

Modeling and Experiments on Mixture Formation in a Hydrogen Direct-Injection Research Engine

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ABSTRACT

Direct injection offers a large number of degrees of freedom, as it strongly influences the mixture stratification process. Experiments on a single cylinder research engine fuelled by H_2 , carried out at Argonne National Laboratory, showed the influence of injection parameters (timing and geometry) on engine efficiency and combustion stability. At low load, when a late injection strategy was performed, an unstable engine behavior was detected varying the injection direction. In order to optimize the mixture stratification process in DI H_2 engines, it is important to understand the physics underlying the experimental results.

A spatially resolved representation of the in-cylinder processes is a useful tool to properly set the injection parameters. Also, the knowledge of the pre-injection flow field is of added value in optimizing the injection process. This paper describes the initial development of a 3D-CFD tool for direct-injection hydrogen engines, including numeric approach, simulation validation, and application to the mixture-formation process for a specific injection strategy.

Simulations were performed by the commercial solver Fluent and the numerical results were compared to laser-based measurements of the fuel distribution in an optically accessible engine. The calculations were found to be reasonably accurate, especially for late injection timings. The simulation results show that intake-induced tumble combines with the jet momentum when the jet is pointed away from the intake valves, which can improve engine operation for early and slightly retarded injection. For late injection timings the engine can fire stably if the injector is pointed towards the spark plug.

INTRODUCTION

Among alternative fuels, hydrogen is considered unique in its potential to reduce overall CO_2 emissions. Its application as an engine fuel has been studied for

several decades and researchers have provided extensive reviews of the available literature [1].

The U.S. Department of Energy set a brake thermal efficiency of 45% and NO_x emissions of 0.07 g/mile as targets for hydrogen internal combustion engines (ICEs). Also, the same power density as that of a comparable gasoline engines is to be achieved [2]. Direct Injection (DI) proved to be a promising approach to help meet the above mentioned objectives [3]. Compared to hydrogen port fuel injection, direct injection allows higher specific power and avoids the risk of backfiring. On the other hand it introduces a higher number of degrees of freedom, mainly due to the injector geometry and injection strategy. Both geometrical and operational injection parameters are critical and need to be optimized to guarantee proper mixture stratification throughout the combustion chamber.

TECHNICAL APPROACH

For this study a simple injector geometry was used to evaluate the effects of the injection strategy on combustion stability. Engine performance testing was performed at Argonne National Laboratory on a 0.5 liter single-cylinder research engine which had been specifically designed for combustion studies and was equipped with a cylinder head that allowed side as well as central injector location. A hydrogen injector with a single-hole nozzle was placed in central location and the fuel jet was oriented in various different directions. Tests were performed at different load points for an array of possible configurations. The influence of start of injection (SOI) and injection direction on combustion stability and engine efficiency was analyzed.

A CFD 3-D numerical model was developed as a tool to improve the understanding of the experimental results. Among other benefits, detailed information of the mixture formation provided by the model is envisioned to guide the experimental activities in optimizing the engine performance. The accuracy of the numerical model in



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predicting the mixture formation process was checked against laser-based imaging in an optical engine at Sandia National Laboratories. After this initial validation, the numerical code was used to help understanding the low load combustion stability issues and operational limitations of Argonne National Laboratory's thermodynamic hydrogen direct injection engine.

EXPERIMENTAL SETUP

OPTICALLY ACCESABALE ENGINE

The optical engine at Sandia National Laboratories is a single-cylinder research engine with optical access of the Bowditch type, i.e., through parts of the liner and pent-roof as well as through the flat-topped piston. Hydrogen fuel is delivered directly into the cylinder through the same injector used for the engine tests at Argonne National Laboratory. Since only pre-spark mixture formation was of interest for this study, the engine was motored and fed with nitrogen as a bulk gas in the intake for all optical experiments. Table 1 summarizes engine and testing parameters. The optical engine and the corresponding validation simulation (see below) were run at 1500 RPM.

The laser-based imaging technique used to measure the in-cylinder fuel distribution is described in detail in [4]. Briefly, acetone is seeded as a tracer into the hydrogen fuel by a high-pressure bubbler. At 100 bar and room temperature, a volume concentration of 0.33% can be reached. A quadrupled Nd:YAG at 266 nm laser excites fluorescence in a plane parallel to the piston. Laser energies of about 100 mJ/pulse and a sheet-forming lens combination with $f = 1500$ mm were used. An $f = 85$ mm, $f/1.4$ camera lens focuses the visible part of the resulting acetone fluorescence onto an unintensified, back-illuminated CCD. Standard background and flat-field corrections were performed to quantify the measurements. For the latter, a nearly homogeneous charge is prepared by injection during the intake stroke. Inhomogeneities in the temperature field, induced by mixing of cold hydrogen and hot bulk gas, are corrected for based on known spectroscopic properties [5, 6] of the tracer and the assumption of adiabatic mixing between fuel and bulk gas.

Table 1: Sandia engine specifications and operating point

Bore	92 mm
Stroke	85 mm
Displacement	560 cm ³
Compression ratio	11
Speed	1500 rev/min ⁻¹
Intake pressure	1 bar
Equivalent fired IMEP	2.5 bar
Global equiv. ratio	≈ 0.25
Injection pressure	100 bar
Injection duration	17.5 °CA

Depending on the crank angle at the time of imaging, images were acquired in up to 5 planes spaced throughout the upper part of the cylinder and pent-roof, as shown in Figure 1. Visible through the piston window are the central 65 mm of the 92 mm bore. A set of images from 100 fueled cycles was acquired per measurement plane. The mean over all images in such a set is considered for comparison with the simulation.

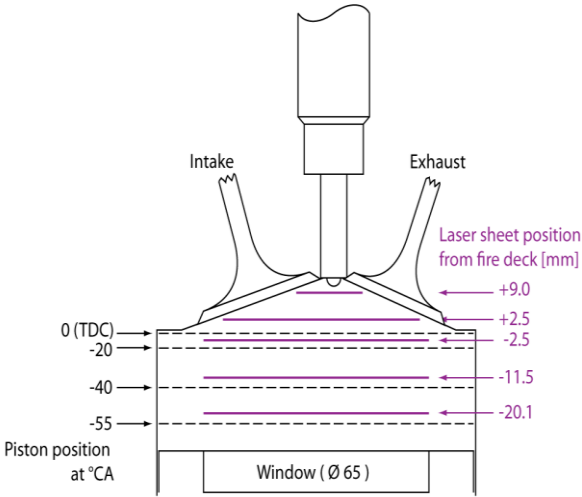


Figure 1: Schematic of the combustion chamber with positions of measurement planes and piston at a several crank locations

THERMODYNAMIC RESEARCH ENGINE

The engine performance tests were performed on a Ford DI H₂ single-cylinder research engine. The main specifications of the engine are summarized in Table 2 [7]. The engine is specifically designed for hydrogen operation and can be operated with hydrogen port injection as well as hydrogen direct injection. Results presented in this paper are based on operation with hydrogen direct injection with central injector location. The hydrogen injection pressure was kept constant at 100 bar for all operating conditions. A hydrogen supply system with an integrated coriolis meter was used to deliver and meter the hydrogen flow to the engine. The injector used for this study is a solenoid-operated injector manufactured by Westport Innovations Inc.

Table 2: Ford Engine specifications [7]

Engine manufacturer	Ford Motor Company
Displacement (l)	0.5
Compression ratio	11.5:1
Bore/Stroke (mm)	89/79.5
Valve Train	4V Dual Overhead Cam (DOHC)
Intake Valve Timing	IVO=15° CA BTDC, IVC=35° CA ABDC
Exhaust Valve Timing	EVO=45° CA BBDC, EVC=10° CA ATDC
Speed Range (RPM)	800-6000
Peak cylinder pressure (bar)	100
Hydrogen measurement	Micro-motion Coriolis Meter
Injector – Direct Injection	Westport

DETAILS OF NOZZLE ALIGNMENT

An injector with a single-hole nozzle was chosen for this study. The injection hole has a diameter of 1.375 mm at an angle of 50° with respect to the injector axis. A schematic of the injector location and the direction of the jet relative to the injector axis are shown in Figure 2. The single-hole design was purposely chosen to simplify the analysis and guarantee a single injection jet without any jet-to-jet interaction inside the combustion chamber [8].

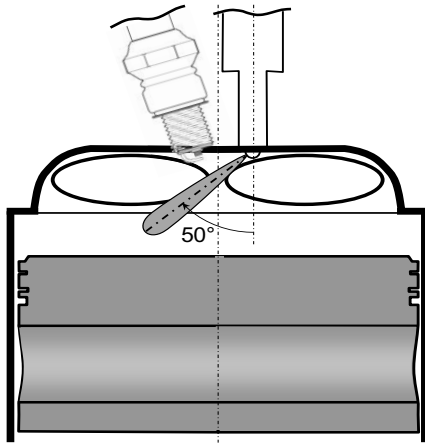


Figure 2: Orientation of the injector jet relative to the injector axis

Various injection directions were investigated as part of this study. The injector with its axis parallel to the cylinder axis could be rotated and clamped down in any radial position (Figure 3). The injection direction is given as an angle relative to the location of the spark plug. Injection directions of 0° , 45° , 90° , 180° , 270° and 315° were investigated. These injection directions can be described as:

- $\phi=0^\circ$ Injection towards the spark plug
- $\phi=45^\circ$ Injection towards the intake valve
- $\phi=90^\circ$ Injection towards the intake quenching zone
- $\phi=180^\circ$ Injection away from the spark plug
- $\phi=270^\circ$ Injection towards the exhaust quenching zone
- $\phi=315^\circ$ Injection towards the exhaust valve

TEST PLAN

In addition to the change in injection direction a sweep of the start of injection was performed for each injection angle, providing further information on the injection strategy's effects on engine performance and combustion stability. In this paper the term *injection strategy* refers to a specific injection configuration and is defined by the injection angle and the start of injection.

The SOI sweeps started with early injection timings, close the intake valve closing (SOI = 140°CA BTDC, or -140°CA in the following), moving towards TDC in increments of 20°CA until the end of injection (EOI)

coincided with spark timing or stable combustion could not been maintained. It was observed that retarding the SOI for certain configurations resulted in misfires and incomplete combustion events with unburned hydrogen exceeding 20,000 ppm. No data were recorded at these points to avoid creation of ignitable mixture in the exhaust and these operating points were considered unstable. The engine speed was kept constant at 2000 RPM while varying engine loads with 2.5, 4, 6 and 8 bar indicated mean effective pressure (IMEP) at MBT spark timing. Detailed results of these tests are reported in [9].

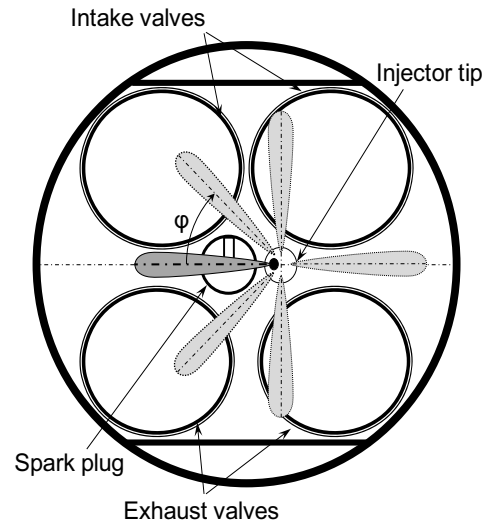


Figure 3: Bottom view of combustion chamber showing the various injector jet directions

NUMERICAL SIMULATION

SIMULATION STRATEGY

To provide a detailed representation of the physical phenomena inside the cylinder, a multi-dimensional CFD approach is usually preferable, especially when the process under investigation is greatly influenced by the engine geometry, as in the case of the mixture formation process in DI engines. For the present study 3-D CFD simulations of the in-cylinder mixture formation were performed using Fluent (version 6.3.35), a commercial software. The computational grids were generated using the Gambit pre-processor of the Fluent solver. The overall strategy of the numerical simulations can be summarized as follows (Figure 4):

- 1) A detailed computational grid (Figure 4a), reproducing the combustion chamber as well as the intake/exhaust valves and ducts, was generated. The purpose for generating this grid was to evaluate the actual flow field development during the gas-exchange phase, before the fuel injection.
- 2) A reduced computational grid (combustion chamber only) was generated in order to focus computational efforts on the compression stroke and the injection process.

- 3) The information on the flow field and physical quantities calculated from the gas-exchange phase were set as initial conditions for the subsequent simulation of compression and injection phase, by means of the reduced grid (Figure 4b).
- 4) For a specific operating condition (engine load and speed), different injector geometries (number of nozzles, nozzle diameter, direction and location) and injection strategies can be evaluated on the reduced grid without the need to re-calculate the in-cylinder flow field (Figure 4c).

The detailed computational grid for the Ford engine consists of about 250,000 cells (at TDC). The overall domain (cylinder and ducts) is mainly characterized by a tetrahedral mesh (deforming zone), with the only exception of the upper valve and piston zones (layering zone), where a hexahedral- or wedge-based mesh was generated. This is to allow for the motion of the valve and piston surfaces. The simulation of the gas-exchange phase starts few crank angle degrees before exhaust valve opening (EVO). The initial conditions for the in-cylinder pressure, intake and exhaust pressure, temperatures, and mass fractions were taken from experimental data. Then, the evolution of the in-cylinder flow field during the exhaust and intake stroke was simulated. Simulations of the gas-exchange process ends around intake valve closing (IVC), just few crank angle degrees before the earliest SOI. Even though for some operating conditions (e.g. SOI = -140°CA) the intake valve is still slightly open (nominal IVC at -145°CA), for purposes of information transfer between full and reduced grids it is assumed to be already closed. The flow-field information and other physical quantities (temperature, pressure, turbulent parameters, density, mass fractions) were stored at the end of the gas-exchange simulation and set as initial conditions for the subsequent compression stroke. Figure 4b, plotting the velocity map in a vertical section through the valve axis, shows the information exchange process at the earliest SOI (-140°CA) from the detailed grid (left side) to the reduced one (right side). To generate the reduced mesh for the Ford engine (in order to simulate the injection and mixture formation) the same topological approach as for the detailed mesh was followed. A layering zone is still present to allow the piston motion. Nevertheless the grid resolution was increased due to the reduced computational time (only the compression stroke is simulated). Different grids were tested (200,000 500,000 and 1,100,000 computational cells, calculated at the beginning of the compression stroke, at -140°CA) to highlight the influence of the grid density on the numerical results. For all the grids, the maximum cell skewness was checked and controlled to be less than 0.9 to ensure the convergence of the numerical solution. To this purpose, for the detailed computational grid, the remeshing algorithm was enabled throughout the deforming zone to allow for a regular mesh during the valves motion. On the other side, numerical simulations on the reduced grid were characterized by a layering

approach only (maximum cell skewness less than 0.85 during the overall piston motion). In Figure 4c a section of the reduced mesh corresponding to the cylinder head is shown. The valve lower surfaces, the spark-plug location, and the nozzle geometry are visible.

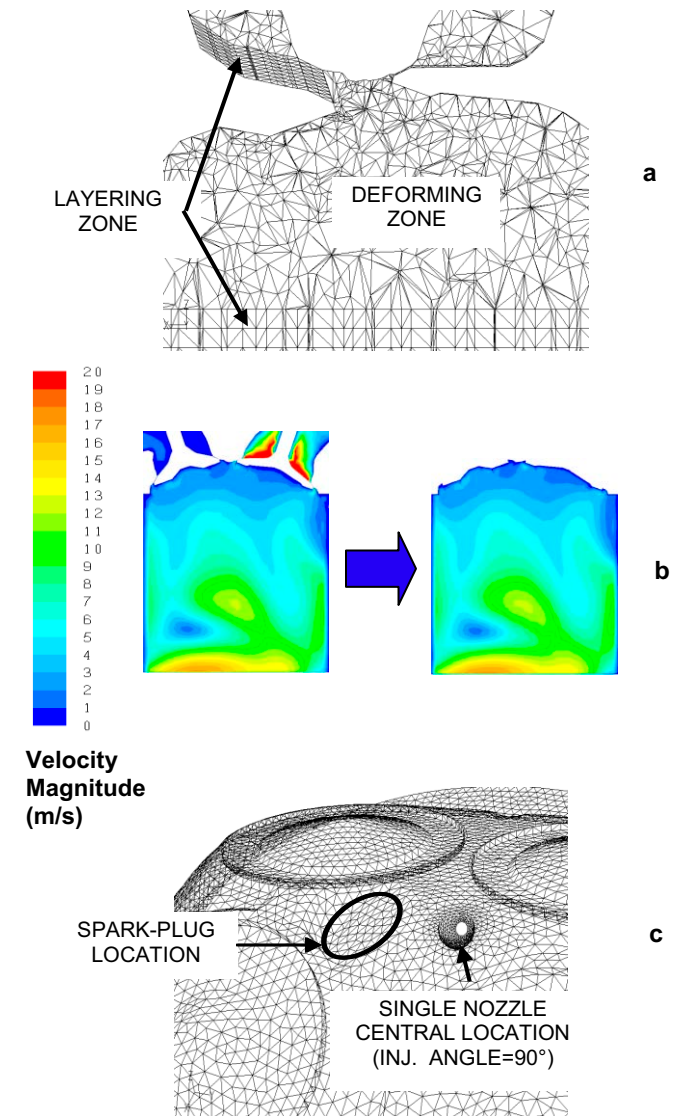


Figure 4: Schematic of the numerical approach:
a) Detailed computational grid;
b) Schematic of the transition from detailed to reduced geometry around IVC;
c) Reduced computational grid and injector geometry

The analysis of the influence of the grid density on the numerical results was carried out on the Ford engine to set the proper number of computational cells for the subsequent validation of the numerical code. Additionally, a study on the influence of the in-cylinder flow field on the overall mixture formation process was performed as well.