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Mixture Formation in Direct Injection Hydrogen Engines: CFD and Optical Analysis of Single- and Multi-Hole Nozzles

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ABSTRACT

This paper describes the validation of a CFD code for mixture preparation in a direct injection hydrogen-fueled engine. The cylinder geometry is typical of passenger-car sized spark-ignited engines, with a centrally located injector. A single-hole and a 13-hole nozzle are used at about 100 bar and 25 bar injection pressure. Numerical results from the commercial code Fluent (v6.3.35) are compared to measurements in an optically accessible engine. Quantitative planar laser-induced fluorescence provides phase-locked images of the fuel mole-fraction, while single-cycle visualization of the early jet penetration is achieved by a high-speed schlieren technique. The characteristics of the computational grids are discussed, especially for the near-nozzle region, where the jets are under-expanded.

Simulation of injection from the single-hole nozzle yields good agreement between numerical and optical results in terms of jet penetration and overall evolution. The 13-hole nozzle creates intense jet-to-jet interaction, with all jets merging into a single effective jet immediately downstream of the under-expanded region. This phenomenon (usually referred as Coanda Effect) is more challenging to the numerical simulation and requires higher level of detail in numerical simulation and grid resolution, with particular regard to the fields near the injector nozzle.

INTRODUCTION

Hydrogen has been researched intensively as a fuel for internal combustion engines (ICEs) for several decades [1,2,3] due to its potential to provide both high engine efficiency and low environmental impact, with NO_X as the only toxic pollutant. One of the main advantages of using hydrogen as fuel in spark-ignition (SI) engines is the wide flammability range, which allows high efficiency in most of the operating conditions while minimizing NO_X emissions. While a large-scale utilization of H_2 is curbed by the well-known challenges associated with production, distribution and on-board storage, hydrogen engines can nowadays show performance that cannot be achieved by conventional SI engines [4,5].

The U.S. Department of Energy started funding experimental activities on H_2-ICEs at Argonne National Laboratory in 2005 with challenging goals, including 45% brake thermal efficiency (BTE) and NO_X emissions of 0.07 g/mile, together with a power density comparable with gasoline engines at a mass-production cost of 30 $/kW [6]. Another important requirement was to avoid unsafe conditions due to irregular combustion (pre-ignition, backfire).

Direct injection is the most promising strategy to meet all the requirements mentioned above [7]. In particular, the risk of backfire can be avoided and the volumetric efficiency losses due to low H_2 density are eliminated, thus allowing the same

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or higher power density than from conventional gasoline engines. As far as efficiency and emissions are concerned, the engine optimization is highly dependent on the mixture formation process. DI engines require great effort in the optimization process since the number of degrees of freedom increases, compared to port fuel injection (PFI). In particular, the injection strategy including engine operating parameters (injection timing) and geometry (injector location, nozzle configuration) has a significant influence on the mixture formation process, which consequently affects combustion and pollutant formation. In addition, jet-to-jet interaction has to be taken into account for multi-hole nozzles.

In order to meet DOE's targets, Argonne National Laboratory has been carrying out intensive research on advanced direct injection and mixture formation concepts [8,9,10] in a single-cylinder engine. An intuitive way to increase engine efficiency is to reduce the individual efficiency losses. To this aim, new injector technologies (piezo-actuated driver) allow performing late injection (thus reducing the losses for compression work) and delivering higher mass flow rates during injection, thus extending the operation range to higher engine load and speed, where the maximum efficiency can be achieved. Moreover, research on DI gaseous engines is extremely focused on optimizing the injection timing (start of injection, SOI) and nozzle geometry to pursuit the “ideal” stratification, consisting of a relatively rich mixture close to the spark-plug and low amount of fuel close to the cylinder walls, at spark timing. This best case scenario would provide high stability during combustion (low COV) due to the enhanced development of the early flame kernels, low NO_X emissions due to highly stratified mixture (rich and ultra-lean mixtures produce much lower NO_X than slightly lean mixtures), and significantly reduced loss for heat transfer to the cylinder walls, which happens to be the highest efficiency loss in almost every condition [11]. Strategies to further reduce NO_X emission like EGR and water injection have also been investigated [12,13], nevertheless DI H2-ICEs have the potential to provide NO_X emissions within the most severe regulation limits without the need for any after-treatment device.

Despite the extensive research in terms of advanced mixture formation, basic experimental activities cannot provide a comprehensive understanding of the physics underlying the in-cylinder processes which significantly affect performance and emissions in a DI engine, where the mixture is internally formed. Laser-based measurements in optically accessible engines can overcome this limitation and provide insight into the mixture formation process. To this end, Sandia National Laboratories have been carrying out optical investigations on a single-cylinder engine with similar geometry Argonne's all-metal engine. Via planar laser-induced fluorescence (PLIF) and particle image velocimetry (PIV), air/fuel mixing and its interaction with the intake-induced flow have been examined for injection from single and multi-hole nozzles [14,15,16].

Optical investigations on ICEs not only offer insight into the in-cylinder processes, but also provide the proper experimental data for the validation of numerical results provided by a Computational Fluid Dynamic (CFD) approach. 3D-CFD investigations of mixture formation have been performed at Argonne National Laboratory with the aim to develop a tool able to provide important input to the experimental testing for the optimization of engine parameters and geometry. Despite the need to constantly verify the accuracy of numerical results by means of the comparison with experimental (and optical in particular) data, a reliable computational code can be used to predict engine performance and drastically reduce production cost for prototypes and testing time. Even operating conditions which may not be easily explored can be simulated and moreover the access to numerical results allows obtaining a wide range of information on the spatial distribution of the most relevant physical and chemical quantities within the cylinder. Accordingly, effort has to be put into ensuring reliability and accuracy of computational codes, which can be assessed by means of validation against experimental data.

This paper expands previous validation work [17,18] by widening the range of analyzed cases, including different injection pressures and different nozzle geometries. Single- and multi-hole nozzles, at high and low injection pressure, are evaluated. Simulations performed in this paper use the commercial code Fluent (v6.3.35) and a Reynolds-Averaged Navier Stokes (RANS) approach to model in-cylinder turbulence. Phase-locked PLIF measurements provide a quantitative comparison for numerical results during mixture formation. In addition, high-speed schlieren images are used to reduce numerical uncertainties related to the injection timing and early-injection transients. Numerical assumptions related to the injection profile are discussed in detail. Grid requirements are also highlighted, with particular regard to the near nozzle domain where the gaseous jet is highly under-expanded due to the high injection pressures. Once validated, the numerical approach will be able to guide the optimization of DI engines fuelled by gaseous fuels like hydrogen, but also natural gas or gaseous blends.

EXPERIMENT

OPTICAL ENGINE

The optical engine is a passenger-car sized, four-stroke single-cylinder research engine, adapted to operate with hydrogen. Large transparent segments make the engine optically accessible for laser-based measurements. Schematics of the relevant optical and mechanical components are shown in Figure la. The engine has a four-valve head with a pent-roof combustion chamber. The piston

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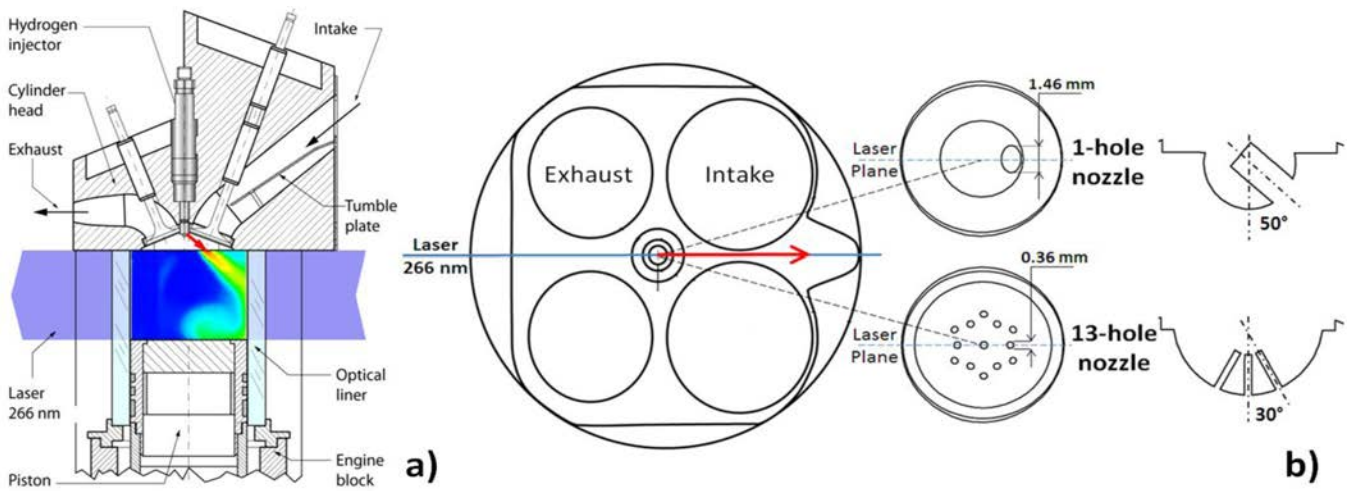

Figure 1. Schematics of engine hardware. (a) Optical engine with measurement plane. (b) Location and targeting of the nozzles with respect to the combustion chamber.

is flat-topped. The intake system consists of two intake ports, one for each valve, both straight and parallel to each other forming an angle of 40° with respect to the fire deck (horizontal). For this study, a full-length fused-silica liner is used, so that the entire volume swept by the piston is optically accessible, but not the pent-roof

The main engine geometrical and operating parameters are given in Table 1. The crank-angle convention used in this paper assigns 0°CA to compression TDC. Thus, crank-angles during the compression stroke are negative. Hydrogen is supplied directly into the combustion chamber via a solenoid injector from Westport Inc. Figure 1b shows the injector location, central between the four valves. Two nozzles are used in this work, the first being a single-hole (1-h) nozzle with a hole diameter of 1.46 mm, aiming at the intake squish region (between the two intake valves) and downward, with a 50° angle with respect the injector axis. The jet axis is aligned with the mirror-symmetry plane of the combustion chamber. The second nozzle (13-h) has 12 holes with a diameter of 0.36 mm at a 30° angle with respect the injector axis and a central hole with a diameter of 0.38 mm

Since the present study focuses on mixture-formation prior to ignition, fired engine operation is not necessary. The engine is motored at a constant speed of 1500 RPM, and nitrogen is supplied as a bulk gas (but treated as air in calculations of the equivalence ratio). The pressure in the surge tank upstream of the intake runner is kept at 1 bar and typical intake temperatures just upstream of the engine head are around 36°C.

In all the examined operating conditions, hydrogen injection is adjusted to obtain a global equivalence ratio of 0.25 (λ = 4.0), or a hydrogen mole-fraction of 0.095. In fired operation, at typical efficiencies, this fuel concentration represents a low-load condition with about 2.5 bar IMEP. The mean fuel flow is measured far upstream of the injector with a thermal mass-flow meter (Brooks SLA5860).

Table 1. Optical engine specifications and main operating parameters

Bore / Stroke / Displacement	92 mm / 85 mm / 565 cm^3
Compression ratio	11:1
Speed	1500 rpm
Intake pressure / Temperature	1 bar / 36°C
Intake Valve Closing (IVC)	-140°CA
Nominal - Actual SOI delay	3°CA (at 1500 RPM)
H_2 Injection Pressure	25 and 100 bar

PLIF MEASUREMENTS

Planar laser-induced fluorescence (PLIF) of gaseous acetone as a fuel tracer is adapted to obtain quantitative images of the hydrogen mole-fraction in the operating engine. The imaging technique is described in detail in previous work [19] and is therefore discussed only briefly here. Gaseous acetone is seeded as a tracer into the hydrogen fuel by a high-pressure bubbler. At 100 bar pressure and room temperature, a volume concentration of 0.33% can be reached. For current purposes, differential diffusion of tracer and fuel is estimated to be insignificant due to the large spatial structures examined here and the high Reynolds number of the post-injection flow. Phase-locked to a particular crank angle, a quadrupled Nd:YAG at 266 nm laser excites acetone fluorescence, which is imaged onto a back-illuminated CCD camera.

Standard background and flat-field corrections are performed to quantify the measurements. For the latter, a nearly homogeneous charge is prepared by DI during the intake stroke. Distortion due to the curved liner is corrected.

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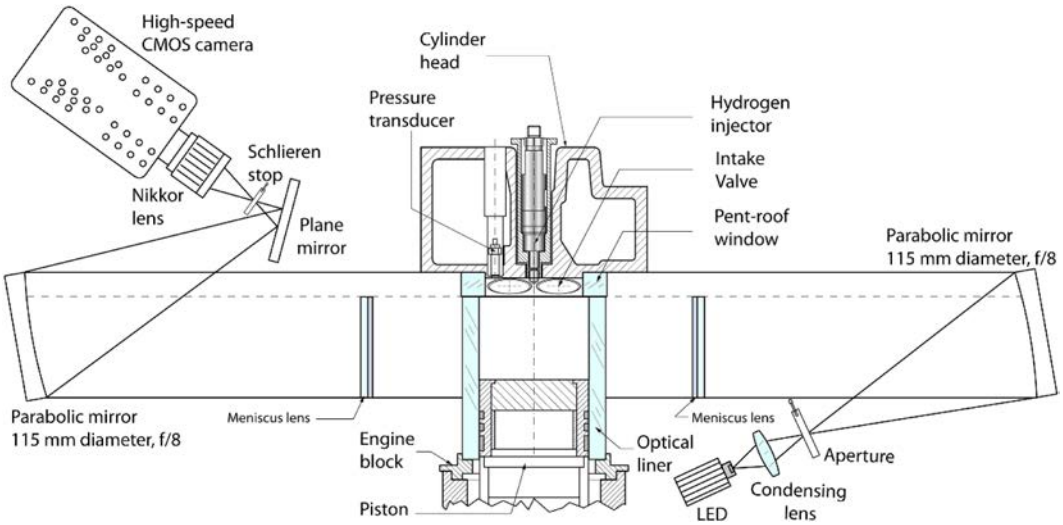

Figure 2. Schematics of the high-speed schlieren imaging technique

Inhomogeneities in the temperature field, induced by mixing of cold hydrogen and hot bulk gas, are accounted for based on known spectroscopic properties of the tracer [20,21] and on the assumption of adiabatic mixing between fuel and bulk gas [22,23,24]. The overall typical maximum error in the ensemble-mean equivalence-ratio fields is estimated to be 25%. Small regions in the images, in particular for early crank angles, may have larger errors because of local window fouling and signal reflections. Ninety images of the hydrogen mole-fraction are collected at each crank-angle. The resulting sequence of phase-locked mean images has already been reported in a previous publication [16] for the case of the single-hole nozzle, while data from the 13-hole injector are presented for the first time here.

HIGH-SPEED SCHLIEREN DATA

Hydrogen-jet penetration is visualized by schlieren imaging with a high-speed camera, illustrated schematically in Figure 2. Since schlieren techniques have been used for many years to visualize density gradients in transparent media [25], only a brief description of the optical system will be given in this paper. The arrangement is that of "focused shadowgraphy" in "Z" layout [25] with the engine's cylinder and pent-roof as the imaged object. Light from a green, pulsed, high-power light-emitting diode (LED) was focused through an aperture with 0.7 mm diameter and collimated by a parabolic mirror with a focal length of 900 mm. After and before passing through the engine, cylindrical correction lenses keep the light collimated. The beam is then focused by another, identical parabolic mirror through a round aperture with 1.7 mm diameter, which acts as a schlieren stop. A camera lens with focal length f = 50 mm projects the resulting schlieren images onto the detector of a high-speed complementary metal-oxide-semiconductor (CMOS) camera (Phantom v7.1). Single-cycle sequences of images are acquired with a temporal frame spacing of 0.5°CA (= 55 μs) and an effective exposure time of 5.5 μs, given by the LED's pulse width. The visual contrast in the schlieren images is enhanced by temporal differentiation, i.e., by subtracting the previous frame from each frame [26].

NUMERICAL SIMULATION

CFD simulations of direct injection of hydrogen and mixture formation are performed using the commercial CFD solver Fluent (version 6.3.35). This study follows a RANS approach combined with a k-ε model to describe in-cylinder turbulence. The quality of the RANS results is not comparable to more detailed approach such as LES or DNS. However, the latter are not computationally affordable yet for engine applications, characterized by large computational domains and high Reynolds numbers. These two main issues significantly increase the grid resolution and consequently the computational time. However, the benefits from performing higher fidelity simulations in the future will be briefly discussed later in the paper. All the formulations of the k-ε model provided by Fluent (k-ε standard, k-ε RNG, k-ε realizable) have been previously tested and showed only slight differences in the numerical results [18]. In this paper, the realizable k-ε is used.

The Gambit software is used as pre-processor to generate the computational grids. The numerical approach followed in this study has been comprehensively documented before [17] and therefore is only briefly summarized here:

- A computational grid for the full engine geometry (including valves and ducts) is used to compute the in-cylinder flow-field during the gas-exchange phase, prior to fuel injection.

- A computational grid of the geometry reduced to the combustion chamber only (including the nozzle geometry) is used to simulate direct injection and mixture formation.

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• The flow field, state variables, and turbulence-model parameters calculated from the gas-exchange phase (step 1) are set as initial conditions for the subsequent simulation of direct injection and mixture formation (step 2).

By this approach, for a specific operating condition (engine speed and load), different injector geometries (number of nozzles, nozzle diameter, direction and location) and injection strategies (injection pressure and timing) can be evaluated on the reduced grid without the need to re-calculate the pre-injection flow-field. Furthermore, the high-pressure DI process with its transient supersonic jet requires higher grid resolution than the simulation of the gas exchange. Accordingly, the two processes are separated and two different grids are used.

This study focuses on hydrogen direct injection and mixture formation, therefore only the part of the cycle calculated with the reduced geometry is considered. However, the in-cylinder conditions (velocity field, physical quantities, chemical species) prior to SOI were previously calculated [17] and are taken into account in the present analysis. The only additionally required information is the boundary condition related to the fuel injection. To this aim, the hydrogen mass flux through the nozzle is calculated from the measured mean mass-flow rate, injection duration, and nozzle diameter, and is set as the mass-flow-inlet boundary condition for the injecting surface. The mass-flow-inlet condition is chosen, due to the lack of information about the instantaneous pressure at the injecting surface. Fuel properties at the critical section might be roughly evaluated by the assumption of sonic flow conditions but the actual pressure and temperature values at the injecting surface are difficult to calculate without explicitly modeling the flow within the injector. Also, the mass-flow-inlet condition has proven to provide more stable numerical solution than the inlet pressure condition. With this choice of inlet condition, the only remaining issue is how to model the jet transient.

The instantaneous mass flow is not experimentally measured. Information on injection current, voltage and needle lift was provided by the injector manufacturer and used to assume the injection profile, which consists of a central, quasi-steady part with linear ramp-up and ramp-down. Figure 3 shows the assumed injection profile for a single-hole jet injected at 100 bar with nominal SOI = −140°CA. The choice of ramp slope and, consequently, of the transient duration is discussed in more detail later. The resulting total mass injected per cycle (proportional to the area under the trace in Figure 3) corresponds to that calculated from the experimental multi-cycle mean hydrogen flow rate (3.46 g/cycle for all cases). At the end of injection (EOI), the boundary condition for the injecting surfaces is changed from mass-flow-inlet to wall. The inlet temperature of the injected hydrogen is set to 300K.

Experimentally, at 1500 RPM a delay of about 3°CA is observed between the injector opening command and the actual start of injection (SOI). Accordingly, for a nominal value of SOI = −140°CA, the mass flux through the nozzle begins at −137°CA. During the compression stroke a 0.5°CA time-step is used for simulation, with the exception of the injection duration, where the supersonic flow requires a smaller (0.1°CA) time-step for stable calculations. The PISO method is used to couple pressure and velocity and the 1st order is chosen as discretization scheme.

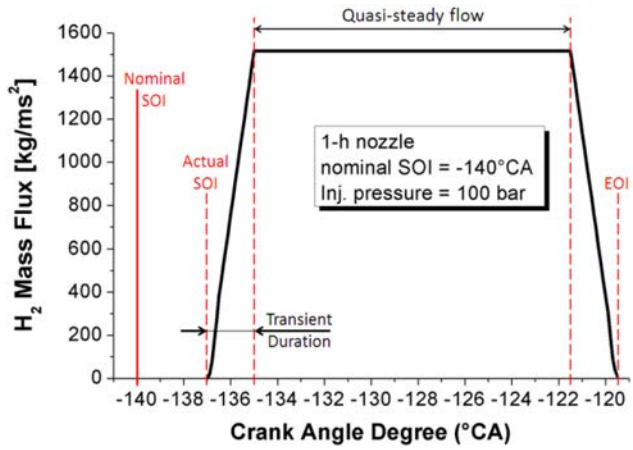

Figure 3. Schematic of the assumed generic injection profile

A detail of the grid resolution in the near nozzle domain is shown in Figure 4. Both (for the single-hole and 13-hole nozzle) the computational grids are optimized to reduce the overall number of cells and maintain the accuracy of numerical results. Accordingly, the overall cell size is slightly increased with regard to previous studies [17,18], while the mesh is locally refined in the proximity of the nozzle. Overall grid resolution (including the boundary layer at the cylinder walls) has a significant influence on numerical results in a direct injection process, however the main influence stems from the cell size within the nozzle and at the nozzle exit [18,27]. Here, the jet is under-expanded and great care in choosing the grid size has to be taken, in order to predict the evolution of the supersonic jet and, consequently, jet penetration. Figure 4 shows that grids for both nozzles are refined near the jet axis for a more detailed analysis of the under-expanded region, but the axial extent of the refined region varies. This corresponds to the different hole diameters (1.46 mm versus 0.36 mm), which leads differently sized under-expanded regions. Overall grid size is 850,000 cells for the 1-h nozzle and 1,200,000 for the 13-h nozzle, both evaluated at IVC.

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Table 2. Examined test cases

	Test Case 1	Test Case 2	Test Case 3
Nozzle	1-h	1-h	13-h
Injection Pressure	100 bar	25 bar	86 bar
Nominal SOI	-140°CA	-137°CA	-140°CA
Actual SOI	-137°CA	-134°CA	-137°CA
Injection duration	17.5°CA	74.5°CA	21°CA

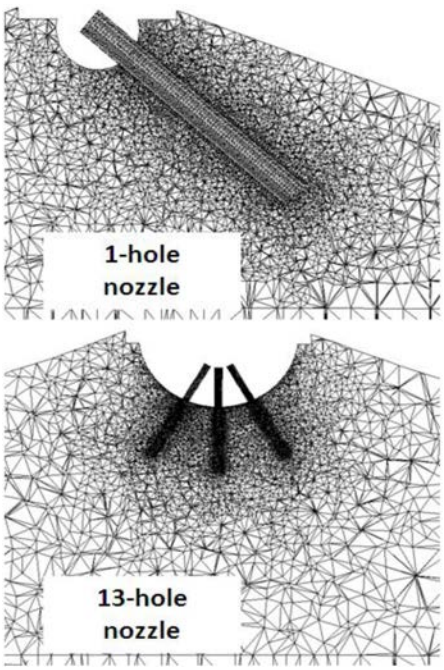

Figure 4. Local refinement in the near-nozzle region for the computational grids used in this study

RESULTS AND DISCUSSION

TEST CASES

Starting from the conditions within the cylinder at IVC (−140°CA), the present analysis focuses on the mixture formation process. As mentioned above, the main engine parameters (engine speed and load, intake pressure) are kept constant for all the examined operating conditions. Accordingly, conditions within the cylinder prior to SOI are identical, with the exception of a slightly different nominal and actual SOI for the low-pressure case. Three cases are analyzed in this paper, as listed in Table 2.

This set of cases provides a proper mix of data to evaluate the mixture formation process, since significant variations in terms of injection pressure, injection duration and nozzle geometry are taken into account. The choice of early injection (SOI = −140°CA and −137°CA) can be emphasized by noting that the most severe conditions to be simulated are those where a significant amount of time is available for the fuel jet to evolve and for mixture formation to occur. Accordingly, the accuracy of the numerical results will be assessed not only in terms of fuel penetration but also in terms of mixture stratification at the end of the compression stroke.

INJECTION PROFILE

In previous studies [17,18], a trapezoidal injection profile, with injection at constant mass flux and 1°CA linear ramp-up and -down, was used. This assumption was accurate enough to yield good agreement between numerical and experimental (PLIF) results along the entire compression. High-speed schlieren data allows evaluating whether the transient modeling is accurate. In Figure 5, two different injection profiles (with 1°CA ramp and 4°CA ramp) are used to simulate the same operating condition (test case 1) and the numerical results in terms of H_2 mole-fraction are compared with schlieren data. The side grid-lines identify the boundaries for the schlieren imaging, therefore a comparison during the transient between CFD and schlieren data is useful only up to −134°CA (the jet reaches the right boundary). Figure 5 shows that the transient influences the jet penetration, in that the slower starting transient yields slower penetration, and that the agreement between modeling and experiments improves with a higher transient duration. However, the transient duration does not significantly affect overall mixture formation, because the differences become negligible at the end of injection (−120°CA). At the end of compression stroke (-30°CA), despite the drastic reduction of the displayed H_2 mole-fraction range, the difference in terms of fuel concentration between the two numerical results is very small.

The comparison with high-speed schlieren data suggests that a transient duration of 4°CA is more accurate in describing the rise of the mass-flow rate through the nozzle in test case 1 (100 bar injection pressure). The same ramp is used to model the transient for test case 2 since the injection pressure is similar (86 bar). For the low-pressure case (test case 3, 25 bar injection pressure), a ramp of 1°CA is chosen, due to the much lower values of maximum mass flux (see Figure 6), in order to assume the same mass flow rise of the high-pressure cases during the transient. The mass-flow is related to the pressure value upstream of the nozzle, therefore the present approach basically consists of assuming linear pressure rise

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up to the quasi-steady flow condition. As mentioned earlier, the choice of a mass-flow-inlet boundary condition for the direct injection process is due to more stable numerical solution as well as to uncertainties about the pressure values at the injecting surface. The code calculates the pressure at the domain boundaries on the basis of the mass flux and temperature (300 K) imposed at the inlet surface.

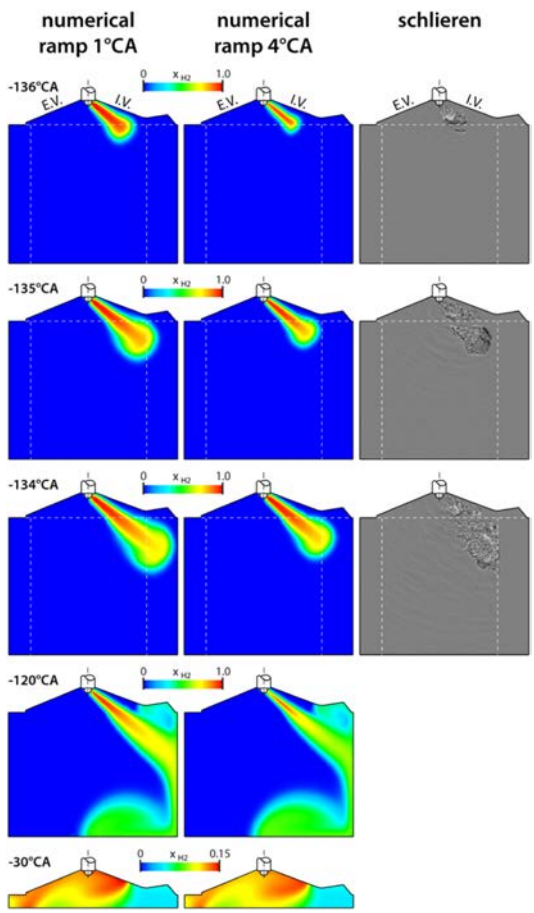

Figure 5. Influence of transient modeling on jet penetration and mixture formation (test case 1)

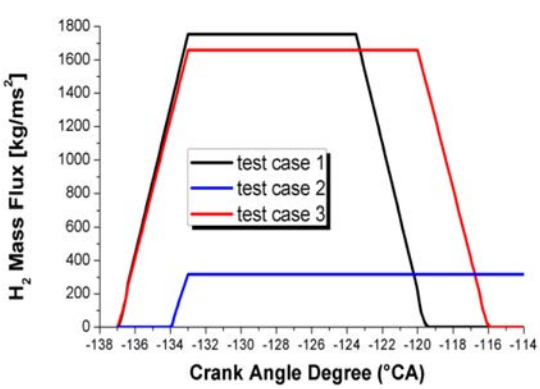

Figure 6. Injection profiles assumed for the examined test cases

SUPERSONIC JET CHARACTERISTICS

The characteristics of the under-expanded jet are calculated based on the mass-flow (imposed), pressure (calculated) and temperature (imposed) upstream of the critical section. If the ratio between injection pressure and ambient pressure is higher than the critical ratio (1.889 for H_2), the flow will be sonic, with the mass flow rate through the nozzle being choked and depending only on the conditions upstream of the nozzle and not on the ambient properties. Figure 7 shows Mach number and absolute pressure in the near-nozzle domain for the three test cases presented here.

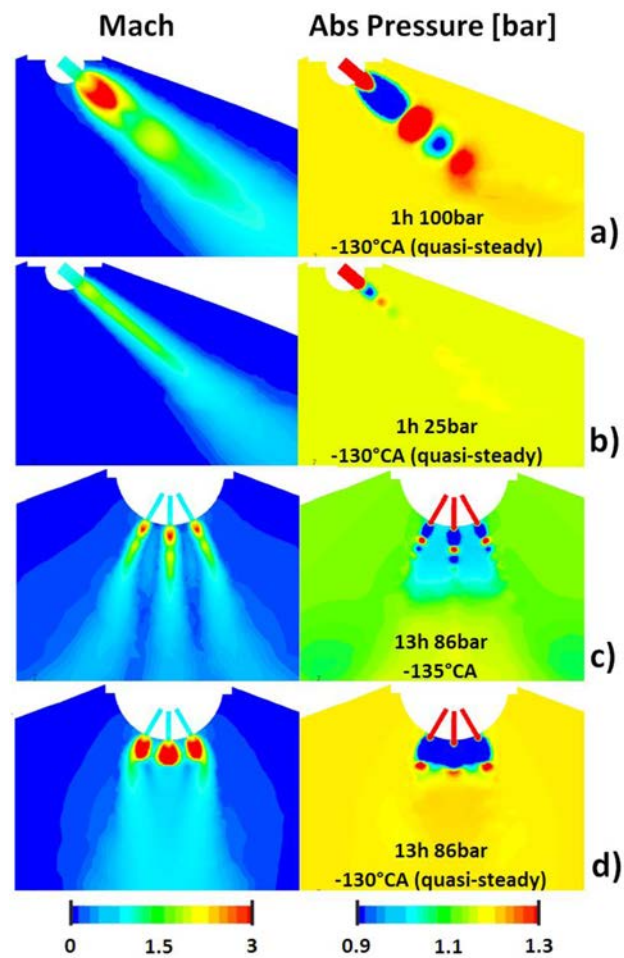

Figure 7. The under-expanded region for the examined test cases. (a) Test case 1, during quasi-steady flow. (b) Test case 2, quasi-steady. (c) Test case 3 during transient, 2°CA after SOI. (d) Test case 3, quasi-steady

In all the examined cases a supersonic region (Ma > 1) can be seen at the nozzle exit, where the pressure switches from the injector conditions to the ambient conditions through a series of shocks along the jet direction. When the jet is highly under-expanded (high injection pressure) the recompression takes place normally through a large Mach disk where the flow switches from highly supersonic (Ma >> 1) to subsonic

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(Ma < 1), which be seen in Figure 7a. The low injection pressure case (25 bar, Figure 7b) does not feature a highly under-expanded jet and a clearly-visible Mach disk, even though small shocks are present and the flow is still supersonic at the nozzle exit. For test case 3 (13-h nozzle), Figure 7c shows the initial formation of separate supersonic flows downstream of each hole, where each jet is highly under-expanded with smaller Mach disks than the ones observed for the single-nozzle hole. This is in agreement with results reported in the literature showing that the Mach disk size is related to the hole diameter [28]. Downstream of the Mach barrel region, the jets interact with each other and subsequently merge into a single jet, due to the Coanda effect [29], which stems from the lack of air entrainment in the jet due to the presence of another jet in close proximity and leads to the formation of a single, bigger under-expanded region (see Figure 7d).

A higher detail of the under-expanded jet is restricted by the significant increase of the local grid resolution, which at the same time affects the size of the whole mesh. In a typical under-expanded jet, the supersonic region is characterized by normal shocks and oblique reflected shocks along the jet direction, where in some cases more than one highly supersonic region is visible. While this phenomenon affects the air entrainment (occurring only in the subsonic region), a previous study [18] has shown that even with a lower resolution mesh of the supersonic region, it is possible to achieve a good agreement with optical data in terms of mixture formation. However, for multi-hole nozzles jet-to-jet interaction may have effects that require the near-nozzle region to be resolved in greater detail than expected from simple downscaling with the hole size.

TEST CASE 1 (1-H 100 BAR)

Figure 8 shows the comparison between numerical and optical data for test case 1 (1-h nozzle, 100 bar injection pressure). As mentioned earlier, a 4°CA ramp is used to model the transient duration, showing good agreement with schlieren images. With the nominal SOI = −140°CA, the first traces of the jet are visible in the cylinder at −137°CA, which agrees with the assumption of actual SOI = −137°CA. The jet penetration in the numerical results seems to match the optical data, even though the actual jet direction is not well captured, as seen in Figure 8 at −135°CA. Apart from tolerances in nozzle fabrication, the jet might also deviate slightly due to the complexities in the flow inside the injector, which are not part of the current calculation. As a consequence, in the CFD results the jet impinges the wall higher compared to PLIF data, with consequent difference in terms of jet penetration at −130°CA.

The assumption of the transient duration can also have an effect on the disagreement at −130°CA. Compared to previous numerical results [17,18], in this paper the injection transient is longer, leading to a “slower” jet penetration at the beginning, which nevertheless matches schlieren data up to −135°CA. Later, the jet is too slow in numerical results, if compared to experiments. This might be an indication that the transient is not perfectly linear.

The post-injection evolution of the hydrogen jet is well captured by numerical simulation throughout the compression stroke, even after the multiple impingements on the cylinder walls. However, two main issues can be highlighted in Figure 8. First, the CFD results can qualitatively capture the fuel distribution within the jet (the region with highest values of fuel mole-fraction is located below the exhaust valve at −70°CA, below the injector at −55°CA and below the intake valve at −30°CA), nevertheless the fuel dispersion is under-predicted, leading to a (quantitative) disagreement in fuel concentration. Overall, the gradient of fuel concentration in the optical data is much shallower than in the CFD results. All the versions of the k-ε model (standard, RNG, realizable) have been previously tested [18] and have provided similar results. Also, tuning of the k-ε realizable model has been performed, showing better (quantitative) results in terms of concentration values but simultaneous loss of qualitative information on mixture stratification [18]. One of the main hypotheses that the authors have developed is that the RANS approach cannot accurately predict the local fuel diffusion, since all scales of turbulence are crudely modeled instead of being directly calculated. This conclusion suggests the use of a more detailed approach (LES) in the future, in order to increase the level of detail and the accuracy of the numerical simulations.

Grid resolution at the cylinder walls might also play a role in the disagreement between experiments and modeling. In this study, the overall grid resolution is decreased compared to a previous study [18], while increased near the nozzle, to achieve higher accuracy within the supersonic jet while avoiding prohibitive computational times. As a consequence, the jet behavior at the cylinder walls might be not well predicted by numerical simulations, and this might influence the fuel distribution in the direction orthogonal to the wall. Wall refinement and the use of a more sophisticated wall treatment are currently under investigation.

It is worth noting that in this study the range of hydrogen mole fraction is dynamically varied during the compression stroke in order to highlight the differences between numerical and optical data. Still, after more than 100°CA, the computational code is able to provide reasonably accurate results in terms of fuel stratification, even though the mixture tends to progressively become homogeneous when the piston approaches TDC.

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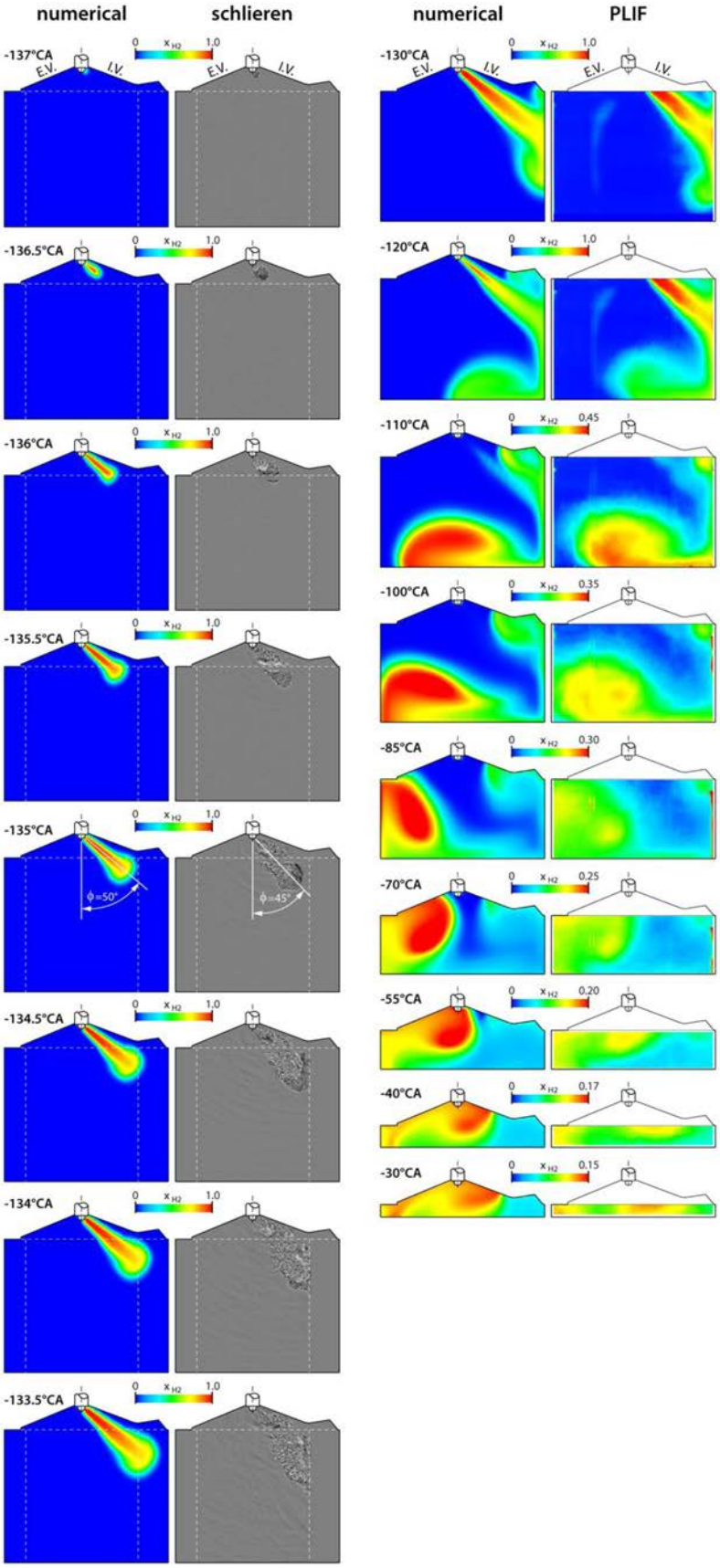

Figure 8. Comparison between numerical and optical (Schlieren and PLIF) data for test case 1 (1-h, 100 bar)

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TEST CASE 2 (1-H 25BAR)

Figure 9 compares numerical and optical data for test case 2 (1-h nozzle, 25 bar injection pressure). The comparison with schlieren data does not show differences between simulation and experiments in terms of jet direction, unlike what is observed for test case 1 (1-h nozzle, 100 bar injection pressure). This suggests that the nozzle internal flow might influence the jet direction as a direct effect of the injection pressure. Also, jet penetrates faster in CFD results than in optical data during early injection (see Figure 9 at −133°CA), while in the PLIF data the hydrogen jet impinges the cylinder walls earlier than in the numerical results (−129°CA). These results may again indicate that the linear-transient model is somewhat lacking and may need refinement, depending on the importance of early jet behavior in the objectives of simulation. It is also possible that these minor differences are due to limited repeatability of the injection process, since PLIF and schlieren images were taken several months apart.

Overall, the agreement during the entire compression stroke is good, suggesting that, when using the same computational grid, the lower jet velocity might play a role in ensuring more accurate results than the 1-h 100 bar case. Results up to −70°CA do not emphasize differences in terms of fuel concentration between optical and CFD data, due to the wide range of values represented (injection is still taking place, since EOI = −59.5°CA for test case 2). However, at −50°CA and −30°CA, where the maximum H_2 mole fraction values are reduced to 0.45 and to 0.2, a good agreement can be observed in terms of fuel dispersion.

TEST CASE 3 (13-H 86BAR)

Figure 10 shows the comparison between numerical and optical data for test case 3 (13-h nozzle, 86 bar injection pressure). This case is extreme, in that the jet-to-jet interaction leads to complete merging of all jets, very close to the nozzle exit. Figure 7d has shown how the jets merging takes place downstream of each Mach disk, where each jet deviates towards its closest neighbor jet and due to the nozzle symmetry all the side jets are pulled towards the central jet. At the end of Mach disk the jet becomes subsonic (see Figure 7c), and that is where each jet suffers from the Coanda effect, since air entrainment is limited by the presence of a close jet. In this zone the requirements for the grid resolution are more stringent and particular care has to be taken when generating the computational mesh, even relatively far from the Mach disk.

The comparison between CFD and schlieren data shows that the assumption of 3°CA delay in SOI is not perfectly verified for this case. Not clearly visible in Figure 10 at −137°CA, the hydrogen jet is already coming out from the nozzle, but the numerical simulation predicts a higher penetration at the beginning of the injection process, up to −136°CA. During the jets' merging (from −136°CA to −134°CA), the resulting single-jet propagates slower in the numerical results compared to optical data. The jet shape in CFD data also does not exactly match the schlieren images. Higher accuracy might be gained by extending the high resolution domain further in the computational mesh, at least to the pentroof - cylinder interface. Still, at −130°CA the penetration in CFD data is slightly higher than in PLIF data. Once again, the assumed injection profile might be another reason for this disagreement.

For this nozzle it is more difficult to use qualitative schlieren images for the purpose of assessing whether the initial transient is modeled with sufficient accuracy. This is because even very early jet penetration is likely to be influenced by the compounded effects of start-up transient and jet merging. Quantitative, high-resolution measurements of fuel mole-fraction may be necessary to separate the modeling insufficiencies that occur simulating both of these phenomena. Turbulence modeling might have a role too. High turbulence at the jet boundaries, clearly visible in the schlieren data and roughly modeled in numerical simulation, might increase the jet-to-jet interaction and slow each jet down. Therefore, the RANS approach in this operating condition might suffer from higher inaccuracy than for the single-hole nozzle cases.

The agreement between simulation and PLIF is again good at −120°CA and −110°CA. Later in the compression, the location of the hydrogen clouds is still well predicted. The rich zones remain located close to the piston during the entire compression stroke. Nevertheless, here the under-prediction of fuel dispersion is even more pronounced than in the previous two cases. The mixture stratification at the end of compression (−30°CA) is not sufficiently well predicted and the lack of optical information in the pent-roof does not improve the quality of the comparison. Experimentally, asymmetry between the two main rich zones can be observed at −40°CA, the richer one being located in the intake quenching zone. The simulation captures the asymmetry, but insufficient dispersion makes this a rough qualitative agreement only.

The multi-hole nozzle represents the hardest case to be simulated, especially when a large number of holes is considered. The complex physical phenomena in the under-expanded region together with the jet-to-jet interaction might lead to inaccurate prediction of the air entrainment in the proximity of the nozzle exit, which might increase the disagreement between numerical and experimental results in terms of fuel dispersion. However, even in this case there is consistency between CFD and optical data in terms of jet penetration and evolution. Future investigations will focus on jet behavior at cylinder walls (wall boundary layers and more sophisticated wall functions) and higher-detail simulations

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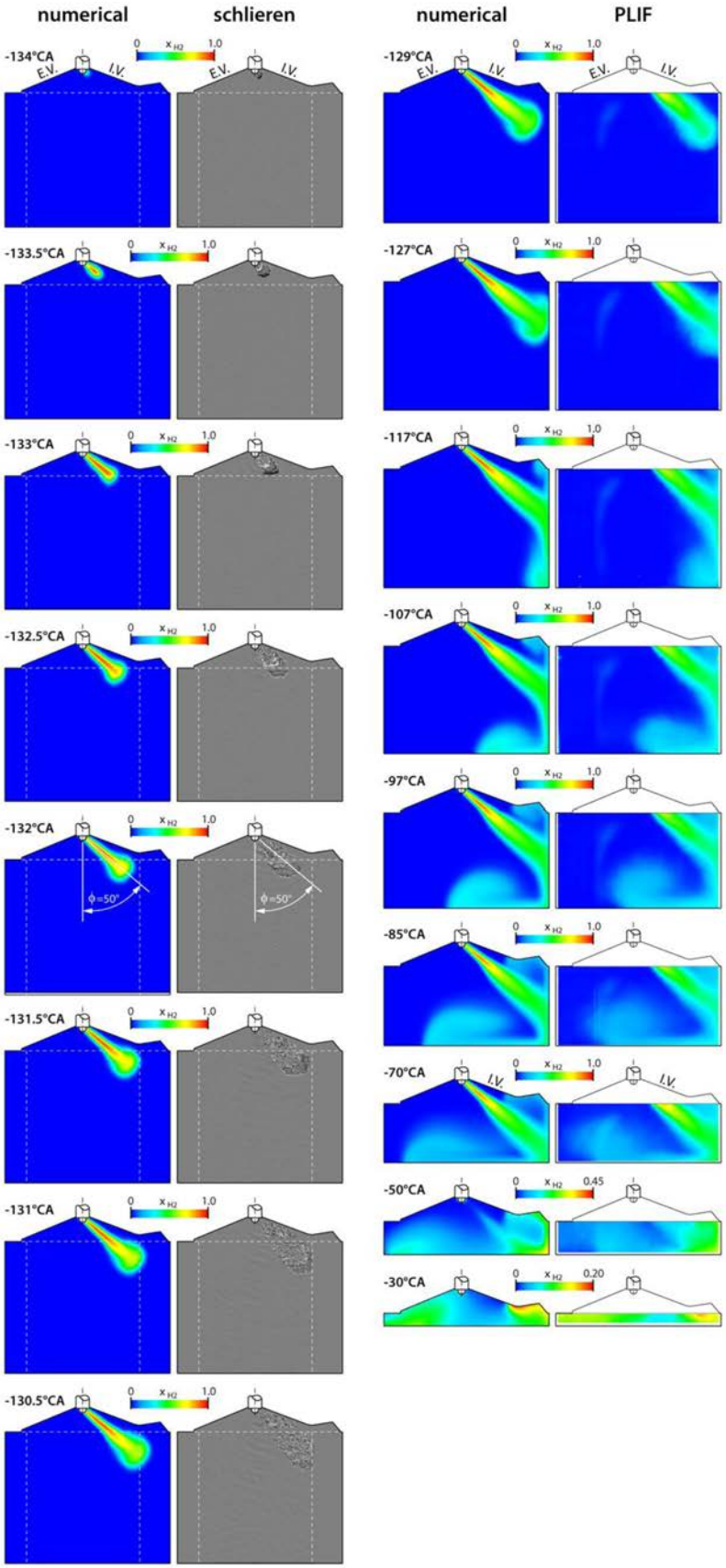

Figure 9. Comparison between numerical and optical (Schlieren and PLIF) data for test case 2 (1-h, 25 bar)

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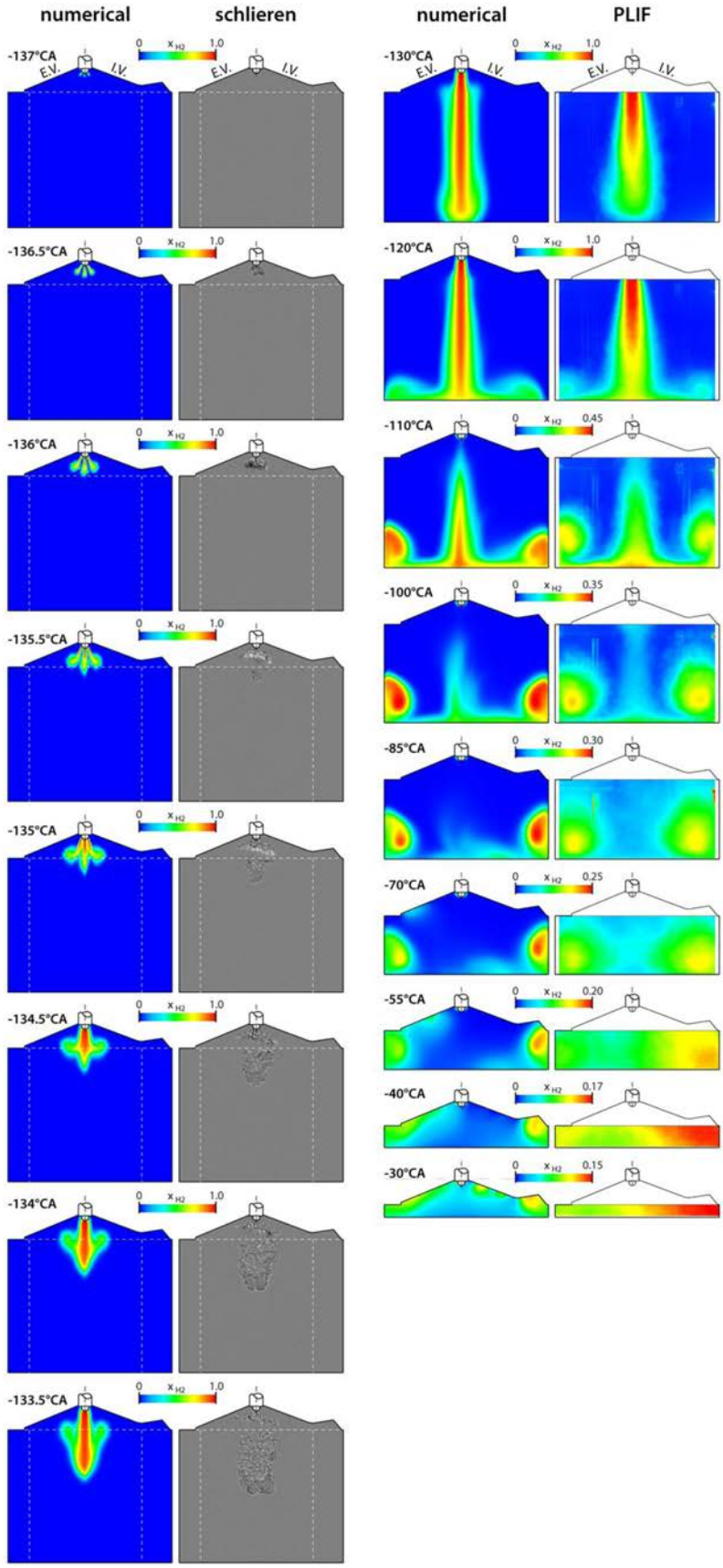

Figure 10. Comparison between numerical and optical (Schlieren and PLIF) data for test case 3 (13-h, 86 bar)

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(higher grid resolution, LES) in order to further improve the numerical predictions.

CONCLUSIONS

A major challenge for a direct injection engine is the optimization of mixture formation. Numerical simulations can become a powerful tool for the optimization of DI H_2-ICEs, however their accuracy needs to be validated by the comparison with experimental data. For mixture formation, the ideal set of data comes from an optically accessible engine.

This paper extends the initial validation of numerical results by a CFD-RANS approach to a wider range of cases, including high and low injection pressure and single- and multi-hole nozzles. Optimized computational grids and the k-ε realizable turbulence model are used and injection profile assumptions are discussed, providing a comprehensive analysis of the main numerical features that need to be taken into account in the simulation of a gaseous fuel DI engine.

The comparison with optical data shows a good agreement in terms of jet penetration and overall evolution for all the cases examined here. The agreement remains good throughout compression, even after multiple impingements with the cylinder walls. Fuel dispersion is under-predicted in all the examined cases, with the highest disagreement for high injection pressure.

The simulation of the multi-hole nozzle shows the least accurate results in terms of both initial jet penetration and final fuel distribution. The hypothesis is that the jet-to-jet interaction occurring in the under-expanded region is not captured with the current level of detail.

Increasing grid resolution along the jet axial direction, using more accurate wall treatment, and performing higher fidelity (LES) simulations to better describe turbulence are identified by the authors as possible keys to improve the accuracy of numerical predictions. However, in the current state CFD already shows remarkable results, making it a useful tool to optimize injection parameters and nozzle configuration in order to increase efficiency and reduce the emissions in a hydrogen-fuelled DI engine.

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NOMENCLATURE

BTE
Brake Thermal Efficiency

°CA
Degree Crank Angle

CCD
Charge-Coupled Device

CFD
Computational Fluid Dynamics

CMOS
Complementary Metal Oxide Semiconductor

COV
Coefficient of Variation

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DI
Direct Injection

DNS
Direct Numerical Simulation

EGR
Exhaust Gas Recirculation

EOI
End of injection

H_2
Hydrogen

ICE
Internal Combustion Engine

IMEP
Indicated Mean Effective Pressure

IVC
Intake Valve Closing

LED
Light Emitting Diode

LES
Large Eddy Simulation

N_2
Nitrogen

Nd:YAG
Neodymium-doped Yttrium Aluminum Garnet

NO_X
Nitrogen Oxides

PFI
Port Fuel Injection

PIV
Particle Image Velocimetry

PLIF
Planar Laser-Induced Fluorescence

RANS
Reynolds-Averaged Navier-Stokes

RNG
Renormalization Group

RPM
Revolution per Minute

SI
Spark-Ignition

SOI
Start of Injection

TDC
Top Dead Center

1-h
Single-Hole Nozzle

13-h
13-Hole Nozzle

Ma
Mach Number

λ
Air/Fuel Ratio

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