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## Natural Gas Fueling: a LES based Injection and Combustion Modeling for Partially Stratified Engines

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### Abstract

The Partially Stratified Charge Spark Ignition (PSC-SI) combustion strategy is envisaged as a way of reducing fuel consumption and therefore polluting emissions; the improved fuel economy is mainly due to lean, stratified combustion, and to the reduction of pumping losses at partial load conditions.

The aim of this work is to explore the potential capabilities of the PSC-SI combustion strategy over a wide flammability air-to-fuel ratio range with a CFD-based computational approach. A validated LES solver has been used to represent the main occurring phenomena into an experimentally implemented Constant Volume Combustion Chamber (CVCC). For different air fuel ratios, both homogeneous and non-homogeneous combustion processes have been simulated in order to compare and emphasize the benefits of the PSC-SI and the impact of the choice of operating conditions.

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### 1. Introduction

Emission regulations and the quest for high performance and low emission spark ignited engines have pushed the automotive industry to trim the operating conditions close to their combustion stability limit. Multi-dimensional modeling has thus become a key tool to predict combustion instabilities, and help in the design process of such engines.

The use of natural gas came also out as a powerful solution in the specific field of spark ignited engines. In fact, on one side the gaseous fuel direct injection gives an increase of thermodynamic efficiency due to de-throttling at partial load, with additional mixing improvement due to the jet

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turbulence production. On the other side, natural gas is itself a very promising fuel intrinsically clean (CO<sub>2</sub> emissions are about 25% lesser than gasoline fed engines with same technology [1]), and whose supply is secure. Moreover, vapor emissions are limited, as well as cold start and low temperature ones, and combustion lean burn flammability limits are much wider than in the case of gasoline homogeneous and heterogeneous charge engines.

Several investigation have been carried out so far, both numerically and experimentally, on the mixture formation process in constant volume combustion chambers as well as in engine ones [2][3][4]. In the numerical studies, RANS based approaches have given reliable results in terms of prediction of global combustion process and engine performance parameters [5][6][7]. During the last years, however, and mainly thanks to the evolution of the computational hardware technology, the LES approach has been increasing its attractiveness also in the case of time-varying geometries (such as IC engines). Different reviews have addressed the capability of LES in analyzing both cold and reactive engines simulation [8][9], based on several work carried out with such an approach [10][11][12].

Based on previous works, this paper is focused in highlighting the role of the ignition model to improve the capabilities of the solver to capture the early stage of the combustion process. As a first step in the current work, a validation of an ignition model has been carried out by directly comparing the numerical results with the experimental data gathered at the University of British Columbia [13].

## 2. CVCC configuration and operating conditions

An optically accessible Constant Volume Combustion Chamber designed and realized at the University of British Columbia [14] was used for comparison with the numerical results.

The spark was provided by a pair of tungsten electrodes with 0.406mm diameter and it was located 10mm downstream of the jet nozzle. The CVCC has a bore of 80mm and a height of 50.8mm. A modified Keihin KN3 CNG/LPG peak-hold port injector was used for the study. The PSC Jet nozzle, and the ignition zone were located along the axis of symmetry of the CVCC. The diameter of the injector nozzle was reduced to 0.571 mm. The injection pressure was fixed at 10 bar (abs.) while the chamber pressure was maintained at 5, 6 and 7 bar (abs.).

In the present study only the case with 7 bar (abs.) pressure is taken into account to represent engine like pressure conditions at the start of PSC injection. The injection duration was set to 9.9 ms leading at a certain mass percentage of Partially Stratified Charge (PSC) injected charge reported as a function of the Air-Fuel equivalent ratio ( $\lambda$ ) in Table 1. The spark timing was imposed at the End Of the Injection (EOI). In order to have a baseline to compare the performance of the PSC-SI combustion strategies homogeneous cases have been also run for the same overall charge conditions.

Table 1. Experimental and numerical operating conditions, and NG charge amounts.

$\lambda$	Total NG charge [mg]	PSC charge [mass %]
1.4	118	0.297
1.6	104	0.336
1.8	93.2	0.375

## 3. OpenFOAM based CFD solver and submodels

An OpenFOAM based CFD solver has been used for the simulation of the compressible, chemically reacting, transient, three-dimensional fluid flows. A One Equation Eddy LES approach is used to

modeling the turbulent flow and mixing while a Partially Stirred Reaction combustion model has been selected to model the partially premixed combustion in order to take into account the interaction between the turbulence and the chemistry, mandatory for the correct description of this particular combustion regime [15]. A Spark-Energy Deposition Model is used to treat the ignition of the mixture. The SnappyHexMesh utility is used to generate the grid of the CVCC which generates 3D meshes containing hexahedra (hex) and split-hexahedra (split-hex) starting from triangulated surface geometries in Stereolithography (stl) format. The mesh well conforms to the surface by iteratively refining a starting mesh and morphing the resulting split-hex mesh to the surface. The specification of mesh refinement level is very flexible and there was really useful to optimize the computational cost, accuracy ratio. It runs in parallel with a load balancing step every iteration. Further details of turbulence and combustion submodels are presented in [16], while some information are given below for the ignition process treatment.

### 3.1. Spark-energy deposition ignition model

To capture the right flame response in the early stage of the combustion, the spark was described as a source term in the energy equation which describes the initial formation of the kernel. Although there are significant simplifications of the spark and the kernel formation physics, it is able to represent the ignition functional dependence on mixture stratification and turbulent field, predicting, for example, failed ignition events if the conditions cannot allow the evolution of the flame.

Deposition of the total spark energy in a spherical volume of diameter of 1mm at the electrode gap simulates the spark discharge (Figure 1). The spherical volume is used to locate the ignition cells and it is kept fixed during the simulation (in terms of volume and location).

The total deposited energy was set equal to 60mJ according to the literature [5][17] and it was divided between the Breakdown and the Arc and glow phases as reported in Figure 1 .

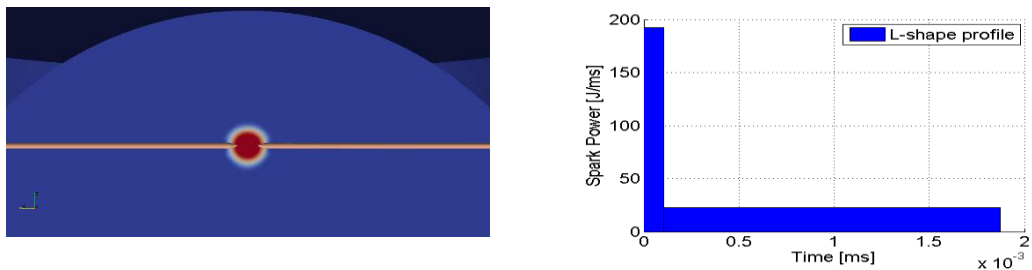


Figure 1: Visualization of kernel energy deposition (left) and spark power energy deposition value temporal distribution (right)

## 4. Computational domain and numerical settings

Figure 2 shows the computational mesh used to represent the CVCC for this study. The average cell size is in the range of 0.8 mm, a recommended value for modelling combustion in engine applications using LES. To better resolve the evolution of the PSC jet and the early combustion event, the mesh was refined to 0.025 mm in the regions closer to the spark electrodes and the central axis, where the PSC injection process takes place. The grid contains 4.4 million hexahedral cells for the injection and 2.3 million hexahedral cells for the combustion simulation, and taking about 1 hour to be generated with 8 Intel® Xeon processors.

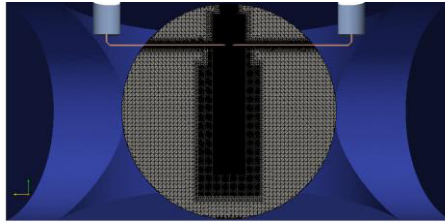


Figure 2 Section of the computational domain of the CVCC.

## 5. Results and conclusions

Before the combustion process (i.e. at the end of the injection process), a good matching between the experimental and the numerical concentration fields has been found: this is key as a careful representation of the jet shape at ignition timing is mandatory to have correct initial conditions for the subsequent combustion process evolution [14].

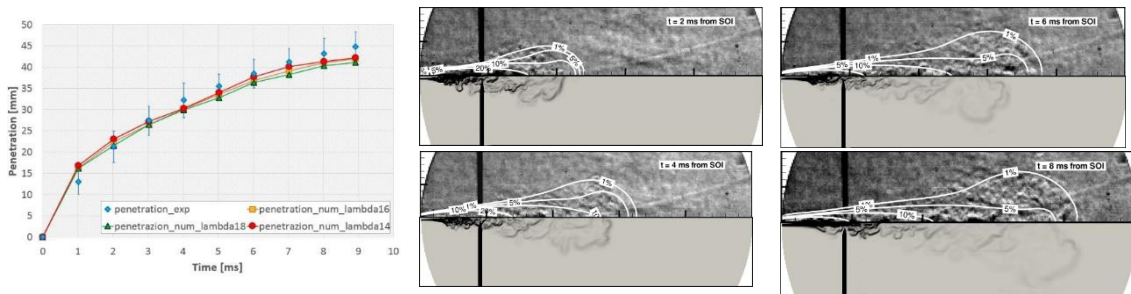


Figure 3: Comparison of jet penetration for all AFR with the experimental penetration (left). Comparison between schlieren images and numerical density gradient for different time of the injection process (right).

The injection simulations were, hence, carried out for all the cases showing no evident differences in terms of jet penetration [Figure 3]; also, the shape of the jet has been well represented as it is evident by comparing the numerical and experimental patterns in Figure 3.

Looking at the combustion process, the presented ignition model shows a great capability of represent the flame behavior in the early stage of combustion, confirming the correct settings of the spark plug energy deposition. Figures 4 (left) show only some realizations for 2 -5 and 10 ms of the numerical results compared to the experimental data, where it is possible to see how both the ignition, the combustion and the turbulent-chemistry interaction models work quite well altogether to give a reliable evolution of the flame front over time.

First, the combustion process of the homogeneous mixture at  $\lambda=1.4$  has been studied to have a baseline case study; then simulations of non-homogeneous mixtures have been done at different lambdas (1.4 and 1.6) and enabling the PSC jet injection (EOI) until  $\lambda=1.8$  (where cases with  $\lambda=1.8$  and homogeneous mixture presented, obviously, misfiring).

All the plots in Figure 4 below show that the Partially Stratified Charge allows for a faster combustion process, that can be appreciated both in the visualization of the flame front propagation (plotted for  $\lambda=1.4-1.8$  referring to PSC and homogeneous cases), and in pressure rising up (Figure 4 (right-up)).

This confirms the PSC SI combustion process as an effective means to improve combustion efficiency and allowing operation at lambdas well above the homogeneous charge flammability limit.

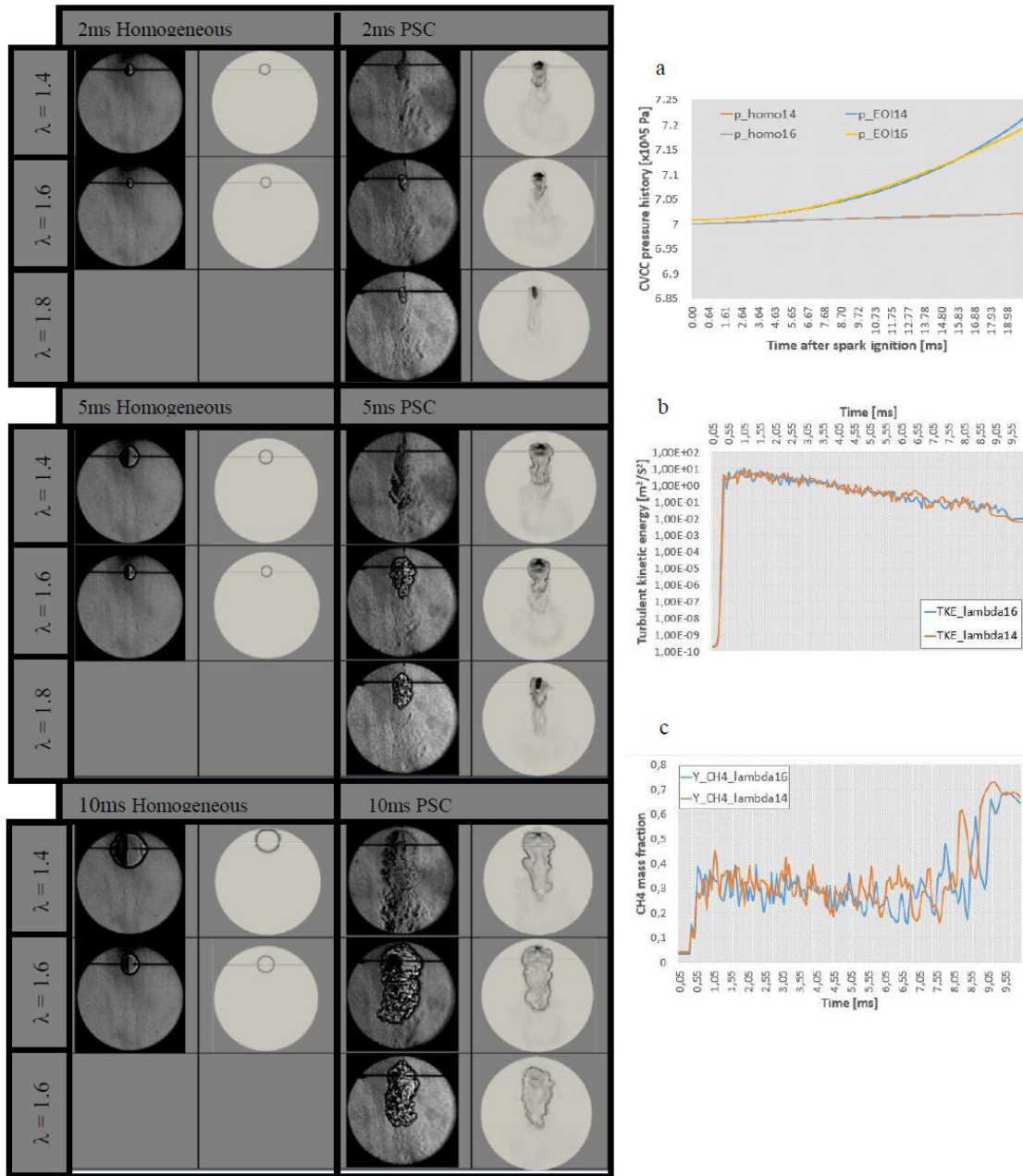


Figure 4: (left) Comparison between Schlieren images and combustion numerical density gradient at 2ms (up) 5ms (center) 10ms (down); (right) Combustion pressure history for all simulated cases (up) Turbulent Kinetic Energy value at the spark location during the injection process (center) CH4 mass fraction at the spark location during the injection process (down)

Figures 4 (right-center and down) show the behavior of the Turbulent Kinetic Energy and the CH4 mass fraction observed between the two electrodes. As it is possible to see in figure a, the value at sparking timing for both the cases is almost similar (i.e. very rich). Also in terms of Turbulent Kinetic

Energy, it is possible to deduce from the Figure b how the PSC jet modifies the local turbulent conditions to enhance the mixing process and give a more stable kernel propagation. After the kernel formation, when the local conditions in terms of turbulent kinetic energy and air fuel ratio can enhance the growth of the flame core, the evolution of flame front is maintained stable also with relatively lean and quiescent mixtures, which is a key aspect of the PSC SI combustion strategy.

Having a reliable model to describe this particular kind of combustion process may also allow important consideration about the timing of the ignition. It is, in fact, well known in literature [14] that a too high value of turbulence near the spark plug could lead to a quenching of the kernel itself, at the same time too low value of turbulence cannot give a proper mixing, eventually leading to misfire. In this context the model could help in choosing the timing and finally allow for reaching a proper balance between these two aspects.

In conclusion, the model has been validated toward an accurate description of the flame front evolution during the early stage of both the homogeneous and the PSC combustion processes.

Important considerations have been highlighted about the capability of the PSC SI combustion strategy to enhance the overall combustion process stabilizing the kernel formation thanks to a coupled contribution of local richer mixture and higher turbulent level in the region close to the spark plug.

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### **Biography**

Lorenzo Bartolucci was born in Rome, Italy, in 1989. He graduated in Energy Engineering from the University of Rome Tor Vergata. He is currently a Ph.D. student in the same university at the department of Industrial Engineering. His fields of interest are CFD modeling of turbulent gas injection and combustion.