

Mixture-Formation Analysis by PLIF in an HSDI Diesel Engine Using C₈-Oxygenates as the Fuel

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ABSTRACT

With increasing interest in new biofuel candidates, 1-octanol and di-n-butylether (DNBE) were presented in recent studies. Although these molecular species are isomers, their properties are substantially different. In contrast to DNBE, 1-octanol is almost a gasoline-type fuel in terms of its auto-ignition quality. Thus, there are problems associated with engine start-up for neat 1-octanol. In order to find a suitable glow-plug position, mixture formation is studied in the cylinder under almost idle operating conditions in the present work. This is conducted by planar laser-induced fluorescence in a high-speed direct-injection optical diesel engine.

The investigated C₈-oxygenates are also significantly different in terms of their evaporation characteristics. Thus, in-cylinder mixture formation of these two species is compared in this work, allowing conclusions on combustion behavior and exhaust emissions. Fuel injection strategy (single and split injection) and in-cylinder air swirl are varied.

Results show that the fuel vapor remains in the peripheral region of the bowl volume near top dead center for 1-octanol, i.e., the region close to the cylinder axis is nearly vapor free. Thus, the peripheral region would provide a suitable glow-plug position. This vapor distribution is basically caused by impingement of liquid fuel on the piston wall. Presumably, wall wetting is also a major reason for increased unburnt hydrocarbon (HC) and CO emissions. Furthermore, the influence of wall wetting can be considerably reduced by using DNBE due to its evaporation and ignition properties. This leads to significantly different precombustion fuel/air mixtures and reduced HC and CO emissions compared to 1-octanol.

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INTRODUCTION

Both 1-octanol and DNBE are interesting biofuel candidates, because they can be produced from lignocellulosic biomass, which is not directly used as a food source ([1] and references therein). A new production pathway was recently developed for 1-octanol [2]. Based on the platform molecules acetone and furfural, 1-octanol can be synthesized even in a one-pot reaction with high yields above 50 %. When separating the process steps, the total yield can even be increased above 90 %. DNBE can be synthesized via etherification of n-butanol [3]. Other biofuel candidates derived from cellulose, hemicellulose, and lignin are furans, tetrahydrofurans, alcohols, ethers, esters, and ketones [1, 3, 4]. These compact molecules have low ignitability. Thus, they may be suitable for spark ignition engines or they have to be mixed with more reactive species for diesel engines [1, 3, 4, 5]. By contrast, 1-octanol and DNBE may even be used as single-component fuels for diesel combustion.

Combustion chemistry was investigated for 1-octanol and DNBE in [6, 7]. These molecules are isomers (C₈H₁₈O), but the oxygen atom is located at the end of the carbon chain in 1-octanol, whereas it is in its center in DNBE. This leads to significantly higher reactivity of

DNBE. The fuel properties are summarized in Table 1 [1]. Note that the cetane number (CN) of 1-octanol is ~34, whereas it equals ~115 for DNBE. According to the definition given in [8, 9], 1-octanol is therefore almost a gasoline-like fuel, whereas DNBE is rather a conventional diesel fuel, in terms of their auto-ignition characteristics. However, the vaporization properties of these fuels are also significantly different, as shown in Table 1. Higher fuel/air-mixing rates are expected for DNBE as compared to 1-octanol, due to the lower boiling temperature and enthalpy of vaporization [10] and/or dynamic viscosity [3] of DNBE. Measurements conducted in a high-pressure combustion vessel demonstrated indeed that the liquid penetration length (LPL) of the jets is significantly larger for 1-octanol compared to DNBE [3, 11].

Numerical simulations indicated that the CN-induced longer mixing time available for 1-octanol does therefore not lead to a reduced mixture fraction at the lift-off length (LOL) at the time of ignition, as compared to DNBE [3]. The air/fuel ratio at the LOL is generally important for soot formation at least under quiescent conditions, e.g. [12, 13, 14, 15, 16, 17]. However, this may be not the case in real

HSDI engines, because air-entrainment into the inner jet core is not necessarily prevented by the diffusion flame downstream of the LOL at high in-cylinder air swirl [5].

Table 1. Properties of investigated fuels at 20 °C ([1] and references therein).

	Unit	1-octanol	DNBE
Boiling temperature	°C	195	141
Heating value	MJ/kg	38.4	38.4
Density	kg/m ³	830	770
Cetane number	-	~34*	~115*
Oxygen content	% m/m	12.3	12.3
Vapor pressure	mbar	0.125	6.4
Surface tension	mN/m	27.5	22.2
Dynamic viscosity	mPas	7.3	0.64
Enthalpy of vaporization	kJ/kg	562	341

*Derived cetane number

Neat 1-octanol and DNBE were used as single-component fuels in a real HSDI engine in [1, 3, 4]. High levels of exhaust gas recirculation (EGR) were applied to achieve low NO_x emissions (according to EU6). Under these conditions, very low soot emissions were found for both fuels over a wide load range. HC and CO emissions were found to be lower for DNBE than for conventional diesel fuel. By contrast, these emissions were slightly higher for 1-octanol compared to diesel fuel. These results are also summarized in the [Appendix](#) for the same operating conditions. [Figure A1](#) also shows that indicated efficiency, cyclic variability of IMEP, and combustion sound level (CSL) are comparable for these three fuels. Hence, these results are overall promising.

In addition, binary fuel blends of DNBE and 2-methyl tetrahydrofuran (2-MTHF) were studied in [4], in order to design an optimal tailor-made fuel. Although the results were promising, a final statement on the optimal fuel characteristics could not yet be made. Thus, a detailed mixture-formation analysis in a comparable optically accessible engine was suggested for these fuels [1, 4]. This is conducted in the present work. In particular, the lowest-load operating condition considered in [1] is also investigated here, because problems associated with starting the engine are expected for neat 1-octanol. They can be potentially solved by a glow plug [8, 18, 19, 20, 21, 22]. Visualization of the fuel distribution around top-dead-center (TDC) is therefore conducted in this work to find a suitable glow-plug position.

Interestingly, the combustion of neat 1-octanol under the current part-load conditions is similar to previously discussed partially premixed compression ignition (PPCI), premixed charge compression ignition (PCCI), and low-temperature combustion (LTC) concepts [8, 9, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34]. Thus, the presented mixture-formation analysis may contribute to the understanding of these concepts. Relatively homogeneous, diluted pre-combustion mixtures are provided by these (and other related) concepts, generally leading to low soot and NO_x but increased HC and CO emissions at low load. The effects of gasoline-type fuels were particularly investigated under such conditions in [8, 9, 27, 28, 29, 30]. Problems with starting the engine or under idle conditions were reported in [8, 9, 19, 20, 21, 29].

OPTICAL DIAGNOSTICS

In this work, tetramethyl p-phenylene diamine (TMPD) is used as a fuel tracer for both the liquid and the gaseous phase. It is a well-known tracer for diesel engine applications [34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49]. It can be effectively excited by a relatively long, readily available laser wavelength (355 nm), in contrast to most other tracers, e.g. [33, 41]. Generally, higher laser power is available at longer wavelength. Laser light attenuation by fouling of optical components also decreases generally with increasing wavelength. Compared to many other tracers [41], only a small amount (~1 % or even less) of TMPD is required in the fuel to get suitable images. Thus, fuel properties are hardly changed.

Since TMPD fluorescence is strongly quenched by oxygen, diesel engines are generally operated with pure nitrogen intake streams for vapor-phase imaging [41]. In the present work, planar laser induced fluorescence (PLIF)-quenching by O₂ is also exploited to distinguish between liquid- and vapor-phase fluorescence. For this purpose, vapor-phase fuel distributions are recorded in pure N₂, whereas liquid-phase fuel images are obtained in air with and without EGR. According to experimental results in [50], it can be estimated that the vapor-phase PLIF per molecule is quenched by a factor of at least 50 near TDC at a pressure of 13 bar compared to the liquid-phase PLIF.

Liquid- and vapor-phase fuel distributions were recorded simultaneously in previous studies using exciplex tracers, such as TMPD combined with another organic molecule [35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48]. However, a relatively high fraction of the second additive is required (~10 %). This method is therefore not applied in this work, in order to avoid the expected effects on overall fuel properties.

The boiling temperature of TMPD is 260 °C. Hence, it is comparable to the one of 1-octanol, as shown in [Table 1](#). Thus, TMPD is expected to be a suitable tracer for 1-octanol (even in the case of wall impingement). By contrast, the boiling temperature of TMPD is considerably higher than the one of DNBE, which is also given in [Table 1](#). Thus, preferential vaporization may be problematic. However, previous measurements by both PLIF and spontaneous Raman scattering indicated that preferential vaporization is negligible in free diesel jets, using six blends with widely varying volatility and enthalpy of vaporization [51, 52, 53]. Thus, TMPD is also expected to be a suitable tracer for DNBE in free jets. However, preferential vaporization of fuel wall films most likely occurs for this blend in the case of wall impingement.

Note also that the LPL of the jets is determined by PLIF for both blends in this work. It is very challenging to detect very small droplets (at the real LPL) by Mie scattering, in particular if they are smaller than twice the light wavelength, due to the dramatically decreasing scattering cross-section in that diameter range [54]. This is a major reason why the LPLs currently measured by PLIF are longer than those previously determined by shadowgraphy [3, 11], as discussed in more detail in the Results and Discussion section.

Quantification of the vapor-phase PLIF is conducted by measurements in a homogeneous, well characterized charge, which is achieved by a number of small injections during the intake stroke, e.g. [33]. More experimental details are given in the following section.

EXPERIMENTAL

In the present study, an optically-accessible HSDI engine and a corresponding all-metal engine are employed. Both engines are identical concerning the injection system (i.e., fuel pump, fuel rail, and injector), and they are also approximately equal with regard to combustion chamber geometry. In Table 2, the corresponding data are shown. (The sac volume, including nozzle holes, of this injector, which is a potential source for injector dribbling [23], is approximately 0.2 to 0.3 mm³.) The fuel injection equipment (FIE) is series production and state-of-the-art. The FIE related data set on the electronic control unit is completely adjustable allowing free adjustment of the injection pattern. In order to minimize effects of retarded combustion on emissions and combustion noise caused by different ignition delays of the fuels in each operating condition, the center of combustion (MFB50) is kept constant by adjusting the start of injection. Further information about the single-cylinder engines is available in [1, 15, 55, 56].

Table 2. Specifications of the single-cylinder engines.

	Unit	All-metal/optical engines
Displacement	cm ³	390
Stroke	mm	88.3
Bore	mm	75
Compression ratio	-	15:1/13.5:1
Valves/cylinder	-	4
Max. cylinder pressure	bar	190/100
Fuel injection equipment	-	Bosch piezo common rail system
Max. injection pressure	bar	2000
Nozzle	-	8 hole, 109 µm, 153°
Hydraulic Nozzle Flow Rate	cm ³ /30sec	310 at 100 bar
Boosting	-	Max. 3.8 bar abs.

The used fuels are 1-octanol (with a tracer concentration of approximately 1.5 % TMPD for the optical engine) and DNBE (with a tracer concentration of approximately 0.1 %, due to limited solubility, for the optical engine). The fuel properties are listed in Table 1.

A sketch of the experimental set-up for the optical engine and the shapes of the optical and all-metal piston bowls are given in Fig. 1. The optical engine is equipped with an elongated piston and ω-shaped quartz glass piston bowl. The curvature of the central bowl surface of the optical engine is reduced as compared to the all-metal engine, in order to avoid strong optical distortion of the images [5, 15]. However, the piston-crown window still causes spherical image distortion, but in the major part of the field of view it is approximately linear.

In order to avoid contact between the piston rings and the inner surface of the window cassettes (for the laser entry and exit) the fire land height is increased. According to [57], the resulting effect on combustion and in particular unburnt hydrocarbon emissions is weak for HSDI engines with combustion in the piston bowl and injection

close to TDC. The compression ratio of the optical engine is about 13.5, whereas the one of the all-metal engine is 15. The decreased compression ratio of the optical engine is a common consequence of modifications for optical access. Differences between optical and corresponding all-metal HSDI engines are discussed in detail in [57, 58, 59] and the references therein. It was concluded that modifications for optical access affect combustion and emissions, but this can be approximately compensated for by adjusting operating parameters such as intake temperature and/or pressure, as conducted in this work.

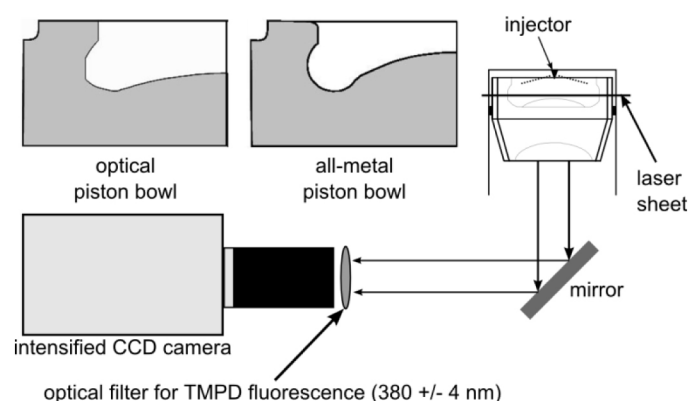


Figure 1. Experimental set-up of optical measurements and piston-bowl shapes of both engines.

The port concept of both engines is described in [60]. It was designed to achieve high flow rates at moderate air-swirl intensity. A parallel arrangement of the valves is employed, allowing high flow rates and a central, vertical injector position. Accordingly, each engine has one tangential and one straight (filling) intake port. Both intake valves have seat swirl chamfers in order to gain high swirl intensity for low valve lift. The valve lift is 8 mm in the present study, and the swirl intensity is enhanced by complete deactivation of the filling port (filling port deactivation, FPD), because this is a widely used method [60]. For the low-swirl condition, the tangential port is deactivated (tangential port deactivation, TPD).

All tests of the all-metal engine are conducted at steady-state conditions. Starting with pure air, the share of exhaust gas introduced into the combustion chamber is increased until lowest NO_x emissions are achieved. In the present study, the test results of pure air and at an EGR-rate corresponding to the Euro 6 NO_x level (0.2 g/kWh) are investigated in the optical engine for the lowest engine load (1200 rpm, 2.6 bar IMEP) used in [1]. For 1-octanol, the effect of the pilot injection is also investigated in both engines for a constant MFB50. The optical diesel engine is operated under fired and motored conditions for a limited number of successive cycles, depending on the operating conditions (fired or motored) and the amount of investigated crank angle (CA) positions, in order to prevent the engine and quartz-glass components from damage. The maximum number of injections is 150 for fired and 400 for the motored conditions. (The images shown in the Results and Discussion section are averaged over 10 single shots for measurements with combustion and over 20 single shots for the measurements in pure N₂ unless otherwise noted.)

Due to this limitation, all operating conditions like engine lubricant temperature, engine speed, intake temperature, and pressure have to be adjusted prior to the first fired cycle (or first cycle with injection, respectively). The intake temperature is about 62 °C for conditions with EGR and 77 °C for conditions without EGR unless otherwise noted. The cooling-water and oil temperature are conditioned to 90 °C. Note that skip firing/injection is not used. The engine speed of 1200 rpm corresponds to the optimum firing frequency (10 Hz) of the Nd:YAG laser.

Since the limited number of fired cycles of the optical diesel engine is insufficient to enable a controlled EGR, a second engine operating on diesel fuel is used to provide external EGR for the fired operating conditions with EGR. The exhaust gas of this engine is mixed with the intake air of the optical engine before entering the supercharger. The concentration of CO₂ in the intake is used as a measure of the inert gas concentration.

The close comparability of the all-metal and optical diesel engine allows the adaption of thermodynamically optimized operating parameters to the optical engine. In the present study, the all-metal research engine is operated at different EGR rates and injection strategies (with and without pilot injection), as noted previously. Relevant fuel and injection parameters are given in Table 3. Note that the start of injection depends on the investigated fuels and EGR rates. Identical injection parameters, such as fuel-rail pressure, start of injection timing, and injection duration, are used for both engines. For operating condition #5, all-metal engine operation data are not available. The investigated conditions are not thermodynamically optimized in terms of center of combustion and load. However, this operating condition can potentially show the influence of the pilot on the main injection.

Table 3. Operating conditions of both engines. The start of energizing the injector (SOE) is given in °CA ATDC (after top dead center). Fuel injection actually starts ~160 μs (=1.2 °CA) after SOE. The injector needs a minimum duration of energizing the injector (DOE) of ~100 μs for fuel injection.

Operating condition	Fuel	EGR-rate	SOE pilot	DOE pilot	SOE main	DOE main
#1	1-octanol	46 %	-	-	-16.5	560 μs
#2	1-octanol	0 %	-	-	-12.0	550 μs
#3	1-octanol	49 %	-21.7	272 μs	-14.6	533 μs
#4	1-octanol	0 %	-11.7	272 μs	-4.7	543 μs
#5	DNBE	55 %	-	-	-3.5	567 μs
#6	DNBE	55 %	-10.5	272 μs	-3.5	567 μs
#7	DNBE	0 %	-8.8	272 μs	-1.8	564 μs

The matching of the operating conditions for both engines is conducted as follows. In a first step of the experiments, the boost pressure of the optical engine is increased by approximately 0.5 bar in order to reach the same pressure near TDC, i.e., at injection timing. (Note that this consequently slightly increases the intake air flow rate.) In addition, the intake temperature is increased (by approximately 30 K and 45 K for conditions with and without EGR, respectively), so that the in-cylinder pressure rise during the early high-temperature combustion phase is approximately equal for both engines under the fired conditions. According to [58], the ignition delay is used as a “thermometer” in the present work. Thereby, not

only the pressure but also the highly relevant temperature in the vicinity of the fuel jets is approximately equal in both engines. The applied method compensates for the lower compression ratio, higher elasticity of the elongated piston, lower metal-surface temperatures, and higher blow-by of the optical engine [57, 58, 59]. The blow-by is likely increased for the optical engine, because the piston rings are run unlubricated in order to reduce window fouling [59]. The metal-surface temperatures are expected to be lower in the optical engine, due to the limited number of fired engine cycles, i.e. the engine is not fully warmed up and stationary conditions are therefore not exactly reached. The lack of piston cooling may lead to higher glass-surface temperature in the optical engine at fired operation, as compared to the all-metal engine [57, 58, 59]. However, this effect is likely offset by the limited number of fired cycles of the optical engine.

DIAGNOSTICS

The laser beam of the frequency tripled Nd:YAG laser (at 355 nm) is formed to a sheet with a width of approximately 15 mm and a thickness of approximately 0.5 mm by three cylindrical lenses and a rectangular aperture. The laser power in the probe volume is approximately 50 mJ. The vertical position of the laser sheet inside the piston bowl and the field of view are illustrated in Fig. 2. The in-cylinder phenomena in the swirl plane are visualized via a fixed mirror in the clearance of the elongated piston. The intensified camera (LaVision, NanoStar) is equipped with an UV objective (f=100 mm) and two optical filters (SemRock RazorEdge 355 nm and bandpass filter at 380 +/- 4 nm).

The camera has 1280 × 1024 pixels. Binning of two pixels in each direction is applied. About 260 × 260 pixels (after binning) are used for the current field of view. The spatial resolution is, however, limited by the optics, in particular the piston window. It is estimated to be about 0.3 mm. The exposure time of the camera is limited by the gate length of the image intensifier, which is 5 μs. The camera has a double-frame option, but it is not applied in this work. The image intensifier is operated at ~1.9 % (for 1-octanol) and 5.6 % (for DNBE) of its maximum gain. Its quantum efficiency at the detection wavelength of the tracer is ~15.5 %. A commercial lens system (LaVision “Enhanced UV Lens”, f = 100 mm, f_# = 2.8) is used for imaging.

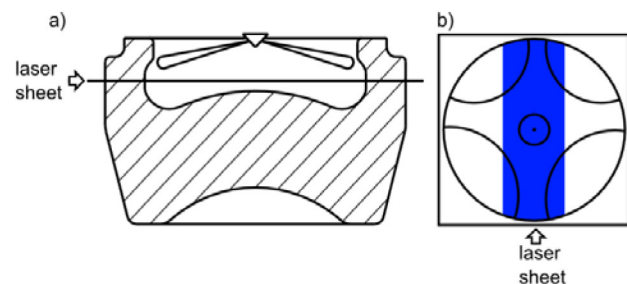


Figure 2. The vertical position of the laser sheet inside the piston bowl (a, side view) and the field of view (b, bottom view). The distance from the cylinder head to the laser sheet is ~10 mm.

If it is assumed that quenching is proportional to pressure and oxygen concentration, it can be estimated that the fluorescence of TMPD is quenched by a factor of approximately 85 for conditions with EGR and 130 for conditions without EGR [50] in the investigated oxygen containing atmosphere. Thereby, the liquid phase of the injected fuel can be selectively visualized under the fired conditions, as noted in the Introduction section. In order to visualize the gas-phase, the fuel is injected into a pure nitrogen atmosphere (motored conditions) with the same ambient conditions of the engine as under the fired operation, i.e. oil and coolant temperatures, boost pressure and intake temperature, injection timing and duration. This method allows the visualization of the liquid fuel distribution and the local fuel concentration in the gas phase. The differences between calibration and the measurement are less than 2 % for the measured pressure as well as the estimated ambient temperature and density (not shown) in the optical engine for all investigated operating conditions. The ambient temperature and density in this optical engine are derived basically from the measured pressure traces [5].

Although gas-phase PLIF measurements are conducted without oxygen, the fuel/air equivalence ratio is quantified for 1-octanol, based on the oxygen content of the gaseous charge in the fired engine.

The applied diagnostics for exhaust-gas analysis at the all-metal engine and in-cylinder pressure measurements in both engines are described elsewhere ([1, 15] and references therein).

RESULTS AND DISCUSSION

Pressure-Trace Analysis and Emissions

The available pressure traces of the all-metal engine and the optical engine under fired and motored conditions, mass fraction burnt (MFB), and the emissions are summarized in Fig. 3 for the operating conditions listed in Table 3. The center of combustion (CA of 50 % MFB) is intentionally approximately constant for all operating conditions and Fig. 3a), b), c), d) show that the pressure traces of the all-metal and optical engines are nearly matched, as described in the Experimental section. In addition, motored and fired in-cylinder conditions are approximately equal before ignition.

The combustion of the pilot and main injections of DNBE (operating conditions #6 and #7) are separately observed as indicated by the pressure traces and the MFB in Fig. 3c)/d)/e). This effect is less distinct for 1-octanol, due to its lower volatility and reactivity, as demonstrated in the following subsections. Note that the MFB is equivalent to the heat release.

Figure 3f) shows that the HC and CO emissions decrease drastically for DNBE as compared to 1-octanol. This will be explained in the following subsections. Soot is not detected for 1-octanol and only a very small amount is found for DNBE.

PLIF Measurements with 1-Octanol

Figure 4a) shows a typical image sequence recorded in the fired engine with 1-octanol under operating condition #1 according to

Table 3. The images are measured within one engine run. In order to suppress interfering signals from the combustion chamber surfaces, a background image is subtracted, which is recorded prior to the data images without injection. Due to strong quenching of TMPD-PLIF in air, Fig. 4a) basically shows the liquid-fuel distribution. Its evolution is clearly observed, although the free jets are only weakly illuminated by surface-scattered laser light, because they are above the laser sheet, as illustrated in Fig. 2. Figure 4a) indicates that the jets impact the bowl wall around $-11^{\circ}\text{CA ATDC}$. This is particularly observed for the jets at ~ 12 and ~ 6 o'clock, respectively, due to the proximity to the laser sheet, which passes through the bowl from the bottom to the top. It is less obvious for some of the other jets, because of very weak illumination by laser light. However, wall impingement is also expected for these jets, due to little jet-to-jet variation of the free jets in Fig. 4a).

Figure 4a) indicates that the LPL is measured correctly by the TMPD-PLIF in the fired engine for the jets at ~ 12 and ~ 6 o'clock, because the formation of fuel wall films is consistently observed for these jets just after wall impingement. The wall films are clearly detected as sharp structures with high signal intensities. This confirms that PLIF signals from the gas phase are negligible during injection in air.

One might think that the determination of the free-jet LPL using TMPD may be affected by formaldehyde (H_2CO) PLIF, which can be detected in the gaseous spray head using the same laser wavelength ([61] and references therein). In principle, some of the potential H_2CO PLIF is transmitted by the current filter combination in front of the camera. However, the analysis of the signal levels obtained under comparable conditions in the authors' lab demonstrate that they are negligible at least for the free jets shown in Fig. 4. Thus, the LPL measurement is not affected by this potential interference.

Note that the LPL observed in Fig. 4a) equals ~ 24 mm at the time of first wall impingement, according to the distance between the nozzle and the wall. This LPL is significantly longer than previously measured values for 1-octanol jets [11]. This can be partly explained by the higher load operating conditions investigated in [11] and also by the Mie-scattering characteristics briefly discussed in the second part of the Introduction section.

Typically, wall wetting is regarded as a problem due to increased PM- and HC-emissions. Neat 1-octanol might evaporate faster due to its lower boiling point as when compared to less volatile components of conventional fossil diesel fuel. However, in the current near-idle load point, PM-emissions are almost below the detection limit based on measurements with an AVL Smoke Meter as well as with an Engine Exhaust Particle Sizer Spectrometer by TSI with 1-octanol. The slight increase in HC- and CO-emission (as compared to conventional diesel fuel) might be caused by the longer ignition delay as well.

Previously, wall wetting by over-penetration of fuel jets was found in light-duty diesel engines under conventional cold-start and low-load [10], as well as PPCI/PCCI/LTC-conditions [23, 25, 31, 32, 33, 34].

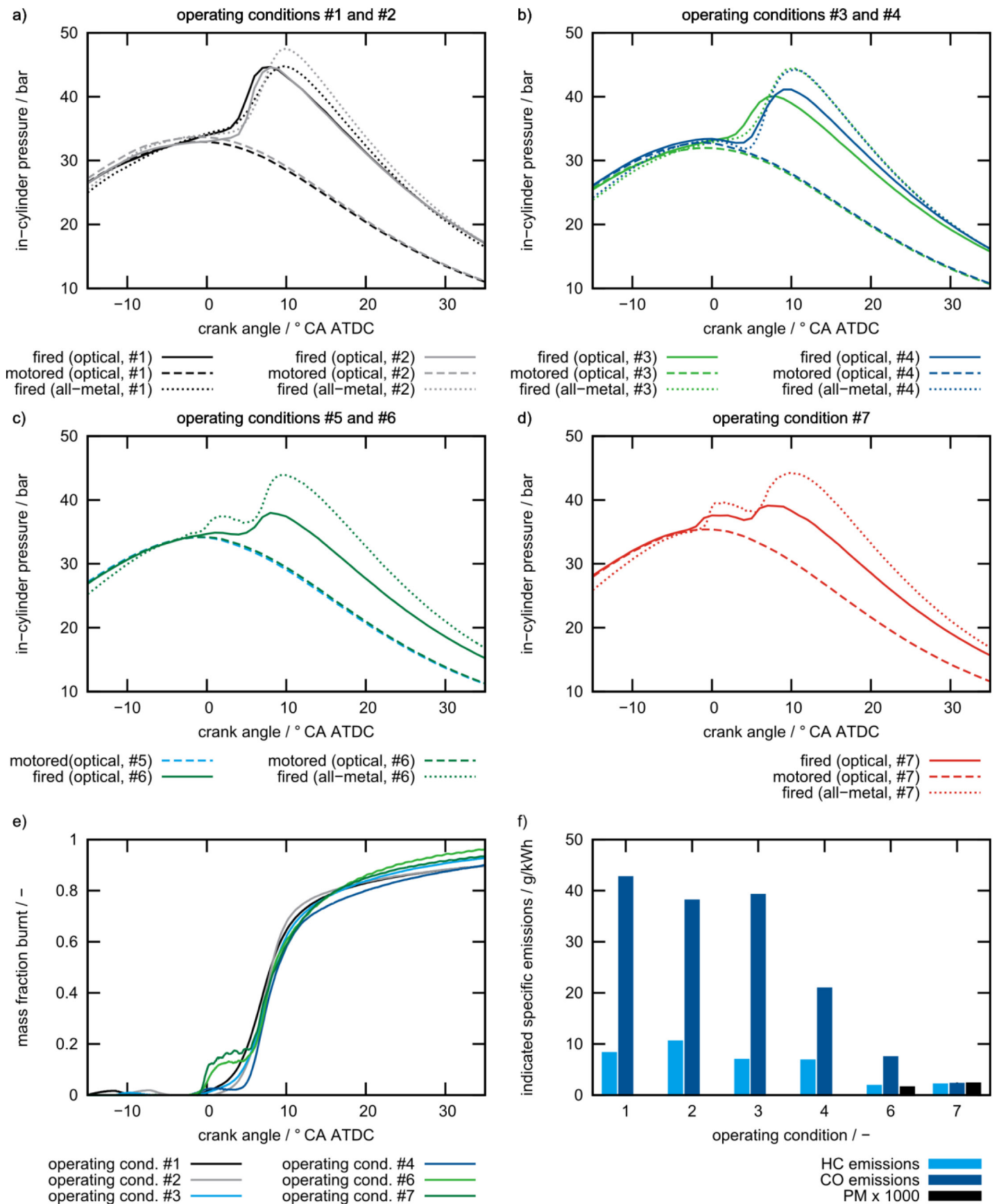


Figure 3. Thermodynamic analysis of the all-metal engine data and pressure traces of the optical engine for the fired and motored operating conditions. In panels a) - d), the solid lines correspond to the fired, the dashed lines to the motored conditions of the optical engine, and the dotted lines correspond to the all-metal engine only. PM: particulate matter.