Partially Stratified Combustion Modeling for Natural Gas Fueled internal Combustion Engines

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Abstract
Lean-burn natural gas fueled internal combustion engines (ICEs) are emerging as a promising strategy to improve thermal efficiency and reduce exhaust emissions. However, as the mixture is leaned out beyond the Lean Misfire Limit (LML), several technical problems are more likely to occur. In order to limit those problems, different solutions have been proposed over the last decade. Among them, the stratification or the partial stratification of the charge has been shown to successfully extend the lean limit with respect to conventional lean burn engines.
During the development and optimization of such strategies, Computational Fluid Dynamics (CFD) is a fundamental tool to thoroughly understand the phenomena occurring during the mixing and combustion phases. In order to reliably simulate the combustion process, a proper model is required which takes account of the Turbulence-Chemistry Interaction (TCI).
In the present work the Partially Stirred Reactor (PaSR) model was used in the numerical simulation of a natural gas fueled single cylinder research engine with RANS approach to analyze the benefits of partially stratifying the mixture around the spark location.

Introduction
During the last decade several technical solutions have been proposed to develop new technologies for a more efficient and clean use of fossil fuels.
Among all the solutions proposed, run the engine at lean air-to-fuel ratios has been accepted as an effective strategy to increase thermal efficiency and reduce emissions [1-3]. Lean operating conditions especially allows for lower flame temperatures thus limiting the nitrogen oxide emissions [4]. Moreover, the thermal efficiency increases significantly, since the ratio of specific heats rises as the mixture is leaned out [5]. Finally, engine load control by varying air fuel ratio allows for further improvement of efficiency.
However, when the mixture is leaned out beyond the Lean Misfire Limit (LML), it is no longer possible to get stable ignition conditions. Misfiring events occur resulting in increased cycle-to-cycle variability, along with higher carbon monoxide and total hydrocarbon emissions [6].
In order to face those issues, several strategies have been proposed in literature; among them, the kernel stability can be increased by stratifying the charge around the spark location, allowing the kernel to mature in a richer mixture. In this regard,

a particular ignition strategy has been developed and patented at the University of British Columbia for natural gas fueled engines in order to extend the lean limit, namely the Partially-Stratified Charge (PSC) ignition system [7].

Computational Fluid Dynamics (CFD) allows for investigating the fundamental phenomena occurring during the injection and combustion processes during engine operation. Under stratified operating conditions taking into account the Turbulence-Chemistry Interaction (TCI) is key for having a reliable simulation of the combustion process [8]. Different combustion models have been proposed in literature so far to evaluate the effects of the mutual interaction between chemical kinetics and turbulent flow structures. Among them, the Partially Stirred Reactor (PaSR) model has proved to provide excellent results both with homogeneous and stratified mixtures into a Constant Volume Combustion Chamber (CVCC) [9, 10].

The purpose of this work is to extend the conclusions drawn for the CVCC, to better understand the beneficial effects brought on by the PSC ignition system under real engine operating conditions. A detailed chemical mechanism has been used to properly take into account the complexity of the methane combustion kinetics. The experimental data provided by the University of British Columbia for a single cylinder spark-ignition research engine have been used for the validation of numerical results.

In the first part of the paper a detailed description of the PSC combustion process has been reported focusing on the effects of the PSC jet on the charge ignition process. Then, the numerical results have been compared with the experimental data, in order to demonstrate the accuracy of the simulated models.

Numerical setup

The numerical simulations have been performed with the software CONVERGE CFD v2.3 [11]. The k-ε RNG has been set for the RANS closure [12]. The Partially Stirred Reactor (PaSR) combustion model [13] has been chosen to take into account the turbulence-chemistry interaction (TCI) coupled with a detailed chemical kinetic mechanism [14]. The basic computational grid has been locally refined with fixed embedding and adaptive mesh refinements (AMR) to provide enough resolution without making the overall cell count prohibitively high. A detailed description of the grid used is reported in Table 1.

Numerical results

A careful simulation of the combustion process allows for understanding the beneficial effects of the PSC ignition system on the engine performance. Figure 1 shows the evolution of the charge ignition and kernel growth processes. Thanks to the stratification of the charge around the spark plug, the ignition process speed is significantly increased if compared with traditional lean-burn engines (Figure 1 (A)). Moreover, the PSC injected fuel is deviated by the lower electrode towards the spark region enhancing the mixing process locally.

Table 1 - Mesh characteristics used for the analysis

Region	Meshing strategy	Grid size
Computational domain	Base mesh	3 mm
Valves	Fixed embedding (cyclic)	0.375 mm
Capillary tube	Fixed embedding (permanent)	0.094 mm
Spark-plug	Fixed embedding (cyclic)	0.094-0.375 mm
Flame front	AMR (cyclic)	0.375 mm

The flame kernel is advected by the velocity field undergoing a rapid growth Figure 1 (B)-(C). This speeding up of the kernel growth allows then for the stabilization of the flame propagation also in an overall ultra-lean operating conditions (Figure 1 (D)).

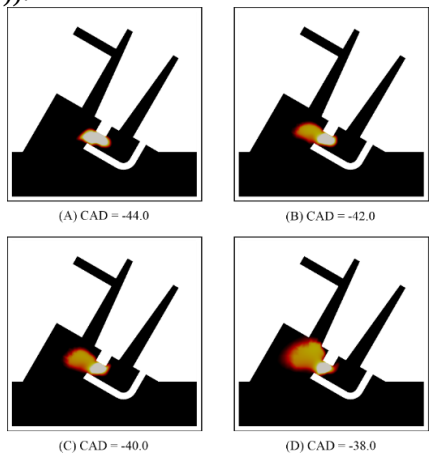

Figure 1. Evolution of the charge ignition.

The typical evolution of the combustion process for a PSC case is shown in Figure 2, where in blue is represented the PSC fuel pocket. At the beginning of the flame propagation, the rich-fuel cloud forms a preferential path for the flame propagation (Figure 2 (A)-(B)). The PSC injection produces thus a third beneficial effect, since it promotes the propagation of the flame kernel into the bulk mixture. When the flame encounters the lean bulk mixture its speed is still relatively high, and thus the propagation proceeds at a faster rate (Figure 2 (C)-(D)).

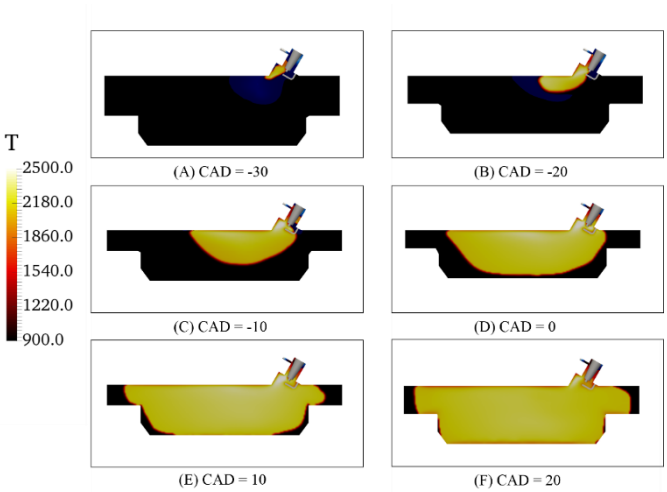

Figure 2 - Numerical results for flame propagation

Comparison with experimental data

Homogeneous charge (λ = 1.53)

The numerical results have then been validated against the experimental data collected at the University of British Columbia for the single cylinder research engine Ricardo Hydra. Figure 3 shows the in-cylinder pressure and the integrated heat released (IHR) versus crank angle for the homogeneous case at λ = 1.53. The solid black and red lines represent respectively the experimental and the simulated mean pressure trace, whereas the dashed lines correspond to the upper and lower bounds of the 95 % experimental confidence interval. The numerical data are almost coincident with the experimental mean data in terms of mean pressure trace while the simulated IHR curve has a slightly lower slope than the experimental one, but it is entirely contained between the two confidential bounds. This indicates that the combustion model is capable of accurately represent the combustion process under the homogeneous ultra-lean operating conditions.

Partially stratified charge (λ = 1.53)

The PSC case with the same air-to-fuel ratio was then tested. Figure 4 shows that the numerical model is capable of accurately predicting the experimental mean trend also under stratified conditions; only minor discrepancies in the vicinity of the peak pressure and in the descending branch of the curve are occurring. It is worth noting that no model tuning has been performed between the homogeneous and the PSC cases, meaning that the model has been able to correctly predict the enhancement in the quality of the combustion process related to the stratification of the charge itself.

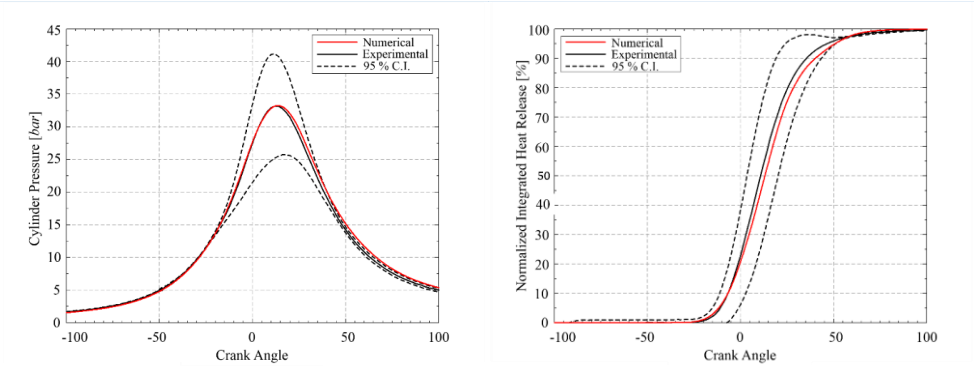

Figure 3 - In-cylinder pressure trace (left) and Integrated Heat Release (right) for λ=1.53 homogeneous case

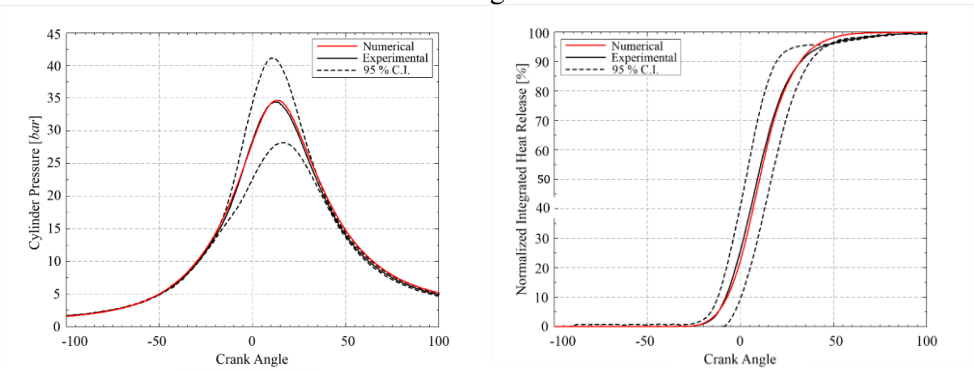

Figure 4 - In-cylinder pressure trace (left) and Integrated Heat Release (right) for λ=1.53 PSC case

The slope of the numerical IHR curve is in excellent agreement with the experimental one in the central portion, but higher values are obtained toward the end of the process. These results confirm the capabilities of the combustion model to handle inhomogeneities of the mixture due to charge stratification and then confirm the possibility to use the proposed numerical framework for the investigation of PSC operating conditions.

Partially stratified charge (λ = 1.68)

The third operating conditions tested was the PSC case with λ = 1.68. The results for this case are shown in Figure 5. The experimental mean pressure trace is close to the numerical one, whereas small discrepancies can be highlighted for the IHR. In particular, the numerical and the experimental curves are almost perfectly superimposed in the first part, but then the slope of the simulated case becomes lower than that of the experimental mean trend.

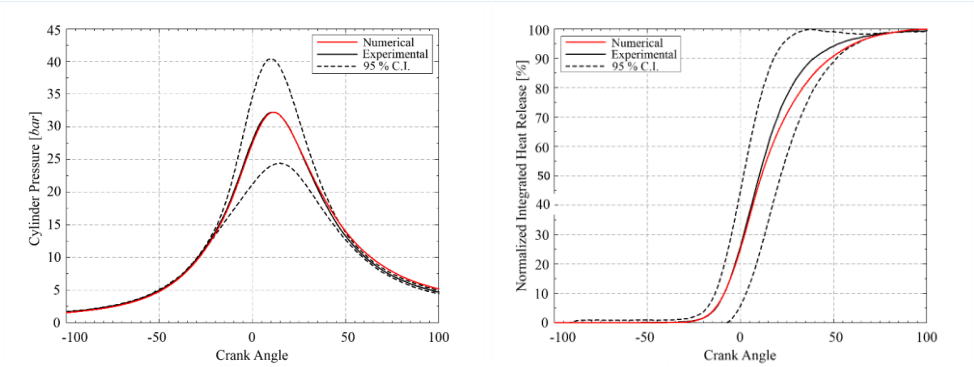

Figure 5 - In-cylinder pressure trace (left) and Integrated Heat Release (right) for λ=1.68 PSC case

This deviation can be attributed to a non perfect representation of the in-cylinder turbulence level during the expansion stroke, giving a small underestimation of the flame front speed.

However, the numerical curve lies within the confidence interval over the entire combustion process duration, and thus the numerical results can be considered reliable. Moreover, these results are indicative of the robustness of the combustion model, whose accuracy is not affected by changes in the relative air-to-fuel ratios.

Conclusions

This study aims at carrying out numerical simulations to highlight the beneficial effects of the Partially Stratified Charge ignition system, trying to understand thoroughly the physical phenomena involved. The PaSR combustion model, combined with a 30-species chemical mechanism, has been validated against experimental data to assess its reliability to represent the combustion process of natural gas mixtures under lean both homogeneous and inhomogeneous conditions. The numerical results are in excellent agreement with the experimental data for both homogeneous and the PSC charge operating conditions, at two ultra-lean air-to-fuel ratios.

Numerical results were entirely contained within the 95 % confidence experimental interval. The results from the PSC case with λ = 1.53 were used to analyze in detail the PSC combustion process with particular focus on the effects of the PSC jet on the combustion process.

The PSC ignition system gives the following three main effects:

1. The formation of a more easily ignitable mixture near the spark-plug, which speeds up the ignition process and makes it independent of the bulk charge composition;
2. The strong interaction between the PSC jet and the flame kernel, which advected by the flow field, increases significantly its growing rate;
3. The generation of a fuel-rich pocket in the vicinity of the electrodes, which forms a preferential path for the flame propagation, helping its penetration into the bulk lean mixture.

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