



## Direct injection of methane in advanced propulsion systems: effects of thermodynamic conditions

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### ABSTRACT

The direct injection of gaseous fuels involves the presence of under-expanded jets due to the high pressure-ratios and the strong gas compressibility. Understanding the physical development of such processes is essential for developing Direct Injection (DI) devices suitable for application in internal combustion engines fueled by methane or hydrogen. In this work a coupled experimental-numerical characterization of a spray, issued by a multi-hole injector, was performed. The experimental characterization of the jet evolution was recorded by means of schlieren imaging technique and then a numerical simulation procedure was assessed using the measurements for validating. A density-based solver, capable of simulating highly compressible jets and developed within OpenFOAM environment, was used to study the effects of thermodynamic conditions on the development of the injection process. The obtained results shed more light on the characteristics of the gaseous spray demonstrating how these features really affects the development of the injection process and the quality of the air/fuel mixture.



## 1) Introduction

The international policies on energy transition and sustainable development aim to reduce greenhouse gas emissions by 2050 and to limit the rise in global temperatures to 1.5°C [1]. The transport sector significantly contributes to greenhouse gases (GHGs) and harmful pollutants emissions. In 2020 the global direct emissions from transportation were over 7 GtCO<sub>2</sub>, namely the 25% of total carbon dioxide emissions for all sectors. The achievement of NZE goal in the transport sector relies in both promoting more efficient modes of transport (modal shifting) and improving the energy efficiency of the actual vehicles. During the transition to NZE, internal combustion engines (ICEs) will still play a fundamental role and therefore it is essential to direct the research towards the development of current low-emission technologies. Among all the available solutions, the use of natural gas (NG) in internal combustion engines represents a concrete possibility for mitigating emissions in the short/medium term [2]. Indeed, compared to liquid fossil fuels, NG presents several advantages including worldwide spreading, low operational costs and low environmental impact due to its lower carbon content than liquid fuels [3].

However, there are two major issues related to the use of NG in actual stoichiometric spark-ignition engines, i.e. low thermal efficiency and high NO<sub>x</sub> emissions due to high combustion temperature. A solution for both problems can rely on lean combustion strategies, as long as it is possible to guarantee the stability of the combustion process and to limit the cycle-to-cycle variations. The direct injection (DI) of natural gas into the cylinder can provide great flexibility in controlling the air/fuel mixture allowing lean combustion strategies, while ensuring the stability of the combustion process [4]. Although already successfully implemented for liquid fuels [5,6], DI for gaseous fuels requires further deepening.

Indeed, to ensure adequate mass flow under each operating condition, natural gas must be injected at high pressure, due to its low density and compressibility. When a compressible fluid is injected at high pressure into the cylinder choked conditions may occur and the subsequent flow is characterized by the presence of shock waves that affect the air/gas mixing process. The strength of the shock waves mainly

depends on the ratio between the pressure upstream of injector nozzle and in-cylinder pressure, namely the net pressure ratio NPR [5,6]. Experimental and numerical investigations on the effects of varying the NPR are fundamental for proper design the fuel injectors [7,8]. In this work the jet issuing from a prototype multi-hole injector designed for DI applications was experimentally and numerically investigated. The experimental measurements provided by schlieren imaging method was used for validating a properly developed numerical model. The last was developed in OpenFOAM framework and it relied in a high-order, density-based solver which resulted being the best choice for reproducing the strong discontinuities occurring due to transient under-expanded flows [9,10]. The numerical investigation was focused on the effect of varying the ambient pressure on the shock waves characteristics.

## 2) Investigation Methodology

The investigations carried out in this paper are finalized to reconstruct the morphology of an under-expanded jet for direct injection in NG engines. In direct injection engines, the chain of events of mixture formation/combustion are strongly affected by such phenomena and so an extensive knowledge of under-expanded jet is necessary. In order to achieve such task, complementary application of experimental imaging and predictive simulations techniques was adopted. A experimental characterization, using schlieren imaging technique, was performed at the STEMS Institute-CNR-laboratories in Naples. Quantitative and qualitative information regarding the whole spray evolution were exploited to setup and validate a CFD numerical approach. Two operating conditions, featuring different thermo-dynamic parameters, were considered for the comparison with experimental data. Then, having verified the validity of the numerical approach chosen, a further condition, involving different nozzle geometry, was analysed. Having a robust numerical simulation code, appropriately validated, allows to investigate different operating and geometric configurations of the injection system, in order to identify the best solution for a more efficient air-fuel mixture formation. For the current study, a prototype high-pressure multi-hole injector has been used, specifically developed for direct injection. (Figure 1).



Figure 1: Silhouette of the high-pressure injector

It must point out that the presence of discontinuities in high-speed compressible flows requires numerical approaches that can capture these features avoiding spurious oscillations. The most widely used methodology involves the adoption of density-based algorithms in order to reproduce the overall jet structure and the above-mentioned phenomena [10–12]. For this reason a high order, density-based solver developed within OpenFOAM environment was adopted. The cases investigated are summarized in the following Table 1.

Table 1: Investigated operating conditions.

	Case 1	Case 2
Ambient Temp. [K]	293.15	293.15
NPR [-]	100	50
Ambient Pressure [bar]	1	0.5
Injection Pressure [bar]	50	50

Cases 1 and 2, whose NPRs were varied changing the ambient pressure ( $p_\infty$ ), were considered for validating the numerical approach.

### 3) Experimental Activities

The apparatus for the experimental measurements was built up at the STEMS laboratories of the National Research Council (CNR) of Naples. Natural gas was injected into a constant volume chamber and the spreading jet images were acquired by the means of mirror-based schlieren “z-type” configuration, as showed in Figure 2.

The tests were carried out into an optically accessible constant volume chamber. Two quartz windows, 80 mm in diameter, permitted the access to a large area of the spreading spray. The pressure inside the chamber was increased by introducing pressurized nitrogen and decreased below the atmospheric value by using a vacuum pump (0.2 bar minimum pressure).

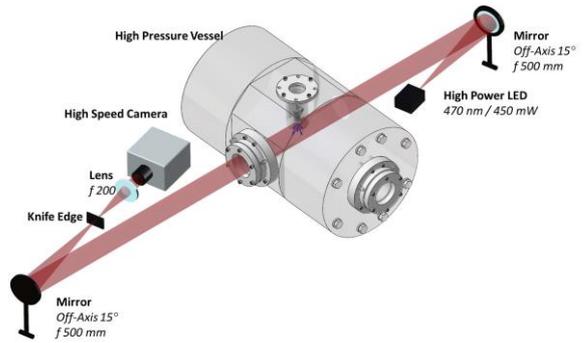


Figure 2: Scheme of the experimental apparatus and optical z-type schlieren configuration

Natural gas, 99.95% purity, was injected by a prototype multi-hole injector. The injection duration was set to 8.0 ms and five repetitions were carried out to ensure the repeatability of the measurements. The source for the schlieren setup was a high-power LED lamp emitting a radiation of 455 nm. The light beam was first collimated through a 15° off-axis mirror (500 mm focal length). After passing through the chamber the collimated beam was deflected and focused by a second off-axis mirror with the same characteristics as the former. A knife-edge mounted at the focus of the second mirror was used for regulating the amount of light detected by a high-speed CMOS camera. The detector worked at 18,000 frame per second with an image window of 448x416 pixels. The camera realized a spatial resolution of 5.5 pixel/mm and a time resolution of 55  $\mu$ s. The acquired images were analyzed by a customized post-processing software, allowing the measurements of axial penetration of the jet. Further details on the experimental apparatus, post-processing routines, and the results of the complete campaign of measurements are provided in [13].

### 4) Numerical Methodology

The presence of discontinuities in high-speed compressible flows, such as shock waves, requires numerical approaches that can capture these features avoiding spurious oscillations. The most widely used methodology involves the adoption of density-based algorithms in order to reproduce the overall jet structure. Such approaches, coupled with a LES turbulence framework, are capable of capturing the initial vortex ring, present at the beginning of the injection, the under-expanded structures and the macroscopic characteristics such as penetration

length and volumetric growth. In present work the solution of the governing equations (mass, momentum and total energy conservation) is performed using the conservative variables ( $\rho$ ,  $\rho u$  and  $\rho e$ ).

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (1)$$

$$\frac{\partial (\rho u)}{\partial t} + \nabla \cdot [u(\rho u) + p] = \nabla \cdot \sigma \quad (2)$$

$$\frac{\partial (\rho e)}{\partial t} + \nabla \cdot [u(\rho e) + p] = \nabla \cdot (\sigma \cdot u) + \nabla \cdot q \quad (3)$$

Considering the intrinsic geometrical complexity of the injector's nozzles simulated unstructured grid is required and so KNP central scheme were chosen together with VanLeer flux limiter (to ensure the simulation stability) [14,15]. Temporal integration was performed using high-order explicit Runge-Kutta 4th [9]. During the generic time step and, for each RK4 step, the  $\rho, \rho u, \rho e$  fields are updated, the relative fluxes recomputed and the turbulence model solved. A complete description of the algorithm can be found in [10,16]. Relying on bibliography, the LES k-Equation turbulence model was selected in order to have an effective representation of the flow field [8,10].

## 5) Simulations Setup

The computational domain is shown in Figure 3. The upper part represents the injector's nozzle which is connected to the injection environment.

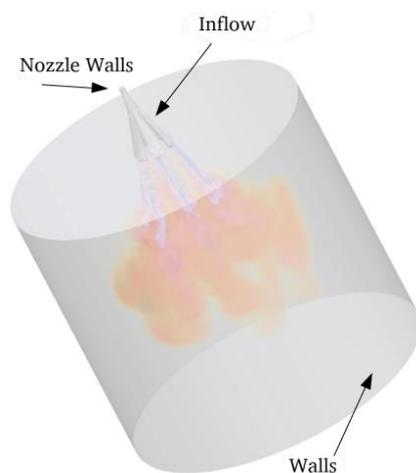


Figure 3: The boundary conditions

The boundary conditions are:

- Inlet: is the section at the top of the divergent ducts where the injected gas enters within the domain. The time-behavior of the total

pressure represented in Figure 4 has been imposed as boundary condition. The value of the total temperature is fixed at 293.15 K. The intensity of the turbulent kinetic energy is fixed at the 0.08. The mass fraction of the entering methane has been fixed to the unity.

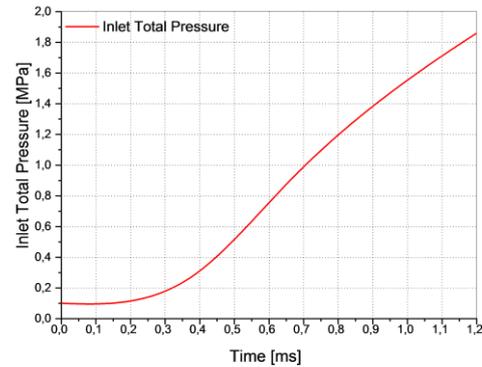


Figure 4: Inflow section pressure temporal behavior

- Walls: walls of the injection environment.
- Nozzle-walls: are the walls internal to the nozzle where a slip condition was set for velocity in order to avoid artificial boundary layers formation

The geometry was discretized with unstructured grids generated using the snappyHexMesh tool embedded in OpenFOAM. The grids had base dimensions of 1.6 x 1.6 x 1.6 mm which were chosen after a mesh sensitivity study performed by the authors in a previous work [16,17]. The meshing strategy was based on the adoption of refinement regions with different refinement levels as shown in Fig. 5.

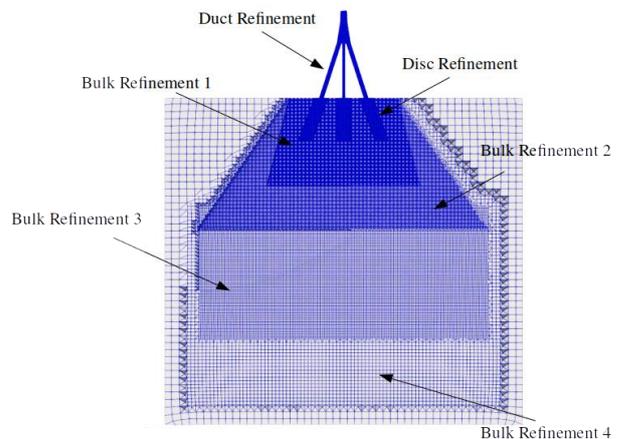


Figure 5: The computational domain grid

The refinement level reported in Table 2 as power of 2. The near-nozzle zone was discretized with elements of 50 $\mu$ m then the

size gradually increased going downstream. The total cell count was of  $\approx 40$  M. The time-step adopted was variable and depended on the Courant number which was limited to the maximum value of 0.8. Numerical results were then post-processed using Paraview software.

Table 2: Refinement regions and respective levels

Refinement region	Level
Duct	5
Disc	5
Bulk 1	4
Bulk 2	3
Bulk 3	2
Bulk 4	1

### 6) Results

To demonstrate the validity of the modeling approach, the simulation results were validated against the experimental data. Figures 6 and 7 show the comparison of experimental and numerical jet penetration over time for the cases 1 and 2 of Table 1.

The penetration length represents the distance between the nozzle exit and the furthest point on the contour of jet, measured along the axis of the spray. The jet’s contour was defined, numerically, by a methane mass fraction equal to 0.1% and from the experimental data performing a proper image post-processing as described in [13, 18]. The penetrations measured from the experimental images and those computed from the simulations are in good agreement and the difference is well within the experimental uncertainty for the whole simulated period. The velocity of penetration for the case 2 is greater in comparison of case 1, as is a direct consequence of the lower ambient pressure which finally brings to a faster penetration.

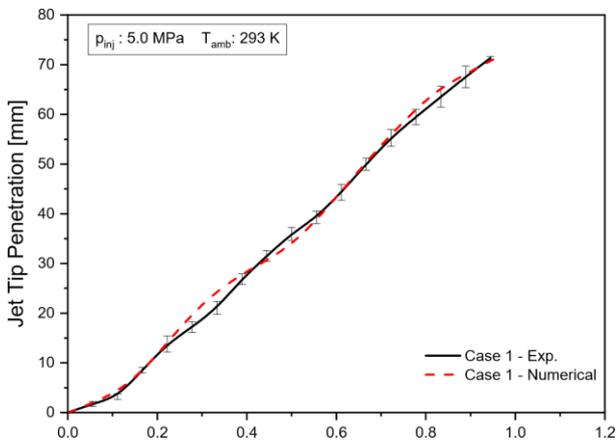


Figure 6: Experimental and numerical axial jet tip penetration vs. time. Case1

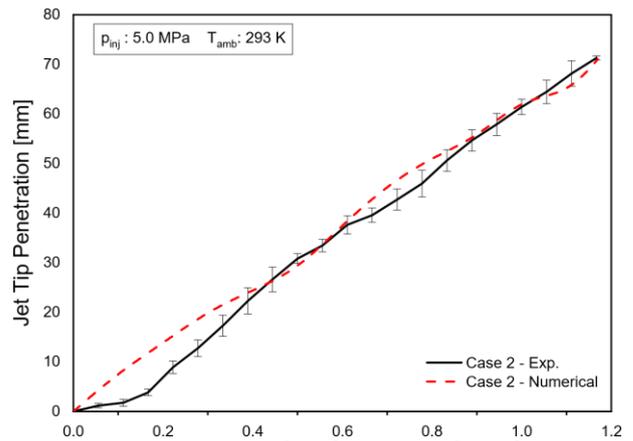


Figure 7: Experimental and numerical axial jet tip penetration vs. time. Case 2.

Figures 8 and 9 show a comparison between experimental and numerical spray’s morphology, for both cases 1 and 2. The numerical results show the volumetric rendering of the logarithm of the density gradient.

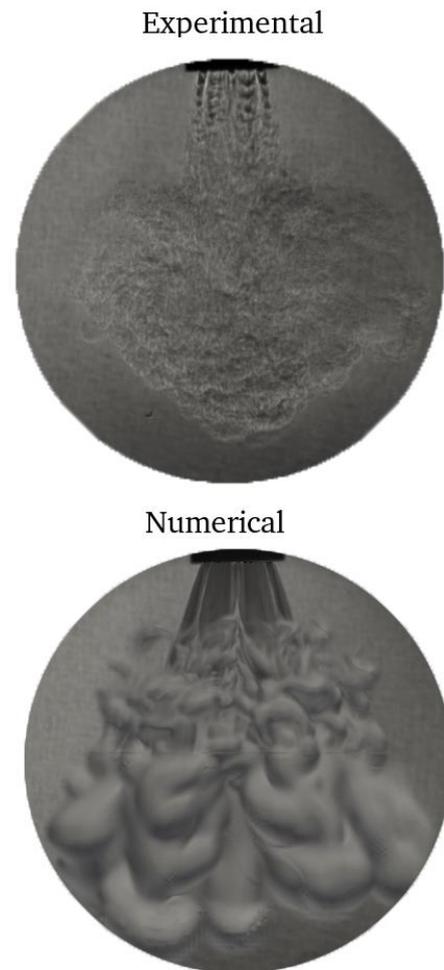


Figure 8: Comparison of experimental schlieren image recorded with the numerical results plotted as methane mass fraction volumetric for Case 1 at  $t=0.9$  ms after SOI.

This comparison allows to understand how the combination of the high order schemes with the LES turbulence framework is capable on reproducing the fluid-dynamics of the high-speed jets for the whole injection period. The higher the NPR is, the narrower the jet becomes (Figure 9, case 2). The experimental images endorse this behavior which is due to higher axial velocity stopping the lateral expansion.

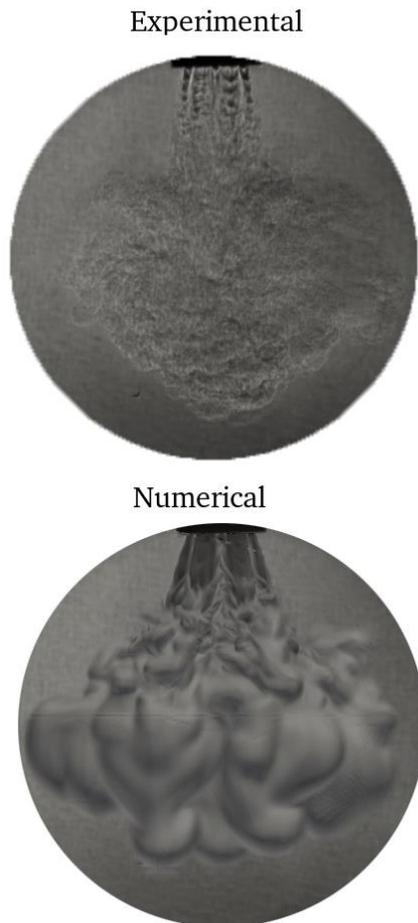


Figure 9: Comparison of experimental schlieren image recorded with the numerical results plotted as methane mass fraction volumetric for Case 2 at  $t=1$  ms after SOI.

Figure 9 is a plot of Mach number across the vertical jet axis, for Case 1 and 2. The location of the Mach disc is highlighted by the jump in Mach number. At the exit from the nozzle the jet is in super-sonic conditions (Mach number equal to 1.5). Moving downstream, the flow becomes subsonic. Indeed, the Mach number decreases sharply to the minimum values (approximately 0.2). The sonic conditions come back at a different distance

considering Case 1 and 2: 12 mm for the first while 3 mm for the latter. A greater shock is recognizable for the case 1 as expected looking at the NPRs.

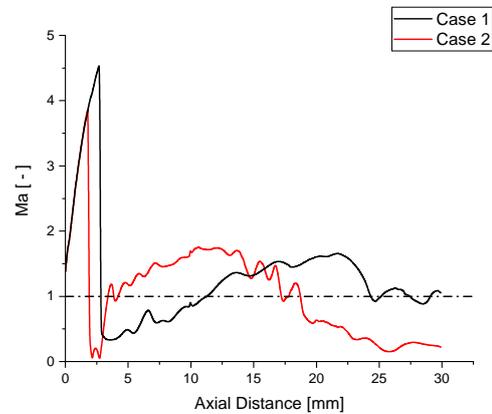


Figure 9: Numerical evaluation of Mach number and of the fuel mass fraction along the jet's axis for the Cases 1 and 2

## 6) Conclusions

The jet issued flow from an innovative, high pressure, multi-hole injector was experimentally and numerically investigated. The experimental study was carried out by injecting methane into a constant-volume vessel using different injection conditions. The images were recorded by means of the schlieren technique and a proper image post-processing. A density based CFD code, featuring LES turbulence and species transport equations, was adopted to simulate the injection process. The model allows a broader understanding of the jet's characteristic and, especially, provides further information concerning the air/fuel mixing. Based on the results, the following conclusions can be pointed out:

- Schlieren imaging technique can be proficiently adopted for characterizing gaseous fuels injections
- Lowering the ambient pressure determine a faster jet penetration with also a wider lateral expansion
- The developed numerical approach is capable of reproducing a spray's morphology observed by means of the schlieren technique and the jet-tip
- The flow discontinuities, as shock waves and Mach discs, are properly captured by the high order discretization schemes chosen.
- Ambient pressure has effect

## List of Symbols

CFD	Computational Fluid Dynamics
CI	Compression Ignition
CNG	Compressed Natural Gas
CVC	Constant Volume Chamber
DI	Direct Injection
DI-CNG	Compressed Natural Gas Direct Injection
DNS	Direct Numerical Simulation
fps	frame per second
GDI	Gasoline Direct Injection
ICE	Internal Combustion Engines
LED	Light Emitting Diode
LES	Large Eddy Simulation
NG	Natural Gas
NPR	Net Pressure Ratio
PDF	Probability Density Function
PECU	Programmable Electronic Control Unit
PFI	Port Fuel Injected
$p_{inj}$	injection pressure
$p_{\infty}$	ambient pressure
PISO	Pressure Implicit Split Operator
RANS	Reynolds-Averaged Navier-Stokes
SI	Spark Ignition
SOI	Start of Injection
TKE	Turbulent Kinetic Energy
TTL	Transistor-Transistor Logic
CH <sub>4</sub>	methane mass fraction

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### تزریق مستقیم متان در سیستم های موتوری پیشرفته: اثرات شرایط ترمودینامیکی

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مخلوط

به دلیل تراکم پذیری بالای گاز و نسبت های فشار بزرگ، تزریق مستقیم گاز موجب ایجاد فواره گازی تحت انبساط می شود. درک صحیح فیزیک این پدیده برای توسعه سامانه های تزریق مستقیم که در موتورهای احتراقی برای تزریق مستقیم متان یا هیدروژن استفاده می شوند، ضروری است. در این مقاله مشخصه یابی کوپل تجربی عددی فواره یک افشانه چند سوراخ انجام گرفت. مشخصه یابی تجربی فواره به کمک روش شیلرین انجام گرفت و محاسبات عددی به کمک نتایج تجربی به دست آمده صحت گذاری شد. حلگر بر پایه چگالی که قابلیت مدلسازی فواره های گازی با تراکم پذیری زیاد را دارد و در محیط نرم افزار Open foam توسعه داده شده است برای بررسی اثرات شرایط ترمودینامیکی روی توسعه فواره مورد استفاده قرار گرفت. نتایج نشان داد که با استفاده از شدت نور زیاد می توان مشخصه هایی از فواره که روی فرآیند تزریق سوخت و کیفیت مخلوط سوخت و هوا موثر هستند را بهتر مشاهده و ارزیابی نمود.



تمامی حقوق برای انجمن علمی موتور ایران محفوظ است.