

Development of HCCI Engines for Dimethyl Ether

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Development of HCCI Engines for Dimethyl Ether



Kim R. Hansen, Troels Dyhr Pedersen and Jesper Schramm

August 2011

Danmarks Tekniske Universitet

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By Kim R. Hansen, Troels Dyhr Pedersen and Jesper Schramm

- Copyright: Full or partial reproduction of this publication is allowed if reference is cited.
- Front page: The DTU team and cars for the Shell Eco-Marathon 2009. The white car had the HCCI two-stroke engine, developed during this project, installed. It won the competition with 589 km/l (gasoline equivalent).
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Preface

This report has been prepared for the Danish Energy Agency. It summarizes the results of the project entitled: "Development of HCCI engines for DME". The project has been financed by "EFP 06".

The chapters about theoretical and experimental studies have been written using the language and terminology typical for this field of research but the introduction and the final chapters have been written in a language focused on communicating the topics to a wide audience to make the report as useful as possible.

A list of abbreviations is included just before the references at the end of the document.

Lyngby, august 2011

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Summary

An HCCI engine combustion concept was evaluated theoretically and experimentally with dimethyl ether (DME) as the primary fuel. DME has very low lubricity and combustion concepts with low injection pressures, like HCCI, are thus preferable since it is difficult to design reliable high pressure DME fuel pumps. The idea behind the study was also that one of the main problems with HCCI operation, namely obtaining correct combustion phasing, could be addressed by mixing a high cetane fuel (DME) with a high octane fuel (methanol). This mixing should take place in the intake manifold just prior to induction of the charge into the engine cylinder in a variable and appropriate ratio in order to provide combustion phasing control.

Using methanol as the high octane fuel is particularly interesting since DME is typically produced by dehydration of methanol. Therefore DME and methanol constitute a cost-effective two-fuel solution for HCCI engines.

The main focus of the research was on combustion phasing control (auto-ignition) and combustion noise. A reduced kinetic scheme for oxidation of DME and methanol was developed based on the detailed scheme for combustion of DME by Lawrence Livermore. The scheme could theoretically validate the concept of methanol for retardation of auto-ignition.

Experiments with combustion phasing control were conducted on a truck-sized diesel engine at NTSEL (National Traffic Safety and Environmental Laboratory) in Tokyo, Japan. It was verified that combustion phasing could be retarded with methanol added to the inlet air. Maximum engine load in HCCI-mode was 50% of the maximum load for the engine in diesel-mode. Fuel consumption for traditional and HCCI operation was comparable. EGR also had a retarding effect on combustion phasing and the equivalence ratio could be brought close to stoichiometric without compromising combustion efficiency when using EGR.

Experiments concerning combustion generated acoustic noise were conducted on a smaller two-cylinder diesel engine at DTU in Lyngby, Denmark. Even though results indicated that multiple smaller combustion chambers in the piston top reduced acoustic noise, the largest noise reduction was achieved with a traditional bowl-in-piston diesel engine design. Increased crevice volumes resulting from applying additional combustion chambers in the piston also reduced the thermal efficiency of the engine.

Student projects at DTU, performed after the start of this EFP-project, showed that it is possible to design a DME fuel pump that could supply up to 150 bars of pressure without resorting to exotic, and thereby expensive, materials and coatings of the contact surfaces. Based on these findings the EFP project group then decided to perform experiments with late injection HCCI operation in a two-stroke engine.

Late injection HCCI is a process where the fuel is introduced into the engine cylinder towards the end of the compression stroke but with fuel injection being completed before the onset of combustion. This is in contrast to normal diesel operation where the fuel is burning as it is introduced into the engine cylinder. In this way sufficient time is available before ignition to achieve a high degree of premixing with air and thereby achieve HCCI-like operation. Injection pressures of approximately 150 bars are necessary in order to do this. In these experiments pure DME was used. No methanol addition was necessary since combustion phasing was controlled by fuel injection timing.

Results for the late injection HCCI two-stroke engine have shown high engine efficiencies and low NO_x emissions but even though combustion phasing is controllable injection timing is critical. Free control of the injection event is necessary to obtain satisfactory operation which in turn means that some form of common rail system is required. At the low injection pressures required (150 bars) such a system may well be feasible.

1. Introduction

1.1 Motivation for the study of dimethyl ether (DME)

DME has been in use for many years as an aerosol propellant. It is a colorless, odorless and non-toxic gas with a vapor pressure suitable for driving for example hair lacquer out of a can. It is also a byproduct that is formed during the production of methanol. In the early 1990's Haldor Topsøe A/S, who designs methanol production plants, considered if it was possible to use this byproduct as an engine fuel. This was tested at DTU and in 1995 a paper was published with the first experimental results using a diesel engine (Sorenson, Mikkelsen 1995). The results showed that DME is an excellent diesel engine fuel with respect to engine efficiency and emissions. With respect to engine durability there were problems because of the very low lubricity of DME and incompatibility with a range of polymers.

These first results generated much interest in the scientific community and the use of DME as a fuel has been explored globally since. Japan, South Korea and China have been at the forefront of this development. The main conclusions regarding the use of DME in engines have not changed much since the original paper from 1995. Significant progress has been made with respect to compatible materials and fuel system design but an off-the-shelf cheap and durable high pressure fuel injection system for pure DME is still not available.

This situation is one of the primary motivations for the studies described in this report: Is it possible to design an engine that can use DME as efficiently as a diesel engine but without the need for a high pressure fuel injection system?

At this point the reader may argue: Why bother with engines in the first place? The future belongs to electric and fuel cell vehicles!

1.2 Electricity and hydrogen vs. hydrocarbons

The energy density of liquid hydrocarbons is much higher than what can be attained with batteries. Energy density is also low for hydrogen which is the best fuel for fuel cells. See Figure 1.

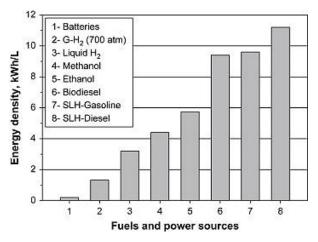


Figure 1 - Volumetric energy densities of selected energy carriers (Muradov, Veziroglu 2008)

This makes hydrocarbons a good choice for vehicles and it is one of the main reasons for them being successful in transportation for the last 100 years. But hydrocarbons from fossil sources are a finite resource and the contribution of CO_2 to the atmosphere from their use is a problem in terms of climate change. On top of this there are problems with other harmful emissions when burning hydrocarbons in an engine such as NO_x and particulates. But these problems are not an unavoidable result of the use of the hydrocarbons themselves. If hydrocarbons could be produced in a sustainable, CO_2 -neutral way and burned in engines without significant harmful emissions they would still be a very efficient way of storing energy in a vehicle. In fact, the high energy density of hydrocarbons contributes to a lower weight of the vehicle and thereby a lower energy consumption to drive it forward compared to a vehicle powered by for example electrical batteries. Three different ways of supplying energy to the transportation sector are illustrated in the following figures.

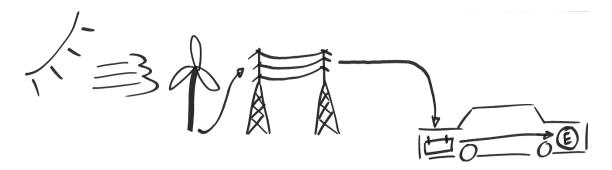


Figure 2 - An electric route: Sun \rightarrow wind \rightarrow grid \rightarrow battery \rightarrow electric motor

The electric route is simple and efficient but there is currently no way of storing large amounts of energy to be used for periods of no wind. The energy density of a vehicle battery is low and battery cost and lifetime are problematic issues.

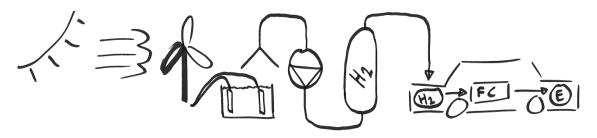


Figure 3 – A hydrogen route: Sun \rightarrow wind \rightarrow electrolysis \rightarrow hydrogen \rightarrow fuel-cell \rightarrow electric motor

The hydrogen route is more complex and less efficient compared to the electric route. Storage of energy is possible but not trivial, especially not in the vehicle. Both the fuel cell and the storage facility for hydrogen in the vehicle are costly at the current state of development.

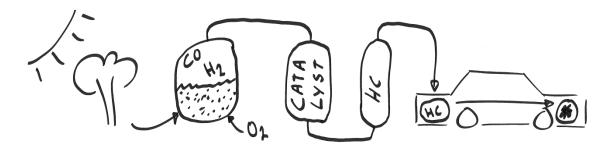


Figure 4 – A hydrocarbon route: Sun \rightarrow biomass \rightarrow gasification \rightarrow hydrocarbons \rightarrow combustion engine

The hydrocarbon route is also less efficient than the electric route but the storage of energy is trivial and the installations in the vehicle are proven and cheap technologies.

There are many other ways of producing energy for vehicles in a CO_2 -neutral way than those illustrated above but the intent is just to show that hydrocarbons are merely energy carriers just like electricity and hydrogen. The major benefits of hydrocarbons are how easy they can be stored and that the distribution systems are in place because they are the ones that are already used today.

Although DME needs to be under a moderate pressure in order to be in its liquid state it is still much easier to handle than liquid hydrogen and the existing infrastructure for liquefied petroleum gas (LPG) can be used for DME with minor modifications.

Figure 4 shows one possible CO_2 -neutral hydrocarbon route: Gasification and conversion of biomass to hydrocarbon fuel. There are a number of other possible hydrocarbon routes. The following section will describe why the authors consider DME to be especially interesting amongst the hydrocarbon energy carriers.

1.3 Well-to-wheel efficiency

If an alternative fuel is to have anything more than academic interest it is necessary to understand and evaluate a number of issues related to its use.

- > Compatibility with engineering materials
- Customer perception
- Economy
- Energy density
- > Harmful emissions during production and use
- Infrastructure
- Safety and health
- Sustainable availability

The list is alphabetically ordered. The political environment will to some extent determine the ranking of some of the issues so it is difficult once and for all to determine the merits of a new fuel. Some of the hard numbers that quantify the technical performance of DME will be defined and discussed in the following section.

DME is best viewed as an energy carrier and not an energy source since it cannot be mined or drilled. The earth's crust or atmosphere does not contain significant quantities of DME.

DME is a synthetic fuel that can be produced in different ways. Energy, carbon, hydrogen and oxygen must be available for this to be possible. This is the case for all synthetic fuels, but DME has a number of advantages over the other synthetic fuels. These will be described here by comparing them to some other alternative fuels.

At first a distinction is made between production of fuel (Well-to-Tank) and consumption of fuel (Tank-to-Wheel). This way of distinguishing between production and consumption is illustrated in Figure 5.

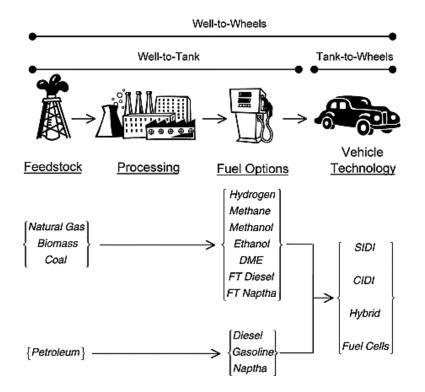


Figure 5 - Well-to-tank-to-wheel (Semelsberger, Borup & Greene 2006)

1.3.1 Well-to-tank efficiency

To evaluate the efficiency of the production the so-called well-to-tank efficiency can be used. It is defined as:

$$\eta_{\text{WTT}} = \frac{\text{energy}_{fuel}}{\sum \text{energy}_{i}}$$

i = energy in feedstock, feedstock recovery, fuel manufacturing, fuel distribution etc.

Figure 6 shows a comparison of well-to-tank efficiencies. DME ranks highest among the energy carriers.

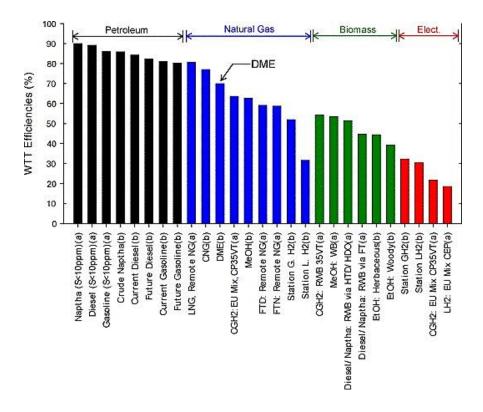


Figure 6 - Well-to-tank efficiencies for different fuels (Semelsberger, Borup & Greene 2006).

Of the fuels derived from natural gas (DME, methanol, naphta, hydrogen, diesel, etc.), biomass or electrolysis, the production of DME is the most energy efficient process (Semelsberger, Borup & Greene 2006).

The process that leads to the high WTT efficiency for DME shown in Figure 6 can be different types of partial combustion of the feedstock into synthesis gas (CO and H_2). Auto thermal reforming is used in the case of natural gas as feedstock. Gasification is used in the case of biomass as the feedstock. The synthesis gas contains the building blocks needed to produce DME (carbon, hydrogen and oxygen) in the following catalytic reactor.

In addition to being more efficient this thermal process used for DME is quicker and requires lower production plant investments than for example the fermentation process used for ethanol production (Consonni, Katofsky & Larson 2009).

1.3.2 Tank-to-wheel efficiency

On the consumption side a tank-to-wheel efficiency for a vehicle can be defined as:

$$\eta_{\text{TTW}} = \frac{\text{energy}_{at \text{ wheels}}}{\text{energy}_{fuel}}$$

This efficiency will be dependent on the vehicle technology used and it is listed as such in Figure 7.

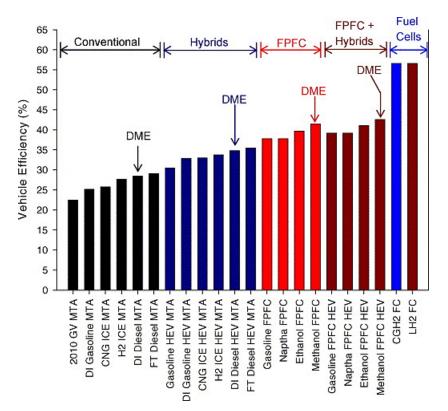


Figure 7 - Tank-to-wheel efficiencies for different fuels (Semelsberger, Borup & Greene 2006)

DME ranges among the best tank-to-wheel efficiencies almost independently of the vehicle technology used. Since both the well-to-tank and the tank-to-wheel efficiency is good the result is an efficient energy carrier. No matter where the energy comes from in the first place, a high well-to-wheel efficiency is a key factor in reducing well-to-wheel greenhouse gas emissions from transportation. The high well-to-wheel efficiency, the clean burning properties and the possibility of producing DME from remote energy sources like stranded natural gas are motivating the use of DME as a fuel.

1.4 Commercialization of DME

When it comes to the wide spread use of alternative fuels there is always a chicken-and-egg situation: as long as there are no vehicles to consume the new fuel the oil companies will not produce it, and as long as the fuel is not available at the pump the car manufactures will not dare to spend money on developing a car for it.

This is probably the major reason why ethanol so far has been the most successful among the alternative fuels. It is possible to cost effectively produce flexi-fuel vehicles that are able to run on both ordinary gasoline and ethanol. Such vehicles are produced in great numbers in Brazil due to the country's high volume production of ethanol from sugar cane.

This leads to the conclusion that if you want to design a new engine type then make sure it can run on traditional fuels. Vice versa, if you are developing a new fuel make sure that it can be used in existing engines.

This report deals with the development of a new engine for a new fuel. For the reasons stated above it is therefore not a report that is likely to be of commercial interest in the short term. But in the long term it will be increasingly difficult to satisfy political and consumer requirements with existing engines and fuels and it will be necessary to go beyond business-as-usual thinking to provide sustainable solutions. Eventually we will also simply run dry of fossil fuels. It is therefore of interest to society to explore what can be achieved with DME given its merits described in this chapter.

Despite the difficulties in introducing a new fuel a consortium of industrial partners in Sweden has made an effort to get started with DME. A significant step forward with respect to sustainable production of DME has been the consortiums opening of a biomass based DME production plant in Piteå, Sweden in 2010.

1.4.1 BioDME

The purpose of the BioDME plant in Piteå, Sweden is the production of DME from lignocellulosic biomass at an industrial scale, and its use as a vehicle fuel as well as for industrial processes.

The project started in 2008 as a demonstration of an environmentally optimized biofuel for road transport, covering the full chain from biofuel production from biomass to the use and testing in vehicles. A fleet of Volvo trucks is testing the DME in order to check engine compatibility, technical standards and commercial possibilities.

The partners involved in the project are:

- CHEMREC has experience in the field of black liquor gasification technology
- Delphi is a leading supplier of diesel injection equipment
- ETC a research and development center with focus on combustion, gasification and biorefining processes
- Haldor Topsøe supplier of catalysts and technology for the refining industry
- PREEM the largest oil company in Sweden
- Total one of the major oil and gas groups in the world
- Volvo one of the world's leading manufacturers of trucks, buses, construction equipment etc.



Figure 8 - BioDME pilot plant in Piteå, Sweden

In 2010 the pilot plant was inaugurated, it has a capacity of about 4 ton DME per day using forest residues as feedstock. During the project four filling stations were built in different locations in Sweden. Moreover, the DME produced will be evaluated for compatibility with materials (rubber, plastic, metals) and to determine the minimum quality to ensure engine durability (DME composition, properties, engine oil requirements etc.). Field tests will take place during 2010 – 2013 with a planned yearly average distance of 100,000 km per truck.

The DME is produced from black liquor through the production of clean synthesis gas and a final fuel synthesis step. Black liquor is an aqueous solution of lignin residues, hemicellulose and inorganic chemicals, obtained as a waste from the Kraft process when digesting pulpwood into paper pulp.

The combustion engine group at DTU was invited to the inauguration in Sweden in September 2010. The 4th International DME Conference was held in Stockholm just prior to the inauguration of the bio DME plant in Piteå. The Technical Review Committee of the conference chose the DTU contribution about DME engine technology as the key technical presentation at the conference (Hansen et al. 2010).

1.5 Motivation for the study of HCCI engine operation

1.5.1 Reduction of harmful emissions

Homogeneous charge compression ignition, or HCCI, is generally regarded as a promising technology for future power train concepts, since it allows an engine to operate with high thermal efficiency and very low emissions of particulate matter and nitric oxides. There are however some drawbacks that still keep the principle from being used in commercial engines. These include a limited load capability, excessive engine noise caused by knocking combustion and the problem of controlling combustion phasing and heat release rate. These areas are the main focus points of the current research.

Several variations of the original HCCI concept have been developed to overcome the problematic issues. Hence names such as PCCI (premixed charge compression ignition), PCI (premixed compression ignition), CAI (controlled auto ignition) etc. are commonly used to denote specific variations of premixed combustion. A thorough description of the various principles is given in (Zhao et al. 2002). The common feature of all these concepts is that they are all low temperature combustion processes which result in lower levels of nitric oxides and particulate matter than the SI and DI combustion principles.

Proprietary names are also emerging as the technologies are implemented in commercial vehicles. Volkswagen have the GCI (gasoline controlled ignition) and CCS (combined combustion system), which are implementations of gasoline and diesel HCCI variants. CCI have been demonstrated in their Touran model, but are not ready for production.

General Motors have developed a technology called Ecotec, which is currently tested in the US model Saturn Aura. The engine uses variable valve timing, direct injection and electric cam phasing to achieve proper timing of HCCI combustion with gasoline.

Mercedes have demonstrated an HCCI engine and calls their technology DiesOtto, which is a gasoline engine with the ability to switch to auto ignition combustion mode. The prototype engine, which was presented in 2008, is a very complex HCCI engine with features such as variable compression ratio, variable valve timing and variable geometry turbo charging.

It is obvious that engines with the abovementioned technologies will be quite expensive, so the question is if the benefit in terms of modest fuel savings can really justify the additional cost to the consumer. It may one of the reasons that despite the efforts to commercialize HCCI, development appears to be slow within the automotive industry. It may be that the interests in commercializing the concepts are not yet large enough to justify the efforts. When looking into the potential fuel savings, figures from 15 - 30 % in part load operation are common guesses. Such savings are fully possible with hybrid solutions as well, although these tend to be even more costly and increase the weight and complexity of the vehicle.

Design changes such as downscaling (both engine and vehicle) or improved aerodynamics are also logical means of achieving the same fuel saving with even lower cost to the consumer, assuming that the consumers can accept smaller cars. Reducing the size of the engine is however often connected with extra costs for pressure charging and other means of maintaining (or even increasing) the engine power, so the resulting cost saving from reduced fuel consumption is most likely offset by the higher cost of the vehicle. Downscaled engines is therefore of limited interest to the consumer.

Given that HCCI is not the only candidate technology for obtaining a better fuel economy, it must be competitive in cost to the other solutions, as well as offering other benefits. A good argument for using the HCCI principle is that it can potentially eliminate the need for expensive after-treatment solutions that are otherwise required to remove emissions of particulate matter and nitric oxides. The only problematic emissions from HCCI combustion are unburned hydrocarbons and carbon monoxide. These are however easily removed by an inexpensive oxidizing catalyst. Such catalysts have a high conversion factor even at low exhaust temperatures, meaning that HCCI engines can easily meet current emission requirements.

The direction of future developments based on the HCCI concept is still largely undetermined. The main reason is the degree of freedom allowed in terms of fuels, injection principles and controlling strategies, which require a large amount of research to cover. Each proposed concept has its own benefits and disadvantages, and so far no concept has made any significant breakthrough that makes large scale production of the engines possible. It is however likely that HCCI engines will be ready for commercial use within a few years, simply because increasing fuel costs make such investments both logical and necessary.

1.5.2 Lower fuel injection pressures

A specific benefit of HCCI operation in connection with DME is that fuel is introduced in the engine manifold and not in the engine cylinder. Manifold fuel injection requires only modest injection pressures and designing durable fuel injection equipment is then easier.

1.6 In short

This report describes work done at DTU in order to explore the possibilities with DME. The title is "Development of HCCI engines for DME". DME has been chosen for investigation since it can be produced sustainably and with the lowest CO2 emissions amongst the alternative fuels. HCCI combustion has been chosen since it produces the lowest levels of harmful emissions.

2. The basics of HCCI combustion

2.1 Combustion principle

The HCCI combustion process concept is based on auto ignition in a lean premixed fuel/air charge. The combustion event is therefore governed mainly by chemical kinetics, which clearly separates it from the diffusion combustion in DI CI engines as well as the flame propagation in SI engines.

The abbreviation HCCI has become a covering term for internal combustion technologies that utilize lean premixed combustion at low temperatures. The temperature region for low temperature combustion starts around 1500 K, which is the minimum temperature required for satisfactory conversion of CO to CO2 in the power stroke. The highest temperature allowed is usually determined by the amplitude of the engine knock. Knocking is a high pitched sound caused by large pressure gradients in the combustion chamber due to very rapid combustion. This limit is reached around 1800-2000 K with DME as fuel, corresponding to an excess air ratio of approx. 2.5. At this temperature level the formation of NO is also increasing notably, thereby reducing one of the important advantages of lean premixed combustion.

2.2 Combustion characteristics

In general, the highly premixed fuel/air charges will burn to completion within a few milliseconds near TDC. The ideal HCCI combustion process is therefore not much different from a constant volume explosion due to the very short duration of the combustion. The term explosion implies that the process is spatially uniform and hence the pressure rise rate is also uniform. Although an explosion is usually connected with destructive events, it does not have any damaging effect on the engine as long as the end pressure is within the design limits of the engine.

With an excess air ratio of 3 or less, the majority of the heat release lies within less than one millisecond in a well-mixed charge. This results in a fast pressure rise rate, typically above 10 bars per one tenth of a millisecond or higher. At this rate of combustion it is common that not all of the charge reacts simultaneously, which can be caused by temperature gradients and uneven fuel distribution in the chamber. As a result, large pressure gradients are created in the combustion chamber. This causes the air to oscillate with high amplitude in the chamber. The frequencies of the oscillations are identical to the resonance frequencies, which may be calculated or determined by computer simulations. The oscillations are similar to those observed in SI engine knock. HCCI knock may - like SI engine knock - be harmful to the engine if the load is high enough; otherwise it may run continuously at knocking conditions without any damaging effects to the piston or cylinder walls. Knocking does however shorten the life of cylinder pressure transducers, since the membranes of the transducer are typically loaded beyond their design specifications when they are impacted by pressure waves.

Part of the energy contained in the pressure waves in knocking combustion is transferred to the engine and causes the engine exterior surfaces to emit acoustic noise. As higher fuel concentrations lead to faster reactions and therefore higher differences in pressure, the acoustic noise is increased with the engine load.

Controlling the rate of combustion is thus a challenge. DME is a so called two-stage fuel. Combustion of DME starts with a series of low temperature chemical reactions that eventually lead to the high temperature reactions where the majority of the heat is released. It is possible to control the low temperature heat release by constraining the development of radicals in the initial phases of the combustion with additives or dual fuel combinations that consume radicals through chain terminating reactions. There is however currently no methods that allow control of the heat release rate in high temperature premixed combustion, which is fully governed by reaction kinetics.

2.3 Combustion phasing parameters

2.3.1 Compression ratio

The most important factor to combustion phasing is the compression ratio. Fuels vary greatly in their auto ignition characteristics. Their individual reaction chemistry gives large differences in ignition delays. Some fuels, such as gasoline and methanol which have high octane ratings, require a high compression ratio and hence temperature to obtain auto ignition. Other fuels, typically those with high cetane rankings such as diesel and DME in particular, have low auto ignition temperatures and low ignition delays. Such fuels require only modest compression ratios to ignite.

2.3.2 Equivalence ratio

The equivalence ratio is also important to combustion phasing. If the equivalence ratio is increased during operation of the engine, the rate of reaction is increased as well due to a higher fuel concentration and a higher temperature increment during combustion. This results in an instantaneous advancement of the combustion phasing. As the temperature of the cylinder liner and piston increase slowly hereafter, the charge reacts even earlier due to increased heat addition. Both the instantaneous and the slower advance of the phasing pose a challenge in terms of maintaining the combustion at an optimum point in the cycle.

2.3.3 Inlet temperature

The timing of the combustion is sensitive to inlet temperature, since the rate of formation of the radicals needed to initiate the combustion is a function of the temperature. The position of the initial part of the heat release may therefore be moved by controlling the inlet temperature. A common approach is to preheat the inlet air. By using a regulated mixture of hot and cold air, the temperature can be regulated on a cycle-to-cycle basis. This approach has been used in a number of studies [8, 9 and 10].

2.3.4 Exhaust gas recirculation

The use of exhaust gas recirculation (EGR) is a well-known method for reducing the nitric oxides in engines in part load operation. The exhaust gas returned to the inlet decreases the specific heat ratio, which means that combustion temperatures will be lowered as well. In diesel engines the usual limit is approx. 30 % EGR, as the oxygen concentration eventually decreases

to a level which reduces the combustion efficiency. This is because the diffusion flame is incapable of consuming all the available oxygen in the cylinder. In HCCI combustion however, it is possible to use much higher quantities of EGR since there are no diffusion flames. It is only required that the equivalence ratio is kept below unity.

The purpose of using EGR in HCCI engines is not to reduce the formation of nitric oxides, although it does have that effect as well on the already low level of nitric oxide formation. The primary purpose is to affect the combustion phasing. If hot EGR gases are used, either as an internal residual gas or an external un-cooled recycled gas, it advances combustion phasing. Cold EGR gas will usually retard the combustion phasing.

The trapped residual gas within the cylinder is sometimes referred to as internal EGR. It has a promoting effect on combustion phasing, due both to its temperature as well as a certain level of radicals. It was used in one of the first successful implementations of HCCI in a gasoline powered two-stroke motorcycle engine, which competed in the Paris-Dakar race. The principle was named Active Thermo-Atmosphere Combustion (ATAC) (Onishi et al. 1979).

2.4 Thermal efficiency

The HCCI concept is, for the time being, only considered practically applicable for part load operation, mainly due to the problems associated with combustion knock and engine noise. It is therefore not possible for an HCCI engine to obtain the same thermal efficiency as an SI or DI CI engine in full load operation. The indicated efficiency is however excellent with HCCI combustion, since it is close to being an ideal Otto process.

Compared with an SI engine in part load operation, HCCI combustion at the same compression ratio is much more efficient. The main reason is that the inlet throttling losses greatly reduces the SI engine efficiency at part load.

HCCI combustion may obtain the same efficiency as a diesel engine at part load, provided that the engine compression ratio is equal to a diesel engine. The diesel engine does not have throttling losses other than that produced by the EGR system. Combustion duration is longer for diesel engines, but the combustion efficiency is very high and the heat loss is low. The HCCI engine combustion efficiency is not as high as the diesel, which offsets the advantage of a faster combustion.

2.5 Emission characteristics

One major advantage of the HCCI concept is that the lean and premixed combustion reduces the formation of harmful pollutants, mainly particulate matter and nitric oxides.

Particulate matter is not formed since the combustion is fully premixed with a large excess of oxygen. Formation of particulate matter from the lubricating oil is still taking place, but the amount of PM related to combustion of lubrication oil is hardly measurable.

As for NO formation it is very low, typically in the order of 10-50 ppm. The combustion temperature is below the level where the rate of production for NO becomes significant. Elevated levels of hydrocarbons from crevice volumes and carbon monoxide are easily dealt with in a simple oxidation catalyst. After treatment systems for HCCI are therefore relatively inexpensive, compared to the cost of particulate filters and catalytic converters.

2.6 Combustion of DME

2.6.1 Combustion stoichiometry

The ideal combustion of DME in dry air is described by the reaction:

$$\lambda \cdot 3 \cdot (3.76N_2 + O_2) + CH_3OCH_3 \rightarrow 3H_2O + 2CO_2 + \lambda \cdot 11.28N_2 + 3 \cdot (\lambda - 1) \cdot O_2 + 1329 \text{ kJ/mol}$$

The stoichiometric fuel to air ratio (λ , FA ratio) is derived:

 $3 \text{ mole} \cdot (3.76 \cdot 28.01 \text{ g} / \text{ mole} + 32.00 \text{ g} / \text{ mole}) + 1 \text{ mole} \cdot 46.07 \text{ g} / \text{ mole} = 411.95 \text{ g} + 46.07 \text{ g}$

$$FA_{S,DME} = \frac{m_{fuel}}{m_{air}} = \frac{46.07 \ g}{411.95 \ g} = 0.1118$$

The equivalence ratio is given as the ratio of the actual FA ratio to the stoichiometric FA ratio:

$$\phi = \frac{FA}{FA_{\rm S}}$$

The typical equivalence ratio in engine experiments with DME is from 0.2 to 0.7.

2.6.2 Physical and chemical properties of DME

Table 1: Properties of DME	
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Chemical formula:	CH ₃ OCH ₃ .
Chemical weight:	46.07 g/mol.
Melting point:	-141 °C
Boling point at atm. pressure:	-24.4 °C
Vapor pressure at 20 °C:	5.1 bars
Critical pressure:	53.7 bars
Critical temperature:	126.9 °C
Heat of combustion, LHV:	28.84 MJ/kg
Heat of vaporization at -20 °C:	410.2 kJ/kg
Auto ignition temperature:	235 °C
Flash point:	-41 °C
Flammability limit in air	3.4-17 vol. %

The data are supplied by Haldor Topsøe A/S. DME has a cetane rating in the range of 55-60. The cetane ranking means that DME has a shorter ignition delay than diesel fuel, which has a cetane ranking of 40-46 (45-50 for premium diesel).

3. Combustion Phasing

In general, controlling the combustion phasing by mechanical means such as variable valve train or variable compression ratio is quite a demanding and expensive solution. From an experimental point of view, such modifications could not be undertaken with the resources available.

An alternative option for controlling the combustion phasing is either to manipulate the fuel ignition properties, or the inlet temperature. DME has a relatively low temperature of auto ignition and a short ignition delay, which effectively limits the compression ratio to about 10. Therefore, to retard the combustion and allow for a higher compression ratio, inlet cooling would be required. While inlet air heating is a common solution used for gasoline and other higher octane fuels when operating in HCCI combustion mode [8], cooling inlet air far below the ambient temperature is a demanding task with potential complications such as ice formation in the inlet. Therefore the best option left for combustion phasing control is to manipulate the fuel ignition characteristics.

To obtain a certain level of insight into the reactions dominating the combustion process, a reduced scheme for the reaction mechanism was developed. This allowed a better overview of the reaction paths, as well as the role of radicals. It also led to an understanding of the special low temperature reactions (LTR) that are observed during HCCI combustion of DME. The low temperature reactions appear for a short time during the compression of the charge, but the reactions terminate as temperature increases further. The reason for this self-terminating behavior is that OH radicals are consumed in a chain terminating reaction parallel to a chain branching reaction. The balance shifts towards the chain terminating reaction as the temperature increases, thereby terminating the reactions which depend on the OH radicals. The OH radical concentration may also be reduced by introducing a second fuel that consumes the radicals. Methanol is one of the fuels that have proven to be very efficient in controlling radical behavior.

Dual fuel operation with DME and methanol formed the basis of the experiments carried out at NTSEL in Tokyo in the summer of 2008. The outcome of these experiments is described in (Pedersen et al. 2010).

3.1 Elementary reaction model

All elementary reactions are modeled using the three parameter form of the Arrhenius expression:

$$k(T) = A \cdot T^{b} \cdot e^{\left(\frac{-E_{A}}{R_{u}T}\right)}$$

with units:

$$T: \mathsf{K}$$

$$E_{A}: \frac{\operatorname{Cal}}{\operatorname{mol}}$$

$$R_{U}: \frac{\operatorname{Cal}}{\operatorname{mol} \cdot \mathsf{K}}$$

The unit of A depends on the reaction type.

The parameters needed to calculate the forward reaction rate coefficient are the frequency factor A, the temperature exponent b and the activation energy E_A . These parameters are supplied for both forward and reverse reactions in the reaction mechanism used to model DME combustion.

3.2 The origins of the detailed reaction scheme

The reaction kinetics of DME is described in details by a reaction scheme named DME 2000 from Lawrence Livermore National Laboratory. The reaction scheme is based on studies on premixed DME/air flames at atmospheric pressure. Extensive documentation is available for this scheme (Curran et al. 1998). Units are in mol, Calories and Kelvin.

Low pressure and Troe fall-off corrections are given for some reactions. The details of these corrections are beyond the scope of this report, but the corrections are included in the simplified scheme for completeness.

3.3 Reducing the mechanism for lean combustion

The full scheme was developed to model both lean and rich flames. Rich flames involve much more complicated reaction paths than lean flames. Reactions leading to the formation of higher hydrocarbons are included, such as ethylene. Since ethylene is believed to be an important precursor to soot, the mechanism can potentially be used to predict soot formation in rich flames. The formation of higher hydrocarbons is however very low at lean and premixed conditions, since the possibility of local rich combustion zones is very limited. Hence there is no need to include these species in the description of lean combustion.

In addition, many reactions which may be relatively important at low temperatures and pressures have insignificant reaction rates when temperature and pressure are elevated.

In order to apply the reaction scheme in CFD models the scheme needs to be simplified without losing its accuracy. The target was that the reaction mechanism should be reduced considerably without affecting the ignition delay, low temperature reaction paths, heat release rate, sensitivity to radical concentrations and composition of products.

There are some commercial tools available that performs automated reduction of reaction schemes. A software called ASRT (Automatic Scheme Reduction Tool) was developed by (Yamauchi et al. 2007) and used specifically for DME. These reduction tools can eliminate elementary reactions from the main paths, which further simplifies the total scheme. The application of such tools was however beyond the scope and purpose of the study, in particular since a major benefit of reducing the scheme is that it creates a fundamental understanding of the reaction paths.

The process of reducing the scheme began by setting up and running a CHEMKIN simulation with the full reaction scheme. CHEMKIN is a program developed for simulation of chemical reactions. The software analyses the mechanism and other data that is supplied by the user and solves the stiff ordinary differential equation system that constitute the problem.

To simplify the detailed reaction scheme, a set of well-known operating parameters were chosen from the functional experimental setup. An excess air ratio of 4, a compression ratio of

10 and an engine speed of 1000 rpm were used. The results from this simulation run were used as the basis for reducing the scheme.

The operating parameters are sufficient to obtain a model that functions well within the operational limits of HCCI combustion. Changes to equivalence ratio are limited due to the narrow temperature interval within which HCCI can be realized. Variation of the engine speed should not affect the outcome either due to the short timescale of the reactions compared to the engine speed. Finally, changes to the compression ratio will only affect the temperature history and thus the timing of the combustion process.

The method used to reduce the scheme was to select only the dominating paths from the fuel molecule to complete combustion products. The dominating carbon containing species were picked out initially, and the paths leading to the formation and destruction of these species were identified.

Besides fuel species the scheme has a number of non-carbon radical reactions. These reactions are between the species: O, H, O₂, H₂, OH, H₂O, HO₂ and H₂O₂. The dominating reactions were selected based mainly on the species rate-of-production. Although concentrations of highly reactive species may be low, their rate of production is often very high. By choosing only those reactions with high rates of production, the scheme for non-carbon radicals may be simplified greatly.

The result from this process was a new scheme with 29 species and 55 reactions. Figure 9 was constructed to illustrate the reaction paths in the reduced scheme. A list of the species names is given at the end of this chapter.

Arrows in the scheme indicate the dominating reaction way. Percentage numbers indicate the approximate distribution on the paths.

The radicals that are placed in the small boxes e.g. [+ OH] denotes that this radical reacts with the radical in the larger box in which it resides. If no radical is in the box, the reaction is by decomposition. An M denotes a third body collision.

References to reaction numbers are to the numbers used in the original mechanism. The reason is that this makes it easier to identify the reactions in the original scheme.

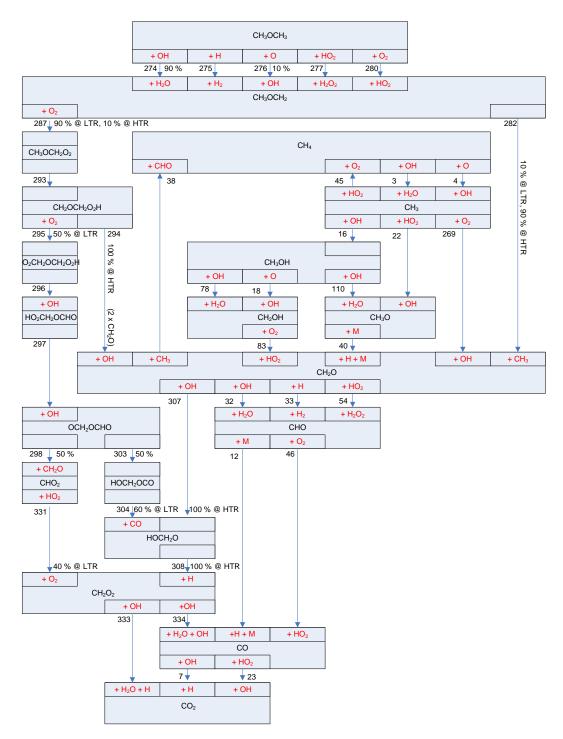


Figure 9 - Reduced reaction scheme for lean combustion of DME

3.4 Comparison of the full and reduced schemes

To evaluate the performance of the reduced scheme against the complete scheme, the two schemes were tested in a CHEMKIN simulation with identical parameters. The heat release and accumulated heat release are plotted in Figure 10 and Figure 11.

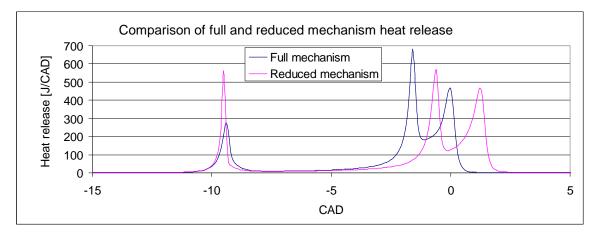


Figure 10 - Simulated heat release for the full and reduced mechanisms

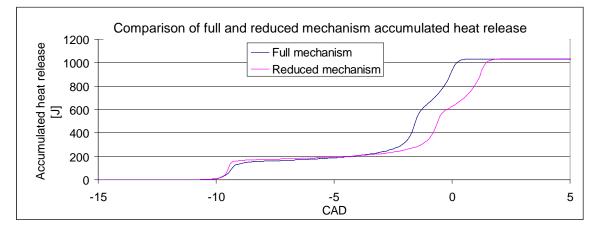


Figure 11 - The accumulated heat release of the full and reduced mechanisms

It is noted that the ignition timing is perfectly preserved with the reduced scheme. All initial reactions with DME were included in the reduced scheme to preserve the mechanism behavior in the first stages of combustion.

The reduced scheme however results in minor deviations in the heat release. The LTR heat release is of shorter duration and with a higher peak in the reduced scheme, but as can be seen from the accumulated heat release the total heat released in the LTR reactions is not very different.

The HTR reactions are slightly delayed and with slightly lower peaks in the reduced scheme. The shape of the two stage HTR combustion is however well preserved, and the final accumulated heat release is identical for the two schemes.

It is found that the reduced scheme is adequately accurate for use in simulations. There is however some potential for improving the scheme in order to match observations better. The most notable deviation between simulations and experiments is in the delay from LTR to HTR reactions, which is often significantly shorter in experiments.

3.5 Reaction paths

3.5.1 Initiation and low temperature reaction paths

Figure 12 shows the temperature and heat release plotted together. The low temperature reactions start at approx. 750 K and are terminated at around 900 K.

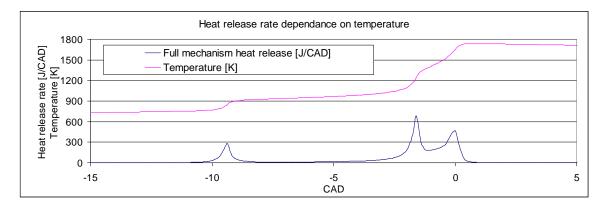


Figure 12 - The heat release dependence on temperature

The LTR is self-terminating due to chain-terminating processes becoming dominating as the temperature increases. This gives the characteristic blue flames, which in case of DME releases a substantial part of the total energy in the fuel.

In experiments, the LTR appears in a very consistent manner. There is very little cycle to cycle variation in both CAD position and magnitude. The development of the LTR heat release is always observed to occur with the same magnitude. This is because the heat release from the LTR is not dependent on initial fuel concentration. The concentration of fuel molecules is not rate limiting; it is the concentration of OH radicals that determines the heat release in the LTR combustion stage.

LTR are of high importance to the subsequent release of the remaining chemical energy. The temperature increase of course means that the reactivity of the gas is increased, but the LTR also creates a few stabile radicals such as hydrogen peroxide (H_2O_2), formaldehyde (CH_2O) and formic acid (HCO_2H), that are ready to proceed to the final oxidation steps to CO and CO₂. Hydrogen peroxide in particular is important, since it becomes unstable as temperature increases, and thereby becomes a source of hydroxyl (OH) radicals.

The initial breakdown of DME occurs by reaction with molecular oxygen. It has a very low conversion rate, but since there are no other active radicals being formed at this temperature it is the only reaction that can produce CH_3OCH_2 initially. Once OH radicals are being produced further down the chain, these radicals are responsible for the major part of the first oxidation step.

There are two major reaction paths from the methoxy-methyl (CH_3OCH_2) radical. The path to the left in the scheme (Figure 9) is the primary at low temperature reactions, while the path to the right is dominating at high temperature reactions (HTR).

The first step in the low temperature reaction (LTR) scheme DME combustion is the formation of the methoxy-methyl radical, CH_3OCH_2 , which is possible by several reactions. The dominating reaction is 274, but to ensure a good prediction of ignition delay it is necessary to include reaction with molecular oxygen as well. Reactions with three other radicals (H, O and HO₂) are also included in the mechanism since they are relevant at higher temperatures.

Initially, reaction 280 is the dominating reaction since there are no OH radicals. It produces CH_3OCH_2 at a very low rate, but the later steps produce OH radicals for reaction 274.

The methoxy-methyl radical predominantly combines with molecular oxygen in reaction 287 during the LTR reactions.

$$#287: CH_3OCH_2 + O_2 \rightarrow CH_3OCH_2O_2$$

Following reaction 287 is reaction 293 in which an H-radical shifts its position in the molecule. This happens almost instantaneously.

$$#293: CH_3OCH_2O_2 \rightarrow CH_2OCH_2O_2H$$

This molecule may now react in two different ways. The first is dissociation which produces one OH radical and two formaldehyde radicals, while the second is the absorption of molecular oxygen:

#294 :
$$CH_2OCH_2O_2H \rightarrow 2 CH_2O + OH$$

#295 : $CH_2OCH_2O_2H + O_2 \rightarrow O_2CH_2OCH_2O_2H$

Initially reaction 295 is dominating. It is followed by reactions 296 and 297:

#296 :
$$O_2CH_2OCH_2O_2H \rightarrow HO_2CH_2OCHO + OH$$

#297 : $HO_2CH_2OCHO \rightarrow OCH_2OCHO + OH$

This reaction path creates two OH radicals. Since one OH radical was consumed initially in reaction 274, the path creates one surplus OH and is therefore chain branching.

As the temperature increases, reaction 294 begins to take a larger share. It produces two formaldehyde molecules. These react with OH to form two HCO in reaction 32.

$$#32: CH_{2}O + OH \rightarrow HCO + H_{2}O$$

Thus one OH radical is consumed overall in this reaction path, which makes it chain terminating. The self-terminating behavior of the LTR reactions is therefore a direct result of the reaction path shifting from a chain branching to a chain terminating path.

The shift can be seen in Figure 13 which illustrates the rate of production of the relevant radicals during the LTR combustion phase. The dissociation reaction (44 in the figure) becomes dominating at around 1.93 milliseconds and continues to increase. The formation of the formyl radical which is chain terminating reaction is seen to increase as well, which causes the net production of OH radicals to become negative and eventually leads to OH concentration being reduced to very low levels.

Following reaction 297, the OCH₂OCHO radical produced may now react in two different ways at approximately equal rates to produce formic acid (HCO₂H). Reaction 298 is followed by reaction 331, in which also formaldehyde is produced:

#298 :
$$OCH_2OCHO \rightarrow HCO_2 + CH_2O$$

#331 : $HCO_2 + HO_2 \rightarrow HCO_2H + O_2$

Alternatively by reactions 303, 304 and 308 which also produce CO:

$$#303: OCH_2OCHO \rightarrow HOCH_2OCO$$
$$#304: HOCH_2OCO \rightarrow HOCH_2O + CO$$
$$#308: HOCH_2O \rightarrow HCO_2H + H$$

This branch in the LTR process ends with the formation of formic acid, which reacts slowly at low temperatures. It is therefore accumulated together with other stabile radicals such as hydrogen peroxide and formaldehyde.

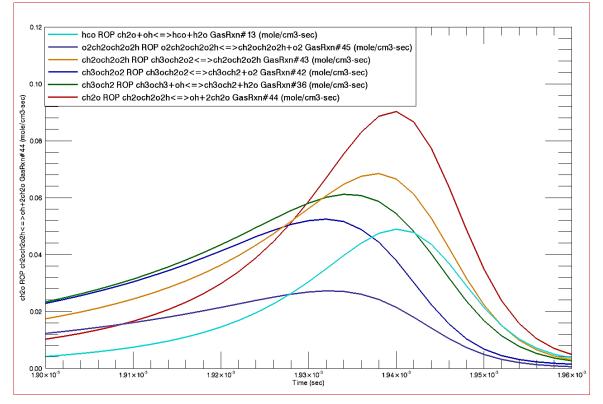


Figure 13 - Termination of the low temperature reactions

Formaldehyde is the intermediate radical with the highest concentration in the interval between the LTR and HTR processes. Formaldehyde appears to have a constant concentration, but it is produced and consumed continuously. Production is mainly through dissociation of the methoxy-methyl radical. Consumption is by reaction 32 that produces HCO, which dissociates by reaction 12, to form CO:

$$#12: HCO + M \rightarrow CO + H + M$$

The continuous production of CO consumes the majority of the available OH radicals and keeps the other possible reactions at low levels. With a limited amount of OH radicals available, the

reaction path consisting of reactions 274, 282, 32 and 12 dominate the interval between the LTR and HTR processes.

The non-carbon radicals interact in a simple way during the LTR process. First the hydrogen produced mainly by reaction 12 combines with O_2 to form HO_2 . The HO_2 then combines with itself, H or OH. Roughly half reacts to form H_2O_2 which accumulates. About half of the remaining HO_2 produces new OH radicals, and the rest is used in the chain terminating reaction.

$$#26: H + O_2 \rightarrow HO_2$$

$$#50: HO_2 + HO_2 \rightarrow H_2O_2 + O_2$$

$$#47: HO_2 + H \rightarrow 2OH$$

$$#49: HO_2 + OH \rightarrow H_2O + O_2$$

As the temperature increases, thermal dissociation of the methoxy-methyl radical (reaction 282) becomes important. The thermal dissociation produces equal quantities of methyl and formaldehyde. The methyl radical mainly reacts with HO_2 to produce CH_3O , which then loses an H in a third body collision and becomes formaldehyde:

$$\begin{array}{l} \#282:CH_3OCH_2\rightarrow CH_2O+CH_3\\ \\ \#22:CH_3+HO_2\rightarrow CH_3O+OH\\ \\ \#40:CH_3O\rightarrow CH_2O+H \end{array}$$

Some CH₃ also reacts with the formaldehyde to produce the methane:

$$#38: CH_3 + CH_2O \rightarrow CH_4 + HCO$$

Methane is accumulated during the LTR process, since the temperature is insufficient for this molecule to be oxidized.

3.5.2 High temperature reactions

The HTR reactions are dominated by thermal cracking of CH_3OCH_2 to CH_3 and CH_2O . The methyl radical may react with the CH_2O to produce CH_4 , which is again oxidized in through various reactions to CH_2O .

HTR reactions exhibit a two stage combustion process, where the heat of reaction of the first stage is mostly from the formation of CO and H_2O , while the second stage is the oxidation to CO_2 . This produces two peaks in the heat release. The pattern is visible in detailed CHEMKIN simulations, but not in heat release analysis of real combustion.

In the first step all remaining fuel is converted to formic acid, HCO and CO. HCO now reacts mainly with O_2 to produce CO:

#46 :
$$HCO + O_2 \rightarrow CO + HO_2$$

The formic acid (HCO_2H) that was produced during the LTR is converted mainly by reaction 333, but also some in 334:

#333 :
$$HCO_2H + OH \rightarrow CO_2 + H_2O + H$$

#334 : $HCO_2H + OH \rightarrow CO + H_2O + OH$

The non-carbon radical activity utilizes the H atom from reaction 333 to produce new HO_2 and OH radicals, as well as converting the H_2O_2 intermediate that was stored during the LTR reactions:

#26 :
$$H + O_2 \rightarrow HO_2$$

#50 : $2HO_2 \rightarrow H_2O_2 + O_2$
#51 : $H_2O_2 \rightarrow 2OH$

The second step is the final oxidation of CO to CO₂.

 $#40:CO+OH \rightarrow CO_2 + H$

The non-carbon radicals act differently in the second step, since now only OH is in demand. The H from reaction 40 is used by reaction 8 to form OH and O. The O is then used in reaction 10 to produce two more OH. Hence a total of three OH are produced for every H supplied. HO_2 , which was produced in reaction 46, combines with roughly a third of the OH in a terminating reaction.

$$\begin{split} \#8: H+O_2 &\rightarrow O+OH \\ \#10: O+H_2O &\rightarrow 2OH \\ \#49: HO_2+OH &\rightarrow H_2O+O_2 \end{split}$$

The overproduction of OH radicals ensures that the rate of CO conversion is mainly limited by the temperature. Any CO existing after the combustion will therefore be due to quenching or crevice volumes, or simply a low combustion temperature. Only a very small concentration of CO is produced due to dissociation of CO_2 , since the temperature is not high enough for dissociation to be significant.

3.6 Manipulating low temperature reactions

3.6.1 Effect of methanol on low temperature reactions

The main purpose of using methanol is to obtain a higher octane rating of the fuel, obtained mainly by increasing the ignition delay of the fuel. In other cases DME has been used as an ignition improver for methanol or other fuels in DI CI engines.

In an HCCI engine both fuels are premixed with the inlet air. The principal role of the methanol is to function as an inhibitor of the LTR heat release. When methanol constitutes about 30 % of the total fuel mass, the LTR heat release is almost eliminated.

The inhibition of the LTR reactions is due to the consumption of OH radicals by reactions 78 and 110, which are the major paths of oxidation for methanol:

#78 :
$$CH_3OH + OH \rightarrow CH_2OH + H_2O$$

#110 : $CH_3OH + OH \rightarrow CH_3O + H_2O$

Both of the radicals formed in the reactions above react to form formaldehyde:

$$#83: CH_2OH + O_2 \rightarrow CH_2O + HO_2$$
$$#40: CH_3O + M \rightarrow CH_2O + H + M$$

The OH consumption by reactions 78 and 110 means that less DME reacts through reaction 274, and thus the chain propagating reaction is reduced.

The advantage of reducing the LTR is that the HTR is delayed proportionally with the LTR reduction. The amount of methanol can thus be used to control the combustion phasing.

The effect of the dual fuel combination with methanol was demonstrated in cooperation with NTSEL in September 2008. The outcome of the experiments is described in (Pedersen et al. 2010). It was found that with about 30 % (mass) methanol added to the intake the combustion could be delayed to shortly after TDC, which improved the indicated efficiency and reduced the pressure rise rate. Furthermore, a change in the combustion towards less knocking could be observed from the engine noise.

3.6.2 Effect of EGR

The use of exhaust gas recirculation (EGR) in diesel engine combustion was introduced to limit the formation of NO by reducing the combustion temperature. By reusing the exhaust gas the specific heat capacity of the gas is increased due to the increase in CO_2 and H_2O concentrations. This reduces the temperature rise significantly. The specific heat ratio is however reduced, which reduces the amount of piston work.

There is a limit to how much EGR may be used in diesel combustion, as the oxygen concentration is decreased with increasing EGR. This reduces the rate of reaction in the diffusion flames and hence slows the combustion. A maximum of approx. 30 % vol. of EGR is normally regarded as the limit for diesel engines. Increasing the amount of EGR will result in excess production of particulate matter and inefficient combustion.

In HCCI combustion, EGR may be used to control the heat release. By decreasing the specific heat ratio, the temperature during compression will also be significantly reduced due to the lower specific heat ratio. This results in a delayed LTR reaction, but it does not reduce the amount of heat released or radicals produced. The second effect of the EGR is that the oxygen concentration is reduced. It was demonstrated that the reaction rate during the last part of the HTR phase could be slowed down, when the initial oxygen concentration was near the stoichiometric limit. The benefit of EGR is therefore that it allows late timing of the combustion and a reduction of the LTR combustion. This means that detonation and engine knock may be avoided. It is however on the cost of efficiency, as the IMEP is reduced significantly.

The effect of EGR was demonstrated at NTSEL in Tokyo in September 2008. The results are described in (Pedersen et al. 2010).

3.7 List of species

Radicals of hydrogen and oxygen

Н	hydrogen atom
0	oxygen atom
H ₂	molecular hydrogen
O ₂	molecular oxygen
ОН	hydroxyl radical
H ₂ O	water
HO ₂	hydroperoxy radical
H_2O_2	hydrogen peroxide

Radicals with one carbon atom

CO	carbon monoxide
CO ₂	carbon dioxide
СНО	formyl radical
CHO ₂	hydrocarboxyl radical
CH ₂ O ₂	formic acid
CH ₂ O	formaldehyde
CH ₂ OH	hydroxymethyl radical
CH₃OH	methanol
CH ₃	methyl radical
CH ₃ O	methoxy radical
CH ₄	methane

Radicals with two carbon atoms

CH ₃ OCH ₃	dimethyl ether
CH ₃ OCH ₂	methoxy-methyl
CH ₃ OCH ₂ O ₂	methoxy-methyl peroxide
CH ₂ OCH ₂ O ₂ H	[unnamed]
$O_2CH_2OCH_2O_2H$	[unnamed]
HO ₂ CH ₂ OCHO	[unnamed]
OCH ₂ OCHO	[unnamed]
HOCH ₂ OCO	[unnamed]
HOCH ₂ O	[unnamed]

3.8 Internal or external EGR

The ideas behind the use of EGR were briefly discussed in the previous section. When the term EGR is used it normally means external exhaust gas recirculation. On a typical four-stroke diesel engine this comprises a pipe connection from the exhaust to the intake with an EGR valve and a cooler. See Figure 14.

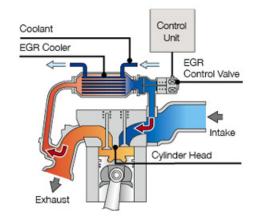


Figure 14 - External EGR system (Hitachi Construction Machinery Co., Ltd 2011)

The EGR valve controls the amount of EGR and the cooler reduces the temperature of the recirculated exhaust gas before it enters the engines air intake. Cooling the EGR results in the lowest flame temperatures and thereby the lowest NO_x emission. The system used to implement external EGR adds significant cost and complexity to an engine system. It would be simpler, cheaper and less error prone if it was possible to avoid this system and achieve EGR by simply retaining the desired amount of exhaust gas in the engine cylinder after the air exchange process has completed. This is called internal EGR. The term "internal EGR" is a little misleading since there is no recirculation to the intake of the engine, but it is used commonly used in the literature. In a four-stroke engine this can be achieved by applying negative valve overlap (Fitzgerald et al. 2010). Alternatively a two-stroke engine can be used since it does not have positive displacement of the exhaust gases. The drawback to internal EGR is that it is not possible to use a cooler. Figure 15 shows a CFD simulation of the cylinder volume of a two-stroke engine with the piston at BDC. The mostly red box on the left of the figure is the start of the exhaust system. The internal EGR is the green, yellow and red nuances in the cylinder volume above the piston. The scavenge port is at the bottom right part of the figure.

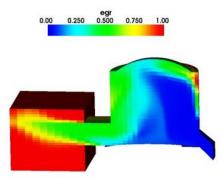


Figure 15 - CFD simulation of internal EGR (Lucchini, Montenegro 2007)

Chapter 4.4 describes the results with an experimental DME two-stroke engine utilizing internal un-cooled EGR.

4. Experimental Studies

A number of experimental studies were carried out to verify the theoretical findings. It was considered unnecessary to include these published papers in this report but the introduction and conclusion of the papers are included below to create an overview of the results.

4.1 HCCI Four-stroke Engine (Pedersen , Schramm 2007)

4.1.1 Introduction

The HCCI combustion process is known to produce little or no particulate matter and low levels of NO_x , while having the potential of a high indicated efficiency at part load operation. In the recent years, the use of DME in the HCCI combustion process has caught the attention of automotive engineers. DME is an interesting fuel for the HCCI process, as it has auto ignition properties superior to normal diesel fuel, thereby ensuring ignition at moderate compression ratios without the need for preheating. Exhaust emissions of unburned DME and lower hydrocarbons as well as CO may be treated in a simple catalytic conversion.

Studies on the application of DME in the HCCI combustion process may be divided into three categories with respect to the supplementary fuel or additive usage. These are studies on combustion of pure DME, studies on additive effects and studies of dual fuel combustion.

Combustion of pure DME has previously been studied by (Zheng, Shi & Yao 2004) at a compression ratio of 17 and engine speeds from 1400 -2000 rpm. Highest imep achieved with pure DME was 3.1 bars. Another study by (Hu et al. 2005) used a lower compression ratio of 10.7 and engine speeds of 1800 and 2000. A bmep of 3.2 bars was achieved in this study. In both of these cases it was concluded that DME is only suitable for part load operation, as higher engine loads causes unacceptable pressure rise rates and knock. (Hu et al. 2006) made a later study were three different compression ratios (8, 10.7 and 14) were used with variation of speed and fuel input. A bmep of 3.5 bars at a compression ratio of 8 was demonstrated in this study.

Hamada (Hamada et al. 2005) have investigated the ignition timing through a study of the formation of OH and HCHO radicals in the low temperature reactions, using a spectroscopic method. A large interval of compression ratios at constant speed (1400 rpm) was used. Useful data on the duration and onset of low temperature reactions were presented here.

The most common finding is that HCCI combustion of DME results in a very limited operability, and that timing of heat release is difficult. The use of EGR is now commonly regarded as a promising strategy to control HCCI combustion of pure DME (Ikemoto, Kojima & Iida 2005) (Ohmura, Ikemoto & Iida 2006), whereas other strategies are concerned with the use of DME in combination with other fuels.

Studies of additive effects include those of (Yamada, Yoshii & Tezaki 2005) who studied the reaction suppression effect of methanol and the reaction enhancing effect of ozone. Ogawa et al (Ogawa et al. 2003) investigated the effect of direct injection of water and methanol in a premixed DME HCCI engine. Studies of dual fuel operation include those of Zheng et al, who have made an extensive theoretical and experimental research on dual fuel combustion of DME

with natural gas, methane and methanol (Zheng, Shi & Yao 2004, Zheng et al. 2004). Sato et al (Sato et al. 2005) also studied the use of DME and hydrogen in combination with methane. Other studies of dual fuel operation include those of Shudo et al (Shudo, Ono & Takahashi 2003), who used a DME-reformed gas as supplement to combustion of pure DME. It was found that control of ignition timing was enabled by varying the amount of reformed DME to pure DME.

4.1.2 Results

• It was possible to achieve values 4.5 to 5 bars of imep both lambda 2.5 and 3, and around 3.5 bars of imep for lambda 4. Normal diesel operation without turbo has an upper limit of 8 bars.

• Indicated efficiencies of up to 40 and 45 percent could be achieved with lambda 3 and 4 respectively, whereas lambda 2.5 resulted in indicated efficiencies up to 35 percent

• The best engine performance with acceptable amplitude of knock was achieved with the leanest charge at 3000 rpm. The combustion delay and low pressure rise rates resulted in a high efficiency, low noise and high imep.

• It was found that the different equivalence ratios used required that the compression ratio was within narrow limits to avoid knock and achieve optimum performance. A compression ratio of approx. 9.2 was found suitable for both lambda 2.5 and lambda 3, while a compression ratio of approx. 11 was required to operate with lambda 4.

• Increasing engine speed generally increases the engine knock. The amplitude of knock was generally unacceptable at 3000 rpm with lambda 2.5

• Emissions of CO and THC are generally low, except for lambda 4 which produced relatively large emission levels of CO compared to the richer mixtures.

4.2 HCCI Four-Stroke Engine Acoustic Study (Pedersen , Schramm 2010)

4.2.1 Introduction

Homogeneous charge compression ignition (HCCI) combustion has a number of advantages such as very low emissions of NO_x and particulate matter, high indicated efficiency and the ability to use a wide range of fuels.

HCCI combustion may be used as a part load option in normal SI and DI engines where low emissions are important. The combustion process is limited to part load primarily due to the reaction rate becoming excessively high when load is increased. As the reaction rate and hence the pressure rise rate increases, the noise level from the engine also increases.

The noise from the engine is caused by large amplitude resonance patterns in the chamber, when reflections of powerful pressure waves transfer energy to the cylinder liner. The energy is transmitted through the engine structure and a small fraction is dissipated as noise, while the rest is dissipated as heat in the structure.

Coupling of pressure waves and reaction kinetics is a common cause for amplification of pressure waves in the combustion chamber. One approach to reducing the noise is therefore to design pistons that prevent this phenomenon.

In this study, DME was used as a fuel. It is used due to its excellent auto ignition properties which makes the fuel usable in engines with compression ratios around 10. DME is a gas with a vapor pressure of approx. 6 bars at 25 °C. It evaporates instantly when injected as a liquid in the inlet manifold, thereby creating a premixed charge. The charge is furthermore homogenized during the intake process and thus the homogeneous charge condition is reached. Since the charge burns homogeneously it does not produce soot. As the charge is furthermore lean, formation of nitric oxides is very low. HCCI combustion of DME is therefore a clean alternative to DI CI combustion as well as an inexpensive option due to a low pressure fuel system. The main challenge is to avoid knocking combustion, which is the subject of this study.

4.2.2 Results

HCCI combustion generated noise is primarily reduced by limiting exposure of the cylinder liner to the combustion. A diesel type piston is most effective in achieving this reduction.

A flat piston type, as commonly used in SI combustion, results in large amplitude pressure waves in the combustion chamber. The exterior noise level is therefore high with this kind of chamber.

A diesel type piston provided the largest reduction in the combustion noise of all tested piston crown geometries. It is believed that the smaller diameter of the bowl in which the combustion takes place is the reason that the combustion does not generate strong pressure waves. The exposure of the cylinder liner is also minimized with this kind of piston, which helps to reduce the noise further.

Two pistons with the compression volume split into 4 and 8 volumes respectively placed in their perimeter were tested. The latter was found capable of reducing the noise, but not the indicated efficiency which suffered from increased heat losses to piston and cylinder liner. The first piston crown increased combustion noise due to Helmholtz resonance between the volumes.

Two pistons with combustion chambers placed as cavities in the top of the piston were tested. One of them had 8 cylindrical cavities and was found capable of similar noise reduction capability as the diesel type piston. The large surface area, crevice volume and possibly the squish region as well, however resulted in a lower indicated efficiency. The second piston had hemispherical chambers in order to reduce the heat transfer and the squish region, but as a result of a more open geometry, combustion noise increased to a level comparable to the flat piston.

The diesel type piston is possibly the best option for obtaining a silent combustion. It may however not be the best option with respect to indicated efficiency, in which case the flat piston design is the best solution.



Figure 16: Flat piston crown



Figure 18: Piston crown with ring shaped chamber



Figure 17: Diesel bowl piston crown



Figure 19: Piston crown with four side chambers



Figure 20: Piston crown with eight side chambers



Figure 21: Piston crown with eight cylindrical chambers

4.3 HCCI Four-stroke Engine – Tokyo, Japan (Pedersen et al. 2010)

4.3.1 Introduction

HCCI combustion is considered to be an efficient alternative to part load SI and CI operation. The main advantage of HCCI combustion is a high efficiency compared to SI part load, and much lower emissions of NO_x and PM than DI.

The efficiency of part load HCCI combustion is usually higher than SI part load since there are no throttling losses. The part load efficiency of HCCI can be comparable to DI CI engines, which has the advantage of a higher compression ratio but also the disadvantage of a slow combustion.

Very low emission levels of NO_x and negligible amounts of particulate matter are inherent effects of the lean and premixed combustion. NO_x formation is kept low due to a uniform low combustion temperature and PM formation is avoided due to absence of fuel rich zones.

CO and HC levels are high and comparable to untreated emissions from SI operation. CO is believed to originate from flame quenching near the combustion chamber walls, and from running the combustion very close to the lean limit. HC is composed of both unburned fuel from the crevice volumes and partially burnt fuel from wall quenching. HC avoids post oxidation due to the lower temperatures in the cylinder and exhaust system. HC and CO emissions are however efficiently reduced in a DOC with surplus amounts of oxygen.

The lowest equivalence ratio that may be applied in HCCI combustion is determined by the minimum temperature, which must be reached to ensure rapid oxidization of CO to CO_2 . This temperature is approximately 1500 K, which means that for the typical range of compression ratios in internal combustion engines the equivalence ratio cannot be less than 0.15 to 0.2. This corresponds approximately to idle condition.

The highest applicable equivalence ratio is usually limited by engine knock which may not surpass a specified tolerance limit. An equivalence ratio of 0.3 to 0.4 is commonly the limit with DME as fuel, depending on the magnitude of knock and pressure rise rates that are tolerated.

An important feature of HCCI combustion is that it relies on auto-ignition. This means that combustion timing depends on both fuel and engine properties, and a proper timing requires that fuel and engine are matched properly. In reality, changing operating conditions and demands for a large operating range means that either engine or combustion chemistry must be manipulated to maintain an optimal operation at all times (Yao et al. 2008). For engines, this usually means changing the effective compression ratio through variable valve timing or similar, whereas combustion chemistry may be changed by mixing fuels with different properties.

DME is an interesting fuel due to its auto ignition characteristics. It has a low temperature of auto ignition and a short ignition delay. The cetane ranking of DME is 55-60, which makes the fuel an excellent alternative to standard diesel fuel which has a cetane ranking of 45-50. The disadvantage of DME is that it has a very low lubricity. This requires that the fuel system components are designed to handle a fuel with no lubrication. In the current study a test engine with a common rail system specifically made for DME is used (Yanai et al. 2008), and the lubricity of DME is increased with a lubrication additive from Lubrizol.

DME is also suitable for HCCI operation in engines with a compression ratio at around 10. If a higher compression ratio is used, some means of delaying the combustion onset must be used to ensure optimal position of the heat release.

In this paper, methanol addition has been used to control the combustion timing in HCCI combustion of DME. The use of methanol in combination with DME has previously been demonstrated by other authors (Ogawa et al. 2003, Zheng et al. 2004, Yao et al. 2006). The common observation is that up to 30 % of methanol by mass is possible before combustion becomes retarded to the point where it fails to complete. The exact amount does however depend on the compression ratio of the engine.

Exhaust gas recirculation can also be used to delay the combustion timing. Some authors (Kanoto , Ohmura & Iida 2007, Yao et al. 2005) investigated the subject. The use of EGR is however a challenge, since it requires a high ratio of EGR to inlet air to achieve the desired effect, as demonstrated in this paper. EGR works mainly by increasing the concentration of CO_2 and H_2O , which increases the specific heat capacity and decreases the specific heat ratio. This reduces the temperature increase during compression and combustion. Secondly, it reduces the amount of oxygen which is normally not desired in diesel engines, meaning they are usually not capable of operating with more than 30 % EGR. In HCCI combustion however, it is possible to operate with much lower oxygen concentrations. It is only required that the concentration of oxygen is sufficient to complete the combustion.

The compression ratio used here (14.5) is much higher than comparable studies with pure DME (Pedersen, Schramm 2007, Kajitani, Hoshimiya & Hayashi 2007). The high compression ratio was selected since it is suitable both for normal DI CI operation and for HCCI operation. This is considered a requirement, since HCCI operation cannot operate at higher loads.

4.3.2 Results

It has been demonstrated that a diesel engine with a compression ratio of 14.5 and a DI common rail system is suitable for dual fuel HCCI combustion. DME was injected directly through the common rail injectors and the methanol was port injected. The effect of high quantities of EGR was also demonstrated.

Combustion timing control was first demonstrated with methanol. The best result was achieved when the equivalence ratio of methanol reached 0.120 at 1000 rpm and 0.076 at 1800 rpm. These quantities ensured complete combustion about 5 CAD ATDC at the respective engine speeds. Increasing the quantity further caused partial combustion and misfire at both engine speeds.

A bmep of 440 kPa was achieved at 1000 rpm and 380 kPa was reached at 1800 rpm with the optimum quantity of methanol. The corresponding brake efficiencies were 0.35 and 0.31 respectively, which is close to the performance of the original engine.

Methanol proved to reduce engine knock to a very low level despite the increased equivalence ratio. It may therefore be used to increase the engine power by enabling higher equivalence ratios.

A disadvantage of the port injection was that a large quantity of the injected methanol was diluted into the lubrication oil. This problem could possibly be avoided by mixing the methanol with the DME at a fixed ratio and injecting the mixture as a whole through the common rail injectors.

EGR was also used to retard combustion timing for a fixed quantity of DME. For EGR percentages up to 65, the delay in CAD was proportional to the EGR percentage. At an EGR percentage of 70 % the rate of reaction was reduced and the heat release appeared around 2-3 CAD BTDC.

Bmep increased with increasing amounts of EGR due to decreased heat losses and less compression work because of the higher heat capacity of the gas when it includes water vapor and CO_2 from the previous cycle. The highest bmep obtained was around 260 kPa at both 1000 and 1800 rpm.

Engine knock was virtually eliminated when the EGR level increased the equivalence ratio close to 1, as the rate of reaction was lowered.

Combustion control of DME HCCI through simultaneous use of methanol and EGR may possibly enable the use of even higher compression ratios than 14.5. This could allow for standard diesel engines to utilize the HCCI combustion process in part load situations.

In general, NO_x emissions were in the 0-30 ppm range. At the operating points with the best thermal efficiencies, the calculated specific emissions of NO_x were close to or less 0.1 g/kWh.

4.4 Late Injection HCCI Two-stroke Engine (Hansen et al. 2011)

A completely different experimental route was explored as well, namely the application of DME in an HCCI two-stroke engine. This has been done in conjunction with DTU's ecocar project. If efficient combustion could be established in a two-stroke engine it would not be such a big problem that the power output would be limited by combustion knock and noise. The low internal friction of the two-stroke engine would make good engine efficiencies possible anyway.

The development of the engine has been a two-step process. The latest version of the engine is described in the following.

4.4.1 Introduction

Most studies of the application of DME in internal combustion engines have focused on DME as a substitute for diesel in conventional diesel engines, typically with cylinder displacements larger than 500cc. In these studies DME is injected at relatively high pressures, typically 200 to 1500 bars. The results have been near-zero soot emissions, equal or slightly lower NO_x emissions than with diesel fuel and high wear rates in the fuel injection system (Arcoumanis et al. 2008, Sato et al. 2008).

This study was performed as a part of ongoing research work at the Technical University of Denmark where an attempt is made to rethink the compression ignition engine so as to fully exploit the chemical and physical properties of DME and to find applications where these properties give special advantages. Motivating the use of DME in the first place is the very high field-to-wheel efficiency that can be attained using DME, produced by gasification of biomass, in a vehicle with a diesel engine (Semelsberger, Borup & Greene 2006, Directive 98/70/EC of the European parliament and of the council 2009).

An earlier publication on the subject (Hansen et al. 2008) describes the engine concept chosen and the first engine test results obtained with an engine built accordingly. The engine was a 50cc piston ported crankcase scavenged two-stroke design. It employed direct injection of DME through a GDI type electronic injector at 100 bars. Fuel line pressure was maintained by pressurization of the fuel tank with helium. Deciding on a two-stroke engine in the first place was based on the line of thought illustrated in Figure 22.

Decision Matrix	Four-Stroke	Two-Stroke
Diesel	NO _x Particulates	Lower NO _x Particulates
DME	Lower NO _x No Particulates	Very low NO _x ? No Particulates

Figure 22 - Engine concept decision matrix

The reason why lower NO_x emissions were expected from a two-stroke engine concept was that the larger amount of residual gas dilutes the trapped cylinder charge. This can reduce the flame temperature and hence the potential for NO_x formation (Gentili 1999, Millo 2007). Since high pressure injection nozzles are not available for 50cc engines the injectors used are from automotive engines. This means that the fuel is injected within a few crank angle degrees. This is the case for both the first concept engine and the second engine which is described in this paper. For both engines the short injection period is followed by an ignition delay with a typical duration of 0.5 ms which is equivalent to 10 CAD at 4000 rpm. If the premixing that occurs before ignition is effective, this method of operation would lead to low NO_x emissions as long as the global air/fuel-ratio is high, due to the low resulting combustion temperatures.

The first engine design proved that it is easy to achieve smooth operation with a DI two-stroke engine operating on DME. The engine was tested at engine speeds ranging from 500 to 6000 rpm. The lower limit given by excessive heat losses that prevented compression ignition and the upper limit given by a limitation in the dynamometer used.

But engine torque was somewhat disappointing reaching a maximum bmep of only 309 kPa at 2000 rpm. Despite the low bmep, engine brake efficiency peaked at 22%, a value that is comparable to fuel injected gasoline two-stroke engines of the same size. That this was possible despite the low engine torque and accompanying modest mechanical efficiency is attributed to the higher compression ratios employed and the resulting higher indicated efficiencies as compared to SI operation. Geometric and trapped compression ratios were 19 and 14 respectively. No particulate measurements were performed but no visible smoke was observed regardless of engine load. NO_x emissions were below 200 ppm at all speeds and loads.

The reason for the disappointing power output was found to be a combination of three factors. Poor scavenging, poor mixture formation and high closed cycle heat losses.

Scavenging

Intake

The fixed geometry of the piston ported air intake arrangement in the original engine design only gave acceptable air flow in a narrow engine speed range and the maximum delivery ratio was measured to be 0.92. In the present study it was decided to change to a reed valve intake arrangement in order to widen the effective speed range of the engine and also increase the maximum delivery ratio. A reed valve is a fast acting one-way valve that responds to the vacuum in the crankcase by opening and allowing air to flow into the crankcase whenever the pressure there is lower than the atmospheric pressure.

Transfer Passages

The cylinder of the earlier engine had two scavenge ports with an area of 216 mm². Increasing the area and thereby lowering the maximum flow speed of the air jets entering the cylinder through the transfer passages can reduce short circuiting to the exhaust port and hence increase the trapping efficiency. It was therefore decided to change to a cylinder with a larger transfer port area.

Exhaust System

Tuned expansion chamber exhaust systems are used with great effect on SI two-stroke engines to improve scavenging. The first engine had a straight cylindrical exhaust pipe instead of a tuned exhaust system. It was decided to devote some effort in this study to experiment with an exhaust system inspired by SI two-stroke engine designs.

Mixture formation and closed cycle heat loss

These two phenomena represent a trade-off relationship. Closed cycle heat loss can be reduced by reducing forced flow due to the piston movement relative to the cylinder head, the so called squish flows. Unfortunately, this will adversely affect the rate at which fuel and air are mixed and thereby the heat release rate. The optimal design will be the compromise that best suits the requirements of the engine application. One way to circumvent this trade-off relationship is to improve mixing by better matching the injector nozzle spray pattern to the combustion chamber geometry and air flow. Some progress in that respect has been achieved on the second engine by using a 7-hole injector instead of the single hole conical spray injector that was used on the first engine.

Engine Design Changes

The second engine was built based on crankshaft, connecting rod, piston and an air-cooled cylinder from a 50cc Peugeot two-stroke SI scooter engine. The remaining parts were custom built based on the experience from the first engine. The primary mechanical changes introduced in order to improve the performance relative to the first engine are listed in Table 2.

Feature	Unit	1st	2nd
Bore	[mm]	38	40
Stroke	[mm]	43	39.1
Displ.	[ccm]	48.8	49.1
CR geo.	[-]	19	22
CR eff.	[-]	14	16
Squish ratio	[-]	0.60	0.60
Inlet port opening	CAD BTDC	50	Reed valve
Exhaust port opening	CAD ATDC	111	109
Transfer port opening	CAD ATDC	129	132
Transfer port area	[mm ²]	216	372
Fuel injector	[-]	Mitsubishi	Bosch
Fuel injector holes	[no.]	1	7
Exhaust	[-]	Cyl. pipe	Expansion chamber

Table 2 – Main parameters for the 1 st and 2 nd eng	ine designs
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The compression ratio of the new engine was increased to improve cold starting. The new engine maintains the use of a solenoid activated plunger pump to supply lubricating oil to the air

intake in the crankcase. It is beyond the scope of this paper to give all the details of the development work that went into the second version of this engine concept. The paper primarily lists the differences between the old and the new design and relevant results of the testing of the new engine design are presented and discussed.

4.4.2 Results

The concept of a small two-stroke engine operating on dimethyl ether has been explored. The present study was conducted because a first prototype engine, described in an earlier publication on the subject (Hansen et al. 2008) had disappointing performance. A second version, also a 50cc crankcase scavenged two-stroke engine with direct injection of DME, was therefore developed and tested. The air flow of the engine was significantly improved by the application of a reed valve intake arrangement and a tuned expansion chamber exhaust system. Compared to the first version of the engine the improvement of the air flow combined with a new fuel injector resulted in a significant increase in maximum engine torque. Increasing the fuel injection pressure from 100 to 150 bars and applying an asymmetric cylinder head further improved engine performance. At the current state of development the maximum engine torque has increased by 46% relative to the first version of the engine. The new engine can operate up to a brake mean effective pressure of 500 kPa but efficiency and emissions deteriorate greatly above 450 kPa.

Approx. 65% of the charge is burnt in a rapid premixed phase and the remaining 35% of the fuel is burned in a slow mixing controlled phase. In the case of the previous engine version, the ratio between premixed and mixing controlled burn was 50/50. The increase in premixed nearly constant volume combustion was found to be the most significant contribution to the increase in indicated efficiency from 29% to 37%. Despite the use of direct injection late on the compression stroke, injection timing is critical and too early injection results in knocking combustion and too late injection results in misfires. At typical operating conditions the injection timing has to be within ± 2 crank angle degrees in order to avoid those phenomena.

The engine was tested from 2000 to 5000 rpm with peak efficiency occurring at 4000 rpm and medium load. Higher engine speeds were not tested but engine power and efficiency are strongly related to engine air flow and tuning intake and exhaust system to a higher engine speed would most likely provide for increased power outputs at good engine efficiency because the premixed combustion is very fast.

Brake efficiency peaks at just above 30%. At loads above 200 kPa bmep and speeds higher than 2500 rpm the efficiency is higher than 28% providing a wide operating range at high engine efficiency. Practical experience with the engine mounted in a vehicle built for a fuel economy competition showed that the engine efficiency is superior to that of four-stroke spark ignition engines of similar size. By now the performance level of the engine corresponds to the initial expectations for the engine concept.

While engine-out NO_x emissions are low, compared to traditional diesel engines, they are still of the same order of magnitude as current emission limits for stationary engines in the EU. As is the case for HCCI engines carbon monoxide and unburned hydrocarbons emissions were significantly higher than for traditional diesel engines. An oxidation catalyst could be considered. Such a catalyst would be effective in removing most of the carbon monoxide but due to the quite low exhaust gas temperatures effective hydrocarbon oxidation could be difficult to achieve. Future combustion development should focus on the reduction of engine-out emission of

hydrocarbons and/or oxidation catalyst performance with respect to hydrocarbons. If the HC emissions could be removed the combined HC and NO_x emissions would be below emission limits.

4.5 Additional information on the late injection HCCI two-stroke engine

Chapter 4.5 gives more detailed information about the performance, emissions and combustion characteristics of the two-stroke engine.

4.5.1 Performance and emission maps for the two-stroke engine

Indicated efficiency, brake efficiency and brake specific emissions are given in the form of engine maps for engine speeds ranging from 2000 to 5000 rpm and engine load ranging from idle to full load. The maps shown in Figure 23 to Figure 28 were made using the asymmetric cylinder head that gave best overall engine efficiency.

Performance maps

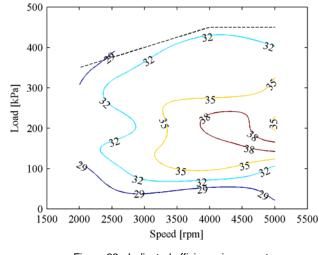


Figure 23 - Indicated efficiency in percent

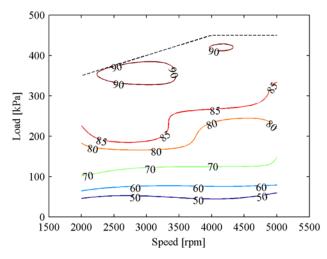


Figure 24 - Mechanical efficiency in percent

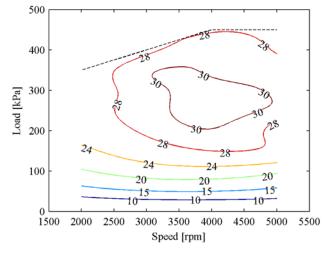


Figure 25 - Engine brake efficiency in percent

Figure 25 shows that the engine brake efficiency is primarily load dependent. Except for the lowest engines speeds if the engine is operated at or above a bmep of 200 kPa the efficiency is higher than 28%. Also seen in the engine maps is the maximum bmep, which peaked at 450 kPa between 4000 and 5000 rpm. This is 46% higher than the maximum bmep achieved with the first engine design. The engine would operate up to 500 kPa, but the limit shown is based on a maximum CO emission of 1% in the exhaust gas. Above this value efficiency and emissions deteriorate fast.

Emission maps

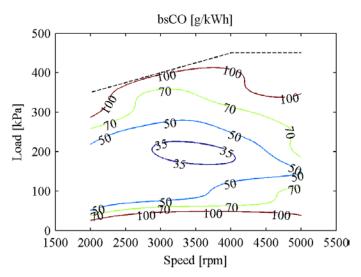


Figure 26 - Carbon monoxide emission

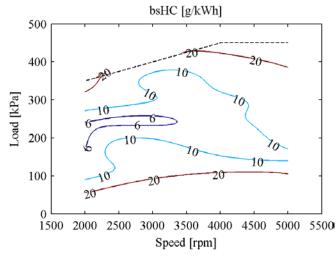


Figure 27 - Unburned hydrocarbon emission

The emission maps of carbon monoxide and hydrocarbons were compared to the maps of an air-assisted direct injection SI gasoline two-stroke engine designed by Piaggio (Nuti 1998). An engine of this type would be the most direct competitor to the developed engine. The Piaggio engine has similar size, port timings and layout as the test engine investigated in this study. The emissions of carbon monoxide and hydrocarbons are on approximately the same level as those of the Piaggio engine. The above mentioned reference did not report NO_x emissions for the Piaggio engine.

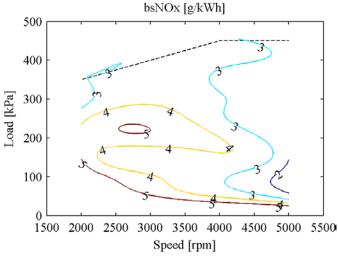


Figure 28 - Nitrogen oxide emission

4.5.2 Comparison to EU emission limits

The emissions were compared to the emission standards currently in force in the EU. Since only hot steady state testing of the test engine mounted in a dynamometer had been performed it was decided to compare with the emission standard valid for non-road engines (Stage III A). Assuming that the test engine is applied to drive an electric generator at 3000 rpm the five mode points that are given in the D2 test cycle of the ISO 8178 standard can be defined. Multiplying the measured emissions at each mode point with the given weighting of the mode points results in the values presented in Figure 29.

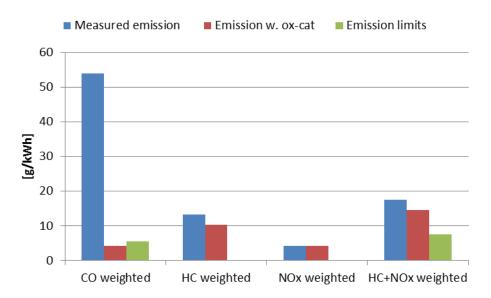


Figure 29 - Comparison to EU emission limits with and without oxidation catalyst.

Figure 29 shows that the engine-out carbon monoxide emission is a factor of ten higher than the emission limit. The sum of hydrocarbons and NO_x is also above the emission limit but only by about a factor of two. Clearly the engine could not be used without a catalyst. The effect of an oxidation catalyst was not tested but estimated by multiplying the measured emissions with the conversion efficiencies of an oxidation catalyst given as a function of exhaust gas temperature in (Nuti 1998). Doing that shows that carbon monoxide can be reduced to a value below the emission limit. Unfortunately this is not the case for the combined hydrocarbons and NO_x emissions. The oxidation catalyst cannot reduce NO_x emissions and has poor conversion efficiency for hydrocarbons at the low exhaust gas temperatures of the test engine that range from 100 to 350 degrees Celsius. A fundamental guestion at the outset of the DME two-stroke engine development was whether engine out NO_x emissions would be very low. Figure 28 and Figure 29 show that NO_x emission are low but still of the same order of magnitude as current emission legislation in the EU. The low levels obtainable in true HCCI operation are not achieved. This indicates that despite the fast fuel delivery and long ignition delays the premixing that occurs before ignition in late injection HCCI is not sufficient to reduce NO_x formation to the levels expected in port injected HCCI-mode. Particulate emissions were measured using a Bosch smokemeter. The result at full load was a reading of 0 on a 0 to 10 scale. This measurement agreed with visual inspection that did not reveal any smoke formation.

4.5.3 Optical access

After the publication of the papers on the two-stroke engine, optical studies were performed in order to better be able to characterize the type of combustion and to see to what extent premixing of fuel and air is happening before combustion.

Pictures of Spark Ignition (SI), traditional Compression Ignition (CI) and Homogeneous Charge Compression Ignition (HCCI) are illustrated in Figure 30.

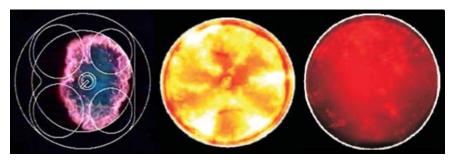


Figure 30 - SI, CI and HCCI combustion

The SI engine burns a premixed fuel-air mixture but where combustion is initiated by the spark plug and progresses through the combustion chamber with the local turbulent flame speed. The CI engine burns the fuel while it is injected creating the yellow sooting diffusion flame that is seen in the central illustration in Figure 30. HCCI is a lean non-sooting combustion that takes place almost simultaneously in the entire combustion chamber.

A cylinder head with optical access was manufactured and high speed color video was taken along the cylinder axis as in Figure 30. Pictures from the videos are shown below illustrating the typical progress of combustion. At a shooting speed of 1200 pictures per second, the resolution is limited to 336 x 96 pixels, thus the picture dimension is quite small. The fuel injector is spraying from the top of the picture and vertically down.

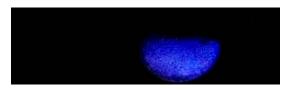


Figure 31 - Initial combustion starts opposite the injector

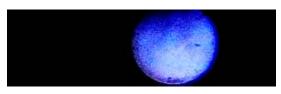


Figure 32 - Combustion quickly proceeds to embrace entire combustion chamber

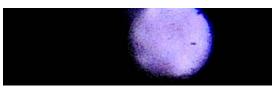


Figure 33 - Combustion finishes with reddish color (colder).

It is clear from these pictures that the combustion is closer to HCCI than traditional diesel combustion, but a completely homogeneous charge is not the case. Figure 31, Figure 32 and Figure 33 indicate there is some variation in the fuel-air mixture ratio across the combustion chamber. The light emission from combustion is stronger from the central lower part of the pictures, indicating a richer mixture of fuel and air there. Because of this partially premixed may be a better description of the state of the charge just prior to combustion. Despite that the charge is only partially premixed the complete absence of the yellow sooting flame typical of diesel combustion (central picture in Figure 30) is noteworthy. It is a key feature of DME combustion.

4.5.4 Concluding remarks regarding the late injection HCCI two-stroke engine

Chapter 4.4 illustrates that it is possible to design and operate a two-stroke engine with late injection of DME and control ignition timing well enough to achieve good engine efficiencies. Although the pictures of the combustion process showed that combustion is premixed to a high degree there is still significant variations in the mixture ratio across the combustion chamber. This results in higher NO_x emissions compared to the four-stroke engine with port injection of fuel in (Pedersen et al. 2010). The two-stroke engine was custom built and especially the matching of fuel injector and combustion chamber is unlikely to be the optimum at this early

stage of development. Better matching would allow for better homogenization and thereby lower NO_x emissions. External EGR or increased amounts of internal EGR could also be tried in order to bring down NO_x emissions.

The power output, measured in terms of brake mean effective pressure (bmep), was at the same level as that for the tested four-stroke engines: approx. 450 kPa. Due to the much lower internal friction of the two-stroke engine this results in an advantage in terms of mechanical efficiency for the two-stroke engine. Mechanical efficiency is defined as:

$$\eta_m = \frac{\text{bmep}}{\text{bmep+fmep}}$$

For the four-stroke engine, with a typical frictional mean effective pressure (fmep) of 200 kPa, this gives:

$$\eta_{m,4s} = \frac{450}{450 + 200} = 0.69$$

For the two-stroke engine, who has a measured fmep of 70 kPa, this gives:

$$\eta_{m,2s} = \frac{450}{450+70} = 0.87$$

A high mechanical efficiency is important in vehicles with a combustion engine and a traditional drive train. The effect on fuel economy by using a two-stroke engine of this type in a passenger car is simulated in Chapter 5.

A disadvantage of the late injection HCCI concept was that the fuel injection pressure had to be raised to 150 bars in order to achieve adequate mixing of fuel and air. Chapter 4.6 describes the progress made with the design of a fuel pump capable of delivering this pressure.

4.6 DME fuel pump

4.6.1 Concept

The first two-stroke engine prototype was tested with a DME fuel rail pressurized by helium to 100 bars. For the second prototype it was decided to also develop and build a DME pump that could supply the fuel rail. Due to the very low lubricity of DME the biggest challenge for engine researchers and manufacturers wanting to test DME has been to devise a reliable fuel injection pump (McCandless, Teng & Schneyer 2000). Typically the solutions have been to modify an existing diesel pump using advanced metal coating techniques and add a lubricant additive to the DME. Typical levels of lubricant addition are 300-1000 ppm. These modified diesel pumps have also had the plunger and barrel section isolated from the plunger actuation mechanism so that the actuation mechanism could be lubricated by ordinary lubrication oil. A different approach is presented in the following section. The basic idea was that it may be possible to use hydraulic type rod seals and avoid any direct contact between plunger and barrel since this engine does not benefit from injection pressures higher than 150 bars. In this way, solutions like advanced metal coatings would be unnecessary and the rod seals would serve, at the same time, to isolate the plunger and barrel section from the rest of the pump mechanism. The details of this design are outlined below.

4.6.2 Design

The pump is a single plunger jerk pump. Cam activated and spring return. Flow control is performed by inlet and outlet one-way valves. Avoidance of metal to metal contact between plunger and barrel is a central idea in the concept. This requires that the plunger is accurately guided relative to the barrel. No metal to metal contact is acceptable. This function is provided by a ball guide unit as shown in Figure 34. Sealing between plunger and barrel is achieved by means of a spring activated PTFE seals.

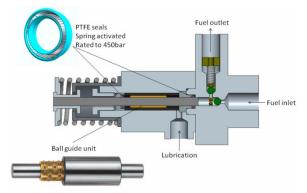


Figure 34 - Cross section of DME pump

Cavitation in the pump inlet and especially around the one-way inlet valve was a concern. If the temperatures of the fuel tank and the pump are the same then any pressure drop across the inlet valve would lead to cavitation. Cavitation would lower the volumetric efficiency of the pump and could only be compensated for by higher feed pressures which would place higher demands on the feed pump. In order to get the lowest possible pressure drop across the inlet valve this is designed as a light plastic ball without spring return. The low pressure created in the barrel during the plunger down-stroke forces the ball away from its seat and inflow of DME commences. During the up-stroke of the plunger the pressure drop reverses direction and the

ball moves back on the valve seat again. The outlet valve functions in the same way but has a return spring in order to achieve quick closing.

4.6.3 Performance

The pump was actuated in sinusoidal motion by an eccentric circular disc mounted on a servo motor. The inlet of the pump was connected to a one liter DME fuel tank on a scale. The DME fuel tank was pressurized with helium at a pressure of 3 bars higher than the DME vapor pressure. A relief valve kept the desired pressure level at the pump outlet. See Figure 35.



Figure 35 - DME pump test setup

The measured volumetric efficiencies are listed in Table 3.

Table 3 - Volumetric efficiency of DME pump

Pump speed	Volumetric efficiency
[rpm]	[-]
500	0.88
750	0.89
1000	0.81

4.6.4 Durability

The rod seal between plunger and barrel facing DME at pressures varying from DME vapor pressure to full rail pressure determines the life of the pump. PTFE seals without fiber reinforcement had a lifetime of less than 5 hours. PTFE seals with carbon fiber reinforcement were tested and lasted longer but still showed signs of critical wear after 10 hours of operation.

A measured leakage flow of 0.3 g/hour flows past the seal contact zone during operation. It was believed that this leakage flow washes away the lubricant in the seal contact zone and was the main reason for the high wear rates. In order to address this issue the front seal facing the DME was mounted oppositely so that the spring faced the lubricant side and the lubrication oil was pressurized to a level slightly higher than the DME pumping pressure. In this way there would continuously be a pressure gradient forcing lubricant into the DME and not vice versa, providing a lubricant film in the seal contact zone. With this concept there has been no critical wear on the seal for the remainder of the test period and the leakage of lubrication oil through to the DME side of the seal is negligible. The test period has included a mixture of dyno testing and testing with the engine in a small urban car used for fuel economy competitions, the latter accounting for the largest share of operational hours. The hours accumulated in the car have not been registered accurately but are approximately fifty hours. In conclusion it can therefore be said that a DME pump using rod seals between plunger and barrel could be a viable solution at the modest injection pressures tested in this study but the design proposed has not accumulated enough hours to draw any final conclusions.

4.6.5 Danfoss

During the project period DTU was approached by Danfoss in California regarding DME pump design. It was interesting for Danfoss to develop a DME pump since the market for DME is expanding and Danfoss has experience in the field. The idea was to suggest this to Danfoss leadership by making an entry into an internal Danfoss business case competition. DTU thought this was an exciting idea given the experience that Danfoss has with hydraulic pumps for low lubricity fluids like water (Danfoss Nessie). DTU supplied data and other information for the business case and it ultimately came in second in the competition. After that it was initially decided by Danfoss management to pursue the development of a DME pump but the project was stopped before significant progress was made. According to our knowledge the primary reason to stop was that the project was considered "high risk" in terms of return on investment given the uncertainty about the growth rate of the DME market.

4.7 Shell Eco-Marathon

In order to test the performance of the late injection HCCI two-stroke engine in a vehicle it was mounted in a small urban car that participated in the Shell Eco-Marathon 2009.



Figure 36 – Competition vehicle with the HCCI two-stroke engine (2009)

The Shell Eco-Marathon is a fuel economy competition for universities held annually in Germany.

The engine was operated at constant load but at varying speed, a method called "coast & burn". While coasting the engine is turned off and while burning the engine is run at peak efficiency load while accelerating the vehicle. This method is used by all competitive participants using internal combustion engines in order to avoid running the engines at a low mechanical efficiency on the parts of the circuit that require little or no power to propel the vehicle.

The car won the Urban Concept car competition in 2009 with 589 km/liter (gasoline energy equivalent) as the result. Second place was awarded to a car with a four-stroke gasoline engine; their result was 343 km/l. The vehicles are not identical but they are built according to the same competition rules and vehicle mass, frontal area and drag coefficient for the two vehicles are very similar. The practical result reflects the high measured efficiency of the test engine.

Since 2009 DTU's ecocar has been using other fuels because the Shell Eco-Marathon did not allow the use of DME starting from 2010. The results since 2009 are shown in Table 4.

Year	Fuel	Result
2009	DME	589 km/l
2010	GTL diesel	348 km/l
2011	Ethanol	509 km/l

Table 4 - DTU results in the Shell Eco-Marathon

The 589 km/liter achieved with DME is a world record that is still standing at the time of writing. It has not, so far, been possible to beat it with the other fuels.

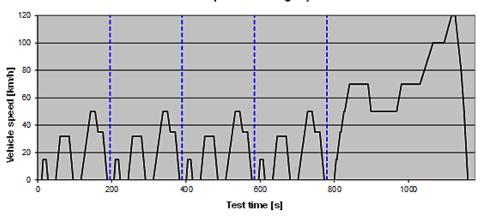
The results for the ecocar are interesting since they are "real life" measurements and can be compared directly with the results of the competitors that are using more traditional engines. The next question that quickly arises is: What would be the fuel economy of a normal passenger car if it was fitted with an engine of this type? This question is considered in chapter 5.

5. Estimation of Passenger Car Performance

In order to investigate the "real world" performance the HCCI two-stroke engine a mathematical model has been developed for that purpose during the project period. It is based on the classical mechanics of a moving vehicle as it is described for example in (Sorenson 2008).

5.1 NEDC cycle simulations

The model is capable of simulating driving cycles such as the New European Driving Cycle (NEDC) which is the driving cycle used by EU to define the requirements for vehicle emissions and fuel economy.



New European Driving Cycle

The model has been run for some existing commercial cars and the fuel economy results are compared with the official numbers in Table 5 in order to evaluate the accuracy of the model.

Car	Test	Simulation	Deviation
	[km/l]	[km/l]	[%]
1998 Citroén Saxo 1.5 diesel	18.9	19.9	+ 5.3
2000 VW Lupo 1.2 turbo diesel	31.3	28.5	- 8.9
2007 Ford Mondeo 1.8 turbo diesel	16.9	17.3	+ 2.4

Table 5 – Comparison of official fuel economy numbers and simulation results:

Without resorting to an actual statistical calculation Table 5 shows that the model is accurate to within approximately $\pm 10\%$. Considering how different the three vehicles are this is a quite good accuracy. It seems that the model includes the most relevant parameters.

The reason why the simulation of the VW Lupo has the largest deviation is probably because it is the most advanced vehicle in terms of energy efficiency. The internal friction in the Lupo

Figure 37 - NEDC cycle

engine has been optimized and it is likely that this is one of the most significant reasons for the deviation since the model uses a traditional friction model for all vehicles.

The model is slightly optimistic with respect to the two more traditional vehicles: The Citroen Saxo and the Ford Mondeo. The reason for this is probably that the model does not take into consideration the detrimental effects on engine efficiency when an engine is started from cold which is the case in the NEDC cycle.

In order to see the effects on fuel economy on the simulated vehicles by switching to an HCCI two-stroke engine a number of choices are made:

- 1. The two-stroke engine displacement is chosen so that the engine torque level is unchanged (the acceleration performance of the car is unchanged).
- 2. The two-stroke engine efficiency is set equal to the efficiency of the 50cc test engine.
- 3. For the turbocharged cars the two-stroke engine is simulated as getting the same relative torque increase as the four-stroke engines get by turbocharging.
- 4. The weight of the vehicles has not been changed. It is assumed that the lower mass of a smaller displacement two-stroke engine is balanced by a heavier DME fuel system.
- 5. The gearing of the car is unchanged.

Table 6 – Fuel efficiency improvement by fitting an HCCI two-stroke engine in a passenger car:

Car	Std.	Two-Stroke	Change
	[km/l]	[km/l]	[%]
1998 Citroén Saxo 1.5 diesel	19.9	23.2	+ 16.6
2000 VW Lupo 1.2 turbo diesel	28.5	31.1	+ 9.1
2007 Ford Mondeo 1.8 turbo diesel	17.3	18.5	+ 6.9

Based on the decisions above it is clear from Table 6 that there would be a fuel efficiency improvement for all three vehicles if they had an HCCI two-stroke engine installed. An interesting trend can also be observed. The improvement is the greatest for the non-turbocharged Citroen Saxo and among the two turbocharged cars it is the greatest for the oldest one. This is no coincidence. The progress in engine technology in recent years has enabled high specific power outputs from small four-stroke diesel engines. Brake mean effective pressures (bmep) in excess of 2000 kPa are now possible. This has a significant impact on four-stroke engine efficiency and thereby vehicle fuel efficiency.

It is difficult to achieve a higher brake mean effective pressure than 800 kPa with a nonturbocharged four-stroke diesel. Poor combustion efficiency and high smoke emissions establish this limit. The situation for the three cars under consideration is shown in Table 7.

Car	bmep	bmep / (800 kPa)
	[kPa]	[]
1998 Citroén Saxo 1.5 diesel	782	0,98
2000 VW Lupo 1.2 turbo diesel	1446	1,81
2007 Ford Mondeo 1.8 turbo diesel	2234	2,79

Table 7 – Absolute and relative break mean effective pressures

The non-turbocharged Citroén Saxo is very close to 800 kPa as would be expected. The VW Lupo is turbocharged to almost twice the specific output. The Ford Mondeo is turbocharged to an even higher degree.

Since the internal friction in an engine is strongly dependent on engine speed but not on engine load this increase in specific output achieved by a torque increase at unchanged engine speeds results in higher mechanical engine efficiencies according to:

$\eta_m = \frac{\text{bmep}}{\text{bmep+fmep}}$

The friction mean effective pressure (fmep) is speed dependent but here a value of 200 kPa has been chosen in order to do a comparison. It is equivalent to the fmep of a four-stroke diesel at an engine speed of 2500 rpm. Using this value the mechanical efficiency at full load can be approximated – see Table 8.

Car	bmep	bmep / (800 kPa)	eta_m
	[kPa]	[]	[]
1998 Citroén Saxo 1.5 diesel	782	0,98	0,80
2000 VW Lupo 1.2 turbo diesel	1446	1,81	0,88
2007 Ford Mondeo 1.8 turbo diesel	2234	2,79	0,92

Table 8 – Approx. mechanical efficiency at full load.

The efficiency of the two-stroke engine can be calculated in a similar way.

Table 9 – Mechanical efficiencies for the two-stroke engine at full load.

Car	bmep 2S	eta_m 2S
	[kPa]	[]
1998 Citroén Saxo 1.5 diesel	450	0,87
2000 VW Lupo 1.2 turbo diesel	813	0,92
2007 Ford Mondeo 1.8 turbo diesel	1257	0,95

Going back and looking at the change in fuel efficiency (Table 6) it is clear that there is a relation between the change in mechanical efficiency and the change in fuel efficiency. This is the major benefit of the two-stroke engine. The lower internal friction enables good engine

efficiencies even though the power output per engine cycle is significantly lower than for the four-stroke diesel engine.

Then why don't we all drive around in cars with two-stroke engines? The improvement in fuel consumption with a two-stroke engine that was computed above is not new knowledge. During the 1990's there was renewed interest in the gasoline two-stroke engine for passenger cars for this very reason. The advent of direct injection systems for gasoline that were capable of quickly creating a homogenous fuel-air mixture made it possible to manufacture efficient direct injection two-stroke engines. But there were a number of issues to deal with that finally stopped further progress for the gasoline two-stroke engine:

- 1. Use of three-way catalyst
- 2. Engine durability

1. Due to the scavenging principle of a two-stroke engine it is impossible to avoid that some of the scavenge air continues directly out in the exhaust pipe. This excess air is not compatible with the operation of a three-way catalyst. Spark ignition combustion of gasoline produces significant amounts of NO_x and since a three-way catalyst could not be used it was not possible to get below emission limits.

2. The two-stroke engine concept with the lowest internal friction, and thereby the best fuel efficiency benefits, uses the crankcase as its scavenging pump. Figure 38 shows a spark ignited gasoline engine but the scavenging principle is the same for crankcase scavenged direct injection engines.

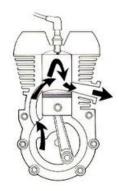


Figure 38 – Crankcase scavenged two-stroke engine

This means that the crankcase cannot be filled with oil as it is in a four-stroke engine. A system called wet sump lubrication. The wet sump crankcase with plain bearings, which is used almost exclusively in car engines of today, has been proven through more than a century to be very reliable. A crankcase scavenged two-stroke engine adds small amounts of lubricant continuously to the crankcase. This oil passes through the crankcase and is eventually burned during combustion and exits with the exhaust gas. The oil does not burn as cleanly as the fuel and oil addition to the crankcase is therefore kept to the absolute minimum required. This marginal lubrication level can give problems related to the durability of the engine and this is an additional reason why car manufacturers have been reluctant to use two-stroke engines.

How do these challenges for the gasoline two-stroke engine apply to the DME two-stroke engine?

1. Since an HCCI engine always operates under lean conditions there will be and excess of air in the exhaust whether the engine concept is two- or four-stroke. A three-way catalyst is therefore not an option in any case. NO_x formation during combustion has to be limited and that is the whole purpose of the HCCI concept.

2. The situation for the DME two-stroke is quite similar to the gasoline two-stroke engine. There is one benefit though. Due to the high vapor pressure of DME compared to gasoline there is very little, if any, wetting of the cylinder wall with DME. This can be the case with gasoline and fuel wetting of the cylinder walls reduce the viscosity of the lubricant film on the walls.

The practical experience during the project has shown no reliability issues with the main components of the DME two-stroke engine.

The obstacles that remain for the HCCI two-stroke engine are wear issues in the fuel injection equipment and that the NO_x emissions are a little too high at the current state of development. The latter is illustrated in Figure 39. Comparison is made to heavy duty vehicles since those values are given in g/kWh and not g/km that is used for cars. The reason why this comparison is better is that the only vehicle that the two-stroke engine has been fitted to is the DTU ecocar. This vehicle has such low fuel consumption that the emission per km is next to zero.

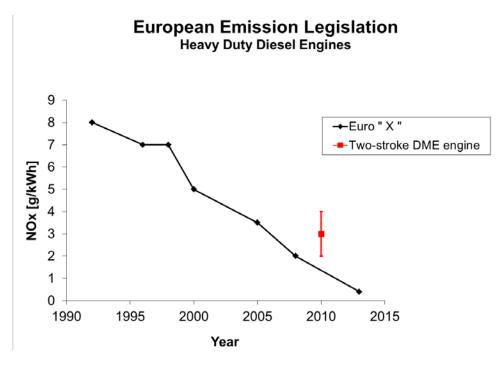


Figure 39 – Emission limits on a g/kWh basis

Figure 39 shows that the two-stroke engine complies with legislation up until 2005. Further work is needed to get below current legislation.

6. Future Work

Some important findings of the project are:

- DME and methanol do constitute a useful dual fuel pair for HCCI combustion.
- The maximum power output for an HCCI four-stroke engine is about half of that of a traditional engine and is limited by combustion knock.
- Although the indicated efficiency is high the lower power output with HCCI results in poor mechanical efficiencies and thereby low total efficiencies.
- The application of late injection HCCI in a two-stroke engine enables the same power outputs per cycle to be reached as with a four stroke engine.
- The lower internal friction of the two-stroke engine then results in an improvement of the total efficiency compared to the four-stroke engine.
- The good fuel efficiency of the two-stroke engine has been proven in a small urban vehicle.
- The two-stroke engine has higher NO_x emissions than the four-stroke engine due to the late injection that makes the fuel-air charge less homogeneous.
- The two-stroke engine requires higher fuel injection pressures than the four-stroke engine.
- High pressure fuel injection of DME remains a challenge.

Four-stroke HCCI engine design is intensely researched across the globe. Not much attention is paid to the improvements possible when combining HCCI combustion with the two-stroke engine concept.

It would be of interest to conduct research in the following fields relating to the HCCI two-stroke engine:

- Test the performance of an oxidations catalyst.
- Improve matching between the fuel injector spray pattern and the combustion chamber.
- Apply known techniques for in-cylinder reduction of NO_x formation.
- Conduct durability testing of the proposed DME fuel pump concept.
- Test the performance of a larger engine.
- Test the performance in a passenger car.

6.1 **DEMØ**

An application for a demonstration project is being prepared at the time of writing. The project has been named DEMØ (DEMonstration af Økobilteknik). The idea is to test different drive train technologies, including the HCCI two-stroke engine concept, on the same vehicle platform. In this way a direct comparison of fuel efficiency and emissions can be conducted. The other drive train technologies are:

- A standard four-stroke turbo diesel engine (the reference case)
- A four-stroke spark ignition ethanol engine
- All electric
- A hydrogen fuel cell
- A serial hybrid system combining a combustion engine and electric motors.

The partners in the project, so far, are:

DTU Mekanik Ecomove Teknologisk Institut Lithium Balance IRD Fuel Cells Inbicon

7. Conclusion

A number of studies were performed in order to find the combustion engine concepts that best deal with the challenges and opportunities encountered when using dimethyl ether (DME) as the primary fuel.

The main challenge with the use of DME in engines is its low lubricity. Focus was therefore on engine concepts without high pressure direct injection since low pressure fuel pumps would be easier to design for DME.

Based on the theoretical and experimental results it can be concluded that DME and methanol can be used with low pressure manifold fuel injection in a homogeneous charge compression ignition (HCCI) engine. The mixture ratio between DME and methanol is then used to control ignition timing which is a major concern with HCCI engine operation. Unfortunately power output was limited by combustion noise to approximately half of that achievable in normal diesel operating mode.

A range of alternative piston top designs were tested in order to reduce the combustion noise and thereby enable higher engine outputs and efficiencies. The traditional bowl-in-piston design, that was the starting point of the studies turned out to be the best, so no improvements could be gained by using alternative piston top designs.

Thermal efficiency and emissions were good but mechanical efficiency low due to the low power output. Focus was therefore turned towards using the combustion concept in an engine type with low internal friction in order to bring the mechanical efficiency back up. A two-stroke engine was designed and built. Due to the operating principle of a two-stroke engine it is not possible to maintain low pressure manifold fuel injection. Injection pressure was increased to 150 bars in order to enable injection shortly before the combustion event. This process is called "late injection HCCI".

The 150 bars required for late injection is still lower than what is needed for efficient operation in traditional diesel mode. The two-stroke engine was built in a very small version so that it could be used in a fuel efficiency competition for students. It turned out to perform well although emissions were significantly worse than with the dual-fuel four-stroke engine initially used. These increased emissions may well be dealt with using a traditional oxidation catalyst but this was not verified during the project period.

Progress was made with the design of a DME fuel pump operable up to 150 bars. At the time of writing the pump concept has been proven to work but the number of testing hours is less than 100.

The results for the two-stroke engine have been so promising that DTU is now seeking funding for a vehicle demonstration project together with a consortium of industrial partners.

List of Abbreviations

ATDC	After Top Dead Center
BMEP	Brake Mean Effective Pressure
BS	Brake Specific
BTDC	Bottom Dead Center
CAD	Crank Angle Degrees
CCS	Combined Combustion System
CFD	Computational Fluid Dynamics
CGH2	Compressed Gaseous Hydrogen
CI	Compression Ignition
CNG	Compresed Natural Gas
СО	Carbon Monoxide
CR	Compression Ratio
DEMØ	Demonstration af Økobiler (Demonstration of Ecocars)
DI	Direct Injection
DOC	Diesel Oxydation Catalyst
EFP	Energisforsknings-programmet (The energy research program)
EGR	Exhaust Gas Recirculation
EtOH	Ethanol
FMEP	Friction Mean Effective Pressure
FPFC	Fuel Processor Fuel Cell
FT	Fischer-Tropsch

FTD	Fischer-Tropsch Diesel
FTN	Fischer-Tropsch Naphtha
G	Gaseous
GDI	Gasoline Direct Injection
HC	Hydrocarbons
HCCI	Homogeneous Charge Compression Ignition
HEV	Hybrid Electric Vehicle
HTR	High Temperature Reactions
ICE	Internal Combustion Engine
IMEP	Indicate Mean Effective Pressure
L	Liquid
LH2	Liquified Hydrogen
LNG	Liquified Natural Gas
LTR	Low Temperature Reactions
MeOH	Methanol
MTA	Manual Transmission
NEDC	New European Driving Cycle
NO	Nitrogen Oxide
NO _x	Oxides of nitrogen
NTSEL	National Traffic Safety and Environmental Laboratory
ОН	Hydroxyl
PM	Particulate Matter
PPM	Parts Per Million

- PTFE Poly Tetra Flour Ethylene
- RPM Revolutions Per Minute
- RWB Residual Wood Biomass
- SI Spark Ignition
- TDC Top Dead Center
- THC Total Hydrocarbons
- WB Wood Biomass

References

- Arcoumanis, C., Bae, C., Crookes, R. & Kinoshita, E. 2008, "The potential of di-methyl ether (DME) as an alternative fuel for compression-ignition engines: A review", *Fuel*, vol. 87, no. 7, pp. 1014-1030.
- Consonni, S., Katofsky, R.E. & Larson, E.D. 2009, "A gasification-based biorefinery for the pulp and paper industry", *Chemical Engineering Research & Design*, vol. 87, no. 9A, pp. 1293-1317.
- Curran, H.J., Pitz, W.J., Westbrook, C.K., Dagaut, P., Boettner, J.C. & Cathonnet, M. 1998, "A wide range modeling study of dimethyl ether oxidation", *International Journal of Chemical Kinetics*, vol. 30, no. 3, pp. 229-241.
- Directive 98/70/EC of the European parliament and of the council 2009, " Relating to the quality of petrol and diesel fuels and amending Council Directive 93/12/EEC", 1998L0070, .
- Fitzgerald , R.P., Steeper , R., Snyder , J., Hanson , R. & Hessel , R. 2010, Determination of Cycle Temperatures and Residual Gas Fraction for HCCI Negative Valve Overlap Operation, Copyright © 2010 SAE International.
- Gentili, R. 1999, "What is the future of the two-stroke S.I. engine", *SAE Technical Paper 1999-24-0069,* .
- Hamada, K., Niijima, S., Yoshida, K., Yoshida, K., Shoji, H., Shimada, K. & Shibano, K. 2005, *The Effects of the Compression Ratio, Equivalence Ratio, and Intake Air Temperature on Ignition Timing in an HCCI Engine Using DME Fuel*, Copyright © 2005 Society of Automotive Engineers of Japan, Inc. and Copyright © 2005 SAE International.
- Hansen , K.R., Dolriis , J.D., Hansson , C., Nielsen , C.S., Sorenson , S.C. & Schramm , J.
 2011, Optimizing the Performance of a 50cc Compression Ignition Two-Stroke Engine Operating on Dimethyl Ether, Copyright © 2011 SAE International.
- Hansen , K.R., Nielsen , C.S., Sorenson , S.C. & Schramm , J. 2008, *A 50cc Two-Stroke DI Compression Ignition Engine Fuelled by DME*, Copyright © 2008 SAE International.
- Hansen, K.R., Nielsen, C.S., Sorenson, S.C. & Schramm, J. 2010, "Development of a Small Two-Stroke Diesel Engine Powered by DME", International DME Association, .
- Hitachi Construction Machinery Co., Ltd 2011, 18 May 2011-last update, *Cooled EGR System* [Homepage of Hitachi Construction Machinery Co., Ltd], [Online]. Available: http://www.hitachi-c-m.com/global/products/excavator/medium/zx240-3/feature_1.html [2011, 7/22].
- Hu, T.G., Liu, S.H., Zhou, L.B. & Chi, Z. 2005, "Combustion and emission characteristics of a homogeneous charge compression ignition engine", *Proceedings of the Institution of Mechanical Engineers Part D-Journal of Automobile Engineering*, vol. 219, no. D9, pp. 1133-1139.
- Hu, T., Liu, S., Zhou, L. & Li, W. 2006, "Effects of compression ratio on performance, combustion, and emission characteristics of an HCCI engine", *Proceedings of the Institution of Mechanical Engineers Part D-Journal of Automobile Engineering*, vol. 220, no. D5, pp. 637-645.
- Ikemoto , M., Kojima , Y. & Iida , N. 2005, Development of the Control System Using EGR for the HCCI Engine Running on DME, Copyright © 2005 Society of Automotive Engineers of Japan, Inc. and Copyright © 2005 SAE International.

Kajitani, S., Hoshimiya, A. & Hayashi, M. 2007, A Study of Low Compression Ratio DME Engine Operated With Stoichiometric Working Gas.

Kanoto, Y., Ohmura, T. & Iida, N. 2007, *An Investigation of Combustion Control Using EGR for Small and Light HCCI Engine Fuelled with DME*, Copyright © 2007 Society of Automotive Engineers of Japan, Inc. and Copyright © 2007 SAE International.

Lucchini, T., Dr. & Montenegro, G., Dr. 2007, 11 June 2007-last update, *OpenFoam for Internal Combustion Engine Simulations, Combustion and Spray* [Homepage of OpenFOAM Workshop], [Online]. Available:

http://www.openfoamworkshop.org/2007/index.php?title=OpenFOAM_for_Internal_Combu stion_Engine_Simulations%2C_Combustion_and_Spray&oldid=1717 [2011, 7/22].

McCandless, J.C., Teng, H. & Schneyer, J.B. 2000, *Development of a Variable-Displacement, Rail-Pressure Supply Pump for Dimethyl Ether*, Copyright © 2000 Society of Automotive Engineers, Inc.

Millo, F. 2007, "Analysis of Different Internal EGR Solutions for Small Diesel Engines", SAE Technical Paper 2007-01-0128, .

Muradov, N.Z. & Veziroglu, T.N. 2008, ""Green" path from fossil-based to hydrogen economy: An overview of carbon-neutral technologies", *International Journal of Hydrogen Energy*, vol. 33, no. 23, pp. 6804-6839.

- Nuti, M. 1998, "Air-Assisted Direct Fuel Injection" in *Emissions from Two-Stroke Engines* Society of Automotive Engineers, Inc., Warrendale, U.S.A., pp. 198-203.
- Ogawa , H., Miyamoto , N., Kaneko , N. & Ando , H. 2003, *Combustion Control and Operating Range Expansion With Direct Injection of Reaction Suppressors in a Premixed DME HCCI Engine*, Copyright © 2003 SAE International.
- Ohmura , T., Ikemoto , M. & Iida , N. 2006, *A Study on Combustion Control by Using Internal and External EGR for HCCI Engines Fuelled with DME*, Copyright © 2006 SAE International and Copyright © 2006 SAE Japan.

Onishi, S., Jo, S.H., Shoda, K., Jo, P.D. & Kato, S. 1979, Active Thermo-Atmosphere Combustion (ATAC) - A New Combustion Process for Internal Combustion Engines, Copyright © 1979 Society of Automotive Engineers, Inc.

Pedersen , T.D. & Schramm , J. 2010, *Reduction of HCCI Combustion Noise Through Piston Crown Design*, Copyright © 2010 SAE International.

Pedersen , T.D. & Schramm , J. 2007, A study on the effects of compression ratio, engine speed and equivalence ratio on HCCI combustion of DME, Copyright © 2007 Society of Automotive Engineers of Japan, Inc. and Copyright © 2007 SAE International.

- Pedersen, T.D., Schramm, J., Yanai, T. & Sato, Y. 2010, *Controlling the Heat Release in HCCI Combustion of DME with Methanol and EGR*, Copyright © 2010 SAE International.
- Sato, Y., Nakamura, A., Takada, Y. & Nakamura, K. 2008, "Development of DME Vehicles and Strategy of Practical Use Penetration", Society of Automotive Engineers of Japan, Inc., Tokyo, Japan, .
- Sato, S., Jun, D., Kweon, S., Yamashita, D. & Iida, N. 2005, "Basic Research on the Suitable Fuel for HCCI Engine from the Viewpoint of Chemical Reaction", .
- Semelsberger, T.A., Borup, R.L. & Greene, H.L. 2006, "Dimethyl ether (DME) as an alternative fuel", *Journal of Power Sources*, vol. 156, no. 2, pp. 497-511.
- Shudo , T., Ono , Y. & Takahashi , T. 2003, *Ignition Control by DME-Reformed Gas in HCCI Combustion of DME*, Copyright © 2003 Society of Automotive Engineers of Japan, Inc.

- Sorenson, S.C. & Mikkelsen, S. 1995, *Performance and Emissions of a 0.273 Liter Direct Injection Diesel Engine Fuelled with Neat Dimethyl Ether*, Copyright 1995 Society of Automotive Engineers, Inc.
- Sorenson, S.C. 2008, *Engine Principles and Vehicles,* 1st edn, Spencer C. Sorenson, Lyngby, Denmark.
- Yamada, H., Yoshii, M. & Tezaki, A. 2005, "Chemical mechanistic analysis of additive effects in homogeneous charge compression ignition of dimethyl ether", *Proceedings of the Combustion Institute*, vol. 30, pp. 2773-2780.
- Yamauchi , T., Matsumoto , A., Takada , Y. & Wakisaka , T. 2007, *Reduction of Detailed Elementary Reaction Schemes by Newly-developed Automatic Scheme Reduction Tool "ASRTâ€*, Copyright © 2007 Society of Automotive Engineers of Japan, Inc. and Copyright © 2007 SAE International.
- Yanai, T., Sato, Y., Kawamura, A., Oikawa, H., Nozaki, S., Noda, T. & Ishikawa, T. 2008, Development and Engine Bench Testing of a Common Rail Type DME Injection System.
- Yao , M., Chen , Z., Zheng , Z., Zhang , B. & Xing , Y. 2005, *Effect of EGR on HCCI Combustion fuelled with Dimethyl Ether (DME) and Methanol Dual-Fuels*, Copyright © 2005 SAE International.
- Yao , M., Liu , H., Zhang , B. & Zheng , Z. 2008, An Investigation on the Effects of Fuel Chemistry and Engine Operating Conditions on HCCI Engine, Copyright © 2008 SAE International.
- Yao, M., Chen, Z., Zheng, Z., Zhang, B. & Xing, Y. 2006, "Study on the controlling strategies of homogeneous charge compression ignition combustion with fuel of dimethyl ether and methanol", *Fuel*, vol. 85, no. 14-15, pp. 2046-2056.
- Zhao, F., Asmus, T.W., Assanis, D.N., Dec, J.E., Eng, J.A. & Najt, P.M. (eds) 2002, *Homogeneous Charge Compression Ignition (HCCI) Engines*, 1st edn, SAE, Warrendale, PA 15096-0001, USA.
- Zheng , Z., Yao , M., Chen , Z. & Zhang , B. 2004, *Experimental Study on HCCI Combustion of Dimethyl Ether(DME)/Methanol Dual Fuel*, Copyright © 2004 SAE International.
- Zheng, Z., Shi, C. & Yao, M. 2004, "Experimental study on Dimethyl Ether Combustion Process in Homogeneous Charge Compression Ignition Mode", *Transactions of Tianjin University*, vol. 10, no. 4.