Design and operation of a high pressure, high temperature cell for HD diesel spray diagnostics: guidelines and results

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ABSTRACT
This paper first compares strengths and weaknesses of different options for performing optical diagnostics on HD diesel sprays. Then, practical experiences are described with the design and operation of a constant volume test cell over a period of more than five years. In this test rig, pre-combustion of a lean gas mixture is used to generate realistic gas mixture conditions prior to fuel injection. Spray growth, vaporization are studied using Schlieren and Mie scattering experiments. The Schlieren setup is also used for registration of light emitted by the combustion process; this can also provide information on ignition delay and on soot lift-off length. The paper further describes difficulties encountered with image processing and suggests methods on how to deal with them. Results are presented that illustrate the wide range of capabilities of this test-rig when combined with high speed video registration, in particular its potential for studying issues related to vaporizing fuel spray dynamics.

INTRODUCTION
A major driver in the development of modern HD diesel engines is the need for increasingly cleaner but conventional CI combustion while retaining the high fuel efficiency of this concept. To realize this, a variety of technological pathways are being investigated: further increased injection pressure, complex multiple injection strategies, further fine-tuning of injector nozzle geometry and introduction of increasing amounts of re-circulated exhaust gas (EGR) [1]. Another promising path towards cleaner combustion is the introduction of different fuel formulations such as GTL, oxygenates and water-fuel emulsions. In the investigation of the potential of these different paths, the study with advanced laser-based diagnostics of the diesel spray combustion process, in dedicated optically accessible test rigs, takes up an increasingly important role both in academia and industry [2,3]. In fact, since 1997 [4] such research by different groups has lead to a new and better understanding of diesel combustion.

The prime requirement of any optical test rig for the study of diesel spray combustion is that it should create ambient gas conditions that are representative of those in a diesel engine during the injection and combustion process. In conventional CI combustion, fuel is injected shortly before TDC. Figure 1 shows the corresponding p and T range for current premium single stage turbocharged HD diesel engines.

The test equipment that most closely resembles the actual engine is the optical research engine (ORE). Such engine typically applies a bow-ditch design with a large window in the piston. Additional access to the combustion chamber is through windows in the liner close to the cylinder head (alternatively also a sapphire ring can be applied) and/or through windows in the cylinder head (sacrificing one or more of the valves). Several of such HD-size research engines have been presented in the literature [5-9]. In these test rigs combustion has been examined at imep levels up to 1.8 MPa, be it with a reduced compression ratio (and therefore lower pressure levels).
the in-cylinder flow field is complex, in-stationary and during compression the piston scrapes off the boundary layer on the cylinder liner and these colder gases are finally squished into the piston “bowl” towards the end of the stroke, thus setting up temperature gradients in the charge.

- spray penetration is in practice limited by the piston bowl radius and typically does not exceed 55 mm; after that spray/wall interaction and spray/spray interaction occur;

- the piston continues its motion during the injection and combustion process.

When aiming to study the basics of diesel spray CI combustion, often the interaction with complex flow phenomena and/or the impact of fuel on piston walls are unwanted phenomena. Then the above characteristics of the ORE are a disadvantage. Because these engines are furthermore complex, expensive to acquire/build and to adapt (towards meeting new research interests) a lot of research is performed on so-called Rapid Compression Machines (RCM). In such a device a piston performs only one compression stroke and is arrested upon reaching its TDC position. Several RCM have been used to study diesel combustion [10-13] and their description in the literature clearly shows how difficult it is to build and to operate and control such a unit. In addition, these machines tend to be noisy and they suffer from strong vibrations at the end of the compression stroke (making the implementation of laser diagnostics more difficult). To illustrate this: for the study of one undisturbed HD diesel spray over a representative period of time the bore of the RCM has to be in the range of 100 mm (or more). In the axial direction the clearance at TDC has to be at least 80 mm. With a typical compression ratio of 17:1 the corresponding stroke becomes 128 cm (in fact, the CR would have to be even higher to compensate for the lower temperatures of cylinder head and of piston surface). To achieve a representative T-level at TDC a mean piston speed of 10 m/s is needed. This asks for high piston deceleration levels. In most cases however, lower CR levels are realized, and this and the above mentioned effects are compensated for by heating the intake charge. As with the ORE this results in lower charge densities and pressure levels (see Fig. 1). Also, as with ORE’s, the compression stroke sets up velocity and temperature gradients in the charge at TDC. But compared to the ORE devices, trapped charge properties can be more accurately determined, at the cost of a longer time between experiments (2 to 10 min).

The rapid cycling machine (RCYM) is a special kind of related test rig (and in fact one of the earliest optical test devices) [14,15]. The RCYM uses a regular piston engine design (often with a 2-stroke side-port-scavenging gas exchange concept) and extends the combustion space with a ~ typically ~ cylindrical combustion chamber that is part of the modified cylinder head. This chamber is made optically accessible from different sides, injection takes place into it, and - by increasing CR - combustion is largely confined to this chamber. With such a device, TDC temperature and pressure levels can cover the full range found in modern diesel engines. Unless a very large displacement (marine type) engine would be used, the corresponding CR however implies a small chamber volume, allowing the study of only one spray within a narrow confinement.

For the study of unconfined diesel spray combustion with no or well-controlled flow interaction usually other devices are used. An interesting concept in this respect

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1 Also Rapid Compression and Expansion Machines have been built (e.g. [12]).
is the constant pressure flow rig (CPFR). Only a few of such rigs are mentioned in the literature [16-20]. In these test rigs a constant flow of hot, pressurized gas is set up in a pipe (with internal thermal insulation). Fuel is then injected parallel and (often) against this flow. Spray evolution and combustion is then observed and studied through multiple windows around the circumference of the pipe. This device allows wide optical access and fast experimentation. On the negative side: maximum T and p levels are limited and the test rig needs ample time to adapt to new target temperature levels. Furthermore, as this approach implies powerful clean air compressing and heating equipment, for HD spray research these tend to be both large and expensive facilities.

An alternative class of test device is the constant volume test cell, where a fixed amount of oxidizer is trapped in a steel vessel at high pressure and heated prior to diesel injection. In the most straightforward approach the walls of the steel vessel are heated towards the target temperature [21, 22, 44]. Even when using special high-strength steels, this approach limits the maximum operating temperature, typically to 900 K. It furthermore also limits the cell volume and maximum pressure level (as also thermal inertia should remain within acceptable levels). By implementing a double wall design it has been possible to realize pressures of up to 80 bar (prior to fuel injection) even for a large cell [23]. As with the CPFR the trapped gas p, T and composition in such constant volume hot cell (CVHC) can be accurately determined. There are however also some drawbacks: optical access is limited (small windows), because of its thermal inertia the time needed to settle to a different target T-level is long, the injector cooling requirement sets up strong temperature gradients inside the cell, the impact of the spray with the hot walls affects the combustion process and similarly, the radiation from these walls might affect the combustion process. To remove this last drawback the fresh charge can be heated in a separate autoclave unit before releasing it into the test cell, which is now heated only to moderate temperature levels (400 – 450 K) [25-27]. The need to keep the temperature of the valves of the charge delivery system below 475 K, together with the relatively cold cell walls, results in an important difference between the autoclave temperature and that of the trapped charge. Typically, with this approach temperatures prior to injection are in the 750-800 K range (in [25, 26] a pilot diesel injection was used to further increase the cell charge temperature to 850 K). As the autoclave has to be at a higher temperature and because its volume has to be considerably larger than that of the test cell (in order to minimize the autoclave pressure level), in practice the cell volume in these units tends to be small and maximum spray observation length typically is in the range of 40-45 mm.

To achieve higher temperature levels and a wider observation range, most constant volume cells nowadays use the pre-combustion technique suggested by Oren et al. [28]: a lean mixture of gaseous fuel(s), oxygen and nitrogen is burnt and the fuel spray is injected into the products of this combustion [29-36, 45, 49]. Controlling the pressure, temperature and composition of the pre-charge as well as the time delay between pre-charge combustion and fuel spray injection gives a very wide range of (p, T)-conditions prior to injection and the possibility to simulate various levels of (simulated) EGR mass fraction. With this technique the full range of (p, T) in Fig. 1 can be covered. This method therefore also allows the study of late cycle injection processes aimed at increasing exhaust temperature or particulate reduction. Such a constant volume pre-combustion cell (CVPC) has the additional advantage that switching between temperature levels is relatively fast. There are however also some drawbacks: the time between measurements is relatively long, the inhomogeneity of the charge temperature can be larger than in an engine, and of course pressure history during combustion and fuel air-mixing are different from a real engine (i.e. given the absence of spray/wall and spray/spray interaction).

Table 1 compares the strengths and weaknesses of the different test devices. Clearly, which optical test rig is most appropriate will depend on the context of the research. In this respect, CPFR, CVHC and CVPC all are more suited for the basic research of free spray combustion.

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2 As an alternative, sometimes the heaters are put inside the test cell, e.g. [24].
TEST RIG DESIGN AND OPERATION

TEST CELL DESIGN AND INSTRUMENTATION

It was the ambition of the internal combustion group in Eindhoven to study the details of the (free) diesel spray CI combustion process and its interaction with injection strategy and fuel quality (with the further aim to validate and improve CFD models of this process). In view of the observations above it was decided to develop and build a constant volume test cell with pre-combustion charge heating. When designing this cell the main requirement was that it would allow the study of combustion of an unobstructed high pressure HD diesel spray during a representative time interval. That implied a minimum jet penetration of at least 100 mm. An additional requirement was that the design would allow (in the future) for the study of spray/wall interaction; and finally it would have to allow for the study of laminar flame propagation at high pressures and temperature of centrally spark-ignited combustible mixtures.

As Fig. 2 illustrates, the design of the cell shows a lot of similarity to that of the test rigs developed at Sandia (presented in 1998 [31]) and at IFP [32,45]. The core is a cubically shaped combustion chamber produced inside a stainless steel cube through spark erosion. The combustion chamber is accessible on each of its sides through a large threaded hole. Each of these holes is fitted either with a window or with a similarly shaped metal plug; these are kept in place with a matching (threaded) retainer. In the current set-up three of the four vertical holes are equipped with a window. The remaining holes are fitted with metal plug units. The horizontal top unit holds the injector with its dedicated cooling jacket (not shown in Fig. 2, ensures an appropriate fuel temperature) and the bottom unit holds a burst disk. The remaining vertical metal unit provides the gas inlet and exhaust valve system. In addition, smaller access holes have been machined in each of the eight corners of the combustion chamber. Each of these holes fits with the outer shape of a generic adaptor.

Table 1: Quality attributes (mostly relative; 0= neutral, + better, - worse) of different optical spray test rigs: optical research engines (ORE), rapid compression machines (RCM), rapid cycling machines (RCYM), constant pressure flow rigs (CPFR), constant volume hot cells (CVHC) and constant volume pre-combustion cell (CVPC).

(*) Not considering the time needed for intermediate cleaning of the windows.

<table>
<thead>
<tr>
<th>Type of optical test rig</th>
<th>ORE</th>
<th>RCM</th>
<th>RCYM</th>
<th>CPFR</th>
<th>CVHC</th>
<th>CVPC</th>
</tr>
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<td>Optical accessibility</td>
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<td>0</td>
<td>++</td>
<td>++</td>
<td>-</td>
<td>+</td>
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<tr>
<td>Similarity to the real engine situation</td>
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<td>-</td>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>Free spray penetration distance</td>
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<td>+</td>
<td>+</td>
<td>+++</td>
<td>++</td>
<td>++</td>
</tr>
<tr>
<td>Control on trapped gas p / T</td>
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<td>+</td>
<td>0</td>
<td>++</td>
<td>++</td>
<td>++</td>
</tr>
<tr>
<td>Control on trapped gas composition (i.e. EGR)</td>
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<td>-</td>
<td>0</td>
<td>+</td>
<td>++</td>
<td>+++</td>
</tr>
<tr>
<td>Flow field impact on combustion</td>
<td>--</td>
<td>(-)</td>
<td>-</td>
<td>0</td>
<td>-</td>
<td>-</td>
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<tr>
<td>Test facility volume</td>
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<td>0</td>
<td>0</td>
<td>++</td>
<td>++</td>
</tr>
<tr>
<td>Time to switch between operating conditions (i.e. T)</td>
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<td>0</td>
<td>0</td>
<td>0</td>
<td>--</td>
<td>++</td>
</tr>
<tr>
<td>Time between tests [s] (*)</td>
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<td>120-600</td>
<td>1</td>
<td>1-3</td>
<td>60</td>
<td>600</td>
</tr>
</tbody>
</table>

Figure 2: 2-D vertical slit drawing of the cell: a. high pressure cell; b. window holder; c. heaters with insulation and aluminum cover plate; d. sapphire window; e. fuel injector; f. thimble; g. inlet valve; h. outlet valve; i. combustion chamber; j. burst disk. Mixing fan, p-sensor, T-sensor and spark plug have access through out-of plane adaptor holes.
Different such adaptors have been made that will either hold a dummy part or a spark plug, pressure transducer, thermocouple or stirring fan.

In view of the high maximum pressure level of 35 MPa (approximately twice the maximum test pressure mentioned in Fig.1; ratio resulting from test procedure, see Fig. 8 and Appendix for motivation/details), special attention was given to the design of the windows and their support and sealing. Different designs have been mentioned in the literature [31,32]. Here a design has been used similar to that of the Sandia unit. The window shape is such that its interaction with the supporting retainer minimizes tensile stress in the window and therefore window thickness. In our design the windows are 50 mm thick and 100 mm in diameter. Thus most of the combustion chamber is visible. Two sets of windows have been made: a set of quartz and a set of sapphire windows. Quartz windows have the advantage of a better transmission of UV light, this is especially of interest when aiming to implement advanced LIF diagnostics or when aiming to detect chemiluminescence of such radicals as formaldehyde. Quartz however has a low resistance to tensile stress and is therefore used only up to maximum cell pressures of 13 MPa. For higher pressures (in practice limited to 30 MPa to protect the piezo-electric pressure transducer) sapphire windows are used. Enclosing the windows between the (shoulder of the) hole in the stainless steel core and the retainer unit puts high demands on the accuracy of all these parts. Small inaccuracies in the alignment of these parts will rapidly lead to a non-uniform load on the window surfaces. That is why the window retainer element was designed in such a way that it will adapt to the remaining small misalignments. Figure 3 compares the effect of a uniform load of 35 MPa on such a window. Shown is the resulting window vertical displacement. For comparison Fig. 3 also shows the displacement of the window in the alternative designs mentioned in [31] and [32]. As the results show, in the new design the window moves uniformly downwards. Consequently the deformation is shifted towards the retainer unit (implying appropriate solutions for maintaining good window sealing). This is further illustrated by the stress distribution given in Fig 3d. As intended the window only experiences compression stresses. Similar calculations were performed aimed at further optimizing the design of the retainer.

To avoid water vapor – from the pre-combustion phase – from condensing on the windows, the cell can be heated using (shielded electrical) heating elements that are fixed to the 6 outer sides of the unit. To limit heat loss to the surroundings the complete unit is covered with a thermally insulating layer and a thin outer aluminum shell. A thermocouple in one of the adaptors is used as part of the closed-loop controlled heating system. The cell wall temperature is typically set at 403 K. This value is chosen as it is high enough to keep the windows free from condensing water vapor but at the same time low enough to allow for maintenance (e.g. cleaning) by hand. Furthermore, at this temperature, non-ideal gas effects during the charging process can be disregarded.

GAS SUPPLY SYSTEM DESIGN AND CONTROL

As shown in Fig. 4, contrary to the approach taken by Oren [28], mixture preparation takes place in the test cell and not in a separate pressure vessel. This was done to avoid the extra costs and security risks of having to store a large quantity of ignitable gas. At the start of an experiment the exhaust valve is opened and the charge of the cell is evacuated by a vacuum pump that is integrated in the exhaust system. When the cell pressure reaches an absolute level of 1 to 2 kPa, the exhaust valve is closed and the different pre-combustion gases are admitted sequentially and in the proper order.
The charging process follows a predetermined algorithm and is done through a set of mass flow controllers. The time between (sequentially) feeding the different gases to the cell is sufficient long to allow these gases to adjust to the temperature of the cell. The charging is slow (typically taking up a total of 300 - 360 seconds), but then again not too slow in order to avoid possible negative effects of (limited) leakage. The cell pressure therefore increases, in steps, in line with the partial pressure of the different components. To check the charging process, the pressure increase in the cell is monitored using an accurate piezo-resistive pressure transducer (Druck PMP 4070) that is positioned upstream of the intake valve. This pressure transducer is protected from the pressure rise in a combustion event because the spark ignition system is automatically disconnected as long as the intake valve is open. The pressure variation in the test cell during pre-combustion and diesel spray injection is measured using a fast piezo-electric pressure transducer: depending on the chamber maximum pressure either a Kistler 7061 (0-200 bar) or Kistler 6041 (0-300 bar) sensor was used. During the filling process the stirring fan is operated to ensure that all the gases are well mixed prior to the pre-combustion event. The fan drive unit is integrated in one of the adaptors and is positioned in one of the bottom corners of the test cell. The fan has 2 blades with a combined diameter of 45 mm and is run at 3000 rev/min. The fan is stopped five seconds before spark ignition because leaving it on during pre-combustion introduced too much variability in the heating and cooling rates.

Of course, as with every piece of high pressure equipment, it is very important to avoid leakage. Great care was taken to ensure this. A particular challenge was sealing the window design: at first a Viton® O-ring was used in a matching cavity between the window and the surrounding metal wall. Although Viton® will withstand up to 490 K (well above the wall temperature) initial pre-combustion tests soon revealed that – with high oxygen concentrations and charge densities above 25 kg/m$^3$ - combustion gases entering the crevices rapidly degraded these O-rings: they started sticking to the windows. Substituting them with Kalrez® rings did not improve on this situation. The problem was solved by protecting the O-rings with a matching solid PTFE “shield”. To further minimize leakage the fan and its shaft are separated with a thin wall from the outside; the shaft of the fan is driven by an electromotor by means of magnetic coupling.

A burst disk limits the actual maximum working pressure to 30 MPa. According to the manufacturer the nominal burst pressure level holds only for pressure rise rates up to 100 MPa/s. During some tests higher pressure rise rates may occur. Under such conditions, pressure levels above 30 MPa will be reached before the burst disk fragmentizes. It is therefore important to empirically confirm the proper behavior of this safety equipment. Furthermore, even when a proper burst disk is chosen, accidents are still possible. In an event of premixed charge auto-ignition, very high internal pressures occurred resulting in window cracking (but not giving away). For this reason the test facility is located in an explosion protected room and operated from a distance.

FIE SYSTEM DESIGN AND INSTRUMENTATION

An in-house common rail fuel injection system has been built. An air driven, single plunger, double acting pump (Resato P160-400-2) feeds the rail with fuel at pressures up to 280 MPa. As it is a positive displacement pump, fuel delivery to the rail will be intermittent, and as a result the rail pressure will fluctuate. This fluctuation is however low frequent (0.2 Hz) and the amplitude of the rail pressure fluctuation does not exceed 2 MPa. The rail is in turn connected to a Common Rail injector. A safety valve will open when the maximum operating pressure of the injector is approached. Through this valve fuel is then returned to the fuel reservoir.

For this study a commercially available injector was selected because of practical reasons: such injectors are easier available and cheaper than custom-made injectors and their design and capability is representative of the actual technology in use. Measurements of rail pressure variation, needle lift profile and fuel injection rate (using a so-called Zeuch chamber) together with AMESIM simulations [37] confirmed that this system provides fuel injections that are highly repeatable and representative of those obtained with commercial systems. Figure 5 shows the complete unit (test cell + FIE equipment + gas supply system components).

Figure 4: 2-D overview of the different components of the gas supply system and of the FIE system: a. fuel reservoir; b. high pressure pump; c. common rail; d. fuel injector; e. mass flow controllers; f. vacuum pump; g. outlet.
The decision to use commercial, multi-hole nozzles and the earlier mentioned requirement of 100 mm observation range implied that only one hole could be tested. To ensure that this hole was no outlier, but typical of the nozzle, the momentum produced by the different holes of the same nozzle was measured in a dedicated test rig, registering the momentum force (in a plane perpendicular to that of the spray axis) in 5° increments for a full rotation around the injector tip. Fig. 6 represents typical results obtained in such a test.

(1) blocking all but one of the holes, (2) use a drainage unit (“thimble”) that collects all but one of the sprays and transfers the corresponding fuel to a drain pipe. As will be shown later the thimble was found to be the best technique. It was therefore retained for all further testing. As shown in Fig. 2, to guarantee the required free spray length the nozzle had to be tilted. The injector cooling jacket was used to keep the fuel temperature in all experiments in the 328-333 K range.

**OPTICAL TECHNIQUES**

To study the evaporating spray a Schlieren setup is implemented as shown in Fig. 7. An AEG 800 W Xenon arc lamp is focussed using a Ø 92 mm lens (f = 600 mm) on a Ø 2 mm pinhole which acts as an extended light source (‘a’ in Fig. 7).

A parallel beam is created by a Ø 100 mm achromatic lens (f = 1000 mm). On the other side of the test cell the beam is focused again by a similar Ø 100 mm achromatic lens onto the second spatial filter. Depending on the situation this is either a Ø 2 mm pinhole or a Ø 2 mm pinhead. For non-reacting sprays the Ø 2 mm pinhole is used, resulting in a dark spray on a bright image background. For reacting sprays a Ø 2 mm pinhead is used and results in a bright spray on a dark image background. The latter approach blocks all of the collimated light and avoids overexposure of the image but at the same time still allows qualitatively good images to determine ignition location and soot lift off length. Images are recorded using a high-speed CMOS Phantom V7.1 camera; this camera is flexible in resolution, varying from 800 × 600 pixels @ 4800 fps up to 32 × 32 pixels @ 150000 fps with a minimum response time of 2 µs. Its dynamic resolution is 12 bit.
and in the tests described here, the spatial resolution for the Schlieren images is 0.39 mm/pixel.

As in [31] the Mie scattering technique is used to visualize the liquid phase of the vaporizing diesel spray. Using a combination of a negative and a positive cylindrical lens, monochromatic light (488 nm) from a continuous-wave Ar+ laser (Spectra Physics 1701) is expanded into a 1.5-2 mm thick laser sheet in-line with the axial movement of the diesel spray. This light is elastically scattered by the fuel droplets that are present in the laser sheet volume. Some of that scattered light is recorded by the Phantom camera which is (as shown in Fig. 7) positioned perpendicular to this sheet. For the Mie-scatter measurements the camera frame rate was typically set at just over 115 kHz (resulting in a long and narrow observation range). To minimize disturbance from other light sources a combination of filters is used to create a very narrow band pass in the range 488±1 nm. The latter filter combination is not shown in Figure 7.

In combustion experiments, the Schlieren set-up not only distinguishes the vaporizing spray but also the light (>315 nm, mainly soot radiation) emitted during combustion is registered. With this info start of combustion (illumination delay) and soot luminosity lift-off length are determined. At present Line-of-Sight laser attenuation (LOSA) is being used to further analyse the soot formation and oxidation process.

**PRECOMBUSTION HEATING**

**PRECOMBUSTION METHOD BASICS**

The principle of the pre-combustion method is illustrated in Fig. 8. The test cell is filled with a lean combustible mixture. This charge is ignited and the ensuing flame propagation process results in a sharp pressure rise. Upon completion of combustion, the cell pressure starts to drop as the hot products lose heat to the cold surroundings. Fuel is injected when the pressure and temperature reach their target values.

In the past different gaseous fuel (mixtures) have been used. The main components however were always oxygen, nitrogen, and (a mixture of) hydrogen, ethylene and/or acetylene. Some basic properties of these fuels are given in Table 2. Obviously these fuels are of interest because they support flame propagation even in very lean mixtures and because they ignite relatively easily. In their pioneering study Oren et al. [28] preferred acetylene (over hydrogen) “as it minimizes water production and thus less heating of the bomb windows is required to prevent condensation”. In early work at Sandia [29], Siebers used ethylene and hydrogen in a ratio of about 1:4. Later [30,31], the Sandia group changed this to a 1:6 mixture of hydrogen with acetylene. Verhoeven et al. [32] applied ethylene with hydrogen in a 1:11.4 ratio (nb. derived from the reported end-gas composition). Others used hydrogen [33,36], and Fujimoto et al. [35] selected acetylene. In none of these studies was the choice explicitly motivated.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>H$_2$</th>
<th>C$_2$H$_2$</th>
<th>C$_2$H$_4$</th>
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<tr>
<td>Lower flammability limit ([@SPT] [% vol])</td>
<td>4.0</td>
<td>2.5</td>
<td>2.3</td>
</tr>
<tr>
<td>Laminar burning velocity (in air @ SPT) [m/s]</td>
<td>2.4$^{[42]}$</td>
<td>1.3$^{[40]}$</td>
<td>0.6$^{[40]}$</td>
</tr>
<tr>
<td>Lower explosion limit ([@SPT] [% vol])</td>
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<td>2.5</td>
<td>2.7</td>
</tr>
<tr>
<td>Auto-ignition temperature [K]</td>
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<td>578</td>
<td>723</td>
</tr>
<tr>
<td>Minimum ignition energy (in air @ 0.1 MPa / 298 K) [mJ]</td>
<td>0.017</td>
<td>0.017</td>
<td>0.07</td>
</tr>
</tbody>
</table>

Table 2: Basic properties of different gaseous fuels.  
SPT= Standard Pressure and Temperature

Of course a prime requirement of the pre-combustion process is that it should deliver products at the appropriate (p,T)-level. At the same time the properties of these products should resemble – as closely as possible – those of the intake charge of a modern diesel engine: mainly air, possibly with some EGR.

In this study we have added one extra component to the pre-combustion charge: argon. By inclusion of this extra component and – to a lesser extent as we will show – by choice of the pre-combustion fuel, properties of the resulting end-gas mixture can be brought in close accordance with those of air (with or without EGR or oxygen enrichment). Since specific heat plays an important role in both vaporization and combustion, we have taken efforts to tune the specific heat as closely as possible to that of air (or - where applicable - to that of a mixture of air with EGR). The low specific heat of argon will compensate the high specific heat of carbon dioxide and water in the end gas. (More details are given in the Appendix). Other parameters that play an important role in spray formation and oxidation process.
Table 3 shows, for a number of charge mixture compositions and one typical selected condition, how these parameters vary with respect to air at a temperature of 1200 K.

<table>
<thead>
<tr>
<th>Mixture</th>
<th>A (%)</th>
<th>B (%)</th>
<th>C (%)</th>
<th>D (%)</th>
<th>E [%vol]</th>
<th>F [%vol]</th>
<th>G [%vol]</th>
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<td>Ref.</td>
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<td>-</td>
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<td>[32]*</td>
<td>[29]</td>
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<td>61.7</td>
<td>55.6</td>
<td>69.3</td>
<td>62.9</td>
<td>64.8</td>
</tr>
<tr>
<td>Ar</td>
<td>0</td>
<td>0</td>
<td>6.7</td>
<td></td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>λ = 1/φ</td>
<td>2.39</td>
<td>2.54</td>
<td>2.61</td>
<td>2.67</td>
<td>3.62</td>
<td>3.86</td>
<td>3.74</td>
</tr>
<tr>
<td>C₀/C_p,air</td>
<td>1.07</td>
<td>1.20</td>
<td>1.04</td>
<td>0.99</td>
<td>1.03</td>
<td>1.08</td>
<td>1.06</td>
</tr>
<tr>
<td>V/V_p,air</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.02</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>k/k_p,air</td>
<td>1.07</td>
<td>1.19</td>
<td>1.04</td>
<td>1.00</td>
<td>1.03</td>
<td>1.08</td>
<td>1.06</td>
</tr>
</tbody>
</table>

These results show that viscosity is hardly affected by the mixture composition choice. But specific heat and thermal conductivity are. This effect is clearly more important for the richer mixtures in this study (these were applied because it was difficult to ignite the leaner mixtures (E to F). Figure 9 compares fuel compositions A-D for specific heat and thermal conductivity over a wider temperature range. This confirms the observations in Table 3. These results in particular speak against the use of pure hydrogen. Similar calculations of the end gas compressibility factor Z showed that for the T-range of interest this effect could be neglected.

**REPEATABILITY OF THE PRECOMBUSTION PROCESS**

The spray growth and combustion process are turbulent and therefore characterized by inherent fluctuations. Obviously, it is important that the charge preparation process does not introduce additional large variations. This was examined and the outcome is shown in Table 4 below. The results refer to two series of 16 (series 1) respectively 18 (series 2) experiments. Clearly, the (fully automated) filling procedure guarantees a high accuracy and repeatability of charge density and composition (air excess ratio λ). The mass averaged (or bulk) temperature was then calculated from the charge density, from the molecular weight of the pre-combustion products and from the instantaneous test cell pressure. As shown in Table 4 also the repeatability of the bulk temperature is high. To maximize the accuracy of this T determination, the piezo-transducer relative pressure data were pegged by setting pressure just before ignition equal to that measured just before intake valve closure with the (± 0.04 % FS) accurate absolute Druck sensor in the intake line (see above). Additional testing confirmed that the piezo-transducer was not suffering from thermal shock. The resulting absolute error on the calculated T was then typically 25 K.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Series 1</th>
<th>Series 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Charge bulk T [K]</td>
<td>795 ±0.1</td>
<td>1188 ±4</td>
</tr>
<tr>
<td>Charge ρ [kg/m³]</td>
<td>16.0 ±0.11</td>
<td>16.1 ±0.09</td>
</tr>
<tr>
<td>λ [-]</td>
<td>2.60 ±0.02</td>
<td>2.61 ±0.01</td>
</tr>
<tr>
<td>O₂ [%vol]</td>
<td>21.0 ±0.2</td>
<td>21.0 ±0.2</td>
</tr>
<tr>
<td>Pₚ₀ [MPa]</td>
<td>120.1 ±0.9</td>
<td>120.3 ±0.5</td>
</tr>
</tbody>
</table>

Table 4. Data on pre-combustion process repeatability

Because of the cooling taking place at the test cell boundaries, the actual temperature of the gas being entrained into the spray will be on average higher (typically 4 %) than this calculated bulk temperature. In addition, the precombustion products exhibit temperature gradients (resulting from flame propagation in a closed vessel, and influenced by the remaining – slow – motion previously set up by the mixing fan). Quantification of these gradients and of their impact on the combustion process is subject of current research.
**PRECOMBUSTION PRACTICALITIES**

When applying the pre-combustion technique some practical issues have to be taken into account. Some important ones are listed below as guideline:

- The order of filling the cell with the different components had to be decided on very carefully. Due to its C-C triple bond, acetylene is unstable, it can explosively dissociate at pressures above 200 kPa. Therefore C$_2$H$_2$ is added first. Next is argon, then nitrogen and, to avoid going into the explosion region, oxygen is added last.

- When selecting a mixture of fuels, preferably small partial pressures should be avoided if possible. This tends to result in – relatively – larger errors in creating the pre-combustion mixture.

- To ignite such lean mixtures (typically $\lambda=2.6$ when aiming at 21%vol O$_2$ products), a powerful ignition system is needed (especially at initial charge densities that exceed 30 kg/m$^3$). Furthermore, the products of the diesel combustion tests tend to foul the spark plug; thus the plug needs regular intermittent cleaning.

- In our research we observed that, already after a relatively small number of tests in simulated air, the injector holes started to show erosion-like damage. Tests in an inert hot gas environment did not show this effect. This problem was solved by putting a TiN-coating on the injector nozzle surface. This treatment was found not to affect the spray behavior.

**IMAGE PROCESSING**

The Schlieren technique visualizes density gradients. Of course such density gradients are set up by the spray. However, also the pre-combustion process sets up density gradients. Towards the edge of the spray the Schlieren produced by the spray and those originating from the pre-combustion will be difficult to discern. Fig. 11 illustrates this for non-reacting sprays

![Figure 10: Effect on commercial diesel nozzle hole of hot oxidizing ambient gas environment.](image)

**Figure 11: Variation of image quality with density; interaction with Schlieren method details.** Top 3 images are for a 2mm pinhole / 2mm pinhead Schlieren filter setting for conditions of respectively (32 kg/m$^3$; 403 K), (25 kg/m$^3$, 611 K), (25 kg/m$^3$, 1180 K). For the bottom picture the pinhead was replaced with a 2.5-3.5 mm diameter ring pass spatial Schlieren filter; test conditions were (32 kg/m$^3$, 1120 K).

Experience showed that for gas densities up to 16 kg/m3 the original pinhole Schlieren filter setting gives acceptable results. The pinhole was replaced with a ring-shaped pass filter for higher density / T conditions. This improved the Schlieren image quality, in particular it helped to separate the spray from the background. Still, for the highest T and density conditions the result is still far from perfect. Additional measures such as increasing the time between fan arrest and pre-combustion spark ignition had little effect. The challenge with analyzing vaporizing spray growth was therefore to develop a robust but accurate method for defining the edge of the spray.

**EDGE DETECTION**

In the past many authors (a.o. [30,31]) have first determined the intensity histogram of the (binarized) spray image. For a dark spray on a bright background this histogram has a peak at high intensities due to the background and one at low intensities due to the spray. The threshold corresponding to the spray edge is then chosen midway between the two maxima. In the set-up
presented here, this approach did not always work well for vaporizing sprays because of local small intensity differences between background and spray (as illustrated in Fig. 11). Furthermore, the abovementioned method is sensitive to variations in light intensities resulting from a.o. details of the Schlieren technique and from fouling of the windows.

For these reasons an alternative edge detection method was used that is less sensitive to these variations. First the image intensity profile \( I(x,y) \) is processed: for every distance \( x \) from the nozzle the light intensity profile is normalized in the \( y \)-direction \( I_{n}(x,y) \). Next a sequence of averaged images, \( I_{n,m}(x,y) \), is created by applying a filter procedure to a window of size \((m \times m)\) pixels at each location. When intensity variance is large, smoothing is limited. When variance is small, the filter performs more smoothing. Then the picture is reconstructed by averaging the smoothed images, \( <I_{d}(x,y)> = \Sigma_{m} I_{n,m}(x,y) \) and finally the spray contour is defined as the position where the averaged intensity \( <I_{d}> \) equals a chosen threshold \( f_{T} \). Interpolation is performed to reach sub-pixel accuracy.

SPRAY ANGLE

The threshold level has an influence on the resulting spray angle. Unfortunately, it is not possible to use one threshold level for all analysis. For each condition (and some separate movies) a separate threshold has to be chosen. The threshold value is varied until it followed the edge accurately. Whether or not this criterion is met, has been decided on by visual inspection. Clearly, there is scope for further improvement in this procedure. As in [30] we determined the spray cone angle for the quasi-steady part of the spray. Because the thimble prevented observation of the spray very close to the nozzle, in practice the spray cone angle was determined in the region between 10 and 45 mm from the nozzle. The surface area between the upper and lower edge of the spray in this region was used to determine an equivalent cone-like geometry.

SPRAY PENETRATION

In [43] a procedure was presented for the analysis of images of non-vaporizing sprays. This method relied on a clear and steep reduction of (laterally averaged) intensity in the tip region with increasing distance from the nozzle. For vaporizing sprays this method fails because at the spray tip region the (normalized) laterally integrated intensity profile slowly decays into the ambient gas zone. Therefore a different approach was taken. As the spray progresses there is a relatively large difference in intensity at the spray tip between the frames. In other words, the spray tip is the only macroscopic part in the recording that changes in intensity that much in such short time. This is illustrated in Fig. 13. At each moment in time the previous image is subtracted from the current one. The spray tip is then defined from the “difference image” as the average position of the five pixels with a defined threshold that lie furthest from the origin in the axial direction. This spray penetration definition was found to be not very sensitive for variations of the chosen threshold values and spray tip position could be determined with an accuracy of 0.2 mm.

LIQUID CORE

Because of air entrainment and vaporization, liquid fuel concentration will decrease with distance from the nozzle, until – at some point – the last droplet has disappeared. The end of the liquid core is defined as that point on the spray axis where the droplet density in a plane perpendicular to the axis drops below a threshold level. When applying Mie scattering to visualize the droplets this corresponds to the point where Mie scattered light intensity drops below a threshold level. The top and middle pictures of Fig. 14 are typical instantaneous images obtained during such experiments. These (and other) pictures seem to indicate that the
liquid core is “wagging” (probably resulting from internal spray dynamics such as vortex shedding).

These internal spray dynamic processes could also explain the large (quasi-steady state) variation of the liquid core end position. To deal with this, all the frames in a recording are averaged yielding an average liquid core intensity profile along the centreline. As can be seen in Fig. 14, the scattered light intensity is high close to the nozzle. It then drops off sharply as most of the droplets disappear, and after that point intensity decreases slowly until it vanishes. In this study the end of the liquid core is defined as the point where the spatial derivative of the scattered light intensity falls off to one third of its maximum value. As this is a relative threshold, it is again less sensitive to window fouling and other disturbances. The actual corresponding distance from the nozzle is again determined by interpolation of pixel values.

Figure 14: Results from Mie scattering experiments. Top: liquid tip break-up phenomena; T=650 K, ρ=25 kg/m³, 9.8 µs between frames. Middle: image of instantaneous liquid core scattering, the red (full) line emphasizes the wave-like behaviour; T=837 K, ρ=16 kg/m³. Bottom: artificially coloured average liquid core picture; T=650 K, ρ=25 kg/m³. Nominal injection pressure: 115 MPa for all pictures; 180 µm nozzle-hole diameter. Scale of both pictures is not the same; bottom picture actual length corresponds to 42 mm.

It should be emphasized that the above mentioned image processing techniques are still subject to study and are not necessarily the best approaches.

**TYPICAL RESULTS**

**MULTIHOLE VERSUS SINGLE HOLE NOZZLES**

When deciding on the best technique to isolate one spray from a multi-hole HD nozzle, two approaches were considered: using a thimble, and blocking all but one of the nozzle holes. Fig. 15 shows the thimble that was used in the experiments. As shown, in this approach, the sprays issuing from all but one of the holes are caught by the thimble. The spray that exits into the test cell is confined within the thimble only up to a distance of 2.8 mm. This is to be compared with the equivalent nozzle diameter \( d_s \sqrt{\frac{\rho_f}{\rho_g}} \); then the dimensionless distance from the nozzle is smaller than 4.

It is known from the literature [46,47] that at these distances the spray is still breaking up into liquid ligaments, entrainment is limited and we therefore assume that this situation is very similar to that of the situation without thimble. In the alternative approach, all but one of the holes was blocked, either by glueing short needles into the other nozzle holes (the length of these needles was small enough to make sure that they did not protrude into the sac volume). For comparison also tests were done where all but one holes was welded.

**Figure 15: Geometry of thimble used to isolate one spray from a multi-hole nozzle.**

It is also known that the literature [46,47] that at these distances the spray is still breaking up into liquid ligaments, entrainment is limited and we therefore assume that this situation is very similar to that of the situation without thimble. In the alternative approach, all but one of the holes was blocked, either by glueing short needles into the other nozzle holes (the length of these needles was small enough to make sure that they did not protrude into the sac volume). For comparison also tests were done where all but one holes was welded.

**Figure 16: Difference in penetration between a spray produced with a blocked nozzle and a nozzle with thimble; \( \rho=9.6 \pm 0.3 \text{ kg/m}^3 \) and \( P_{inj}=83 \pm 7.5 \text{ MPa} \) (different T: 750/915/990/1100 K).**

For both approaches (thimble and blocking), spray cone angle and penetration were measured. Penetration results are shown in Fig. 16. Clearly, penetration is fastest for the blocked version. Experiments with another (nominally similar) nozzle showed that the spray from a “blocked” nozzle had an almost 10 % higher momentum force than the average spray momentum of the
corresponding regular nozzle. Of course the last result may be because that one hole was an outlier. However, AMESIM calculations indicated that blocking all but one of the nozzles resulted in a faster pressure build-up in the nozzle sac-hole, a faster needle lift and a higher pressure at full needle lift. These calculations also predicted an increased momentum flux. All this seems to confirm that the “blocking” approach modifies the injection process. At these same conditions the spray angle measurements gave a spray angle of 18.2°± 2.5° for the thimble version and an angle of 15.8°± 2.5° for the blocked nozzle (same edge detection threshold level selected). As fuel vaporization is mixing limited, a wider spray angle would result in a smaller liquid core length. This is confirmed by experimental results as shown in Fig. 17. A possible explanation for these observations would be that blocking the holes changes the flow field inside the nozzle sac and in the nozzle hole itself, reducing in-hole cavitation. Experience has shown that this tends to correlate with a reduced spray angle [48].

- The limited accuracy of determining the spray tip penetration

Fig. 18 shows the spray penetration determined from 11 consecutive experiments. As shown, variation of testing conditions was small. The spray penetration tests demonstrated more variation than expected, on the other hand similar variations were registered by other researchers.

![Figure 17: Liquid core length with a blocked nozzle (top curve) versus a nozzle with thimble (bottom curve).](image)

In view of these results the thimble method was retained (notwithstanding its practical implications such as faster fouling). The above results furthermore suggest that studying multi-hole nozzles is to be preferred over research on single-hole nozzles.

VARIABILITY IN SPRAY PENETRATION

It is to be expected that there will be variability in spray penetration between different tests under nominally identical conditions. The reasons for this variability are:

- "nominal identical" test conditions in reality show a variation in the charge conditions at the start of injection (see Table 4 on the repeatability of the pre-combustion technique) but also a variability in the rail pressure. Originally this variation was larger (e.g. Fig. 16) but after some modification the average rail pressure now shows a 3-4 % max. variation.

![Figure 18: Spray penetration vs. time for 11 experiments; shown are power fit curves \((x=a.t^b)\). Variation is in the order of ± 8.3 %. All tests at 794< T[K]< 803, 31.5<p [kg/m³]<32.2 and 118< P_inj[MPa]<124.](image)

This observation is important when considering the fact that often correlations are used to predict spray penetration (in particular when designing for minimal spray wall wetting in advanced PCCI combustion development). Very few of such studies consider the variability and uncertainties that are intrinsic to these correlations. Further study of this variability is ongoing.

CONCLUSION

1. The design of a constant volume test cell using pre-combustion for charge preparation is presented and explained in detail.

2. Guidelines are given for window (holder) design and sealing, and for many other design and operation details of the cell.

3. It is shown that adding Argon to the pre-combustion mixture allows preparing end-gas products that more closely resemble real engine charge properties.

4. Schlieren image processing methods are described that have proven to work well in a situation where spray edge detection is difficult because of high background disturbance. This situation mostly occurs when gas density increases.
5. Test results confirmed that multi-hole nozzles have a different behavior from single nozzles and that to isolate one spray of a multi-hole nozzle it is better to use a thimble than to block all but one nozzle hole.

ACKNOWLEDGMENTS

The financial support of technology foundation STW is gratefully acknowledged, as well as the in-kind contribution of DAF Trucks N.V. and the valuable contributions of Roel Peters, Rob Vallen, Mohamed Douch, Robert Klein-Douwel, Miao Yu, Marc Willekens, Madan Bindraban, Gerard van Hattum, Gerard van Hout and Hans van Griensven.

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ACRONYMS. SYMBOLS
λ Air excess ratio = 1/φ
φ Equivalence ratio
CI Compression Ignition
CPFR Constant Pressure Flow Rig
CR Compression Ratio
CVHC Constant Volume Hot Cell
CVPC Constant Volume Precombustion Cell
EGR Exhaust gas recirculation
FIE Fuel Injection Equipment
GTL Gas-To-Liquid synthetic fuel
HD Heavy-duty
Mathematically, the determination of the pre-combustion mixture composition can be cast into a system of equations for the input masses of fuel, O\textsubscript{2}, N\textsubscript{2} and Ar. Targets to be met are total density (\( \rho_{\text{set}} \)), adiabatic flame temperature (\( T_{f}^{\text{ad}} \)), remaining oxygen mass (\( m_{\text{OX}}^{\text{fin}} \)), and specific heat at a specified temperature. For the adiabatic flame temperature we have argued in the main text that it should satisfy

\[
T_{s} = T_{u} + f(T_{p} - T_{u}),
\]

where \( T_{s} \) is the maximum temperature during injection (lower values are possible by waiting longer) and factor \( f \) is an empirical value (for which we use 0.5) denoting that the cooling process should be at least halfway before injection. The equations become

\[
\sum_{i} m_{i}^{\text{ini}} = \rho_{\text{set}} V = m \quad (A.2)
\]

\[
\sum_{i} m_{i}^{\text{ini}} u_{i}(T_{i}^{\text{ini}}) = \sum_{i} m_{i}^{\text{fin}} u_{i}(T_{i}^{\text{ad}}) \quad (A.3)
\]

\[
m_{i}^{\text{fin}} = m_{i}^{\text{ini}} + s_{i} m_{i}^{\text{fin}} \quad (A.4)
\]

\[
c_{p} = \sum_{i} c_{p,i}(T_{i}) \frac{m_{i}}{m} \quad (A.5)
\]

The subscript \( i \) denotes each component. The specific internal energy (\( u_{i}(T) \)) as well as the specific heat (\( c_{p,i}(T) \)) of each component is evaluated from the Burcat tables [8]. In the limit of complete combustion the mass-based stoichiometric coefficients \( s_{i} \) are simply obtained from the global fuel consumption reaction:

\[
C_{x}H_{y} + (x + \frac{y}{4})O_{2} \rightarrow xCO_{2} + \frac{y}{2}H_{2}O \quad (A.6)
\]

For combusting spray experiments (i.e. fuel-lean pre-combustion) this approach will not lead to large errors. However it can simply be generalized to account for incomplete combustion and dissociation through replacing equation A.4 by minimization of the Gibbs free energy. This results in:

\[
\sum_{i} m_{i}^{\text{ini}} = \rho_{\text{set}} V \quad (A.2)
\]

\[
\sum_{i} m_{i}^{\text{ini}} u_{i}(T_{i}^{\text{ini}}) = \sum_{i} m_{i}^{\text{fin}} u_{i}(T_{i}^{\text{ad}}) \quad (A.3)
\]

\[(dg)_{f_{\text{set}},p} \leq 0 \text{ with } g = g(\rho, T, m_{i}) \quad (A.7)\]

It should be noted however that the equilibrium composition will change during cool-down towards the desired state and the resulting temperature at the actual state will need to be re-evaluated (i.e. average molar mass will change).