

# Numerical Simulation of Gasoline and n-Butanol Combustion in an Optically Accessible Research Engine

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## ABSTRACT

Conventional fossil fuels are more and more regulated in terms of both engine-out emissions and fuel consumption. Moreover, oil price and political instabilities in oil-producer countries are pushing towards the use of alternative fuels compatible with the existing units. N-Butanol is an attractive candidate as conventional gasoline replacement, given its ease of production from bio-mass and key physico-chemical properties similar to their gasoline counterpart. A comparison in terms of combustion behavior of gasoline and n-Butanol is here presented by means of experiments and 3D-CFD simulations. The fuels are tested on a single-cylinder direct-injection spark-ignition (DISI) unit with an optically accessible flat piston. The analysis is carried out at stoichiometric undiluted condition and lean-diluted mixture for both pure fuels. Numerical simulations are carried out on the same operating points and a dedicated set of detailed chemistry simulations are used to accurately predict laminar flame speed for both gasoline and n-Butanol at selected engine-relevant conditions. Moreover, a method to accurately fit target results is presented and it is applied to obtain a polynomial form of laminar flame speed for both fuels. Mixture preparation and combustion development are carefully analyzed to explain the experimental evidence and to argument the differences between the two fuels, as well as the fuel-specific tolerance to mixture leaning. Finally, conclusions are drawn to summarize the obtained results and to outline the foreseen advantages of using n-Butanol as gasoline substitute in modern SI engines.

**CITATION:** Breda, S., D'Adamo, A., Fontanesi, S., D'Orrico, F. et al., "Numerical Simulation of Gasoline and n-Butanol Combustion in an Optically Accessible Research Engine," *SAE Int. J. Fuels Lubr.* 10(1):2017, doi:10.4271/2017-01-0546.

## INTRODUCTION

The rise in fuel prices and the need to reduce ground-transported generated emissions to improve urban air quality have brought fuel-efficient, low-emissions powertrain technologies at the top of vehicle manufacturers' and policy makers' agenda. Furthermore, political instabilities in oil-producer countries have encouraged the production of fuels from domestic renewable resources in order to reduce the dependence on petroleum based products. Nowadays biofuels production is widely promoted around the world (for example, 10% of transportation fuel should be derived from biofuel by 2020 in the EU) thanks to the chance to obtain them from non-edible residues of food and plants, or lignocellulosic biomass, overcoming issues related to food supply [1,2,3].

The use of bio-alcohols has been studied in both Spark Ignition (SI) and Compression Ignition (CI) engines. In the SI units, thanks to the high octane ratings and flame speed, alcohols such as ethanol or methanol allow to improve engine thermal efficiency while reducing knock tendency [4,5], generally resulting in lower regulated

emissions [6]. In CI engines, different applications are reported in literature ranging from blending alcohol with diesel or biodiesel [7,8] to the dual fuel concept with port injection [9]; in general and for all the applications a reduction in particulate emissions is obtained.

Focusing on SI engines, a new generation of highly downsized units with specific power outputs around or above 150 HP/litre are nowadays emerging. Such performance targets can be reached, for a fixed fuel octane rating, using high-boosting, direct injection and high compression ratios and adopting unconventional strategies such as water injection or cooled EGR [10,11]. From this point of view, bio-alcohols are particularly attractive fuels in view of the different physical and chemical properties listed in Table 1. Thanks to the higher octane number and vaporization heat, pure methanol and ethanol are more effective than gasoline in reducing engine knock tendency; nevertheless, their poor energy density combined with the very low air-to-fuel stoichiometric ratio makes the adoption of these two fuels not convenient in reducing fuel consumption. In the

drawback of these two alcohols compared to gasoline is the increased corrosive action on distribution pipelines which reduces the compatibility with existing power units.

From this point of view high-carbon alcohols, such as n-Butanol, are very attractive due to their higher energy density and air-to fuel stoichiometric ratio, much closer to the gasoline values. This means that, under the same lambda index, n-Butanol is able to release about the same energy compared to gasoline, with an increase of the total fuel mass of about 30%. The same result can be obtained using methanol and ethanol, although an increase in the total fuel mass of 125% and 60% would be required, respectively. Moreover, thanks to its molecular structure, n-Butanol can be blended with both gasoline and diesel and it shows lower corrosive action. All these features enhance the compatibility of this fuel with the existing power units. However, the much lower n-Butanol latent heat of vaporization, RON and MON numbers, make pure n-Butanol less effective than methanol and ethanol in improving knock resistance. Such drawback can be counterbalanced by the faster burn rate, leading to better knock resistance for n-Butanol compared with a RON 92 commercial gasoline, as showed in previous studies [12,13].

Another important factor in the evaluation of new fuels for the currently made SI power units is the performance in terms of regulated and not-regulated emissions. The effect of n-butanol on emissions was found to be comparable to that of ethanol [14] and, thanks to special control strategies such as dual injection, the reduction of unburned hydrocarbons levels in the exhaust stream can be further improved in both WOT (Wide-Open Throttled) and part load operations [15,16]. Other studies from the authors revealed that the beneficial effects in the use of n-Butanol on emissions and engine power output increase when charge dilution through cooled EGR was employed. Compared to gasoline, n-Butanol featured higher rate of heat release and shorter flame development periods with EGR while in undiluted operations a change of the fuel resulted in practically same in cylinder pressure [17].

Despite the above advantages, there are also some potential issue in the direct use of n-Butanol in modern DISI engines related to the higher viscosity and lower vapour pressure of n-Butanol compared with gasoline; this may lead to problems in terms of mixture preparation and fuel deposit formation especially at part load conditions, due to low charge and wall temperatures. In PFI engines, the incomplete fuel evaporation can drop down the fuel conversion efficiency [18]; in DI engines fuel deposits and high charge stratification can slow-down combustion velocity and be responsible of an increase in soot and unburnt hydrocarbons emissions [19].

In DISI engines combustion development, knock onset and emissions are strictly dependent on charge stratification. Moving from fuels with fast evaporation rate, such as methanol, to less evaporating ones such as gasoline or n-Butanol, for a fixed injection system and phasing, a very different fuel distribution in the combustion chamber is formed. Such an effect can hardly be observed in experiments, where charge stratification is not fully known. This may hinder a complete understanding of the potential advantages of the adoption of an innovative fuel in terms of combustion development, emissions and knock resistance. It may be difficult to distinguish what are the

effects of the different fuel properties (mainly, its attitude towards vaporization and mixing) from those linked to combustion development and/or emission formation. To this aim, CFD (Computational Fluid Dynamics) can be a useful tool to better understand the reasons behind observed behaviours in the instrumented engine, identifying critical issues and moving the engine design and calibration towards the optimal solution for each type of fuel.

Table 1. Properties of Gasoline and Alcohols [12,17].

| Fuel                                 | Gasoline                        | Methanol           | Ethanol                          | n-Butanol                        |
|--------------------------------------|---------------------------------|--------------------|----------------------------------|----------------------------------|
| Molecular Formula                    | C <sub>4</sub> -C <sub>12</sub> | CH <sub>3</sub> OH | C <sub>2</sub> H <sub>5</sub> OH | C <sub>4</sub> H <sub>9</sub> OH |
| Lower Heating Value [MJ/kg]          | 42.9                            | 20.08              | 26.83                            | 32.01                            |
| Density @ 20 °C [kg/m <sup>3</sup> ] | 744.6                           | 791.3              | 789.4                            | 810                              |
| Research Octane Number [-] RON       | 92                              | 111                | 108                              | 96                               |
| Motor Octane Number [-] MON          | 82                              | 88.6               | 90                               | 78                               |
| Latent Heat of Vaporization [kJ/kg]  | 373                             | 1098               | 838                              | 584                              |
| Self-Ignition Temperature (°C)       | 300                             | 470                | 474                              | 385                              |
| Stoichiometric Air-to-Fuel Ratio     | 14.46                           | 6.43               | 8.94                             | 11.12                            |

The aim of the present work is the development and validation of a 3D-CFD method to simulate the behaviour of different fuels; such procedure is applied to an optically accessible DISI engine. In particular, two different fuels are compared in this analysis: a commercial RON 95 gasoline and n-Butanol at two different operating conditions. The first is a throttled condition at stoichiometry, while the second is a WOT condition with lean mixture. In particular, in order to improve the combustion model predictive capability, laminar flame speed (LFS) is calculated through detailed chemistry with a validated mechanism and a method to accurately fit the target results is applied to obtain a polynomial form for LFS of both fuels. This developed methodology allows to analyze the different combustion behaviour of a wide set of different fuels and it is very promising in order to better understand pros and cons in using innovative pure fuels or blends. Due to the peculiarity of the optically accessible simulated engine, the presence of non-negligible crevices (between the transparent piston and cylinder walls) and blow-by mass flow rate are taken into account in the simulations in order to improve the consistency of the results. Thanks to the accurate CFD framework it is possible to explain potential issues in using n-Butanol as well as to suggest strategies to improve engine performance with such an innovative fuel.

## INVESTIGATED ENGINE AND EXPERIMENTAL RESULTS

The research unit used for the experiments is a single cylinder DISI engine (Fig.1) where the cylinder head of a 4-cylinder, 16 valves commercial unit is coupled to the optically accessible cylinder block. The engine is equipped with a side mounted side injector (between

the intake valves) and the injection pressure is set to 100 bar; the spark plug is centrally located. The main geometrical engine characteristics are briefly recalled in [Table 2](#).

The optical access is ensured through an 18 mm-thick fused silica window fixed on the piston crown featuring a Bowditch design with a 45 degree UV-enhanced mirror fitted within the hollow piston and the reflected natural flame emission was recorded with an ICCD camera as reported in [Figure 1](#) and [2](#). The digital imaging was performed in two acquisition modes: sequential and repetitive. The first allowed following the inception and propagation of the flame from spark ignition until late combustion through 100 acquisitions corresponded to 100 consecutive CADs. In the repetitive mode, 100 acquisitions were carried out at the same CAD. Specifically, in this work 15 CAD ASOS and 30 CAD ASOS were selected in order to evaluate the cyclic variation of the flame in the early stage of combustion up to the optical limit. After the detection, the flame images were analyzed by a procedure developed in Vision of NI. More details on the acquisition and post-processing procedure applied to optical data can be found in [\[20\]](#).

The engine is un-lubricated in the optically accessible part and the sealing between the transparent piston and the cylinder walls is ensured through bronze-Teflon rings: these allow a non-negligible blow-by flow rate during the compression and the power strokes. The distance between the piston crown and the first ring is about 40 mm and a 0.5 mm thickness is measured, leading to a crevice volume of approx. 4.8 cm<sup>3</sup>, which represents a non-negligible portion of the combustion chamber (about 12%). These dimensions were measured at ambient temperature and can be expected to vary during combustion due to dilatation of all components that determine the aforementioned volume. Nonetheless, they give an idea into the extent of the phenomena of mass transfer from the combustion chamber to the top-land region.

The other issue of blow-by is more difficult to evaluate, but a calibration procedure based on motored pressure traces was found to ensure good results in this respect [\[21\]](#).

**Table 2. Single cylinder SI engine characteristics.**

|                       |                     |
|-----------------------|---------------------|
| Displacement          | 399 cm <sup>3</sup> |
| Bore                  | 79 mm               |
| Stroke                | 81.3 mm             |
| Connecting Rod Length | 143 mm              |
| Compression Ratio     | 10:1                |

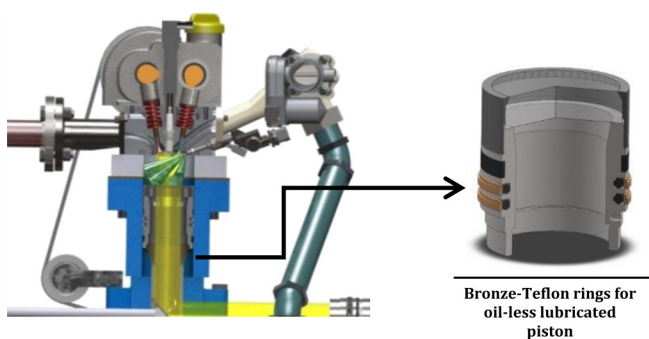


**Figure 1. Optical access design (left) and transparent piston (right).**

Coolant temperature was maintained at 330-335 K, at the upper limit recommended for the uninterrupted sealing rings. Intake air temperature was about 310 K in both WOT and throttled operation while the intake pressure changes around an average value of about 1 and 0.7 bar respectively. In order to easily estimate the fuel conversion efficiency for each investigated operation, the same fuel quantity is injected for the two intake pressure settings (different for the two fuels); a lambda value close to stoichiometry is adopted for throttled operation and a lean flammability limit one is analysed for the WOT condition.

Moreover, the injection phasing is fixed for all the cases at 300 CAD (Crank Angle Degrees) bTDC (before Top Dead Centre) while the injector opening time is increased when switching from gasoline to butanol, in order to compensate the combined effect of lower stoichiometric air-to-fuel ratio and higher density of butanol. Injection duration ranges from 2.3 to 2.9 ms respectively. 200 consecutive In-cylinder pressure traces are acquired for all the operations while the optical analysis is carried out on the last 100 cycles. The experiments are repeated three times for all the operations. Engine speed and spark timing were fixed and equal to 2000 rpm and 30 CA bTDC respectively, for both operating points. For a clearer identification, all the cases selected for this work are resumed in [Table 3](#).

**Table 3. Test Conditions.**

| Case Name      | Fuel     | Intake Pressure[bar] | Lambda | Spark Timing |
|----------------|----------|----------------------|--------|--------------|
| GASOLINE-WOT   | Gasoline | 1 bar                | 1.35   | 30 CA bTDC   |
| GASOLINE-THROT | Gasoline | 0.7 bar              | 1.05   | 30 CA bTDC   |
| BUTANOL-WOT    | Butanol  | 1 bar                | 1.35   | 30 CA bTDC   |
| BUTANOL-THROT  | Butanol  | 0.7 bar              | 1.05   | 30 CA bTDC   |

From a first analysis of the experimental results reported in [Figure 2](#), it is noticeable that butanol presents slower combustion development during both ignition and main flame propagation, despite the fact that higher burning velocity would be expected. The CAD of 50% mass fraction burned is always retarded in both throttled and WOT operation, and this delay in the combustion progress starts from the ignition phase, as visible from the longer 0 to 10% combustion duration. Such an effect leads to lower in-cylinder pressure peak for the butanol cases, while the indicated performance (IMEP) is almost equal in throttled mode and lower in WOT, compared to gasoline. The largest differences between the two fuels are measured in terms of IMEP coefficient of variation (COV). As known, when increasing the lambda value, combustion progress becomes less stable and this produces higher COV, as confirmed by the experiments. However, the rate of COV increase is higher using butanol under the same mixture leaning. Given the expected higher burning velocity for alcohols, such evidence can hardly be explained by the test-bench raw data analysis.

In fact, both outcomes are in contrast with the expectations for an alcohol-fed unit. The object of the presented CFD analyzes is therefore to model the details of mixture preparation and combustion development for both fuels in order to understand what are the reasons behind this behavior.

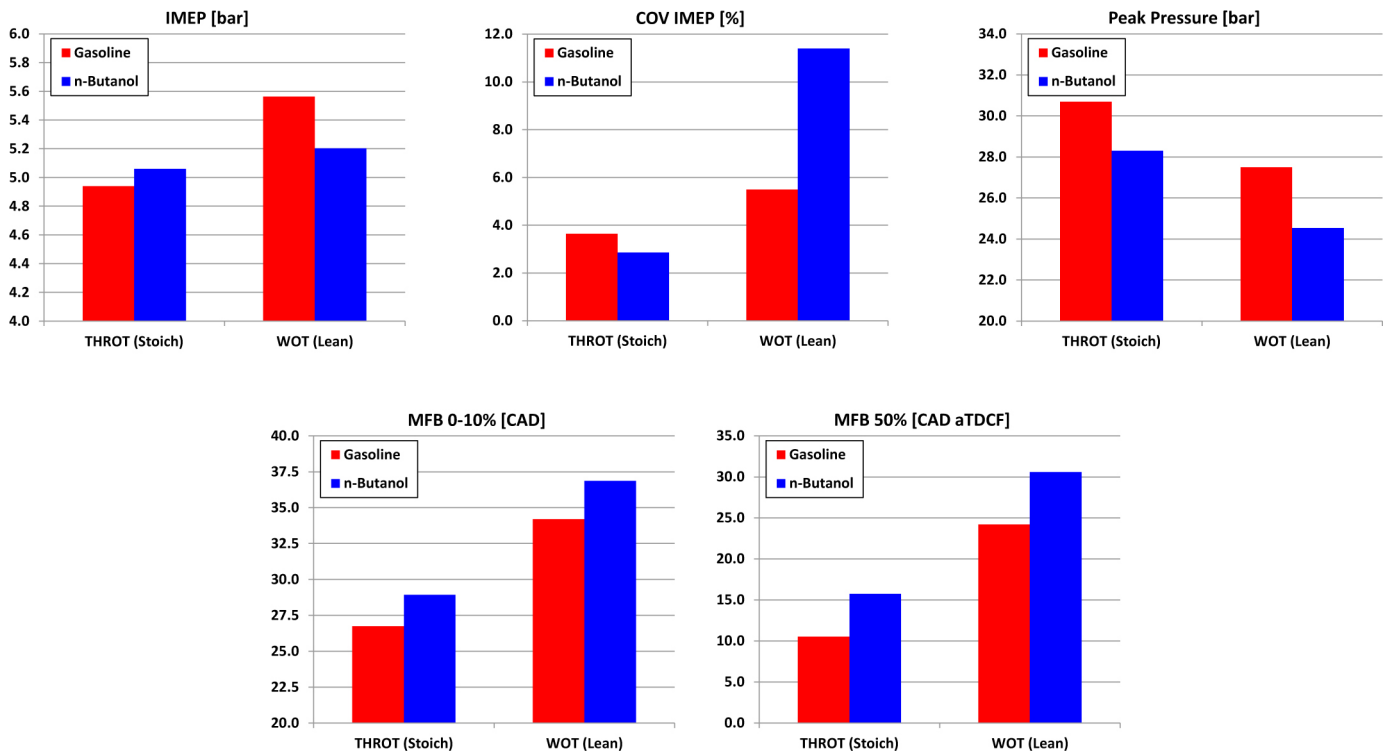


Figure 2. Experimental results related to overall thermodynamic parameters.

## CFD MODEL

The 3D CFD analyzes presented in this paper are carried out by means of a customized version of STAR-CD v4.22, licensed by SIEMENS. In order to reduce the computational effort, the 3D model covers only half of the combustion chamber, plus one intake and one exhaust port, thanks to the geometrical symmetry of the engine. The piston crevice is modelled as a hollow cylinder of 40 mm length and 0.5 mm thickness as in the real geometry and the mesh size in this region is 0.1 mm. The total number of fluid cells ranges between 1.2 and 0.4 million cells at BDC and TDC respectively. In [Figure 3](#) the full grid at TDC, details of the mesh of the ground J-electrode of the spark plug and the crevice are reported.

All the calculations are carried out in a RANS framework and the adopted turbulence model is the k- $\epsilon$  RNG for compressible flows. Time-varying pressure and temperature boundary conditions are applied at the intake and exhaust port, while an unsteady mass flow rate is applied at the bottom of the crevice in order to consider the blow-by flow rate ([Figure 3](#)). All the boundary conditions are derived from a tuned 1D model of the engine. In the 1D framework, the charge blow-by is modelled with a simplified approach, connecting the cylinder with the ambient through a network of three channels with a length equal to the crevice height. The channel diameters are chosen to have the same area of the circular crown between the piston and the cylinder walls. This area is strongly reduced by the presence of the sealing rings, as reported in [Figure 4](#) and it is modelled in the 1D code by splitting the crevice volume through orifices. No direct measures of the blow-by mass flow rate are available, so the orifice diameters are tuned in order to match the in-cylinder pressure trace in terms of peak pressure and phasing in motored conditions at intake charge pressures. The blow-by model was validated against experimental measurements and previous work by the authors [33].

Thanks to this simplified representation of the flow in the crevices it is possible to quantify the blow-by mass flow rate during the engine cycle. The resulting mass flow and temperature boundary conditions at the end of the first crevices channel are applied at the crevice bottom in the 3D model, as reported in [Figure 4](#).

The blow-by and the crevice modeling are not a standard practice in in-cylinder simulations of current production engines because the blow-by mass flow rate and the crevice volume can be neglected without dramatic effects on the result accuracy; conversely, in the analyzed research unit these effects are not negligible. This is confirmed by the results of the 1D simulations reported in [Figure 6](#) for the throttled and WOT operations with gasoline. Neglecting the blow-by mass flow rate an overestimation of the in-cylinder pressure peak is visible for both the operations; the same can be observed for the in-cylinder pressure during the power stroke, which leads to a relevant overestimation of the indicated performance (IMEP). It is important to underline that these results are obtained in the 1D framework using the experimental value for the intake air pressure, temperature, compression ratio and lambda. The combustion development in 1D is not calculated but superimposed using the experimental burn rate, and the lower heating value of the fuel is the same as that used in the experiments. Using the blow-by diameter tuned under motored conditions and comparing the simulated in cylinder pressure traces with the simulated one the agreement with the experiments is notably improved for both operations and with both fuels. In [Figure 5](#) the trend of the blow-by mass flow rate during the compression and power stroke is also reported for both operations; the direct dependence of this mass flow rate on the engine load is clearly visible: an increase of the in-cylinder pressure trace leads to an increase of the blow by mass flow rate.

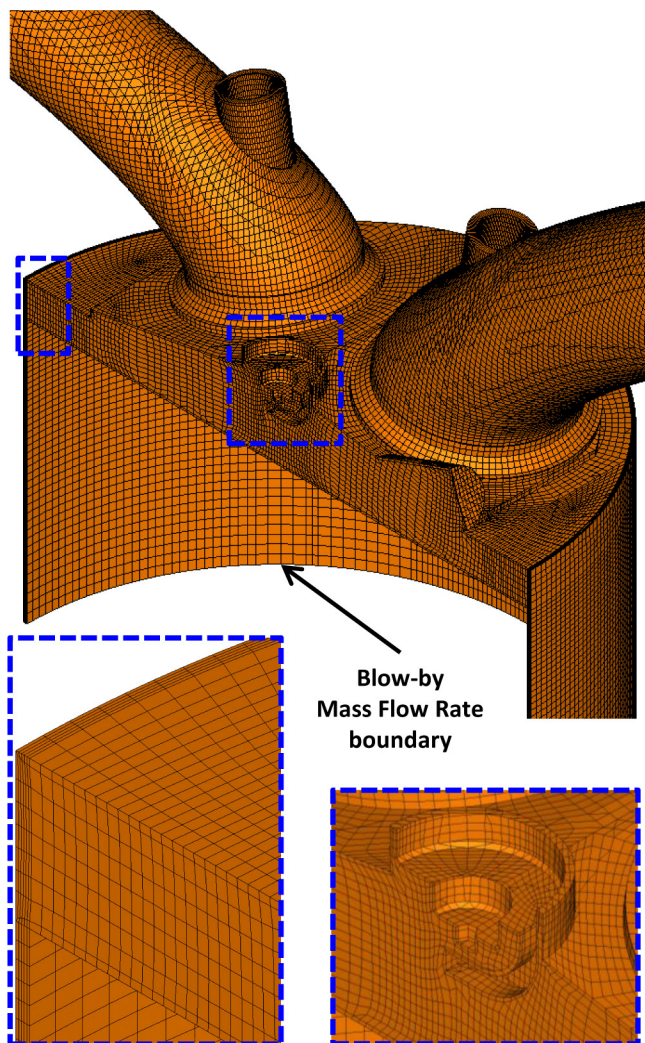


Figure 3. Computational grid.

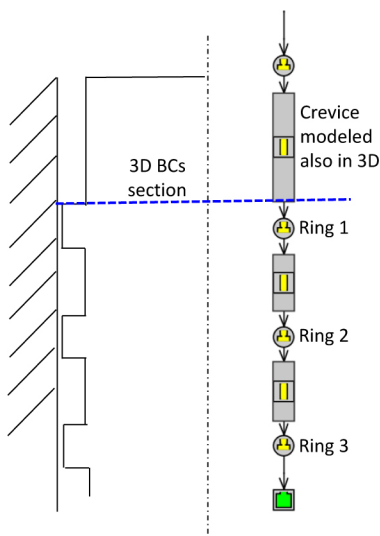


Figure 4. Schematic representation of crevices between piston and cylinder walls (left) and their modeling in 1D (right).

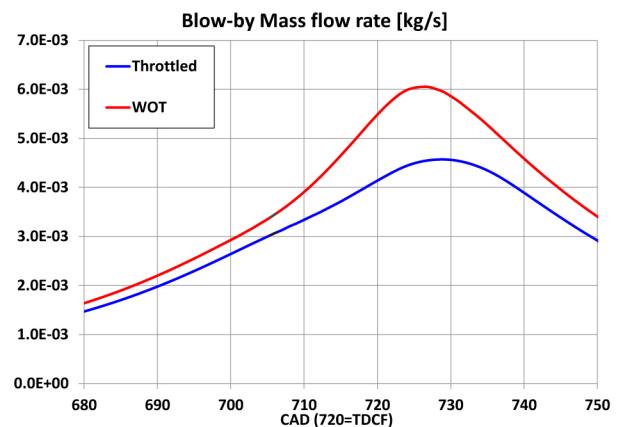
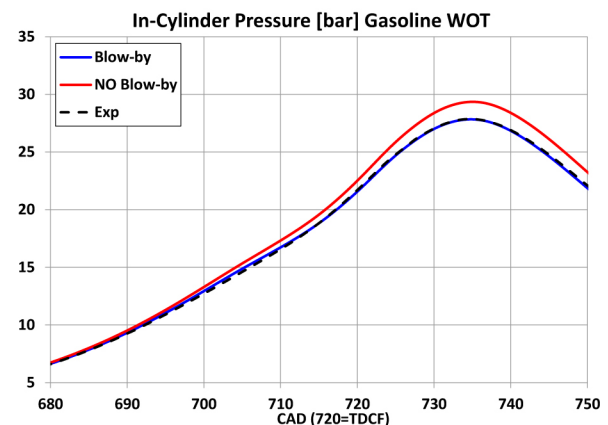
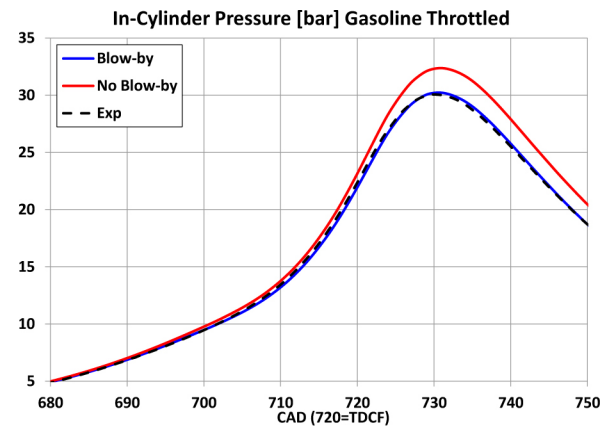


Figure 5. Effects of blow-by modeling in 1D framework.

### Spray Modelling

The correct representation of the 6-hole full-cone GDI spray evolution is a key aspect in the CFD simulations since it plays a fundamental role in mixture preparation. This in turn affects the mixture laminar flame speed and thus the combustion development. The nominal nozzle length and diameter of the injector adopted in the experiments are 0.14 and 0.196 mm respectively, while the orientation of the six nozzles is sketched in Figure 6. The multi-hole liquid spray is modeled using a Lagrangian approach, where the primary atomization is replaced by a distribution of numerical parcels whose size is represented by a purposely-calibrated Rosin-Rammler distribution [22] and whose velocity is derived, as a function of the

nozzle diameter, from a prescribed experimental instantaneous mass flow rate reported in Figure 7 for both fuels. The effective nozzle diameter, used to estimate the spray characteristics at the nozzle exit, is estimated using the Kuensberg 1-D model [23].

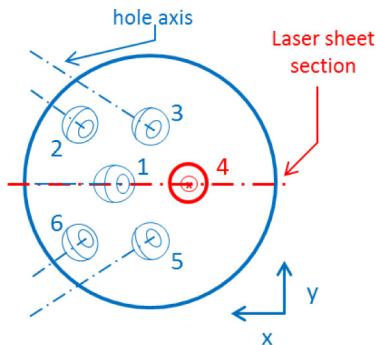


Figure 6. Nozzle axes orientation.

The injector was tested in a quiescent vessel using gasoline and butanol under two different injection pressures, i.e. 50 and 100 bar. The analysis of the experimental results reveals small differences in terms of spray penetration and fuel mass flow rate using the two different fuels, as shown in Figures 7 and 8. Due to the similar spray behavior, the same spray model tuning is maintained for both fuels; as visible in Figure 8, where the comparison between the experimental spray penetration and the CFD results is reported for both injection pressures and both fuels, the predicted spray penetrations closely matches the experiments.

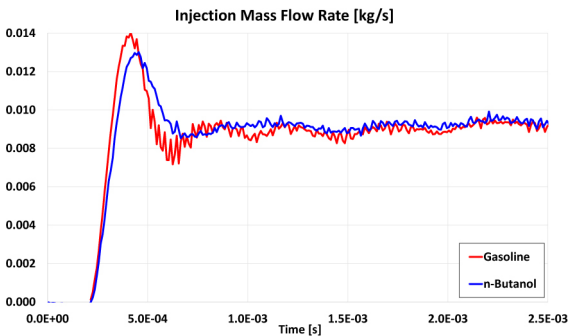


Figure 7. Instantaneous mass flow rate for both Gasoline and n-Butanol.

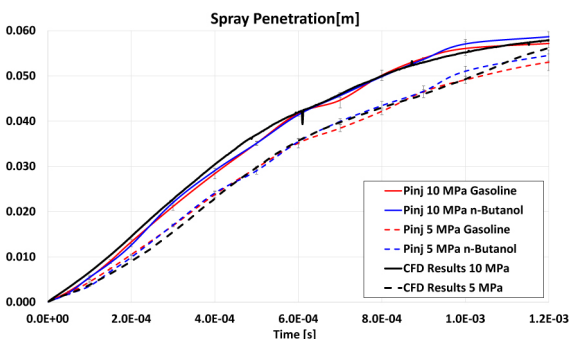


Figure 8. Numerical and experimental results on spray penetration for both Gasoline and n-Butanol.

## Combustion and Heat Transfer Modelling

The adopted combustion model is the ECFM-3Z [24] which was widely used in previous publications by the authors [5,10,25] and whose capability to simulate partially premixed combustion realizations is fundamental for the present analysis. The model is based on the flamelet hypothesis, considering a laminar flame profile embedded in a turbulent flow regime. In the standard practice the laminar flame speed of the fuel is derived from correlations available in literature [26,27]. Polynomial functions are used to fit unstretched laminar flame velocities from experiments at extremely different conditions (low pressure and temperature) from those typically experienced in engines. Therefore, the polynomial fits are largely extrapolated from their field of validation to simulate engine combustion. Such extrapolation can lead to unfeasible LFS trends such as LFS peaks for extremely rich mixtures at engine-like pressure levels, as shown in Figure 9.

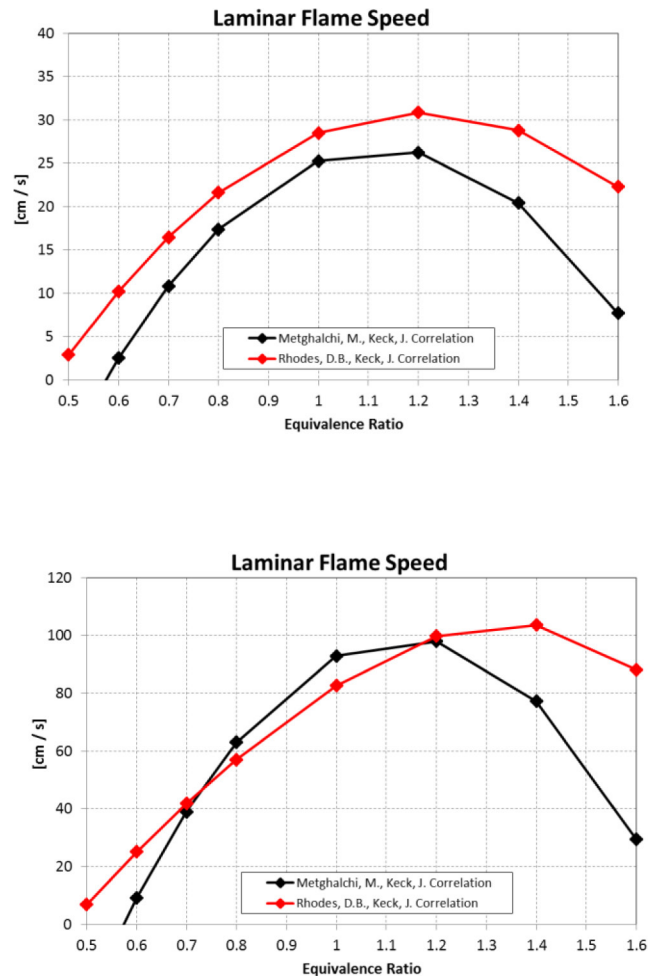


Figure 9. Laminar flame speed from [26] and [27] for 1 bar, 300 K (top) and for 30 bar, 700 K (bottom).

To avoid such issues and to improve the model accuracy, a new methodology, described in details in the following paragraph, is developed to estimate the fuel-specific LFS through chemical kinetics

calculations and to fit the calculated data at engine relevant conditions. Such procedure also overcomes the unavailability of LFS correlations for alternative fuels, such as n-Butanol.

As for spark ignition, a relatively simple algebraic model based on a Flame Surface Density (FSD) deposition after a kernel growth delay is used [28]. Uniform wall temperatures are applied at each engine component facing the combustion chamber and a model developed and validated within the research group is adopted to take into account for wall heat transfer [25].

## METHODOLOGY FOR LAMINAR FLAME SPEED

Laminar flame speed is a fuel-air mixture property depending on pressure, unburnt temperature, air-to-fuel ratio and residual presence. It is a fundamental property of reacting mixtures and it serves as input in many CFD flamelet combustion codes, such as the ECFM-3Z. Given the mentioned predictive error due to large extrapolation of standard fits, an alternative method is developed and applied in this study. Validated chemical mechanisms for laminar flame speed of gasoline surrogate and n-Butanol have been published by several research groups. In this study, gasoline surrogate is modelled based on the mechanism proposed by Dirrenberger et al. [29], consisting of 304 species. A ternary blend of n-Heptane/iso-Octane/Toluene (13.7/42.9/43.4 mole fraction) is implemented in the DARS-Basic chemistry solver to obtain 1D flame profiles and to predict laminar flame speed at selected engine-typical conditions. As for n-Butanol, the Frassoldati et al. [30] mechanism is used, involving 317 species and being validated for oxidation of butanol isomers and LFS simulation.

A fitting procedure is adopted to obtain new polynomial forms built upon flame speed simulations at engine conditions. The procedure follows the approach proposed in [31], where the assumption is made that flame speed dependence on pressure, temperature and equivalence ratio can be expressed by a commonly used power-law relationship such as that in Eq. 1 once accurate forms for  $s_{L,0}$ ,  $\alpha$  and  $\beta$  are given. The effect of residuals will be discussed separately at the end of this section.

$$s_L = s_{L,0} \cdot \left(\frac{T}{T_0}\right)^\alpha \cdot \left(\frac{p}{p_0}\right)^\beta \quad (1)$$

Several correlations for LFS are based on this assumption, such as [26,27,32]. In this study, the LFS simulations serve as virtual experiments of flame speed, then  $s_{L,0}$ ,  $\alpha$  and  $\beta$  have to be fitted on these results. A fifth order logarithmic polynomial form is used as functional fitting form, Eq. 2.

$$s_L = \left[ \sum_{i=0}^5 a_i \cdot \log(\phi)^i \right] \cdot \left(\frac{T}{T_0}\right)^{\sum_{i=0}^5 b_i \cdot \log(\phi)^i} \cdot \left(\frac{p}{p_0}\right)^{\sum_{i=0}^5 c_i \cdot \log(\phi)^i} \quad (2)$$

This relationship is still based upon the power-law expression (Eq. 1), although the definition of  $s_{L,0}$ ,  $\alpha$  and  $\beta$  follows a 5<sup>th</sup> order logarithmic function of the equivalence ratio through the coefficients  $a_i$ ,  $b_i$  and  $c_i$  respectively. The  $a_i$  coefficients describe the equivalence ratio dependence of LFS at reference conditions, and they are grouped in the  $\bar{A}$  vector, which is determined by a least square minimization of the system (Eq. 3):

$$\begin{bmatrix} s_{L,0}(\phi_1) \\ s_{L,0}(\phi_2) \\ \vdots \\ s_{L,0}(\phi_n) \end{bmatrix} = \begin{bmatrix} 1 & \ln(\phi_1) & [\ln(\phi_1)]^2 & \cdots & [\ln(\phi_1)]^5 \\ 1 & \ln(\phi_2) & [\ln(\phi_2)]^2 & \cdots & [\ln(\phi_2)]^5 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \ln(\phi_n) & [\ln(\phi_n)]^2 & \cdots & [\ln(\phi_n)]^5 \end{bmatrix} \cdot \underbrace{\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}}_{\bar{A}} \quad (Eq. 3)$$

Similarly, the flame speed dependence on temperature and pressure (hereafter  $s_{L,pT}$ ) is expressed by the six  $b_i$  and the six  $c_i$  coefficients, grouped in the  $\bar{B}$  vector and determined similarly by a least square minimization of the system (Eq. 4). The  $\bar{L}_{TP}$  is composed by  $\bar{L}_T$  and  $\bar{L}_p$  matrices (Eq. 5 and 6), illustrated as separate for the sake of clarity.

$$\begin{bmatrix} \ln\left(\frac{s_{L,pT}(\phi_1)}{s_{L,0}(\phi_1)}\right) \\ \ln\left(\frac{s_{L,pT}(\phi_2)}{s_{L,0}(\phi_2)}\right) \\ \vdots \\ \ln\left(\frac{s_{L,pT}(\phi_n)}{s_{L,0}(\phi_n)}\right) \end{bmatrix} = \underbrace{\begin{bmatrix} \bar{L}_T & \bar{L}_p \end{bmatrix}}_{\bar{L}_{TP}} \cdot \underbrace{\begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \\ c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}}_{\bar{B}} \quad (4)$$

$$\bar{L}_T = \begin{bmatrix} \ln\left(\frac{T}{T_0}\right) & \ln\left(\frac{T}{T_0}\right) \cdot \ln(\phi_1) & \ln\left(\frac{T}{T_0}\right) \cdot [\ln(\phi_1)]^2 & \cdots & \ln\left(\frac{T}{T_0}\right) \cdot [\ln(\phi_1)]^5 \\ \ln\left(\frac{T}{T_0}\right) & \ln\left(\frac{T}{T_0}\right) \cdot \ln(\phi_2) & \ln\left(\frac{T}{T_0}\right) \cdot [\ln(\phi_2)]^2 & \cdots & \ln\left(\frac{T}{T_0}\right) \cdot [\ln(\phi_2)]^5 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \ln\left(\frac{T}{T_0}\right) & \ln\left(\frac{T}{T_0}\right) \cdot \ln(\phi_n) & \ln\left(\frac{T}{T_0}\right) \cdot [\ln(\phi_n)]^2 & \cdots & \ln\left(\frac{T}{T_0}\right) \cdot [\ln(\phi_n)]^5 \end{bmatrix} \quad (5)$$

$$\bar{L}_p = \begin{bmatrix} \ln\left(\frac{p}{p_0}\right) & \ln\left(\frac{p}{p_0}\right) \cdot \ln(\phi_1) & \ln\left(\frac{p}{p_0}\right) \cdot [\ln(\phi_1)]^2 & \cdots & \ln\left(\frac{p}{p_0}\right) \cdot [\ln(\phi_1)]^5 \\ \ln\left(\frac{p}{p_0}\right) & \ln\left(\frac{p}{p_0}\right) \cdot \ln(\phi_2) & \ln\left(\frac{p}{p_0}\right) \cdot [\ln(\phi_2)]^2 & \cdots & \ln\left(\frac{p}{p_0}\right) \cdot [\ln(\phi_2)]^5 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \ln\left(\frac{p}{p_0}\right) & \ln\left(\frac{p}{p_0}\right) \cdot \ln(\phi_n) & \ln\left(\frac{p}{p_0}\right) \cdot [\ln(\phi_n)]^2 & \cdots & \ln\left(\frac{p}{p_0}\right) \cdot [\ln(\phi_n)]^5 \end{bmatrix} \quad (6)$$

The outlined procedure allows to determine the set of eighteen coefficients needed to define a polynomial form as in Eq. 2.

The simulated LFS data for gasoline and n-Butanol, as well as the fitting coefficients for both fuels, are reported in Table 4. The results of the fitting forms given by the outlined procedure are depicted in Figure 10, where a satisfactory agreement is observed against target data from chemical kinetics simulations. The target data for the fitting procedure are calculated at engine-relevant conditions (EC), which are reported in the legend in Figure 10. The higher LFS for n-Butanol is clearly visible in Figure 10 and 11 for all the analyzed conditions with respect to the gasoline counterpart, while both fuels show a peak LFS for equivalence between 1.0-1.1 at all conditions.