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3D Simulation Methodology for n-Butanol Combustion in an optical accessible research GDI Engine

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Abstract

The strict political regulations in terms of engine tailpipe emissions and reduction of fossil fuel dependency are pushing forward the study of alternative fuels; these fuels must be suitable for currently available engines, in order to allow quick and inexpensive replacement. The alternative fuel chosen for this analysis is n-Butanol; being its key physico-chemical properties similar to those of commercial Gasoline, it does not require relevant changes in engine design and operation and therefore it is suitable for currently produced units. The paper describes the modeling and characterization of spark-ignited combustion of n-Butanol in comparison with that of conventional Gasoline. The comparison is made by means of 3D CFD simulations and experimental tests, carried out on a single-cylinder optically accessible engine characterized by a flat and transparent piston. The engine is equipped with direct injection and makes use of a current production engine head. The operating conditions used in the experiments are reproduced in the CFD simulations, in order to validate the CFD model and to provide additional insight to the experimental observations. The numerical simulation outcomes replicate with a good accuracy the experimental test results and they help to better understand the behavior of the alternative fuel during the combustion process. The adopted modelling methodology can therefore be used for further investigations such as exploration of different engine operations through virtual DOE of both operating and functional parameter variations.

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Keywords: n-Butanol; Combustion; Optical access engine; 3D; CFD

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Nomenclature

b/a TDC	Before/After Top Dead Center
CAD	Crank Angle Degree
CFD	Computational Fluid Dynamics
COV	Covariance
DI	Direct Injection
DISI	Direct Injection Spark Ignition
ER	Equivalence Ratio
FSD	Flame Surface Density
IMEP	Indicated Mean Effective Pressure
LFS	Laminar Flame Speed
MFB	Mass Fraction Burnt
SOI	Start of Injection
UHC	Unburned Hydrocarbon

1. Introduction

Environmental policies developed in the last 25 years, especially in EU, are characterized by the constant and significant lowering of engine-out emission limits. The purpose is to achieve the ambitious goal of a 60% reduction in emissions by 2050 compared to 1990 [1]; such policy is seen as a countermeasure to face the increase and strong variability in the oil price due to the inexorable depletion of raw material and the poorly established political conditions of the oil producing countries (the price in 2050 will be doubled compared to 2005 [2]).

The above mentioned aspects are impacting relevantly on the technological development and the design of current and next generation internal combustion engines. The need for reduced tailpipe emissions have determined, at first, a more complex engine structure, due to the simultaneous implementation of many different solutions such as direct injection (DI), turbocharging, variable valve actuation, all aimed at increasing engine thermal efficiency, and reducing fuel consumption [3,4,5]. Secondly, the need to reduce the dependency on petroleum-based products has pushed towards the complete or partial substitution of gasoline and Diesel with alternative fuels.

A critical issue in gasoline replacement is the compatibility of any alternative fuel with the existing units: physico-chemical properties of the replacing fuel must guarantee its usability in pre-existing hardware; hence no major modification related to the engine architecture will be needed.

Bio-alcohols are particularly attractive as gasoline replacement: the main advantages are the reduced greenhouse gas emission, including the carbon dioxide, the easy production from common biomass sources and the higher flame speed and octane ratings [6,7]. Thanks to these properties [Table 1] it is possible to expect a theoretical increase in engine thermal efficiency due to the shorter flame development duration or the possibility to increase the volumetric compression ratio without penalties in terms of engine knock tendency.

On one side, high carbon alcohols such as n-Butanol are more similar to gasoline in terms of heat of vaporization and air-to-fuel stoichiometric ratio compared to more traditional low carbon alcohols, thus overcoming issues related to cold start ignition and higher fuel consumption [8,9]. On the other side the very low volatility of this kind of fuels can lead to poor mixture preparation and fuel deposit formation in GDI units, increasing soot and UHC emissions especially at part load operations. Previous studies [10,11,12,13] clarified the crucial relevance of mixture quality in DISI engines, and the effect of charge stratification on combustion development and emissions. In particular, it was highlighted that the very low mixture homogeneity at the spark time using n-Butanol leads to combustion velocity slow down and soot production increase compared to gasoline despite the promising chemico-physical similarity.

Complex aspects such as mixture preparation, fuel deposits formation and flame development can be fully understood trough CFD analyses, provided reliable methodologies can be adopted to predictively represent the engine behavior when moving the engine design and calibration towards the optimal solution. The purpose of previous studies [10,13] was the development and validation of accurate CFD tools able to reproduce the behavior of the optically accessible research unit using different fuels and injection strategies. In particular, in order to improve

the engine performance in terms of pollutant emission and burn rate using n-Butanol as gasoline replacement, different injection strategies were numerically and experimentally tested. The available measurements are now used to further validate the developed methodology, using the CFD analyses to explain more in depth the reasons behind the measured behavior.

Table 1. Key properties of Gasoline and Alcohols

Fuel	Gasoline	Ethanol	Methanol	n-Butanol
Molecular Formula	C_4-C_{12}	CH_3OH	C_2H_5OH	C_4H_9OH
Lower Heating Value [MJ/kg]	42.9	20.08	26.83	32.01
Density @ 20 ◦C [kg/m^3]	744.6	791.3	789.4	791.3
Research Octane Number [-] RON	92	111	108	96
Latent Heat of Vaporization [kJ/kg]	373	1098	838	584
Stoichiometric Air-to-Fuel Ratio	14.46	6.43	8.94	11.12

2. The Research Engine

The experimental analyses are carried out using an optically accessible DISI available at the Istituto Motori of the National Research Council of Italy. The optically accessible cylinder is coupled with the head of a 4-cylinder, 16 valve commercial power unit (Fig. 1). The optical access is obtained through an elongated hollow transparent piston (Bowditch design [14]). A 18 mm-thick silica window fixed in both the piston and the cylinder extended liner ensures the image capture, which is obtained using a 45 degree UV-enhanced mirror placed inside the hollow piston. The engine features a centrally located spark plug and a wall-guided injection system characterized by a 6-hole injector placed between the intake valves. The sealing between the transparent piston and the cylinder is ensured by bronze-teflon rings, nevertheless during compression and power strokes a non-negligible blow-by flow rate is observed. In Table 2 the main geometrical engine characteristics are reported, while a more detailed description of the experimental lay-out can be found in [15].

Table 2. Experimental Engine Data

Displacement	399 cm3
Bore	79 mm
Stroke	81.3 mm
Compression Ratio	10:1

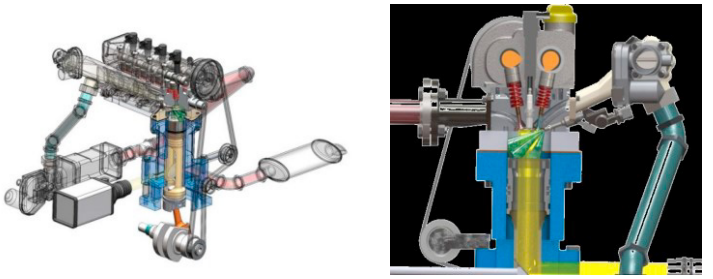

Fig. 1: Optically accessible Engine

The engine is tested at partial load conditions at 2000 rpm with an intake pressure and temperature of 0.7 bar and 310K respectively. Spark advance is fixed for all the operations and equal to 30 CAD bTDC. Fuel delivery is characterized by 100 bar injection pressure and 2.7 ms duration (corresponding to 32.5 CAD), ensuring a global relative air-fuel ratio close to stoichiometry. Three different injection phasings are tested, namely SOI 260, SOI 300, SOI 330 CAD bTDC. Mixture stoichiometry and in-cylinder pressure are monitored respectively through an exhaust gas oxygen sensor and a piezo-electric sensor; in both cases the sensor features an accuracy of ±1%; crank angle resolution was set at 0.2 CAD.

3. CFD Model

The 3D-CFD analyses are performed trough a customized version of STAR-CD v4.22, licensed by SIEMENS-PLM. Thanks to the engine geometrical symmetry, the computational domain covers half of the combustion chamber. The total number of fluid cells ranges between 0.4 and 1.2 million at TDC and BDC respectively. As

mentioned above a non-negligible quantity of fuel and air leaks out from the combustion chamber. For this reason, the piston crevice is accurately modelled as in the real geometry (40 mm length and 0.5 mm thickness) with a mesh thickness of 0.1 mm.

CFD calculations are carried out in a RANS framework with the k-ε RNG turbulence model for compressible flows. An algebraic model is used for spark ignition, based on the deposition of a volume of enfamed gases after a kernel delay growth [16]. A Lagrangian approach is used for the liquid spray simulation, in which a distribution of numerical parcels reproduces the primary atomization: a pre-calibrated Rosin-Rammler distribution is used to determine the size of the parcels [17] while their velocity is calculated coupling a fixed experimental and instantaneous mass flow rate with the nozzle diameter value; the latter is obtain through the Kuensberg 1D model [18]. A tuned 1D model of the entire engine based on a phenomenological turbulence model [19] provides the time-varying pressure and temperature boundary conditions, which are applied at both the intake and exhaust ports. In order to take into account the blow-by mass flow rate mentioned above, both the crevice and three bronze-teflon ring regions are modelled. Thanks to this it is possible to obtain, from the 1D model, a time-varying mass flow rate to be applied at the bottom of the crevice in the 3D model.

The engine components facing the combustion chamber are characterized by uniform wall temperatures (180 °C for the dome, 230 °C for the piston and 150 °C for the liner) and the wall heat transfer is calculated through a model developed at the University of Modena [4,20,21]. NOx rate of production is calculated resolving the extended 3-step Zeldovich mechanism while no further refining action was taken in account for other pollutant predictive model, such as soot formation and oxidation.

As for the combustion process, the ECFM-3Z model is adopted [22]; given the assumption of a sequence of local laminar flames embedded in a turbulent flow regime to represent the turbulent flame, the Laminar Flame Speed (LFS) become a mandatory input. Laminar flame speed values for conventional fuels can be calculated through empirical correlations available in literature [25], but for alternative fuels, such as n-Butanol, not so consistent correlations are available. Therefore, the development of a new methodology in order to calculate LSF for n-Butanol is needed.

LFS value are calculated at different engine conditions in terms of pressure and unburned temperature through chemical kinetics calculations, and accounting for the flame speed dependence on pressure, temperature and equivalence ratio. For n-Butanol LFS calculation the Frassoldati et al. [26] mechanism is used, involving 317 species and being validated for oxidation of butanol isomers and LFS simulation.

Then a polynomial form is obtained through a fitting procedure. In Fig. 2 (left) the chemical kinetic calculations and experimental data are reported for n-Butanol at different physical conditions and equivalence ratios. As reported in the error map on the right side of the Fig. 2 the relative error introduced by the fitting procedure is always lower than 10%. More details about the proposed approach for the fuel specific laminar flame speed can be found in [10].

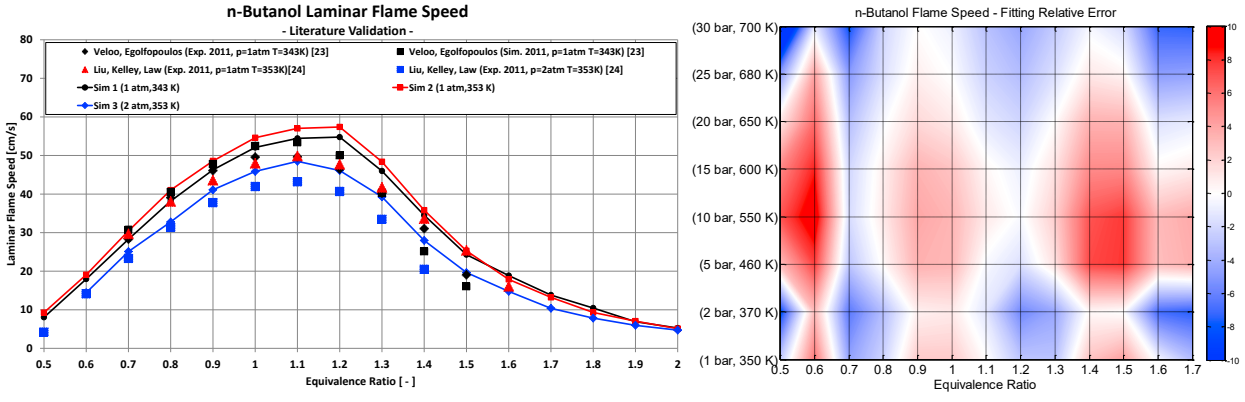

Fig 2. Calculated and experimental n-Butanol laminar flame speed (left), Fitting relative error (right)

4. Experimental Results

From a rough analysis of the experimental data reported in Fig. 3 it is possible to conclude that the "SOI 300" case is the best among the three tested strategies. The results for case "SOI260" show a slowdown of combustion, a significant reduction in the peak pressure, as well as a drop in the engine performance in terms of IMEP, all this sided by a decrease of combustion stability (high IMEP CoV). Shifting ahead the SOI of 40 CAD causes a delay of about 15 CAD in MFB 50% and the first stage duration (MFB 0-10%) is 8 CAD longer. This results is expected considering the shorter time available to the fuel evaporation delaying the injection, which leads in turn to a less homogeneous mixture at spark time; as a consequence a slower and less stable combustion process is measured.

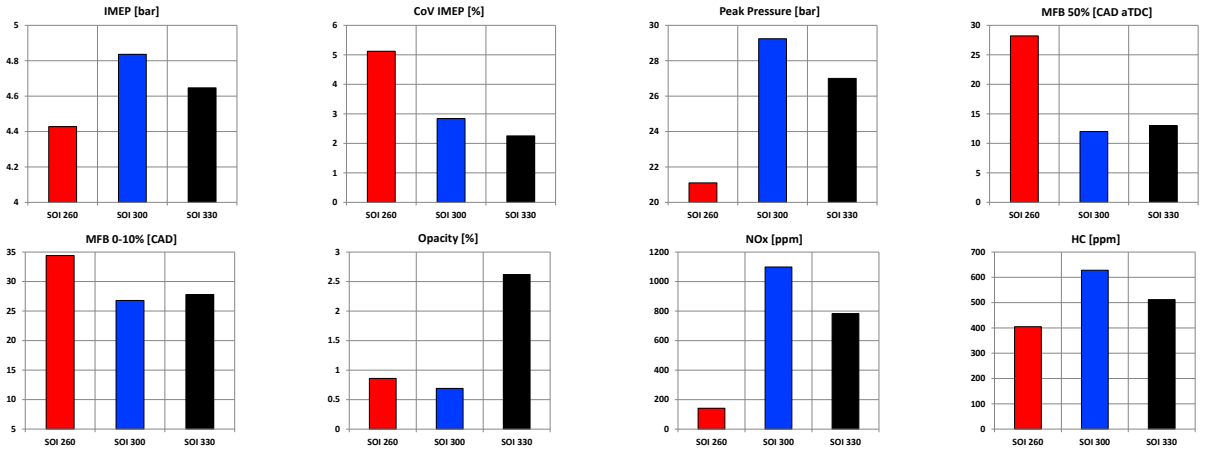

Fig. 3. Experimental results

The case "SOI330" shows no major differences compared to "SOI300": a decrease in terms of pressure peak, combustion speed and engine performance is still present, however the main difference concerns the higher soot production, due to the interaction between the fuel spray and the combustion chamber walls. As mentioned before mixture quality is a key factor in a DISI engine and a detailed investigation of the effect of different injection strategies, in particular for low volatility fuels such as n-Butanol, is crucial in order to well understand in which conditions the poor mixing disadvantage will overcome the advantageous high laminar flame speed. Thanks to the CFD analyses, it is possible to highlight the physical factors governing the early flame onset and subsequent propagation, i.e. it is possible to rank advantags and drawbacks of a given injection phasing. As for emission formation, thanks to the optically accessible engine it is possible to analyse both the propagation preferential direction of the main flame and the onset of favourable locations for secondary diffusive flames. The latter hold crucial relevance in terms of soot production.

5. CFD Results and validation

3D-CFD Results for the three injection strategies reproduce well the experimental test data and the trend variations for all the tested conditions. In Fig. 4 it is possible to observe the drop in pressure peak and combustion slowdown, in terms of MFB 50% CAD value, for the delayed case "SOI260", while the difference between "SOI300" and the advanced "SOI330" is less evident but still present. The model is able to reproduce the experimental measurements in terms of in cylinder pressure traces, flame area and preferential flame front direction.

The experimental ensemble-averaged enflamed area is calculated through the acquired images of actual combustion events. In CFD, a threshold value of 0.5 for the combustion model progress variable, that allows to separate the unburnt mixture from the burnt gases, is used (Fig. 4). The comparison is valid until the flame reaches the optical limit (equal to the 65% of the engine bore). The experimentally observed asymmetric flame propagation for "SOI260" and "SOI330" cases is a direct consequence of the different fuel distribution in the combustion chamber, strongly affecting the local LFS.

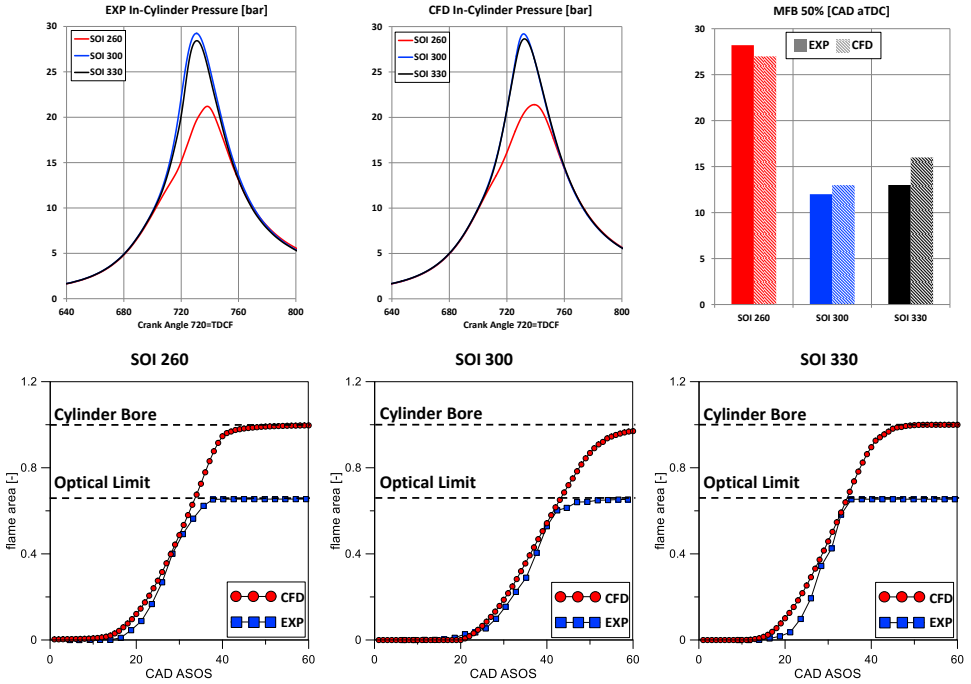

Fig 4. Experimental and CFD In-cylinder pressure traces and MFB-50% (top), and comparison between experimental and CFD flame area (bottom).

Such experimental evidence is confirmed by the CFD results reported in Fig. 5 and Fig. 6, the intermediate SOI (300) is the one showing the higher fuel homogeneity, leading to a more symmetric LFS field and flame propagation. Conversely, the very lean mixture pocket in the intake side and in the exhaust one using as SOI 330 and 260 respectively leads to a very low local LFS, and this is responsible for the notably asymmetric flame front development. Fuel distribution in the combustion chamber not only affects the preferential flame propagation, but also the emission formation. Focusing on soot formation, thanks to the optical access, diffusive flames at the end of the combustion process are analysed and reported in Fig. 7 for the three different SOIs (left). As visible, the local probability of diffusive flames is higher for SOI 330 and it is located in the exhaust portion of the combustion chamber, while it is lower and towards the intake side for the SOI 260 case. This result is a direct consequence of the fuel distribution in the combustion chamber considering that, according to combustion fundamentals [27], diffusive flame are promoted by rich mixture spots. This analysis represent a further validation of the proposed CFD methodology, which proves to be able to well predict not only the combustion velocity but also the fuel distribution in the combustion chamber.

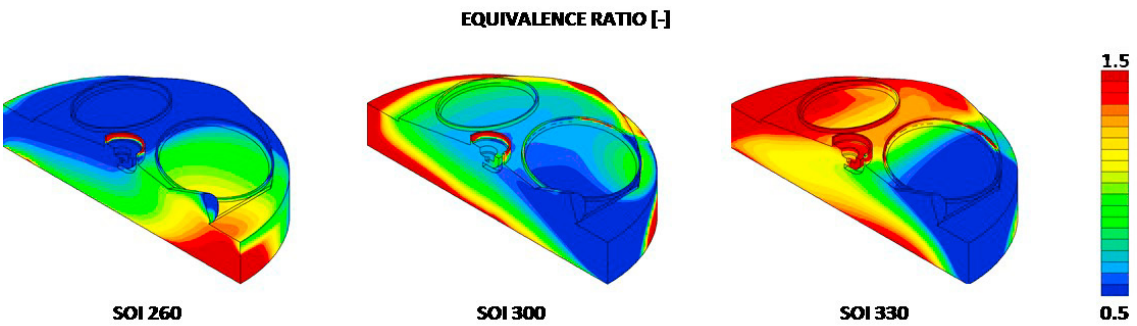

Fig. 5. CFD Equivalence ratio at spark time.

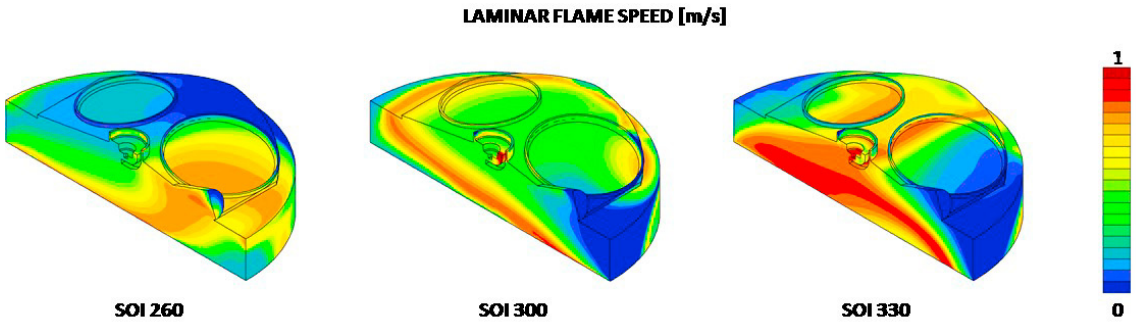

Fig. 6. CFD Laminar flame speed fields at spark time.

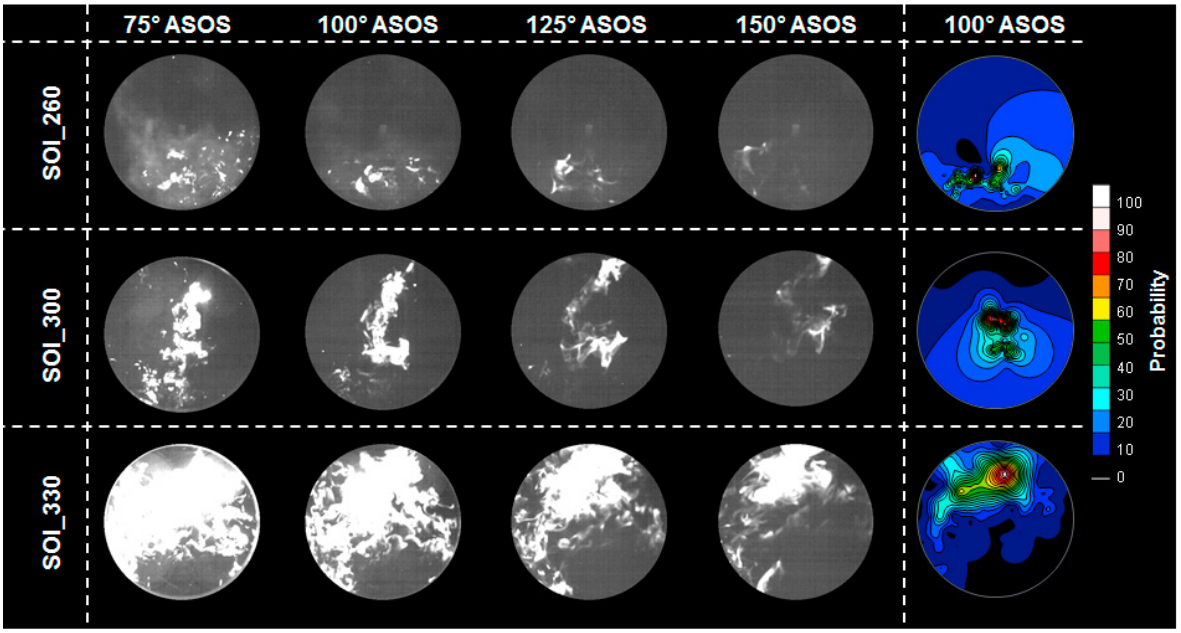

Fig. 7. Cycle-resolved images detected in the late combustion phase and probability density distribution of diffusive flames at 100° CAD After Start Of Spark (ASOS).

6. Conclusion

The need to reduce pollutant emissions and fuel consumption simultaneously increasing engine thermal efficiency is one of the major goals of policy makers and engine manufacturers. Moreover, concerns related to fossil-fuels are promoting a growing interest towards bio-fuels. The use of bio-alcohols as gasoline replacement in SI engines is widely studied trough experimental campaigns showing the advantages in using such kind of fuels in reducing engine knock tendency and pollutant emissions. Well-established methodologies for the CFD simulation of these innovative and often not fully known fuels are currently not available. The aim of this work is the development and validation of a reliable CFD methodology for mixture formation and combustion simulation of any fuel type. In this paper the developed methodology is validated using n-Butanol as gasoline replacement in an optically accessible research engine, tested under different injection strategies. The results show the reliability of the proposed methodology, which is able to reproduce with a reasonable accuracy the experimental evidences. In particular, a possible critical issue in the use of n-Butanol as gasoline replacement in DISI units was identified in previous works [10] in the poor mixture quality, which is responsible for a combustion velocity drop down an increase in combustion instability and soot formation compared to gasoline. In the current work different injection strategies are

experimentally and numerical tested in order to improve mixture quality, but both experiments and CFD show a worsening in terms of engine performance and pollutant emissions. The use of delayed injection strategies leads to very inhomogeneous mixture responsible for very low performance and combustion stability while early injection strategies leads to a strong increase in soot formation.

Thanks to the developed and validated CFD methodology a higher number of more complex injection strategies will be numerically evaluated in the future in order to identify the numerical optimum, moving the engine design and calibration towards the best possible solution.

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