissions from the E3 cycle, factoring in weighing, are presented in Table 9. Additionally, during testing, it was observed that both soot and sulfur oxides emissions were negligible, and the efficiency was on average 42% for the ISO 8178 E3 cycle.

Table 9 Weighted specific power and emissions from the optimization of the MeOH97 engine according to the E3 cycle with weighing [paper II].

Specific emissions and Power:	E3
Weighted power (kW)	286
NO_x (g/kWh)	2.0
HC (g/kWh)	0.5
CO (g/kWh)	0.6
CO_2 (g/kWh)	667

Achieving these results, without the use of an aftertreatment system, underscores the great potential of methanol CI engines emissions. Additionally, the absence of an aftertreatment system not only simplifies the engine design but can also translate into significant cost savings. This emphasize the attractiveness of CI methanol engines as a sustainable alternative for heavy-duty applications.

Following the certification process, the engine was installed in the Pilot 120SE pilot boat in Sweden, where it underwent rigorous testing in real-world conditions, including varying weather conditions spanning winter and summer. Remarkably, the engine performed well without encountering any major issues. Additionally, it successfully passed acceleration tests with margin, further validating its reliability and performance under demanding operational conditions.

4.2.2 Comparing to diesel and MeOH100

The analysis of the MeOH97 engine provided valuable insights, but further investigation into this fuel blend was deemed necessary. As a result, this thesis further explored the MeOH97 fuel blend by conducting tests on MeOH97, MeOH100, and diesel using the previously described research engine, see

Experimental setup section. When comparing MeOH97 to MeOH100, the impact of the ignition improver becomes clearer, while comparing to diesel enable an assessment of whether MeOH97 can perform comparatively to the fuel it aims to replace.

For the ignition improver Beraid 3555M was used, as it was the same as used in the pilot boat. It is a non-ionic polyethylene glycol derivative specially developed for alcohol fuels and has shown in previous tests to perform well compared to other ignition improvers [89].

The experiments partially followed the E3 cycle, similar to the MeOH97 engine certification. However, due to limitations of the research engine, the two highest loads were not tested. Instead, a lower load point was added. As explained earlier, methanol exhibits CI issues in colder conditions, making it interesting to test lower loads. The testing conditions are outlined in Table 10.

Table 10 Experimental conditions for testing MeOH97 against MeOH100 and diesel, with Mode 3 and 4 from the E3 cycle [paper III].

Mode	**3**	**4**	**5**
IMEPg [bar]	13.4	8.8	5
Speed [rpm]	1600	1260	950
Injection pressure [bar]	880	690	520
Boost pressure over ambient [bar]	0.5	0.25	0
CA50 [CA aTDC]	Highest Eff.	Highest Eff.	Highest Eff.
IMEPg COV [%]	Below 3	Below 3	Below 3

Intake heating was employed to achieve stable combustion through a coefficient of variation (COV) below 3% for indicated mean effective pressure gross (IMEPg). The resulting temperatures used are depicted in Figure 4, illustrating the significant intake heating required for stable combustion of MeOH100. However, as load and speed increased, the need for heating decreased, approaching the temperatures of MeOH97 and diesel. Where MeOH97 exhibited no need for intake heating for the modes tested in the E3 cycle. However, at the added low load condition, some additional heating was necessary. This suggests that there are limitations to how much the 3% ignition improver can assist neat methanol combustion. Nonetheless, in the development of the MeOH97 engine, a pilot injection was utilized at the lowest loads, a concept previously discussed as beneficial for methanol CI. This indicates that additional techniques are necessary for MEOH97 low load combustion but strategies are available that are sufficient. It's worth noting that only a single injection strategy was used for simplicity in these tests, leaving room for further investigation.

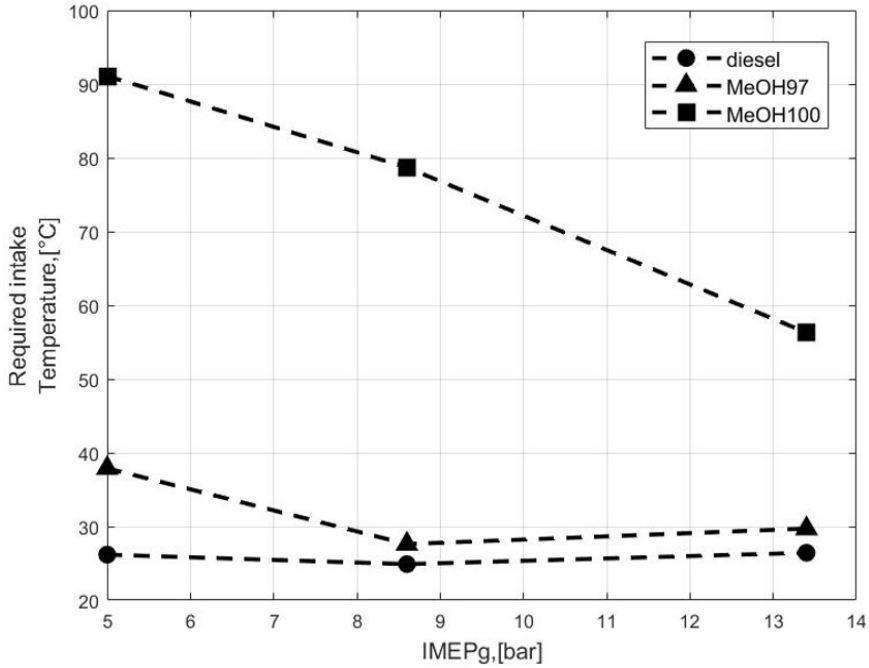

Figure 4 Used intake temperature for testing MeOH97, MeOH100, and diesel, at the three modes (indicated here by load) [paper III].

To better understand the differences in combustion characteristics between methanol and diesel, as well as the impact of using intake heating and an ignition improver, the observed ignition delay times can be used, see Table 11. At the lowest load/speed, both methanol fuels demonstrate comparable ignition delay times or even shorter ones than those of diesel. However, as load/speed increases, the ignition delay times gradually approach each other. This behavior at the lowest load is intriguing, as methanol is generally characterized by longer ignition delays compared to diesel [90]. To gain a better understanding of these observations, pressure and temperature conditions at ignition are plotted in Figure 5 across all tested modes and fuels, observing an approximate 200-250 K higher overall temperature for MeOH100 compared to diesel, which is the effect of using intake heating and higher compression ratio. It's important to note that these temperature conditions are calculated from the cylinder pressure, rather than being direct temperature measurements and that they represent overall temperatures in the cylinder. Consequently, local variations in temperature can occur, particularly for methanol due to its cooling effect at injection, which can lower local temperatures and influence the ignition delays. When comparing the temperature data from Figure 5 to the autoignition temperatures listed in Table 3 (738 K for methanol and 483-502 K for diesel), it becomes evident that the temperatures are sufficiently high for

autoignition upon injection. Therefore, what primarily governs the ignition delay is the local temperature and the chemical kinetics of the fuels involved. To get deeper insights into the underlying mechanisms governing ignition delays and offer a more comprehensive understanding, numerical calculations of ignition delays were investigated, as performed by Parsa and Verhelst [90], plotted in Figure 6. Parsa conducted a study on the ignition delays of n-heptane and methanol in various proportions using a constant volume batch reactor numerical setup in Cantera. The focus was on pilot-ignited dual-fuel engine conditions, which differ from the experiments conducted here. Nonetheless, some of Parsa's findings can help explain the differences in ignition delay between methanol and diesel observed in this study, especially as a 95% methanol case was investigated, and n-heptane has ignition characteristics similar to that of diesel. In Figure 6, a noticeable difference is observed between 95% methanol and n-heptane, which will henceforth be referred to as the methanol and diesel cases. For methanol, the ignition delay line appears almost straight in the displayed format (logarithm scale for ignition delay time versus the inverse of temperature), while diesel exhibits a dip/plateau around 1.2 1000/T. This shows methanol to have a longer ignition delay than diesel under operating conditions above 1 1000/T. However, in the present study, methanol benefits from higher in-cylinder temperatures due to intake heating and a higher compression ratio. These conditions shift the methanol cases further to the left in the figures, potentially allowing the ignition delay to fall below that of diesel. This is likely the explanation for the results in mode 5. As load/speed increases, in-cylinder conditions feature higher temperatures, which leads to further reductions in the ignition delays of all fuels. However, the results obtained here suggest that the reduction is higher for diesel, to the extent that ignition delay times become similar at mode 3. With higher temperature the relevant ignition delay time is found further left in the plots of Figure 6, from which it can be seen that the difference will decrease with higher temperature, especially considering the scale is logarithmic. However, it does not fully explain why methanol and diesel as equal ignition delay times, as methanol has hotter in-cylinder conditions and should so have a shorter ignition delay time. This can instead be explained by local differences in in-cylinder conditions, where the cooling effect of methanol injection likely plays a crucial role in lowering the local temperatures, which in turn increase the ignition delay.

Another intriguing observation from Table 11 is the similarity in ignition delay times between MeOH97 and MeOH100, despite the different conditions illustrated in Figure 5. Also, both fuels exhibit a similar cooling effect upon injection and should so have similar local condition. This makes the impact of adding an ignition improver to methanol's autoignition chemical kinetics evident, showing an overall lower temperature of more than 100 K at ignition. This can be seen to be equivalent to lowering the ignition delay line of methanol in Figure 6. Further, what makes this observation particularly interesting is the magnitude of the improvement. With just the 3% ignition improver, significant differences are observed compared to MeOH100. This finding warrants further investigation into how various proportions

of ignition improver alter the fuel blend properties. Further, in Figure 6 the impact of the intake heating on methanol ignition delay becomes more clear. As the scale is logarithmic small changes in temperature, when the combustion happens at lower temperatures, can greatly impact the ignition delay time.

Table 11 Ignition delay times in ms (and CAD) for all modes and fuels, based on heat release and start of injection, estimated to be 0.4 ms after the start of the injection current signal.

Mode	**3**	**4**	**5**
Diesel	0.3 (2.9)	0.5 (3.8)	1.0 (5.7)
MeOH97	0.2 (1.9)	0.3 (2.3)	0.5 (2.9)
MeOH100	0.3 (2.9)	0.3 (2.3)	0.5 (2.9)

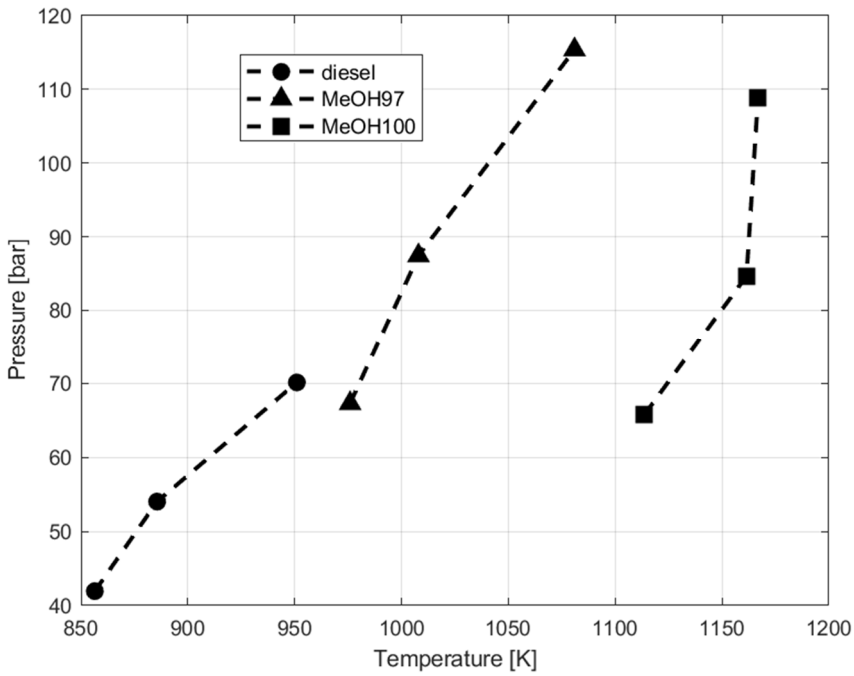

Figure 5 Calculated temperature-pressure plot of start of combustion conditons for all three fuels and modes, with higher load/speed points going up in the plot.

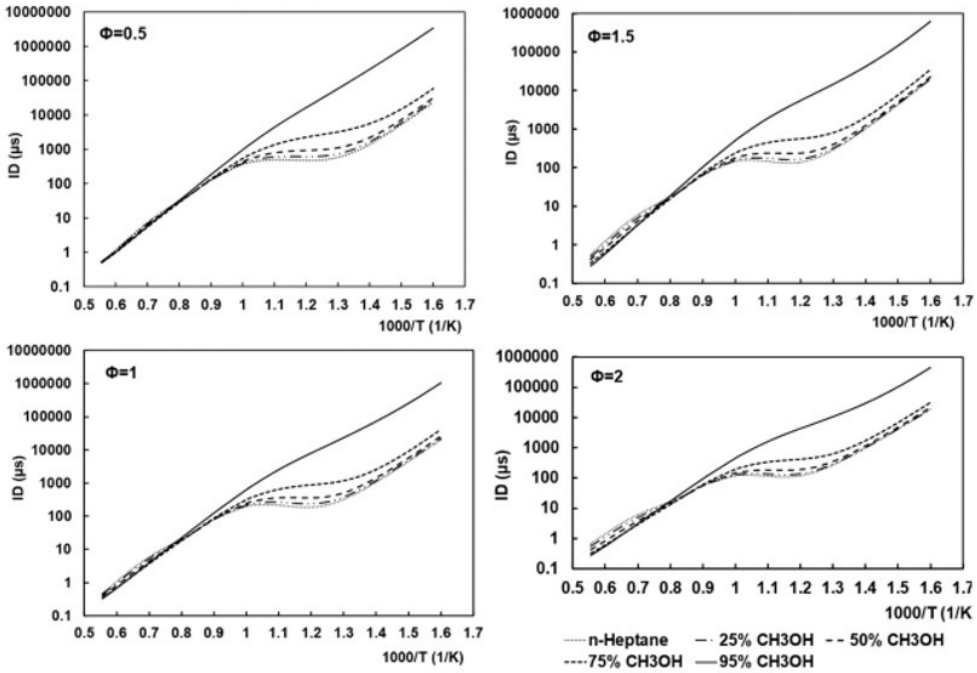

Figure 6 Numerically calculated ignition delays plotted versus inverted temperature for several equivalence ratios, performed by Parsa and Verhelst [90].

Another result from this study that was of interest, was that the efficiency of both methanol fuels was comparable to that of diesel when testing modes in the E3 cycle. However, similar to the stability issues a notable steep drop in efficiency was observed for both methanol fuels, for the additional lower load test point, indicating problematic conditions for methanol CI. This decline in efficiency was attributed to lower thermodynamic efficiency, particularly due to higher heat losses, see Figure 7. These heat losses were discussed in paper III and were reasoned to be caused by combustion occurring closer to the piston bowl, partially caused by the smaller combustion chamber, resulting in increased heat transfer to the piston. However, it is also an effect of the high heat of vaporization of methanol, which effectively extracts energy from the surrounding air, showing as a loss in heat. Gainey et al. Gainey et al. saw this effect during experiments conducted on wet ethanol 80 (comprising 80% ethanol and 20% water by mass), which shares a similar heat of vaporization with neat methanol, using an engine of 0.423 liter/cylinder at high load operations [91]. They observed a drop in efficiency when going from HCCI to mixing-controlled combustion and this was tracked to arise from wet ethanol 80 having a heat of vaporization close to 6% of its lower heating value. Therefore, a significant thermodynamic efficiency drop results when injected near TDC. This was due to the heat absorption from fuel heating and vaporization, resulting in a heat

transfer loss. While this effect also occurs with diesel, the difference is that the heat of vaporization compared to the lower heating value of diesel is much lower, rendering the effect negligible. Gainey et al. [92] quantified this "cooling potential" of a fuel to clarify this, and defined an equation based on the fuel's heat of vaporization divided by its stoichiometric air/fuel ratio. Essentially, this "cooling potential" parameter quantifies the temperature drop caused by evaporating a stoichiometric mixture of a given liquid fuel. Furthermore, Gainey et al. utilized 0-dimensional thermodynamic engine modeling to quantify the magnitude of this thermodynamic penalty, demonstrating around a 2 percentage point decrease in efficiency when the heat of vaporization was changed from zero to the actual value of wet ethanol 80. This effect aligns with the findings here, as there is a significant increase in heat transfer losses observed with both methanol fuels compared to diesel. Notably, given that cylinder conditions are the coldest at lower loads, the relative impact of the temperature drop is higher, potentially explaining why this phenomenon is particularly pronounced at lower loads. Additionally, the higher loss exhibited by MeOH97 compared to MeOH100 could be due to the same effect as the in-cylinder conditions are colder for MeOH97 as observed in Figure 5. However, further investigation into the effects of load, speed, and in-cylinder conditions is warranted to comprehensively understand this effect.

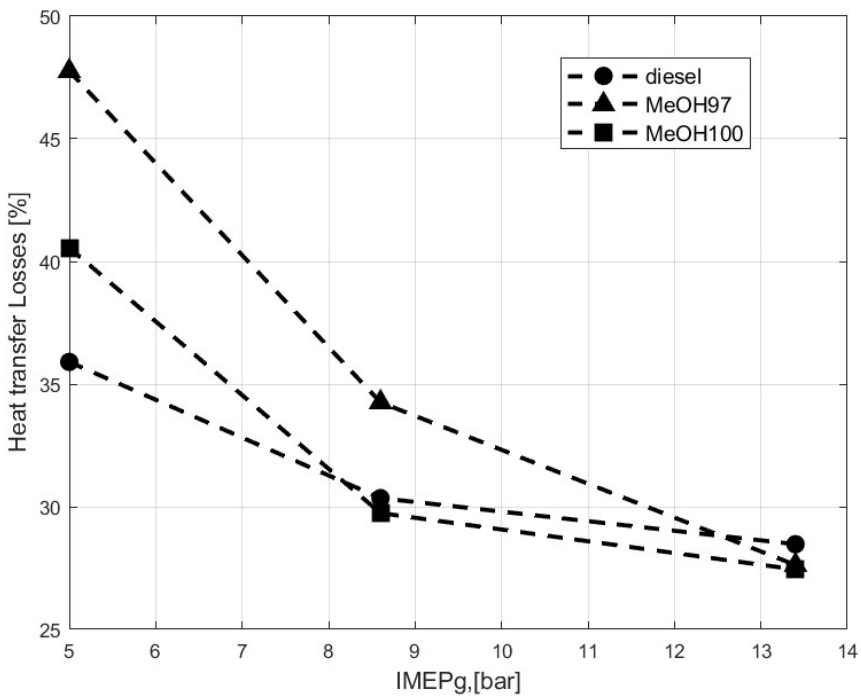

Figure 7 Calculated heat transfer losses for diesel, MeOH97 and MeOH100, through all tested modes (indicated here by load) [Paper III].

In terms of emissions, both methanol fuels exhibited similar values, with CO emissions below the Euro VI standards in most conditions, comparable to diesel. However, they showed higher levels of unburnt HC compared to diesel, but on the flip side there was a notable reduction in NO_x emissions ranging from 20% to 60% compared to diesel across the different modes, see Figure 8.

Comparing these results to those of the MeOH97 converted engine, it becomes evident why the previously discussed MeOH97 engine achieved NOx certification without the need for aftertreatment. As shown in Figure 8, NOx emissions significantly decrease towards higher load modes, suggesting that extrapolating to even higher load modes not tested here would likely meet the IMO Tier III limit. This is particularly beneficial considering that the weighting of the different modes in the certification process place more weight on higher load modes, which are therefore favorable for methanol fuels. Furthermore, formaldehyde (HCHO) emissions from methanol were found to be limited to single ppm values.

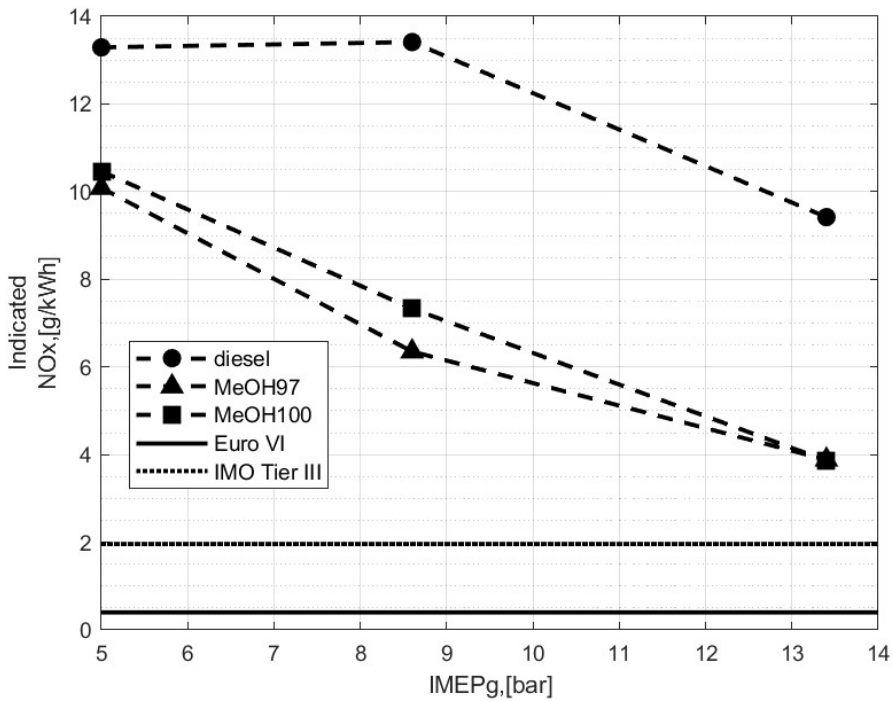

Figure 8 Indicated NO_x emissions from testing MeOH97, MeOH100, and diesel, at the three modes [paper III].

These results, albeit limited in the parameters tested, explains the reasons behind the good performance of MeOH97 in the NO_x certification and its achievement of diesel-like average efficiency in the E3 cycle. Furthermore, the results indicate that

even MeOH97 requires additional combustion aiding techniques at the lowest loads and the diminishing necessity for intake heating of MeOH100 with increasing load and speed. Suggesting that if an engine concept can facilitate low load MeOH100 CI, the requirement for ignition improvers can potentially be removed. This suggests the potential of using an on-demand system for ignition improver blending. By utilizing double fuel tanks in a vessel, one for methanol and one for ignition improver, and blending them as needed depending on operational condition, this could potentially save money for a vessel operator as the more expensive ignition improver is only used when needed.

4.3 Improving low load methanol CI

Following the literature review, various options for facilitating low load MeOH100 CI were identified, however, significant knowledge gaps were highlighted with need for further research. Notably, a higher CR and the use of a pilot injection was seen as potential methods to facilitating low load MeOH100. Accordingly, this thesis investigated these areas, with the investigation of CR in Paper IV and of pilot injection in Paper V. The objective was to determine the extent to which these factors could aid low load MeOH100 combustion and how design parameters impact their effect.

4.3.1 Increased compression ratio

Upon reviewing the literature, it becomes evident that an increased CR, relative to that of a standard diesel engine, holds promise through enhancing in-cylinder temperatures and so potentially improving methanol CI. Consequently, this concept was adopted in the conversion of the MeOH97 engine. However, this thesis sought to investigate the impact of an even higher compression ratio, as the one used with MeOH97 was apparently not enough for stable MeOH100 CI.

The methodology involved utilizing the research engine, described in the experimental section, to examine three distinct conditions: firstly, operating at a 6 bar IMEPg load with the original diesel piston featuring a CR of 17.3; secondly, replicating the load condition with a higher CR piston, set at 40; and thirdly, employing the 40 CR piston at a reduced 3 bar IMEPg load to assess performance under lower load conditions.

During testing at the initial condition, it became apparent that relying solely on intake heating to autoignite MeOH100 at a CR of 17.3 was insufficient, as the heater's capacity was limited, achieving a maximum temperature of 140°C. Consequently, a fixed pilot injection was introduced, enabling stable combustion of MeOH100. This pilot injection was retained in the higher compression scenarios to

maintain methodological consistency, and the results demonstrated that the elevated compression ratio took away the need for intake heating. Moreover, it was observed that stable combustion could be achieved even without the pilot injection with the 40 CR piston and 3 bar IMEPg load.

However, the utilization of the high compression ratio piston presented challenges due to the substantially increased crevice-to-volume ratio, resulting in an eighteen-fold rise in CO emissions and a reduction in combustion efficiency of over 5 percentage points due to incomplete combustion. Although this issue was somewhat mitigated at the lower load condition due to reduced fuel injection, it remains a significant concern. Furthermore, the high compression ratio led to excessively high pressures, severely constraining the operational range of an engine equipped with such a piston.

Therefore, while increasing the compression ratio offers advantages in terms of heat addition and potentially enhanced thermodynamic efficiency, it must be weighed against the risks of increased unburnt emissions and the limitation of maximum pressure. This underscores the conclusion that while some form of increased compression ratio is beneficial for CI methanol combustion, it cannot singularly address methanol's challenges at low loads without severe drawbacks. Hence, it should be complemented with other concepts and be carefully designed, as exemplified in the previous MeOH97 study, which utilizes an intermediate CR of 26. Another option would be to adopt a variable compression ratio setup, or variable valve timing together with a high CR, varying the effective compression ratio to match it to the needed temperature while avoiding engine limitations.

4.3.2 Pilot injection

A pilot injection was employed in the prior study demonstrating its potential in facilitating MeOH100 combustion where it would otherwise fail. Despite not needing a pilot injection with the implementation of a high CR, its continued use yielded better results than without it, with a 1.3 percentage point increase in gross indicated efficiency. Furthermore, the utilization of the pilot injection led to notably smoother combustion, as evidenced by the rate of heat release (RoHR) depicted in Figure 9. In the figure a small heat release following the pilot injection is seen, the heat from this results in a reduced ignition delay for the main injection which decreases the portion of premixing before combustion, as seen by the much shorter ignition delay. This causes the combustion to be more diffusive and so more smooth, which can be compared to the no-pilot heat release showing more premixing in turn giving rise to a more rapid premixed combustion. Additionally, experimental observations noted a reduction in noise levels when a pilot injection was added. This underscores the beneficial role of a pilot injection, even in circumstances where it is not necessary for achieving stable ignition.

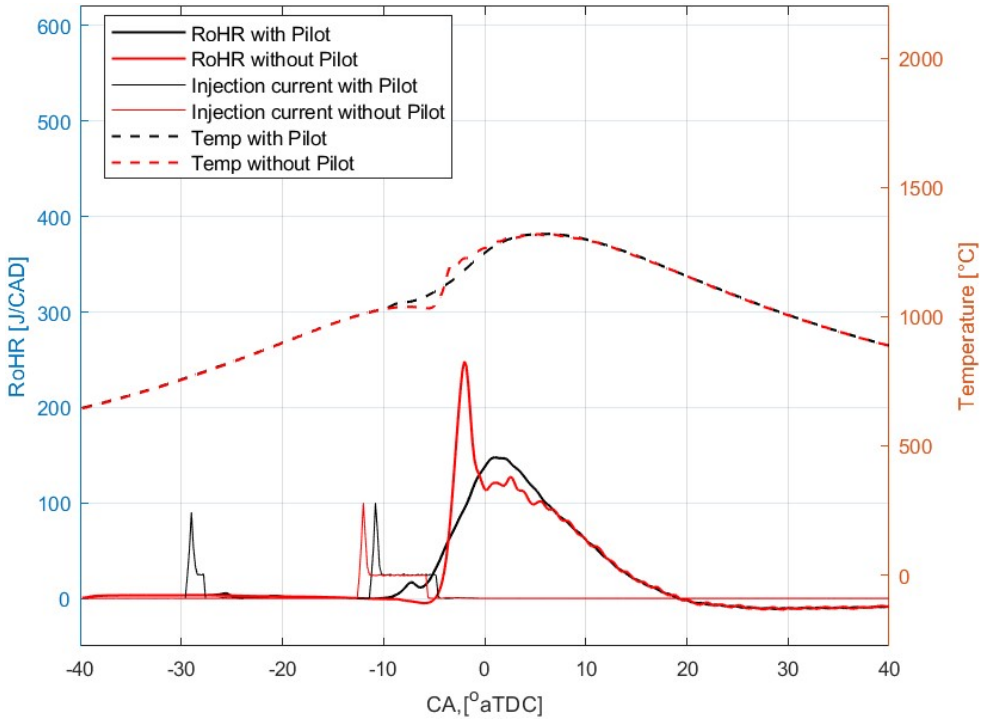

Figure 9 The RoHR, calculated temperature and injection current for MeOH100 CI using a 40 CR piston, with and without the use of a pilot injection at 3 bar IMEPg [Paper IV].

Building upon the previous results, it is evident that pilot injection holds significant potential for enhancing low load methanol CI. However, the optimal timing and size of the pilot injection have not been comprehensively explored, as highlighted in the literature review. Consequently, as part of this thesis, an investigation into pilot timing and size was undertaken in Paper V to clarify their impact on combustion dynamics.

This investigation utilized a similar experimental setup as employed in testing the MeOH97 fuel blend, see Experimental setup section, focusing on the low-load operating conditions of Mode 5, characterized by 950 rpm speed and 5 bar IMEPg load. Pilot injection timing and length were systematically varied, as outlined in Table 12 and Figure 10. For comparison, a single injection of MeOH100 was also employed, with intake heating utilized as needed to ensure stability below 3% COV of IMEPg.

Table 12 Pilot injection settings investigated [paper V].

Pilot injection timing, dwell [CAD aTDC]	3, 5, 10, 15, 20, 25
Pilot injection length [µs]	250, 375, 500
Main injection timing [CAD aTDC]	Set to achieve a fixed CA50
Main injection length [µs]	Set to achieve a set load

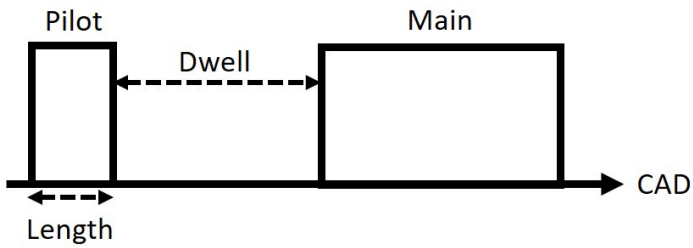

Figure 10 Explanation of the dwell and injection length parameters used in the study.

The study unveiled that a dwell time ranging between 15 to 20 CAD paired with a pilot injection length of 250 to 375 µs, translating to a pilot to main injection ratio ranging from 0.18 to 0.27, yielded favorable results across all investigated combustion parameters. These settings exhibited the highest efficiency, lowest emissions, and stable combustion. In comparison to a single injection of methanol, these optimized settings improved efficiency by 5 percentage points, marginally improved CO, CO_2, and HC emissions, and reduced NO_x emissions by approximately 20%. Notably, these improvements were achieved at an intake temperature 36°C lower than a single injection, while still achieving a 50% reduction in the COV of IMEPg, underscoring the potential of a well-designed pilot injection strategy. To further investigate the combustion characteristics associated with pilot injection, the RoHR was for all cases were investigated. It was observed that a shorter pilot injection duration or a shorter dwell time between the pilot and main injections resulted in the integration of the pilot burn into the main heat release, yielding a characteristic "hump" in the heat release profile. Conversely, longer injection durations and dwell times led to the pilot burn occurring independently, resulting in a two-stage heat release pattern. This phenomenon is illustrated in Figure 11, which depicts the four RoHR cases corresponding to the aforementioned optimal pilot injection combinations. In the shorter heat release scenarios, the pilot burn is integrated into the main release, while in the longer durations, the pilot burn precedes the main burn. This observation suggests that both a pre-burn of the pilot and an early burn with the main injection burn can be beneficial. The observed two-stage heat release pattern aligns with the explanation of how the pilot injection concept should work, leveraging the first heat release to facilitate the subsequent main burn, and it is seen in Figure 11 that the pilot fuel reaches ignition conditions

approximately 7-8 CAD bTDC. However, in the shorter injection duration scenarios, the fuel from the initial injection does not ignite at 7-8 CAD bTDC, and can so be expected to interact with the fuel from the subsequent injection instead. This interaction is attributed to the pilot injection being too small to produce an ignitable mixture, resulting from becoming too lean. Consequently, upon the main injection, a lean mixture with sufficient temperature to autoignite is already available in the cylinder. This is very interesting as it works differently compared to the classical pilot injection concept, but has here been shown to be equally efficient. Comparing the pilot RoHR plots to a single injection RoHR as depicted in Figure 12, it is clear that the use of a pilot injection avoids most of the rapid burning premixed combustion that happens with a single injection. Instead, a majority of the injected fuel mass is consumed through mixing-controlled combustion. This renders a more stable combustion process with a lower rate of heat release which in turn contributes to reduced NO_x through colder combustion conditions.

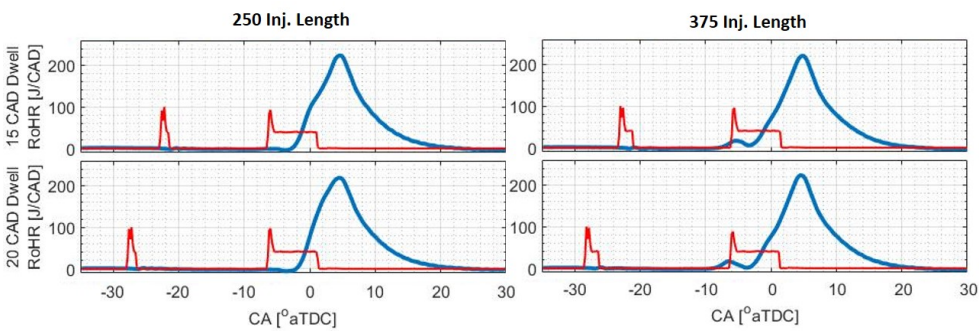

Figure 11 RoHR of the optimal configuration when using a pilot injection, with 15 and 20 CAD dwell and 250 and 375 µs length, with RoHR in blue and normalized injection current in red [Paper V].

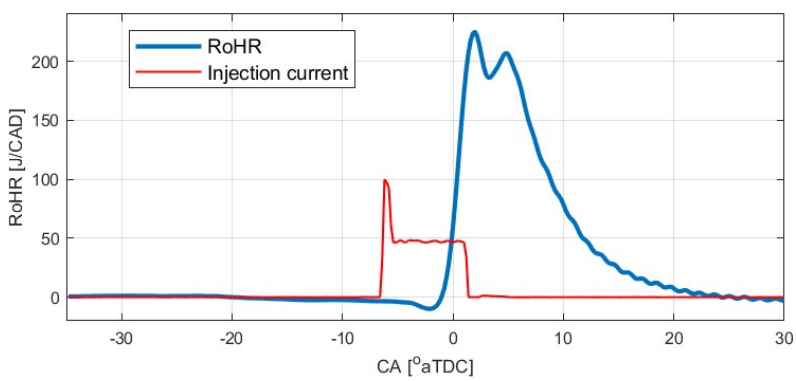

Figure 12 RoHR from a single injection of neat methanol at 950 rpm speed and 5 bar IMEPg, with 97°C intake temperature.

To further understand the effect of the two pilot combustion cases a comparison to a CFD study by Pucilowski et al. [93] gives further insight. Pucilowski performed numerical simulations, using experimental data, through Unsteady Reynolds averaged Navier-Stokes simulations of methanol injection at different injection timings. The study aimed to enhance understanding of methanol combustion behavior by investigating variables such as local equivalence ratio and temperature within the combustion chamber. Figure 13 presents two plots with the temperature and equivalence ratio distributions for 2 and 4 CAD after methanol injection. The heat of vaporization of methanol is observed to influence the distribution of local temperature after injection. This effect is more pronounced in the richer regions of the combustion chamber, where a greater amount of fuel has evaporated and absorbed heat, resulting in a greater temperature reduction. Consequently, autoignition conditions occur earlier in leaner regions rather than in richer ones, causing an ignition delay before the mixture reaches autoignition conditions. This allows more time for the fuel to form a premixed mixture before combustion onset. This causes a rapid start of combustion as evident with a single injection in Figure 12.

Pilot injections, however, mitigate this delay either through pre-burning or by achieving a combustible mixture earlier. Specifically, with a 250 µs pilot injection, a very lean mixture forms in the combustion chamber before the main injection, as seen by the lack of pre-burn, this can be seen to be equivalent to an upward movement of the plots in Figure 13 (arrow 1). This shortens the formation time to achieve an ignitable mixture and so reduces the ignition delay, which in turn reduces the premixed combustion. Additionally, the initial cooling effect is partially offset by the already hot pilot fuel, this leads to an early heat generation creating a "hump" in the heat release profile. Subsequently this early burn facilitates the remainder of the main injection and contributes to improved overall combustion stability. On the other hand, a larger pilot with a 375 µs injection provides sufficient fuel to create a combustible mixture, resulting in a pre-burn and so increased temperature before the main injection. This is equivalent in Figure 13 to a shift of the plot to the right (arrow 2), making the fuel mixture meet autoignition conditions earlier, reducing ignition delay, reducing premixed combustion and enhancing combustion stability.

Further numerical studies of this kind to confirm the observed effects and provide detailed insights into combustion processes would be of interest together with exploring intermediate parameter values between 15 to 20 CAD dwell and 250 to 375 µs. This would give a better understanding of how the pilot burn evolves between the two cases of burn characteristics, and if there is an even better case.

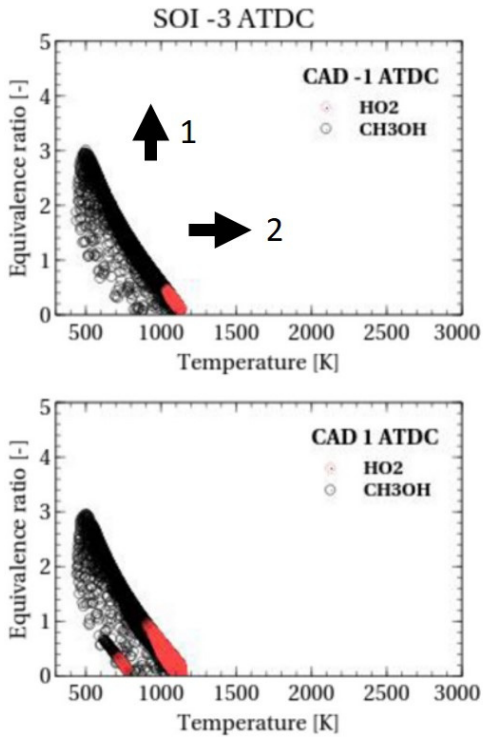

Figure 13 Scatter T-Phi maps after methanol injection at -3 CAD aTDC, with the dark color indicating methanol, while the red shows HO_2 which indicates combustion. Based on plots from Pucilowski [93] and modified here with the addition of arrows. Arrow 1: The effect on the plot when the pilot is not pre-burnt before the main injection. Arrow 2: The effect on the plot when the pilot is pre-burnt before the main injection.

Through this investigation, it has been demonstrated that an increased compression ratio, within reasonable bounds, coupled with a well-designed pilot injection strategy, can substantially contribute to achieving stable MeOH100 CI. This is evident from the results in Table 13, which compares the outcomes of the experiments conducted in this thesis under Mode 5 conditions. Although MeOH100 with a pilot injection exhibited superior stability, it used higher intake temperature compared to MeOH97 employing only a single injection strategy. However, it's also worth noting that MeOH97 exhibited the lowest efficiency, both of which might have been improved with a pilot injection, albeit untested in this thesis.

Table 13 also shows how using MeOH100 employed with the most effective pilot injection combination and with an increased compression ratio of 26, demonstrated efficiency and CO emissions comparable to diesel, alongside the lowest NO_x emissions at 62% of the diesel value. However, notable concerns persist regarding the higher HC emissions observed across all methanol cases, likely caused by higher

portions of fuel in crevices, albeit being lower when employing a pilot injection. This emphasizes the significant impact of a pilot injection and advocates for its inclusion in the design of MeOH100 engines.

Table 13 A comparison between different tested fuels and combustion aiding concepts at similar conditions of 950 rpm speed and 5 bar IMEPg load. The pilot injection case is with 20 CAD dwell time and 250 µs injection length.

Concept [Paper] → Measurements ↓	**Diesel [III]**	**MeOH97 [III]**	**MeOH100 [V] Single Injection**	**MeOH100 [V] Pilot Injection**
Gross IE [%]	41.6	29.6	31.7	36.3
Intake T [°C]	26	38	97	61
COV of IMEPg [%]	1.3	2.7	2.9	1.4
CO [g/kWh]	0.6	0.8	0.7	0.6
CO_2 [g/kWh]	654	898	756	737
HC [g/kWh]	0.4	2.1	1.8	1.7
NO_x [g/kWh]	13.3	10.1	10.3	8.3

5 Conclusion

5.1 Summary

This thesis has explored, analyzed, and tested various engine concepts aimed at achieving stable single-fuel methanol compression ignition (CI), starting with a literature review aimed at finding the most promising concepts to achieve this. The use of ignition improver, increased compression ratio, and pilot injection were all found to show potential and were therefore further investigated in this thesis. Another concept found to have high potential, but not tested here, was the use of a glow plug, particularly for addressing the start-up issue of neat methanol. Moreover, the use of exhaust gas recirculation was also found to be interesting as methanol does not have a NOx-soot trade-off and can potentially (further) lower NOx emissions without major penalties.

The investigation of the use of ignition improver with methanol demonstrated its viability in CI engines with minimal modifications through an analysis of a converted engine, made to run on methanol with 3% ignition improver. The results showcased comparable performance to diesel in terms of efficiency, coupled with lower NOx and significantly reduced soot emissions. Moreover, it was observed that the need for ignition improver was primarily pronounced in colder, lower load conditions. Nevertheless, given that ignition improver is an expensive additive requiring an extra blending stage in the supply of the fuel, it would ideally be minimized in use. The tests showed significant improvements in ignition delay characteristics with the addition of ignition improver and it was proven to a viable way of achieving single-fuel methanol CI.

Further, in this thesis increased compression ratio and the utilization of a pilot injection strategy were explored as means to enhance low load neat methanol CI. An increased compression ratio was utilized in the ignition improver test, and did aid in achieving stable methanol combustion. However, that compression ratio was not enough to have stable CI of neat methanol by itself. Therefore, a significantly higher compression ratio of 40 was tested, which was proven to be sufficient to achieve stable CI of methanol at low loads. This compression ratio, however, came with significant drawbacks, including higher unburnt emissions due to a greater crevice to volume ratio and elevated peak pressures, potentially limiting higher load operations. Consequently, it was proven that increasing the compression ratio cannot singlehandedly facilitate methanol CI while maintaining the operation range

of an engine. A solution could instead be to use a moderately increased compression ratio with other techniques or by utilizing some technique to achieve a variable effective compression ratio.

Using an intermediate compression ratio, the same as the one in the ignition improver experiment, the use of a pilot injection strategy was then investigated and it was demonstrated to reduce NOx emissions by approximately 20% compared to a single injection of methanol and 62% compared to diesel. This emphasized the significant impact of a well-timed pilot injection and that it should be included in the design of MeOH100 engines. In the experiments, two different ways of utilizing a pilot injection were observed, one where the pilot burns before the main injection and so ads enough heat to facilitate the main injection vaporization and ignition. The second observation was that the pilot could be so small that the fuel/air mixture ended up being too lean to ignite, but that it still aided by speeding up the time for the main injection fuel to achieve an ignitable air/fuel ratio. By doing so the combustion could start earlier and could so precede the full cooling effect of the main injection.

The findings presented here, together with the insights from the literature review, led to the conclusion that it does not seem to be possible to achieve stable neat methanol CI using only one concept. Instead, a combination of concepts should be used to achieve stable combustion. From this thesis, an increased compression ratio combined with a pilot injection was proven to be beneficial and should be used as a base for further testing.

5.2 Future work

The research of this thesis has highlighted the need for further exploration in several different directions.

Investigating the needed ignition improver percentage across a broader range of operational conditions could determine whether an on-demand ignition improver blending process would be beneficial for real-world engine operation. Additionally, further experimentation involving different ratios of ignition improver compared to ignition delay characteristics could offer deeper insights into how the fuel blend properties change with varying percentages of ignition improver.

Further, this thesis highlighted the need for further exploration of combining neat methanol technologies, with especially the concepts glow plug, increased compression ratio, EGR, and pilot injection that have shown individual potential in some conditions but not full operation length compatibility. Understanding how these concepts interact when used simultaneously could possibly significantly improve methanol compression ignition. Additionally, there's a gap in research

concerning methanol's performance at higher loads, especially after modifications have been made to address low load issues as these modifications might negatively affect higher load operations.

5.3 Thesis contribution

This thesis has contributed with:

- A review of existing literature on CI single-fuel methanol concepts which identified several concepts with the potential to facilitate methanol compression ignition, including ignition improver blending, increased compression ratio, pilot injection strategy, glow plug utilization for startup, and exhaust gas recirculation. However, it also identified several knowledge gaps, emphasizing the need for further research into these concepts.
- Analysis of methanol with 3% ignition improver fuel blend through real-world testing and research engine experiments. Analyzing the performance of the MeOH97 fuel blend and comparing it to diesel and neat methanol, revealing a significant improvement in chemical kinetics regarding ignition delay time and showing the high readiness of the technology.
- Investigation of increased compression ratio, examining to which degree a significantly increased compression ratio can aid neat methanol compression ignition at low load operations. The findings indicated that while an increased compression ratio can indeed facilitate neat methanol combustion, it also imposes limitations on the engine operating range. Thus, it should be employed in conjunction with other concepts to avoid limiting the engine operation.
- Study of the use of a pilot injection and its impact on low load neat methanol compression ignition, including the effect of varying dwell time and pilot injection length. The results demonstrated significant benefits of a well-timed pilot injection, with exclusively positive effects on neat methanol compression ignition.
- Based on the review and research conducted, recommendations were provided regarding the most promising concepts for further investigation, including pilot injection, increased compression ratio, glow plug utilization, and exhaust gas recirculation.

Overall, this thesis has expanded the understanding of methanol compression ignition and laid the groundwork for future research in this field.

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Appendix

The following equations were used to calculated the presented mean effective pressures (MEP), efficiencies (η), rate of heat release (RoHR) and measurement uncertainty (δq).

The fuel mean effective pressure (FuelMEP), i.e. the total chemical energy contained in the injected fuel, was calculated using the fuel flow (m_f), the lower heating value of the fuel (Q_{LHV}) and the engine's displaced volume (V_d), according to equation 1.

$$FuelMEP = \frac{m_f Q_{LHV}}{Vd} \tag{1}$$

The combustion efficiency, i.e. how efficiently the fuel is converted into useful heat, was calculated using the exhaust emission with heating values (i), their molar mass (M_i), wet concentration (x_i), lower heating value ($Q_{LHV,i}$), molar mass of products (M_p), lower heating value of the fuel ($Q_{LHV,f}$) and air to fuel ratio (A/F), according to equation 2.

$$\eta_{comb} = 1 - \frac{\sum_i \frac{M_i}{M_p} x_i Q_{LHV,i}}{\frac{Q_{LHV,f}}{1+A/F}} \tag{2}$$

The heat mean effective pressure (QMEP), the total usable heat after the fuel injection, was calculated using FuelMEP and η_{comb}, according to equation 3.

$$QMEP = FuelMEP * \eta_{comb} \tag{3}$$

The gross indicated mean effective pressure (IMEPg), the usable work after heat losses, was calculated by integrating the pressure (P) over the volume (V), from 180 CAD bTDC firing to 180 CAD after TDC (aTDC) firing and dividing it with the displaced volume (V_d), according to equation 4.

$$IMEPg = \frac{1}{V_d} \int_{TDC-180}^{TDC+180} p\, dV \tag{4}$$

The gross indicated efficiency, was calculated using IMEPg and FuelMEP, according to equation 5.

$$\eta_{gross\ Ind.} = \frac{IMEPg}{FuelMEP} * 100 \tag{5}$$

The thermal efficiency, was calculated using IMEPg and QMEP, according to equation 6.

$$\eta_{therm} = \frac{IMEPg}{QMEP} * 100 \quad (6)$$

The exhaust mean effective pressure (ExhMEP), the heat losses to the exhaust, was calculated using the exhaust mass flow (m_e), specific heat capacity of the exhaust (C_p), exhaust temperature (T_{exh}), ambient temperature (T_{amb}) and displaced volume (V_d), according to equation 7.

$$ExhMEP = \frac{Qex}{V_d} = \frac{\mathrm{me}C_p(T_{exh} - T_{amb})}{V_d} \quad (7)$$

The heat transfer mean effective pressure (HTMEP), the heat losses from heat transferred to the engine, was calculated using QMEP, IMEPg and ExhMEP, according to equation 8.

$$HTMEP = QMEP - IMEPg - ExhMEP \quad (8)$$

Heat transfer losses were calculated using HTMEP and FuelMEP according to equation 9.

$$HT_{Losses} = \frac{HTMEP}{FuelMEP} * 100 \quad (9)$$

Exhaust losses were calculated using ExhMEP and FuelMEP according to equation 10.

$$Exh_{Losses} = \frac{ExhMEP}{FuelMEP} * 100 \quad (10)$$

The rate of heat release was calculated using the specific heat ratio (ɣ), pressure (P) and volume (V), according to equation 11.

$$RoHR = \frac{\gamma}{\gamma - 1} P \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dp}{d\theta} \quad (11)$$

The lambda (λ) value was calculated using two equations. Equation 12 using the fuel mass (m_f), air mass (m_a) and the stoichiometric air-fuel ratio of methanol (A/Fs).

$$\lambda = \frac{\frac{ma}{mf}}{\mathrm{A/Fs}} \quad (12)$$

While equation 13 used measured gaseous emission, with a, b and c representing quantities of C, H and O in the fuel, x being the concentration of wet species in the exhaust gas.

$$\lambda = \frac{1}{2\left(a + \frac{b}{4} - \frac{c}{2}\right)} \left(\frac{a}{axHC + xCO + xCO2} * (cxUHC + xH2O + xCO + 2xCO2 + xNOx) - c\right) \quad (13)$$

A simplified specific heat ratio was used to estimate the heat capacity (ɣ) during compression and expansion by using equation 14, with the temperature (T) and an initial ɣ0 decided from the equivalent ratios during experiments [38].

$$ɣ = ɣ0 - \frac{T-300}{1000} * 0.0813 \quad (14)$$

The temperature was calculated from equation 15, using measured pressure (P), calculated volume (V) and their initial condition at intake valve closing denoted with a 0.

$$T = \frac{PV*T0}{P0*V0} \quad (15)$$

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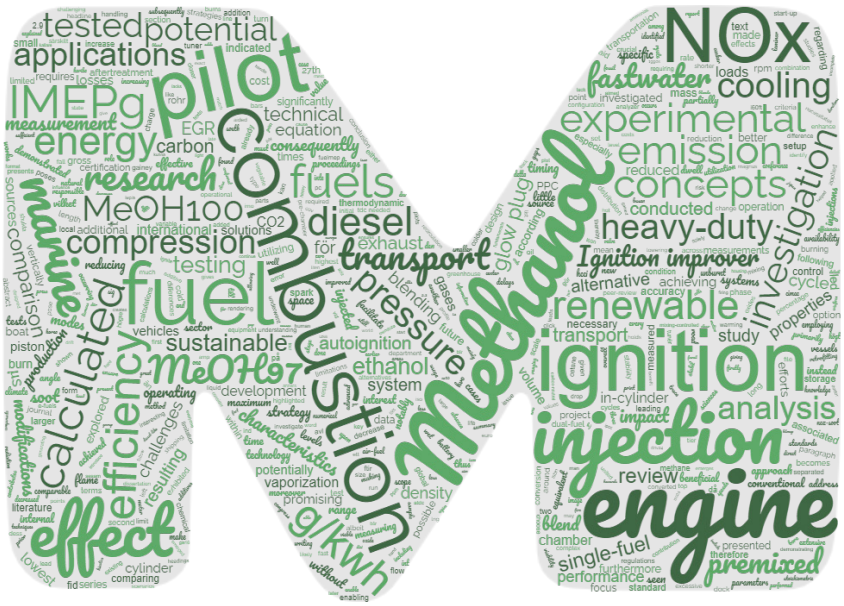

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