

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 H₂ 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 H₂-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 H₂ density are eliminated, thus allowing the same

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 pursue 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 1a. The engine has a four-valve head with a pent-roof combustion chamber. The piston

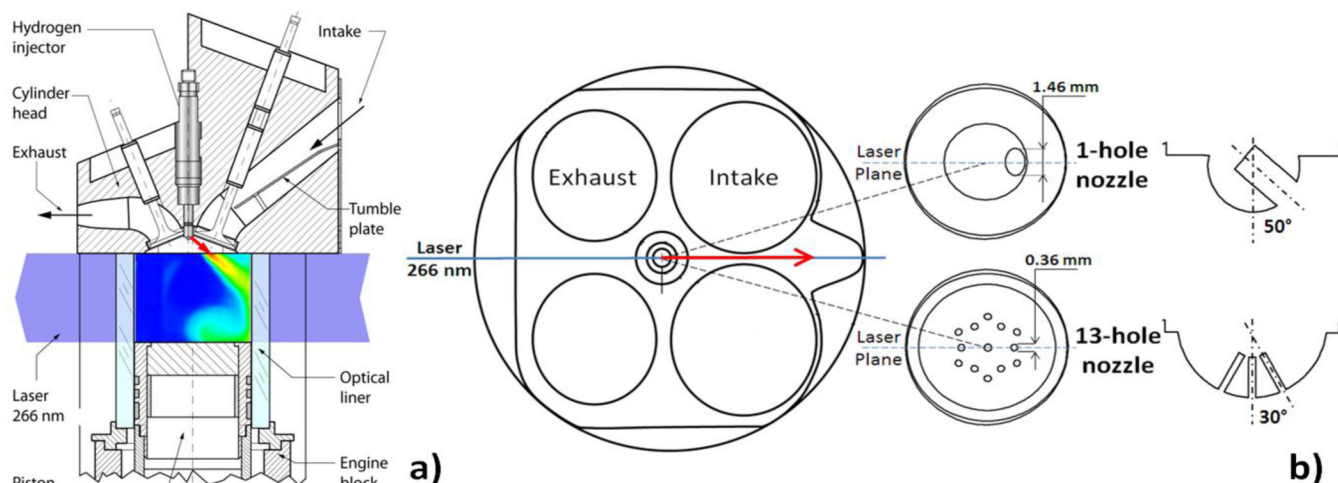


Figure 1. Schematics of engine hardware. (a) Optical engine with measurement plane. (b) Location and targeting of the nozzles with respect to the combustion chamber.

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 ($\lambda = 4.0$), 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

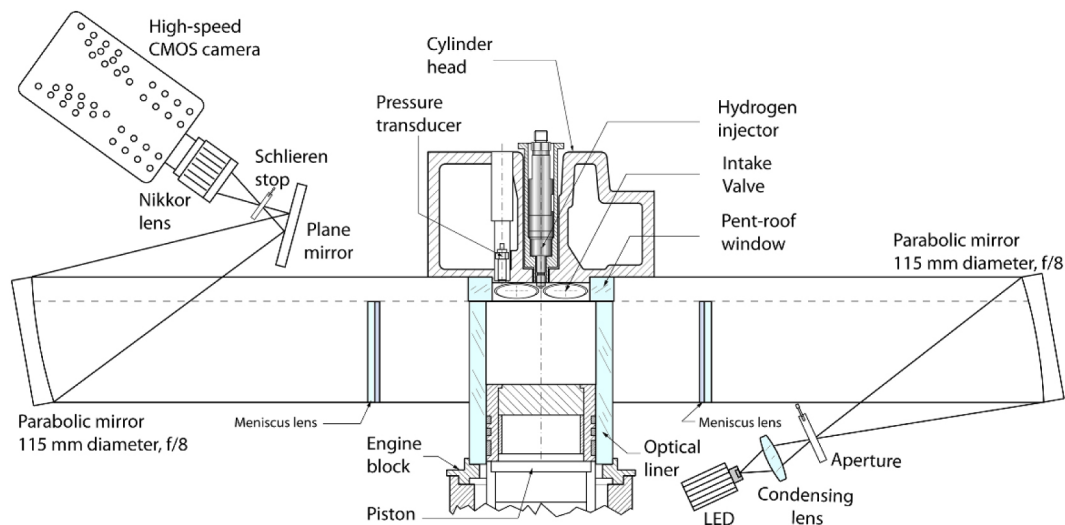


Figure 2. Schematics of the high-speed schlieren imaging technique

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 ($= 55 \mu\text{s}$) and an effective

exposure time of $5.5 \mu\text{s}$, 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 $k-\epsilon$ 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 $k-\epsilon$ model provided by Fluent ($k-\epsilon$ standard, $k-\epsilon$ RNG, $k-\epsilon$ realizable) have been previously tested and showed only slight differences in the numerical results [18]. In this paper, the realizable $k-\epsilon$ 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.

- 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.

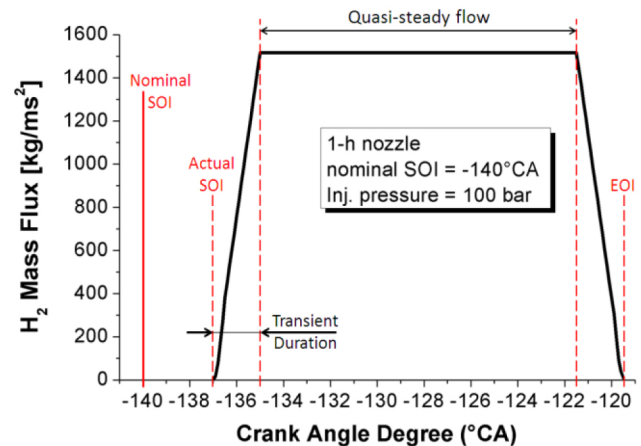


Figure 3. Schematic of the assumed generic injection profile

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.