

Formation of Unburned Hydrocarbons in Low Temperature Diesel Combustion

Sylvain Mendez, Julian T. Kashdan, Gilles Bruneaux,
Benoist Thirouard and Franck Vangraefschep
IFP

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ABSTRACT

Low temperature combustion is a promising way to reach low NO_x emissions in Diesel engines but one of its drawbacks, in comparison to conventional Diesel combustion is the drastic increase of Unburned Hydrocarbons (UHC). In this study, the sources of UHC of a low temperature combustion system were investigated in both a standard, all-metal single-cylinder Diesel engine and an equivalent optically-accessible engine. The investigations were conducted under low load operating conditions (2 and 4 bar IMEP). Two piston bowl geometries were tested: a wall-guided and a more conventional Diesel chamber geometry. Engine parameters such as the start of injection (SOI) timing, the level of charge dilution via exhaust gas re-circulation (EGR), intake temperature, injection pressure and engine coolant temperature were varied. Furthermore, the level of swirl and the diameter of the injector nozzle holes were also varied in order to determine and quantify the sources of UHC. It was found that for the wall-guided combustion chamber geometry, the formation of liquid films and their subsequent emission was a significant source of UHC. In the conventional Diesel combustion system liquid films did not seem to exist under warmed-up, steady-state engine operation and therefore are not believed to be a significant source of UHC emissions. Overall the major source of UHC in low temperature combustion appeared to be bulk quenching in over-lean regions rather than fuel partial oxidation in locally over-rich zones. Bulk quenching is characterized by incomplete fuel oxidation in regions of the combustion chamber where the combination of local temperature, equivalence ratio and charge dilution is inadequate for fast oxidation reactions. Indeed, the local temperature is too low to allow complete oxidation despite the excess of oxygen. In contrast, partial oxidation occurs in over-rich

zones where fuel oxidation is limited due to a lack of available oxygen. A detailed analysis of the experimental data revealed that the level of UHC emissions correlated well with the heat release peak. Finally, a conceptual representation of the bulk-quenching mechanism is proposed which is primarily based on consideration of the effects of mixing. This conceptual model is useful for understanding the various phenomena involved in bulk quenching and the impact of engine settings and configurations on UHC emissions.

INTRODUCTION

To reach future emission regulations which include very low NO_x and soot levels, new combustion modes are being investigated.

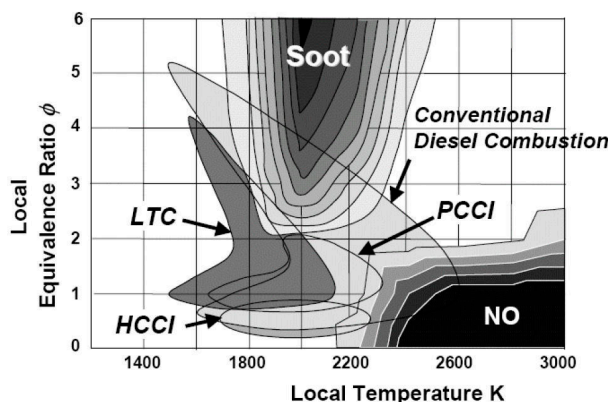


Figure 1: Conventional Diesel and other combustion processes in relation to the NO_x and Soot-forming zones – Figure from Neely, et al, SAE Paper 2005-01-1091

These new combustion approaches are called Homogeneous Charge Compression Ignition (HCCI) [1],

Premixed Combustion Compression Ignition (PCCI) [1] or Low Temperature Combustion (LTC) [2-4]. All these combustion modes try to avoid high local equivalence ratio and/or high local temperature in order to limit soot and NO_x formation (Figure 1) and [5]. One way to achieve low local equivalence ratio and low local temperature is to use engines with low compression ratios (CR), typically 14:1 or lower and high EGR rates. These specific conditions allow long ignition delay and thus enhanced air and fuel mixing resulting in reduced equivalence ratios. High dilution associated with reduced CR leads to low combustion temperatures.

The implementation of these combustion modes in production engines still faces significant challenges. In particular, the operating range where these specific combustion modes may be applied is limited and, as a consequence, the emission benefits integrated over standard driving cycles [7-8] are also limited. Moreover, controlling the combustion noise and maintaining efficiency comparable to today's direct injection Diesel engines is very difficult [8]. Another major issue related to these combustion modes is to control and limit the CO and UHC emissions [8-9]. In particular at light loads, low temperature combustion lead to a significant increase of UHC in comparison to a conventional combustion system. This is a major issue since the Diesel oxidation catalyst system may not fully oxidize the unburned species into CO₂ due to low exhaust temperature. In particular, CH₄ which requires high temperature in the catalyst device to be completely oxidized turns out to be a significant contributor to UHC emission in a LTC Diesel combustion system [10-11].

Until recently, the data available in the literature on the origin of UHC in Diesel engines was limited because the level of UHC emissions is very low in a conventional Diesel combustion system. With the development of low temperature combustion modes, a strong need for investigation and understanding of the UHC sources has arisen. In this context, it is interesting to perform a literature review of the known origins of UHC in spark-ignition engines and Diesel engines. Spark-ignition engines with indirect injection lead to a homogeneous charge in the combustion chamber that can be compared with the partially homogeneous charge obtained in LTC mode. Therefore identifying the sources of UHC emissions in spark-ignition engines is also interesting for LTC. The main mechanisms responsible for UHC emissions in spark-ignition engines reported in the literature are [12-13]:

1. Combustion chamber crevices (small volumes with narrow entrances where flame cannot penetrate). These crevices are volumes between piston, piston rings, and cylinder wall, threads of the spark plug, crevices of valve pockets, head gasket space.
2. Absorption and desorption in engine oil. This is absorption of fuel vapor in the oil film during intake and compression stroke and desorption of fuel vapor

from oil film during combustion and expansion stroke.

3. Deposits on the combustion chamber wall. Deposits on the combustion chamber wall due to mileage increase UHC emissions. This is due to a mechanism of absorption/desorption of fuel vapor and deposits.
4. Flame-quenching (wall and bulk). Incomplete reactions due to a cold wall (wall quenching) or excessively low temperature in the combustion chamber (bulk- quenching)
5. Incomplete combustion due to lack of O₂ (over-rich regions) that does not allow oxidation of UHC products

For Diesel engines and HCCI engines, numerous studies [13-14-15-16-17-18-19-20-21-22-23-24-25] also report a complete or a partial inventory of UHC origins that can be summed up as follows:

1. Combustion chamber crevices (similar to spark-ignition engines)
2. Formation of liquid films
Formation of fuel liquid film on the combustion chamber that can survive after combustion and be released during the exhaust stroke
3. Wall flame-quenching (similar to the spark-ignition case)
4. Bulk-quenching / Over-leaning: excessively low local equivalence ratio and temperature that do not allow oxidation reaction
5. Under-mixing: over-rich zones due to under-mixing of fuel in air leading to O₂ deficit which would otherwise allow oxidation of UHC (included fuel retained in the injector nozzle sac volume)

All these phenomena contribute to a certain degree to the global UHC emissions. Nevertheless, it should be kept in mind that UHC emissions are the result of UHC formation and post-oxidation (when temperature, O₂ concentration and residence time are sufficient).

After having analyzed each UHC source found in literature, it has been decided to investigate the following UHC origins that seem to be the major sources of UHC in low temperature Diesel combustion:

1. Combustion chamber crevices
2. Wall quenching
3. Liquid fuel films
4. Bulk quenching / Over-leaning
5. Under-mixing

This paper is a synthesis of different studies carried out at IFP since 2002. Each phenomenon previously identified as a source of UHC has been investigated with an all-metal single-cylinder Diesel engine and/or an equivalent optically-accessible engine to better understand UHC mechanisms.

EXPERIMENTAL SETUP

ENGINES SPECIFICATIONS

The results presented in this paper are a compilation of several studies conducted at IFP which were performed on different engines, each with their own characteristics. All the engines tested are a single-cylinder type derived from a 4-cylinder PSA 2.0 liter engine. Table 1 describes the common engine specifications for all engines used.

Bore x Stroke	85 x 88 mm
Displacement	499 cm ³
Valve / cylinder	4
IVO / IVC (lift of 1 mm)	17 CAD / 193 CAD ATDC
EVO / EVC (lift of 1 mm)	203 CAD / 17 CAD BTDC

Table 1: Common specifications of engines

Table 2 presents the specifications of each engine used to conduct the various studies discussed in this paper.

Engine number	# 1	# 2	# 3	# 4
Type	all-metal	all-metal	all-metal	optical
CR	14:1	14:1	14:1	14:1
Bowl Shape	Wall guided	Toroidal	Toroidal	Wall guided & Toroidal
Swirl ratio	1.1	1.7	2.2	1.1
Injector type	CRI2 VCO	CRI2 VCO	CRI2 VCO	CRI2 VCO
Nozzle holes	6 holes	6 holes	6 holes	6 holes
Nozzle static flow rate	420ml	340ml	340ml	420ml
Nozzle spray angle	60°	152°	152°	60°

Table 2: Particular specifications of engines

The fuel used for all the tests (except for liquid fuel film measurements and optical visualizations for which the corresponding fuels will be presented later) is a Diesel Fuel that meets European Norm EN 590 (maximum sulfur level of 50 ppm).

UHC SAMPLING AND MEASUREMENT REPEATABILITY

Engine-out UHC emissions were measured using a conventional flame-ionization detector (FID) analyzer.

The emissions sample was extracted downstream of the exhaust surge tank and exhaust backpressure valve. The sampling line was heated and maintained at a constant temperature of 180°C to avoid exhaust gas condensation between the exhaust pipe and the UHC analyzer. Since gas sampling was performed downstream of the exhaust valves, there is a possibility that the heavier UHC fractions may remain in the exhaust line upstream of the sampling location. As a consequence, the heavier UHC fractions might not be accounted for in the UHC emissions values presented in this paper. Nevertheless, it should be noted that excellent measurement repeatability was observed which gives confidence in the overall emissions behavior for the experiments reported here.

HEAT RELEASE AND IN-CYLINDER TEMPERATURE COMPUTATION

The heat release was calculated by using the first thermodynamic law and the Woschni heat transfer model [26]. The in-cylinder pressure was measured by a combustion chamber pressure sensor mounted in the glow plug location.

In-cylinder temperature was estimated by using the ideal gas law ($P.V = m.r.T$) for each crank angle. Gas mass trapped at IVC was determined with air flow rate, EGR rate measurements and internal residual burned gas rate was assumed to be 5%.

STUDY OF UHC EMISSIONS COMING FROM CREVICES OF THE COMBUSTION CHAMBER

As has been shown previously [20], the volume between piston, cylinder wall and piston rings seems to be the major source of UHC among all crevice volumes for spark-ignition and HCCI engines. To evaluate the influence of the geometry of the piston topland on UHC emissions for low temperature combustion, a specific piston geometry has been designed. This specific geometry included a circular groove machined into the piston crown (Figure 2). The volume of the groove was defined to be equal to the volume of the topland. As a result, the final topland volume was double compared to the reference topland geometry.

To maintain the same CR for the piston with the increased topland volume minor adjustments were made to the piston bowl volume without affecting the bowl shape. By adopting this approach, it is assumed that these modifications do not influence the injector spray/mixture preparation and subsequently auto-ignition and combustion behavior.

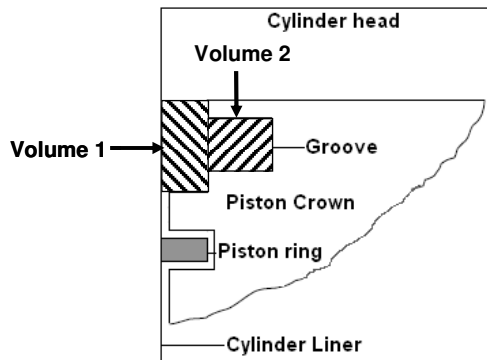


Figure 2: Specific Topland geometry with groove

To determine the influence of topland geometry on UHC emissions, a SOI sweep was conducted while keeping all other parameters constant (equivalence ratio, EGR rate, intake temperature...). The SOI sweep was performed for both the reference topland geometry and the modified topland geometry, for two bowl shapes (wall-guided engine #1 and conventional #2) and two engine operating conditions (1500 rpm – 2 & 4 bar IMEP). Engine settings for these operating points are given in Table 3 and Table 4.

Table 3: Engine operating conditions for engine #1

Engine #1		
Speed [rpm]	1500	1500
IMEP [bar]	2	4
Equivalence ratio	0.45	0.71
Intake temperature [°C]	70	70
Intake pressure [bar]	1.015	1.15
EGR rate [%]	45	45
Exhaust Pressure [bar]	1.10	1.25
Injection Pressure [bar]	1000	1000

Table 4: Engine operating conditions for engine #2

Engine #2		
Speed [rpm]	1500	1500
IMEP [bar]	2	4
Equivalence ratio	0.44	0.71
Intake temperature [°C]	70	70
Intake pressure [bar]	1.015	1.15
EGR rate [%]	52	45
Exhaust Pressure [bar]	1.10	1.25
Injection Pressure [bar]	500	1000

WALL-GUIDED COMBUSTION CHAMBER GEOMETRY

The SOI sweep was realized firstly with a wall-guided combustion chamber mounted on engine #1. The wall guided combustion chamber is composed of a combustion chamber with a specific central tip associated with a narrow spray angle. This design leads to significant spray-wall interaction. In some cases, the injected fuel jets are guided along the bowl shape, from the piston tip to the bowl lip [27-28]. The wall-guided combustion chamber geometry is represented in Figure 3.

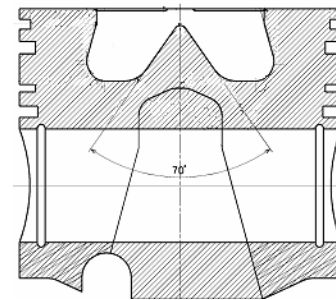


Figure 3: Wall-guided geometry with an additional crevice in the piston crown

The SOI sweeps were conducted over a wide range from 10 to 75 CAD BTDC to significantly change the fuel distribution in the combustion chamber. It is probably reasonable to assume that a homogeneous air/fuel mixture is achieved for the very early SOI timing of 75 CAD BTDC. Additionally for such early injection timing, fuel sprays impinge on the top of the piston as illustrated by Figure 4 and as a consequence part of the fuel is believed to reach the piston topland.

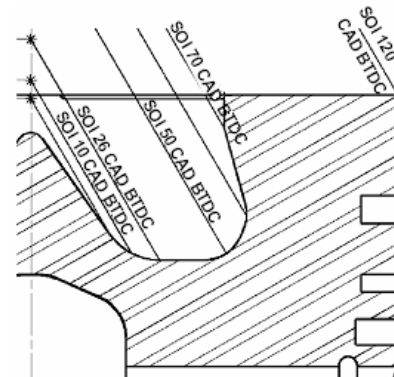


Figure 4: SOI theoretical spray impingements for wall-guided combustion system – Engine #1

SOI sweep results (Figure 5) show that the groove in the piston crown does not seem to have a significant impact on UHC for both loads tested (2 and 4 bar IMEP). Even at the earliest SOI (>65 CAD BTDC) no significant differences in the UHC emissions are observed between the reference and the modified piston topland geometries.

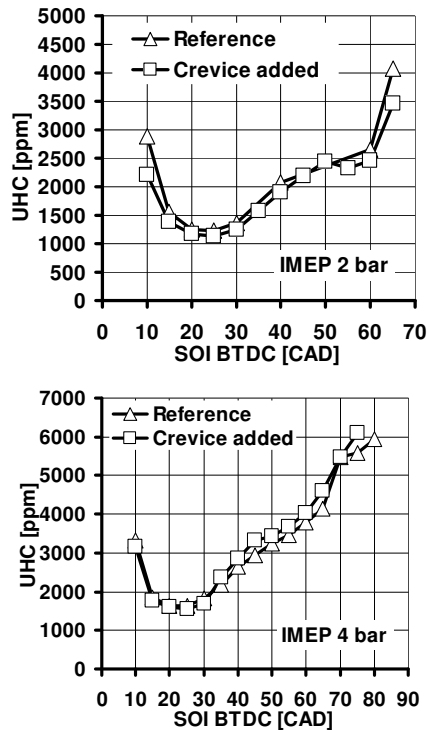


Figure 5: SOI sweeps – Influence on Topland geometry on UHC emissions – 1500 rpm 2 & 4 bar IMEP – Engine #1

CONVENTIONAL COMBUSTION CHAMBER GEOMETRY

A SOI sweep was also performed with the conventional combustion chamber geometry. In order to avoid oil dilution as a result of fuel sprays impinging directly on the cylinder liner, the earliest SOI was set to 35 CAD BTDC. As a consequence, the SOI sweep ranged from 10 to 35 CAD BTDC. For this geometry tests were performed with engine #2. Figure 6 shows the geometry used.

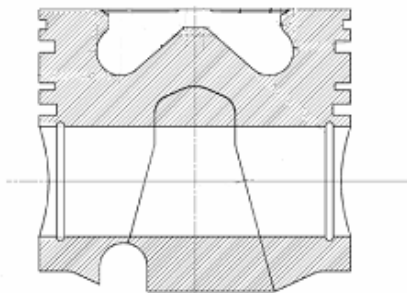


Figure 6: Conventional chamber geometry with an additional groove machined into the piston-top land crevice region

Figure 7 shows the theoretical spray trajectories for each SOI tested. At the earliest SOI, fuel impinges at the top of the bowl and on the top surface of the piston crown. As a result, an SOI of 30 CAD BTDC is expected to enhance the effects of the topland geometry, if there is an effect of topland crevice with this engine configuration.

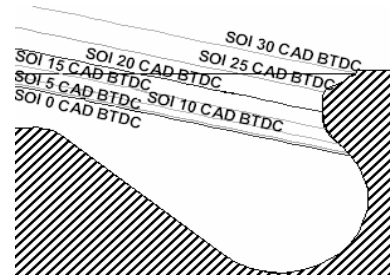


Figure 7: SOI theoretical spray impingements for conventional combustion system – Engine #2

SOI timing sweeps performed at IMEP 2 and 4 bar show that the UHC emissions are very similar for both the reference and the modified piston geometries (Figure 8). This result was verified for all the SOI timings tested including a very early SOI timing (35 CAD BTDC).

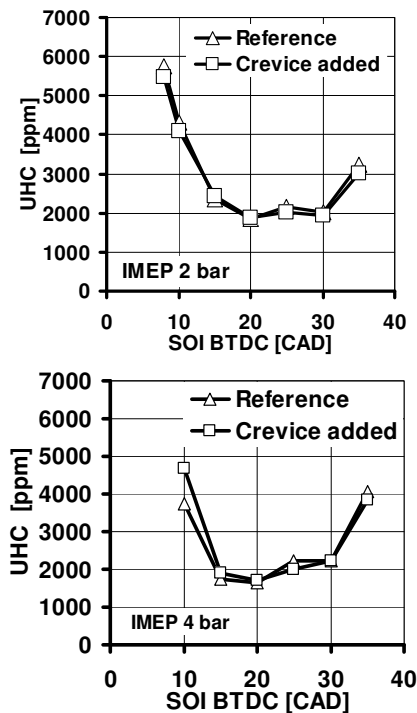


Figure 8: SOI sweeps – Influence on Topland geometry on UHC emissions – 1500 rpm 2 & 4 bar IMEP – Engine #2

SOI timing sweeps performed for wall-guided and conventional combustion chamber geometries at 2 and 4 bar IMEP did not reveal a difference in UHC emissions related to the piston-top land crevice volume. As a consequence, for the engines, loads, combustion chamber geometry and SOI tested, the piston-top land crevice volume was not found to be a significant source of UHC emissions in LTC mode. Despite long ignition delays (from 20 CAD to 70 CAD) and early SOI timings that lead to spray impingement out of the piston bowl,

fuel did not seem to be trapped in the top-land volume. These results differ from those obtained with HCCI [20-21] and spark-ignition [13] engines where fuel is injected during intake stroke.

STUDY OF WALL QUENCHING

Wall quenching results from the slowing down of the chemical reactions near to the combustion chamber walls due to a temperature drop induced by the cold walls. Wall quenching is generally considered to be a potential source of UHC for spark-ignition engines where the flame originates from the spark-plug and propagates toward the combustion chamber walls. In Diesel engines with low temperature combustion using long ignition delays, fuel has more time to mix with air and diffuse through the combustion chamber than with conventional Diesel combustion. So, for low temperature combustion, the fuel / air mixture can reach the walls and combustion completeness may be affected by wall-quenching.

To evaluate the influence of wall-quenching on UHC emission the coolant temperature was reduced from 90°C to 40°C with engine #1. It has been shown [30] that decreasing the cooling temperature reduces the wall temperature but also reduces the piston temperature due to thermal conduction effects. As a consequence, even if Diesel combustion is largely confined within the piston bowl rather than in the vicinity of the cylinder walls, the authors believe that imposing a significant decrease in the coolant temperature will primarily induce wall-quenching effects. Initially, all other engine settings were kept constant and only the engine coolant temperature was varied. As a consequence, combustion was significantly retarded due to the increase in ignition delay and decrease of combustion speed (Figure 9 and Figure 10). As the combustion process is significantly affected by the variation of coolant temperature, this test is not relevant to identify the effect of wall-quenching on UHC emissions. A second test was thus performed.

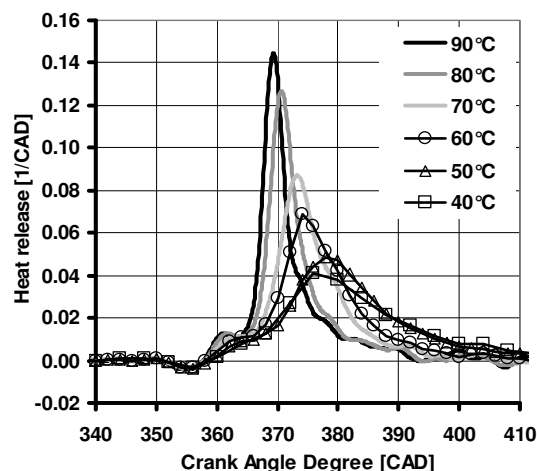


Figure 9: Influence on combustion of engine coolant temperature – 1500 rpm – IMEP 4 bar – Engine #1

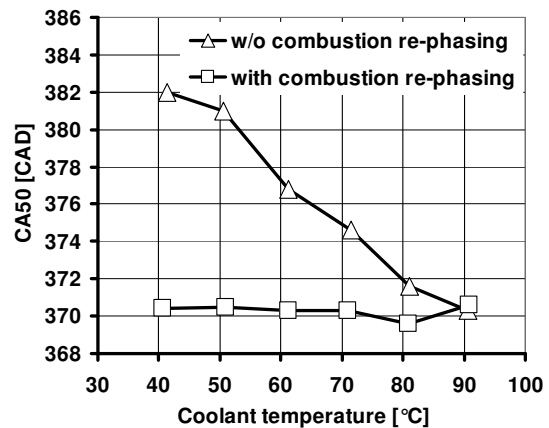


Figure 10: Combustion phasing with and without re-phasing vs. coolant temperature - 1500 rpm – IMEP 4 bar - Engine #1

During this second test the engine coolant temperature was varied while care was taken in order to ensure that the constant combustion phasing (CA50 – crank angle for which 50% of total fuel is burned) was maintained constant. Combustion re-phasing was achieved by adjusting the intake temperature. This was necessary in order to ensure that the bulk gas temperature within the combustion chamber was not affected by variations in the engine coolant temperature. This approach thus enabled us to study solely the effects of changes in the wall temperature and the impact on emissions. The intake pressure was also adjusted to maintain a constant intake mass flow rate and equivalence ratio (Figure 10). As a result, the impact of wall-quenching on UHC emissions could be evaluated by varying the engine coolant temperature at constant combustion phasing so as to ensure that the combustion process does not jeopardize the interpretation of the results.

Figure 11 shows the UHC emissions obtained for each test. When all settings are kept constant except for the coolant temperature, the UHC emissions increase significantly with a decrease in coolant temperature. UHC emissions rise by approximately a factor of 3.5 between 90 and 40°C of the coolant temperature. By slightly adjusting the intake temperature and pressure, it was possible to maintain constant combustion phasing for each coolant temperature tested. In this case, the UHC emissions are less sensitive to coolant temperature than the case without steady CA50. Indeed, UHC increase is limited to a factor of 1.5 for the same coolant temperature range.

Without maintaining a constant combustion phasing, when the coolant temperature decreases, combustion is retarded into the expansion stroke and the in-cylinder temperature is considerably reduced. It is well-known that UHC and temperature are well correlated [13-17-19]. Since maximum in-cylinder temperature decreases with coolant temperature because of delayed combustion timing, the UHC curve describes two effects: a probable wall-quenching effect and a temperature effect related to combustion phasing. It shows that this testing method is not appropriate to analyze the isolated effect of wall-quenching phenomena.

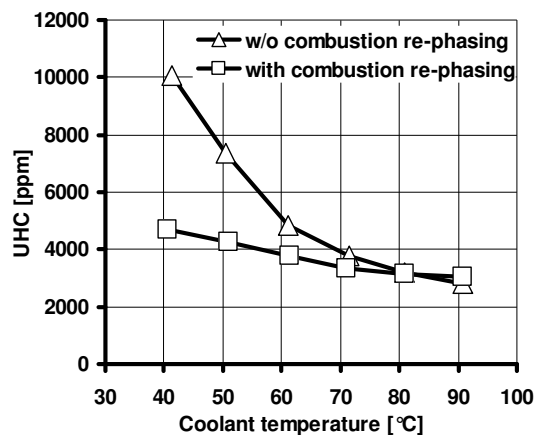


Figure 11: UHC emissions for coolant temperature reduction

On the other hand, when combustion phasing is maintained constant for the range of coolant temperatures studied and by adjusting both the intake pressure and temperature, wall-quenching will probably be the major phenomena impacting the UHC emissions when coolant temperature is varied.

Varying the coolant temperature while maintaining constant combustion phasing shows that wall-quenching could be a significant source of UHC emissions. In particular, for coolant temperatures lower than 70 °C, UHC emissions increase significantly. This could certainly be an issue for engine startup even under ambient conditions and for the urban part of the NEDC cycle where the catalyst device is not warm enough to oxidize unburned species.

On the other hand, for coolant temperatures in the range 70 °C to 90 °C, UHC emissions are very similar. Comparable levels of UHC emissions for coolant temperatures in the range 70 °C and 90 °C seem to indicate that wall-quenching effects are stabilized.

STUDY OF LIQUID FUEL FILMS

To investigate the presence of liquid fuels, a multi-fuel approach and LIF visualizations were performed [29].

WALL-GUIDED GEOMETRY

Multi fuel approach

Two fuels were tested on the all-metal engine: a standard Diesel fuel and a higher volatility Fischer Tropsch/kerosene blend. The blend of 90% kerosene and 10% of a Fischer Tropsch fuel was formulated so as to maintain a similar cetane number compared to the standard Diesel fuel. The objective here was to perform engine tests using two fuels of varying volatility but similar combustion characteristics in order to evaluate the contribution of fuel film formation as a source of UHC emissions. The fuel properties are summarized in Table 5.

Table 5: Fuel specifications of the standard Diesel fuel, kerosene/Fischer Tropsch fuel blend and dodecane used in experiments on the all-metal and optical access engine

Distillation temperatures	Standard Diesel	Kerosene /FT blend	Dodecane
Initial boiling point	173 °C	194 °C	216 °C
10% distillation temperature	200 °C	199 °C	
50% distillation temperature	272 °C	219 °C	
90% distillation temperature	331 °C	257 °C	
Final boiling point	352 °C	297 °C	216 °C
Cetane number	51	51	80
Lower heating value	46.11 MJ/kg	46.53 MJ/kg	47.39 MJ/kg

This table also displays the fuel properties of dodecane which was used for the tracer-LIF imaging experiments performed on the optical access engine together with 5-nonanone tracer (1% by mass). Dodecane is a high-volatility fuel since its boiling point (216 °C) is at the lower end of the distillation curve of standard Diesel fuel (typical boiling points of Diesel fuel are in the range 175 to 350 °C). Therefore in order to compensate for this high volatility, as well as for the higher wall temperature obtained in an optical engine (caused by the difference in thermal properties of the wall material), appropriate strategies were adopted on the optical engine so as to ensure that the combustion chamber wall temperature can be considered comparable to conditions encountered in the all metal engine. Those strategies might require the use of skip-firing strategies and/or adjustments of the engine coolant temperature in order to decrease the chamber wall temperature. More details of such strategies are provided in [30]. As a result, LIF visualizations were performed in order to study liquid fuel film formation as presented later.

UHC emissions data obtained on the all-metal engine #1 equipped with a wall-guided piston geometry are shown in Figure 12 for a wide range of SOI timings.

Several notable features can be observed. Firstly, for SOI timings in the range of 330 to 350 CAD, Figure 12 reveals very similar UHC emission levels for the two fuels. It should be noted that for this range of SOI timings, liquid film formation is expected to be minimal since significant spray-wall interaction occurs which results in a guiding effect of the fuel-air mixture, thus enhancing mixture preparation. In contrast however, for SOI timings in the range of 300 to 330 CAD, significant discrepancies are observed in terms of the engine-out