

## A CFD Study for Spray Characteristics of CNG Fuel

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### Abstract

Compressed natural gas has various advantages as an automotive fuel compared to that of gasoline and diesel. Natural gas is economical, has better knock resistance, a wider range of flammable air fuel ratio, as well as lower carbon monoxide, carbon dioxide and hydrocarbon emissions. In CFD calculation, the comparison with optical data shows a good agreement in terms of jet penetration and overall evolution for all the cases examined here. From these results, CFD proves to be a useful tool to optimize injection against environmental parameters and nozzle configuration in order to increase efficiency and reduce the emissions in a CNG-fuelled DI engine.

**Keywords:** CNG(Compressed Natural Gas), CVC(Constant Volume Chamber), DI(Direct Injection), CFD(Computational Fluid Dynamics), HCNG(CNG + H<sub>2</sub>)

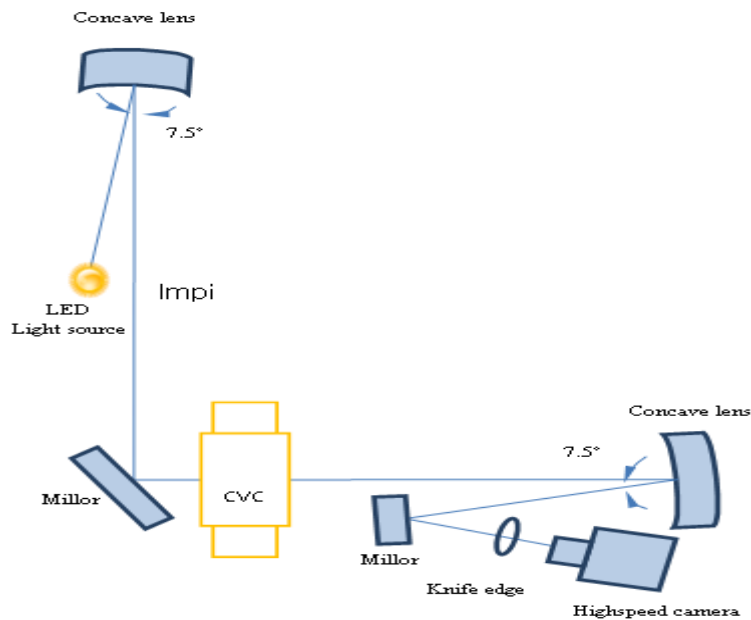
### 1. Introduction

Increase of automobile demands throughout the world facilitates the development of the engine performance depending on the applied fuels. A CFD study was done on a diesel engine applied by dual-fuel (diesel-CNG, diesel-H<sub>2</sub>) for the better mixture formation characteristics of gas injector. This study investigated how the mixing rate of gases fuel was affected by gas injection pressure and location of gas injector at a constant speed (1500-1800rpm) [1].

Meanwhile, comparative evaluations of injection and spray characteristics of a diesel engine using biodiesel blends were made [2]. In bio-diesel, boiling point is higher and longer penetration and fuel impingement is stronger with the increase of bio-diesel contents. Specially, the cetane numbers for bio-diesel blends are important factors for the combustion performance. In premixed ignition, the fuel is introduced with intake air so that homogeneous air-fuel mixture may form. The ignitability of this method depends on the global equivalence ratio. Differently, in gas-jet ignition, CNG is introduced directly into the engine combustion chamber. The overall mixture is stratified by retarded fuel injection (close to ignition timing). This method relies on local combustible mixture near the ignition position, resulting in high ignitability [3]. In addition, the relation of combustion chamber geometry and gas injection and mixing was studied by [4]. The characteristic of CNG direct injection was investigated in SI engine by numerical and experimental approach [5-7]. In order to achieve a more reliable

combustion, HCNG(CNG assisted by hydrogen) fuel was applied, where HC emissions were reduced by 100ppm without increasing CO and NOx[8]. CFD and optical study was made to investigated mixture formations indirect injected hydrogen engine [9].3-D computational fluid dynamics investigations of mixture formation have been performed by several researches with the aim to develop a tool which is 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 the comparison with the experimental data, a reliable computational code can be used to predict engine performance and drastically reduce production cost for prototypes and testing time shows that CFD is useful tool to optimize injection parameters and nozzle configuration in order to increase thermal efficiency and reduce the emissions in hydrogen fuel direct engine. This study aims to understand spray characteristics of CNG fuel engine and a CFD simulation technique is employed to obtain fundamental properties regarding overall mixture formation of direct injected CNG fuel inside a constant volume chamber.

3D-CFD investigations of mixture formation have been performed by several researchers [10-13].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. CFD is 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. The environments considered were quiescent with two individual series of tests consisting of igniting and non-igniting scenarios. For these scenarios a gas-jet was visualized using high-speed imagery and with the combustion event and products analyzed for the igniting scenario. To justify the experimental work CFD was employed to help develop more optimized and favorable ignition and injection timing and combustion phasing.



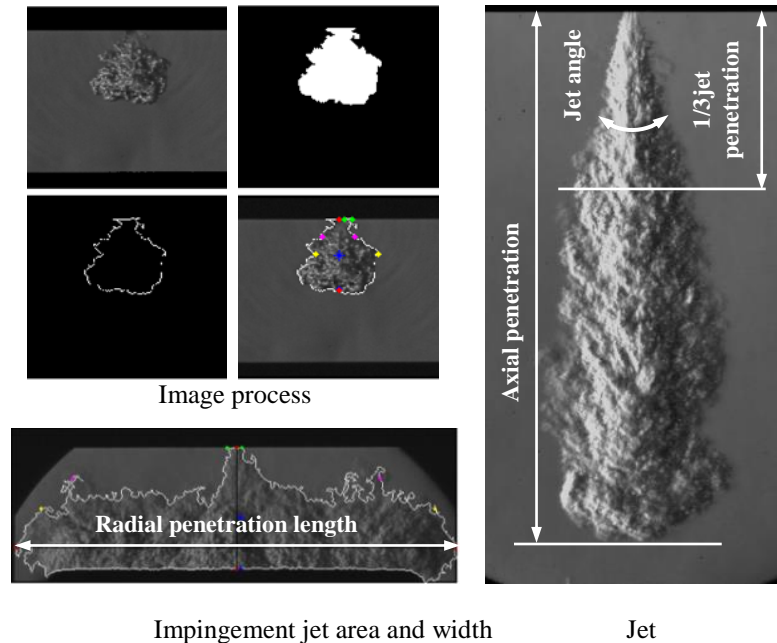
**Figure 1. Schematic Diagram of Schlieren Optical System**

## 2. Schlieren Optical Approach

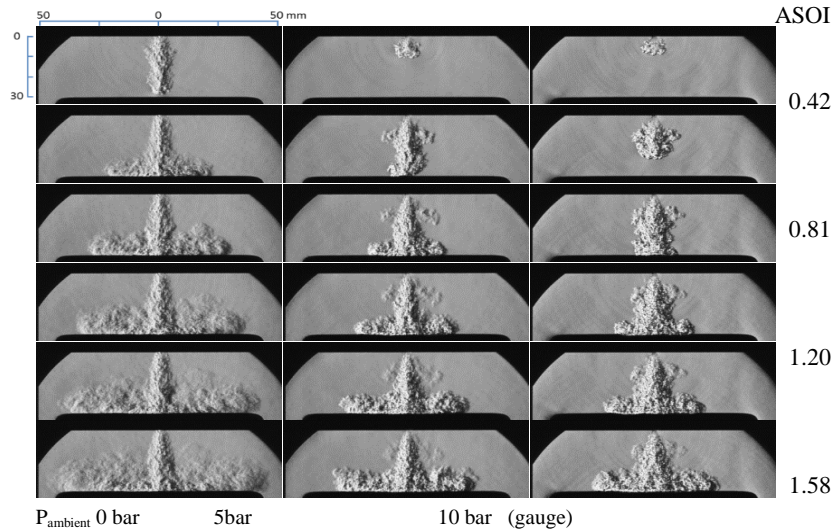
Gas-jet structure is visualized by Schlieren imaging with a high-speed camera, illustrated schematically in Figures 1 and 2. Schlieren techniques have been used for many years to visualize density gradients in transparent media, and is a convenient method of detailing the global flow structures of jets as a continuous, non-intrusive measurement (Settles 2001). Light from a white light-emitting diode (LED) was transmitted through an aperture with 1 mm diameter and collimated by a parabolic mirror with a focal length of 1524 mm. The light-rays are then focused by another parabolic mirror and blocked about half by a knife-edge which is placed at the focal point. A camera lens with focal length  $f = 50$  mm projects the resulting Schlieren images onto the detector of a high-speed (CMOS) camera (Phantom Miro).

In-house image processing was developed to help quantify the structural properties of the gas-jet. Features extracted include: physical boundaries, area, spread angle, axial and radial penetration, symmetry, jet walk and a host of other structural properties to better quantify the development of the jet and its interaction with its environment. The process of extraction is somewhat as follows: a background image is selected and a mask is created to provide a region of interest to which an interrogation image is then over-laid by the resultant subtraction leaving only useful flow information.

Through a series of filters a boundary is defined around the jet. The appropriate level of threshold intensity is critical in selecting this boundary accurately. This process is substantially more difficult for low contrast (low fuel density and thus low refractive index) images where the difference in foreground and background is minor. For this reason at images near SOI additional ROI masks were added for a more locally refined interrogation.



**Figure 2. Image Processing and Measurement Method**



**Figure 3. Schlieren Images of the Transient CNG Impingement Jet under different Ambient Pressure ( $P_{ini}$ : 85bar,  $T_{ambient}$ : 20°C)**

This boundary serves as the foundation for most other processes. From this point the maximum axial penetration is defined from the nozzle tip to the furthestmost extension along the jet axis. Similarly, the radial penetration is defined as the maximum jet width. Uniquely, these are not single-pixel investigations, rather the average of the neighboring pixels (+/- 5) from the local maximum. This local maxima method proved to be more statistically sound and robust against local perturbations.

Finally, the jet penetration proved to be the most difficult aspect. As the jets ensemble very quickly; within 60-100 $\mu$ s (1-2 frames) aSOI due to the Coanda effect, the variability of the spread angle is quite high. To overcome this several methods were used with the most accurate and repeatable method found to consist of taking the average jet width from the nozzle to 1/3 of the penetration. The average of these several hundred points gave the most accurate representation of the jet spread. A sample of the process is shown as below.

### 3. Visualization of CNG Impingement Jet

Figure 3 shows a Schlieren images of the transient CNG impingement jet under different ambient pressure ranging from 0.0~10 bar (gauge) with the injection pressure of 8.5 MPa. Also, Figure 4 shows results of projected jet area and radial penetration from the images. Impingement wall is located 30mm from the injector tip.

From these results, after approximately 0.42 ms from the injection signal, the injected fuel penetrated to the wall and impinged on it at atmospheric condition.  $P_{ambient}$  increase to 5 and 10 bar, gas jet collision interval to the impingement-wall is delayed 0.3ms each approximately. Also, two large vortexes on both sides of spray centerline are shown and rotating in the opposite direction. As  $P_{ambient}$  increase, radial penetration and projected area decrease apparently.

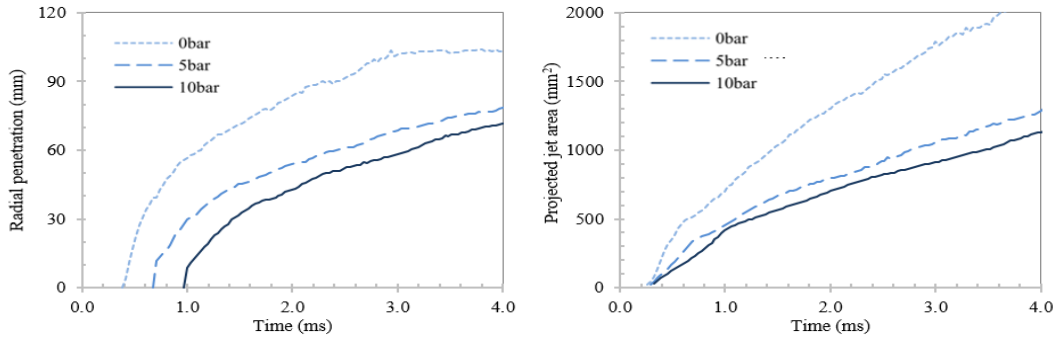


Figure 4. CNG Impingement-jet Radial Penetration & Impingement-jet Area

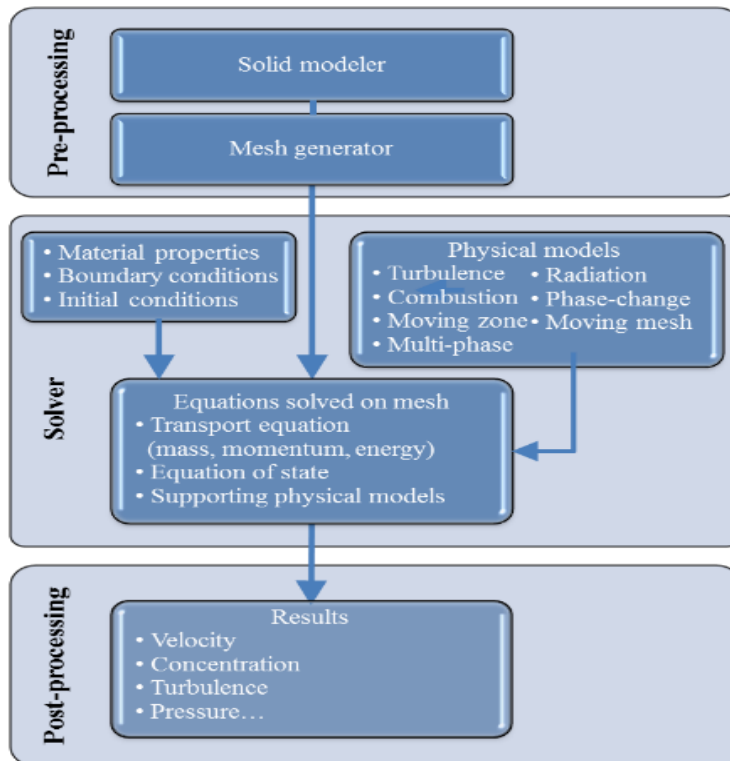


Figure 5. Processing Diagram of CFD Analysis

#### 4. Computational Analysis

To provide a detailed representation of the physical phenomena inside 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. In this research, CFD simulations of direct injection of CNG fuel are performed using the commercial CFD solver Fluent (version 6.3). A first step for modeling of mixture formation, the Gambit software is used as pre-processor to generate the computational grids. A computational grid for the full engine geometry is used to compute the cylinder flow field during the gas exchange phase prior to fuel injection. The flow field, state variable, and turbulence model parameters calculated from the gas-exchange phase are set as initial conditions for the subsequent simulation of direct injection and mixture formation. Then the equations of conservation for mass, momentum, energy and chemical species are

solved for every cell within the physical grid by the finite volume method, using a power law interpolation. The calculation steps are schematically illustrated in Figure 1 and the equation for conservation of mass, momentum as follows

Equation (1) is the general form of the mass conservation equation and is valid for incompressible flows.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m(1)$$

$\rho$ : density

$S_m$ : the mass added to the continuous phase from the dispersed second phase

Conservation of momentum is an inertial (non-accelerating) reference frame is described by:

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = -\nabla p + \nabla \cdot (\bar{\tau}) + \rho \vec{g} + \vec{F}(2)$$

$p$  : static pressure,

$\bar{\tau}$ : stress tensor

$\rho \vec{g}$ : gravitational body force,  $\vec{F}$  : external body forces

Conservation of energy is described by:

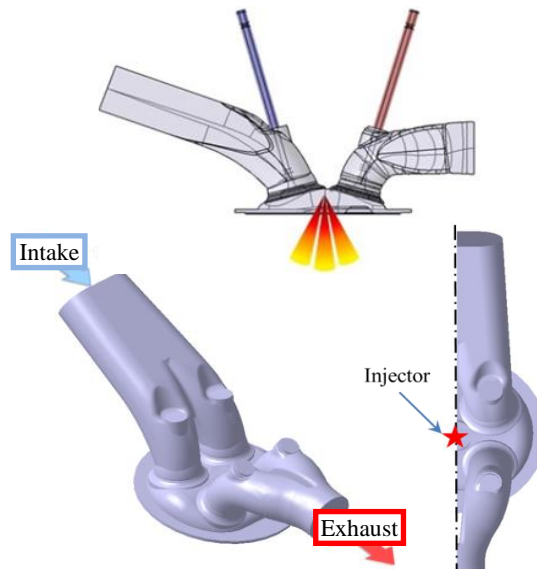
$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = -\nabla \cdot (\sum_j h_j J_j) + S_h(3)$$

$E$ : total energy per unit volume,

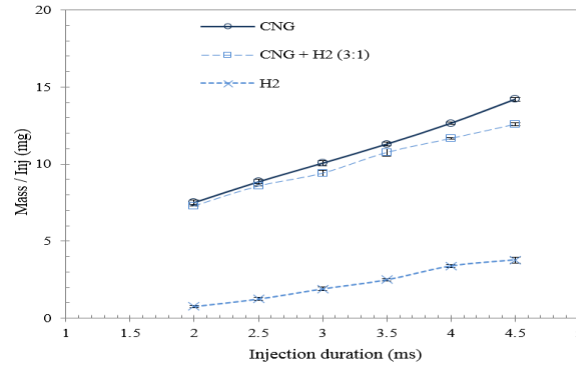
$h_j$ : sensible enthalpy

$J_j$ : diffusion flux of species

$S_h$  : heat of chemical reaction, and any other volumetric heat sources



**Figure 6. Computational Geometry of Cylinder Head and Ports**



**Figure 7. Mean Mass Flow Rate versus Injection Duration**

The detailed computational grid for the engine consists of about 300,000 and 500,000 at TDC and BDC respectively. The simulation starts at intake valve opening (IVO) and the gas-exchange process ends around intake valve closing (IVC). The flow-field information and other physical quantities such as temperature, pressure, turbulent parameters, density, and mass fractions were stored at the end of the gas exchange simulation and set as initial conditions for the subsequent compression stroke. Further details of simulation conditions are summarized in Table 1. Figure 6 depicted a cross sectional and three-dimensional geometry of the engine cylinder head. Injector is located at the center of the head. The CNG mass flux through the nozzle is calculated from the measured mean mass-flow rate as shown in Figure 7. And it is set as the mass-flow-inlet boundary condition for the injection. The resulting total mass injected per cycle is set as 15mg/cycle.

**Table 1. Engine Specification and Calculation Conditions**

Bore × Width (mm)	86 × 96	
Displacement	4 Cylinder 2L	
Compression ratio	11:1	
Injection pressure (bar)	85	
Injector	Direct injector ( $\phi$ 0.19mm, 6 hole)	
Injected CNG	10 and 23 mg/cycle (equivalent to BMEP 2 and 8bar)	
Injection Timing (Crank Angle)	10 mg/cycle	BTDC 90°
	23 mg/cycle	BTDC 150°
Engine Speed (RPM)	2000	
Crank AngleStep Size(deg)	0.25	
Crank Radius (cm)	46.5	
Valve timing (Crank Angle)	IVO	BTDC 10°
	IVC	ABDC 40°
	EVO	BBDC 45°
	EVC	ATDC 5°

## 5. Computational Results

The 3-D numerical model has been applied to the simulation of methane direct injection into a constant volume chamber and an engine with real-like moving piston. In this context the effect of ambient conditions and injection timing has been studied on mixture homogeneity and distribution inside the cylinder with flat piston head configurations. Figures 8 and 9 show the calculated images and plotted penetration respectively. The numerical simulation predicts a higher penetration, narrower jet angle at the beginning of the injection process under atmospheric condition. The comparison with optical data shows a good agreement in terms of jet penetration and overall evolution for all the cases examined here. Meanwhile, the penetration in CFD data is slightly different in the beginning of injection. This is because even very early jet penetration is likely to be influenced by the compounded effects of start-up transient and the jet-to-jet interaction. Also, in this calculation pure CH<sub>4</sub> is used because multi-component fuels such as CNG fuel are still different in CFD calculations. But it is clear that results are roughly well modeled in numerical simulation from Figure 10.

The results of engine simulation are shown in Figures 11 and 12. Injection is set as BMEP 2(10mg/cycle) and 8bar (23mg/cycle) at 2000rpm respectively. Section A-A is the horizontal cross-section of the clearance volume 1mm below the lower face of cylinder head. At low load conditions (injection timing: BTDC 90° CA), this mixture can reach the upper volume at TDC and 10° ATDC which is relatively near the spark position. But it shows an in-homogenization at the end of compression process. Although there seems a need in more justification between combustion chamber geometry and injector, especially regarding cylinder head shape and spark plug location. This kind of justification necessitates more studies. Turbulence at the jet boundaries is clearly visible and roughly modeled in numerical simulation. At high load condition (injection timing: BTDC 160° CA), it provides enough time for mixture homogenization even. Therefore, an ignitable mixture is located in a broad region around the spark plug with a local equivalence ratio of about 1.0. In this study, only flat piston was used, but it is necessary to study more sophisticated piston head and cylinder head functions in order to further improve the numerical predictions.

**Table 2. Fuel Properties**

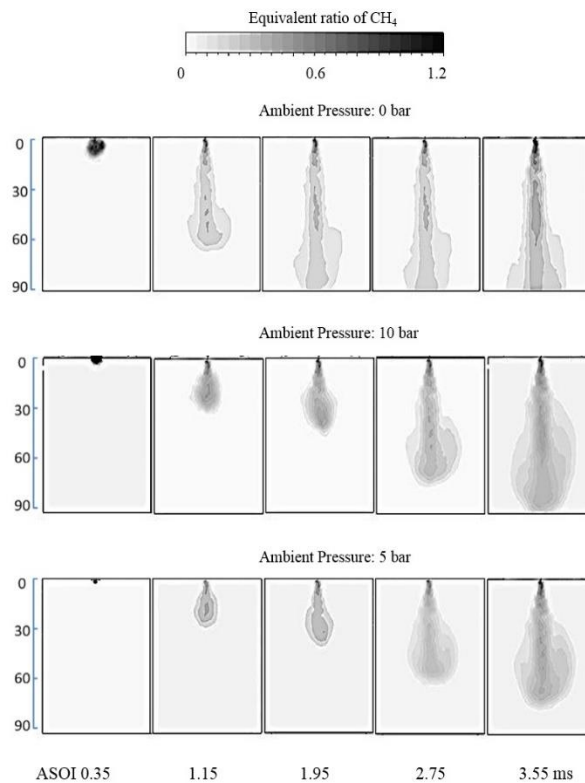
Fuels Property	Gasoline	CNG
Molecular formular	C <sub>8</sub> H <sub>18</sub>	CH <sub>4</sub> (≥90%)+...
Molecular weight	≈100	≈16
Specific gravity(kg/ℓ)	0.750	0.423
Lower heating value (MJ/kg)	42~44	54.7
Boiling point (°C, 1 atm)	35~210	-162
Stoichiometric Fuel/Air	14.7	17.3
RON /MON (Research / Motoring Octane Number)	92 / 83	130 / 125~130
Energy Density(MJ/ℓ )	31.83	7.88



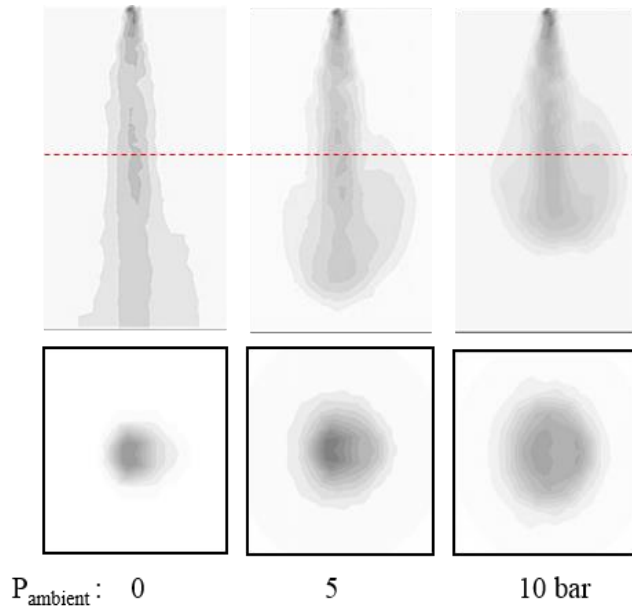
## 6. Conclusions

A major challenge for a direct injection engine is the optimization of mixture formation. The jet patterns of CNG fuel was investigated by using computer simulation. The characteristics of injected jet flow in a cylinder and flow distribution is simulated in an engine using CFD code as well. Numerical simulation can become a power tool for the optimization of DI CNG engine, however their accuracy need to be validated by the comparison with experimental data. Based on the observation of the qualitative flow visualization for the characteristics of injected flow distribution, following conclusions were obtained.

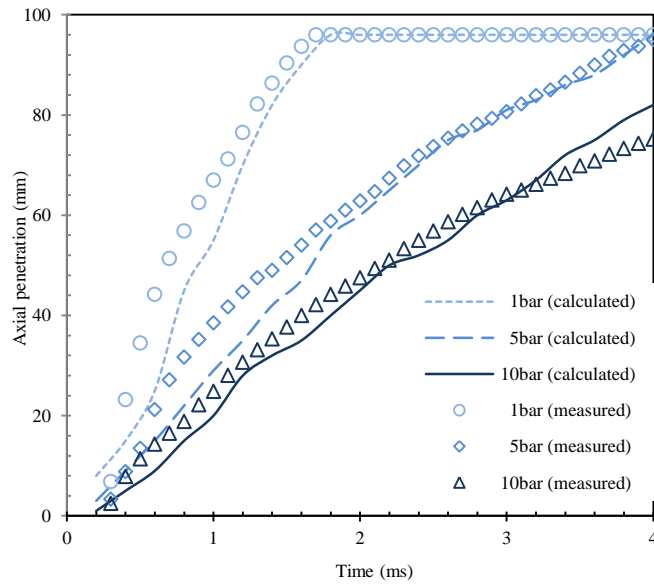
- 1) This research extends the initial validation of numerical results by CFD approach including high and low ambient pressure. The comparison with optical data shows a good agreement in terms of jet penetration and overall evolution for all the cases examined here.
- 2) The simulation of the multi-hole nozzle shows the least accurate results in terms of both initial jet penetration and final fuel distribution. However, in the current state CFD already shows remarkable results, making it useful tool to optimize injection parameters and nozzle configuration in order to increase efficiency and reduce the emissions in a hydrogen-fuelled DI engine.



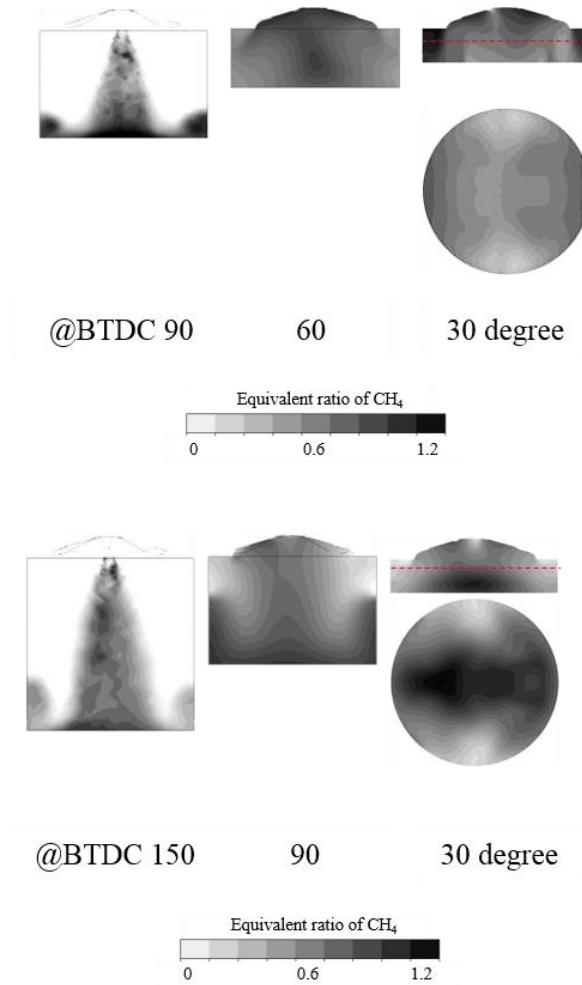
**Figure 8. Transient Modeling on CH<sub>4</sub> Jet Penetration and Mixture Formation in a Constant Volume Chamber ( $P_{inj}$ : 85bar,  $T_{ambient}$ : 20°C)**



**Figure 9. Enlarged Cross Sectional Images of Gas Jet (view,  $P_{inj}$ : 85bar,  $T_{ambient}$ : 20°C, @ASOI 2.75ms)**



**Figure 10. Comparison between Numerical and Experimental Result ( $P_{inj}$ : 85bar,  $T_{ambient}$ : 20°C)**



**Figure 11. CH<sub>4</sub> Mixture Formation in Engine Cylinder (CH<sub>4</sub>: 10mg & CH<sub>4</sub>: 23mg)**

## Acknowledgements

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