

Influence of the Local Mixture Characteristics on the Combustion Process in a CAI™ Engine

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ABSTRACT

Among the existing concepts to help improve the efficiency of spark ignition engines on low load operating points, Controlled Auto-Ignition™ (CAI™) is an effective way to lower both fuel consumption and pollutant emissions at part load without major modifications of the engine design. The CAI™ concept is founded on the auto-ignition of a highly diluted gasoline-based mixture in order to reach high indicated efficiency and low pollutant emissions through a low temperature combustion.

Previous research works have demonstrated that the valve strategy is an efficient way to control the CAI™ combustion mode. Not only the valve strategy has an impact on the amount of trapped burnt gases and their temperature, but also different valve strategies can lead to equivalent mean in-cylinder conditions but clearly differentiated combustion timing or location. This is thought to be the consequence of local mixture variations acting in turn on the chemical kinetics.

In the present study, 3D CFD computations and optical diagnostics are combined to explore the local mixture differences due to the choice of valve strategy. The mixture characteristics are then linked to the experimentally observed differences in terms of auto-ignition location and timing, combustion duration and pressure rise.

The results provide an insight into the effects explaining the suitability of the Negative Valve Overlap (NVO) strategy for low CAI™ loads and the capability of the Exhaust Gas Re-Breathing (EGRB) strategy to reach higher loads.

INTRODUCTION

The present concerns about environment and long-term fuel availability are powerful incentives and above all bases for legal demands for more efficient and less polluting power sources for transportation. Even if

various emerging new concepts exist, the short and mid-term powertrain concepts are still based on internal combustion engines (ICE) and most of the time on hydrocarbon-fuelled ICE.

Present series engine concepts are most of all either gasoline-fuelled spark ignition engines or Diesel-fuelled compression ignition engines. Because the spark ignition engines combine simplicity, a low purchasing cost and low running costs, they are the world's most widely sold power sources for passenger cars. Nevertheless, for the European market, Diesel-fuelled engines have become a major part of total sales thanks to a decisive advantage in the eyes of the customers, i.e. a lower fuel consumption combined with lower fuel purchasing prices. On the other hand, the Diesel-fuelled engines naturally suffer from higher pollutant emissions, which leads to the implementation of complex and expensive after-treatment devices.

The fuel consumption penalty for spark ignition engines is mainly due to the load control through throttling. Among the existing concepts to help improve the efficiency of spark ignition engines on low load operating points, Controlled Auto-Ignition™ is an effective way to lower both fuel consumption and pollutant emissions at part load without major modifications of the engine design [1-3]. Therefore, the spark ignition engines' drawback can be reduced while keeping the engine simple and relatively cheap to build and run.

The CAI™ concept is founded on the auto-ignition of a highly diluted gasoline-based mixture in order to reach high indicated efficiency and low pollutant emissions through a low temperature combustion. To promote auto-ignition in an engine with limited compression ratio, a source of thermal energy is required. Besides, in order to avoid the large pressure rises related to the auto-ignition of a fully premixed mixture, a dilution media is needed to slow down the chemical reactions. The simplest way to combine the need for thermal energy and for dilution is to trap a part of the hot burnt gases from the preceding

engine cycle in the cylinder. The use of the burnt gases from the preceding engine cycle is what differentiates CAI™ from the other HCCI concepts [1]. It also induces a cycle-to-cycle coupling due to the dependency of the auto-ignition occurrence and timing on the amount and thermodynamic conditions of these trapped burnt gases [4-5].

The CAI™ combustion mode as generally all HCCI concepts is theoretically based on the rapid oxidation of a homogeneous mixture of air and fuel [6]. Nevertheless, in real engine configurations, a perfect homogeneity of species and temperature fields is impossible. Various previous research works from a wide range of authors have demonstrated the existence of different levels of heterogeneity in HCCI engines [1, 7-13]. Particularly, for gasoline PFI engines which should allow to create fairly homogeneous mixtures, these heterogeneities are of prime importance because they drive the auto-ignition timing and location as there is no way to act on the mixture once the intake valves are closed.

The ability of the heterogeneities to control the auto-ignition timing and the consequent combustion has been recently pointed out as an efficient way to gain control on such combustion as gasoline HCCI [12]. The most promising benefit presently put forward is the control of the pressure rise, its reduction allowing for an extension of the load range towards higher loads. In these results, the temperature heterogeneity is the main driving force as the chemical kinetics controlling auto-ignition and subsequent combustion are highly sensitive to this parameter. In the present study, we aim to determine until which limit the temperature field is the only driving force and if some species field heterogeneity could become another effective way to improve our control on the CAI™ combustion mode.

To reach these goals, two totally different valve strategies are used to trap the desired amount of burnt gases: Negative Valve Overlap (NVO) and Exhaust Gas Re-Breathing (EGRB). The strategies have an impact on the mean in-cylinder values but also on the local distribution of these quantities. The links between the valve strategy, the mixture and the auto-ignition as well as the various combustion parameters are studied combining optical diagnostics and 3D CFD computations.

OPTICAL DIAGNOSTICS TOOLS

A brief description of the relevant optical diagnostics tools used in the present study is provided below. For more complete information, the reader should refer to [7].

The used optical diagnostics aim to study two distinct aspects:

- the degree of mixture heterogeneity and its possible influence on the combustion process;

- the evolution of the combustion process itself.

Therefore, dedicated methods are chosen for each purpose, namely Laser Induced Fluorescence (LIF) imaging for mixture characterisation and direct visualisation of the chemiluminescence emitted during the combustion process.

VISUALISATION OF SPECIES DISTRIBUTION

Planar Laser Induced Fluorescence is used to image the species distribution in the combustion chamber. Several studies [7, 14] concluded that acetone is an appropriate fuel tracer because of its good resistance to thermal decomposition and the limited oxygen quenching of acetone fluorescence in CAI™ running conditions.

Depending on the thermodynamic conditions and the excitation wavelength, the fluorescence emission of acetone may exhibit a significant temperature dependence. Spatial fluctuations in the fluorescence signal may be attributed to composition and/or temperature variations in the mixture distribution. In the present application, the recycled burnt gases being significantly hotter than the air, the heterogeneities between fresh and burnt gases are somewhat amplified by the fluorescence dependency on temperature.

Excitation is realised with the fourth harmonic of a Nd-YAG laser (266 nm). A laser sheet formed with 90 mJ laser pulses is passed through the cylinder head side windows along the pentroof axis of the combustion chamber (see Figure 1). PLIF images are captured through the transparent piston crown with an intensified CCD camera (Princeton 12-bit Pentamax or 12-bit USS LaVision) and an 80 mm Nikkor lens.

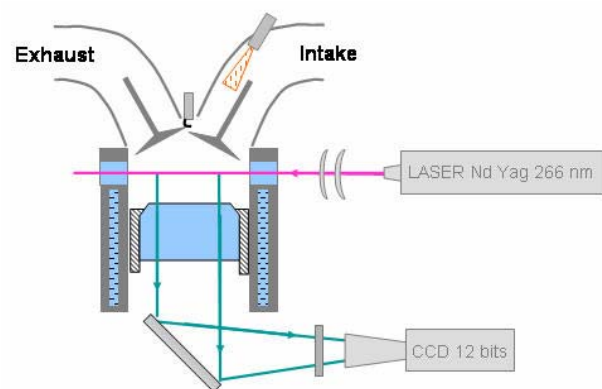


Figure 1 : Scheme of the experimental arrangement for LIF visualisation

To visualise the fuel distribution, acetone is mixed with the fuel and the fuel distribution is considered proportional to the acetone fluorescence.

To visualise the residual gas distribution, acetone is atomised and mixed with air 2 m upstream the cylinder head thanks to a Venturi type diffuser. The residual gas

distribution is consequently the negative of the fresh gas distribution, itself considered as proportional to the acetone fluorescence.

FUEL FOR LIF IMAGING

PLIF imaging requires a non-fluorescent fuel to avoid fluorescence spectral interference, which prevents from using commercial RON 95 fuel. Because of its strong resistance to auto-ignition, iso-octane, which is the most common substitute for gasoline, cannot be used in the present study. A series of Primary Reference Fuels (PRF) have been tested in the NVO configuration to determine the most relevant one based on the comparison of the mean in-cylinder pressure trace with that produced by the commercial RON 95 gasoline. As depicted in Figure 2, the most suitable PRF is the PRF 65, which confirms that the octane number is not an appropriate indicator of the fuel auto-ignition ability in CAI™ operating conditions [15-17].

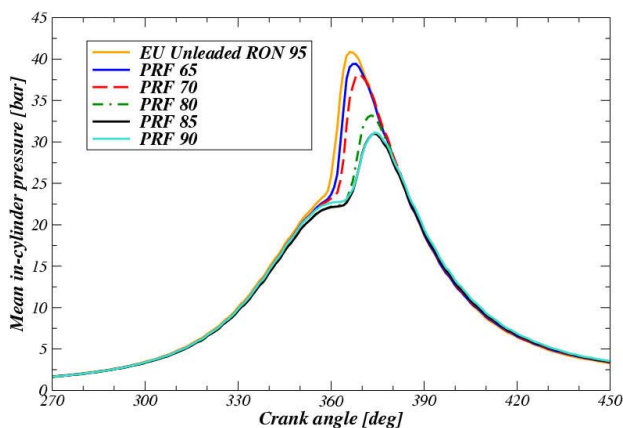


Figure 2 : Comparison of pressure traces for Primary Reference Fuels and commercial RON 95 gasoline

To retain consistency throughout the entire study, all the experimental and numerical results presented in the following are obtained with PRF 65 as fuel.

COMBUSTION VISUALISATION

The temporal and spatial development of the CAI™ combustion process is monitored by direct observation of the naturally emitted light. A 12-bit high speed intensified CCD camera (USS LaVision) and a 105 mm UV Nikkor lens are used to image the chemiluminescence emission from the hot reacting gases. In [7], Thirouard et al. demonstrated that the chemiluminescence intensity is approximately proportional to the local reaction rate. Consequently, the reaction rates obtained through the numerical analysis can be compared to the chemiluminescence imaging. Because of the observation set-up (light collection through the transparent piston crown), the observed chemiluminescence is the integration of the emitted light intensity along the chamber height. The same type of integration is performed for the computed reaction rates in order to provide relevant comparison data.

COMPUTATIONAL FLUID DYNAMICS TOOLS

The main CFD tool used in the present study is a 3D CFD code. Nevertheless, a 1D CFD code is also used to simulate the entire test bed in order to provide the relevant initial and boundary conditions and to avoid the need for multicycle calculations. These tools are commercial tools developed at IFP and integrated in the AMESim platform [18]. They are shortly described below.

THE 1D CFD CODE AND ITS ROLE

The IFP-ENGINE library is a 1D CFD code dedicated to the simulation of engine systems. A variety of sub-models representative of the most relevant engine components are available such as pipes, injectors, cylinder heads, combustion chambers, turbochargers... With these, a sketch describing in detail the test bed is created (see Figure 3) in order to define the initial and boundary conditions for the 3D CFD calculations.

The goal is to dispose of sufficiently accurate initial conditions to avoid a multicycle calculation with the 3D CFD code. Replacing the multicycle 3D CFD calculation by a multicycle 1D CFD calculation followed by a unique cycle calculation with 3D CFD is really efficient to save computational time if the accuracy of the 1D CFD calculation results is carefully checked.

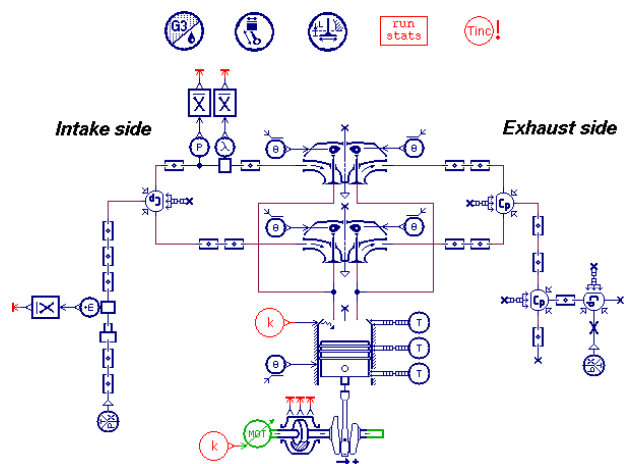


Figure 3 : Single-cylinder engine sketch built with IFP-ENGINE

This procedure is valid for all types of engine operation strategies but is especially efficient with CAI™ combustion mode as the auto-ignition process is extremely sensitive to both the in-cylinder species concentrations and the in-cylinder thermodynamic conditions. Consequently, for such engine conditions a multicycle calculation either with 3D CFD or with 1D CFD is absolutely necessary to claim to reach a certain level of predictivity. Multicycle calculations with 3D CFD alone have already been demonstrated [13] and its accuracy has been proved. The combination of 1D and 3D CFD calculations is developing [19-20] but its use for CAI™ combustion mode simulation is still limited [4].

THE 3D CFD CODE

IFP-C3D [21] is a 3D CFD parallel code solving the Navier-Stokes equations using an ALE-extended (Arbitrary Lagrangian Eulerian) finite volume method on unstructured and conformal hexahedral meshes. For turbulent combustion, the 3-Zone Extended Coherent Flame Model (ECFM3Z) is used [22]. The auto-ignition prediction and the influence of chemistry on reaction rates are provided by the TKI auto-ignition model [23].

The ECFM-3Z combustion model

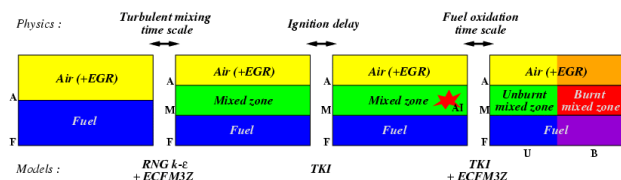


Figure 4 : Description of the ECFM3Z model and its interaction with other models for each mesh cell

The principle of the ECFM3Z model, which blends the ECFM and CFM3Z approaches into a unique combustion model, is detailed in Figure 4 for compression ignition operating conditions. A more complete description is available in [22].

In order to correctly represent the local mixing process, the ECFM3Z model includes a description of the local stratification by considering three regions of mixing: one region contains only pure fuel (region F), the second region contains fresh air plus any additional EGR (region A) and the third region contains a mixture of the latter two (region M). During injection, the evaporation of the spray droplets leads to a source of mass in region F. The fuel and air (+EGR) from regions F and A mix with the help of turbulence to form region M. The mixture in region M may then auto-ignite after a delay depending on the local thermodynamic conditions. When the auto-ignition delay is reached, combustion in region M starts, thereby dividing it into two sub-zones: a fresh (or unburned) gas zone and a burnt gas zone. As the mixed fresh gases in region M are oxidised following auto-ignition, the formed hot products are added to the burnt gas side of the mixed region.

The TKI auto-ignition model

To numerically study the CAI™ combustion mode, an auto-ignition model is needed which has to provide the auto-ignition delay and an accurate description of the subsequent chemistry reactions. Indeed, a precise knowledge of the reaction rates is needed to correctly predict the pressure rise during combustion since this is a limiting factor for the higher loads in the CAI™ operating range. The latest version of the TKI auto-ignition model [23] meets all these requirements.

The Tabulated Kinetics of Ignition (TKI) auto-ignition model [23] relies on tabulated auto-ignition variables

deduced from detailed chemistry calculations performed with the Senkin code, which is part of the Chemkin package. The detailed mechanism has been generated by the Département de Chimie Physique des Réactions (Nancy, CNRS) for mixtures of n-heptane and iso-octane [24]. This mechanism contains 1992 reactions between 416 species. The 3D model variables are calculated once and for all for 68400 different initial thermodynamic conditions and are stored in look-up tables. The fresh (or unburned) gas quantities that are used as input parameters of the auto-ignition lookup tables are the temperature, the pressure, the Fuel/Air equivalence ratio, the rate of dilution and the octane number.

Figure 5 shows an example of the temperature profile predicted by the TKI model and a comparison with the temperature profile computed with the detailed chemistry mechanisms. In this example, the thermodynamic conditions lead to a first part of the combustion controlled by the cool flame. To represent this phenomenon, two auto-ignition variables are defined: the auto-ignition delay τ and the portion C_1 of fuel consumed by the cool flame. Then, main ignition is modelled based on reaction rates ω_{c_k} tabulated as a function of the progress variable. When the thermodynamic conditions lead to the absence of the cool flame effect, C_1 is simply zero and the combustion is entirely described with reaction rates.

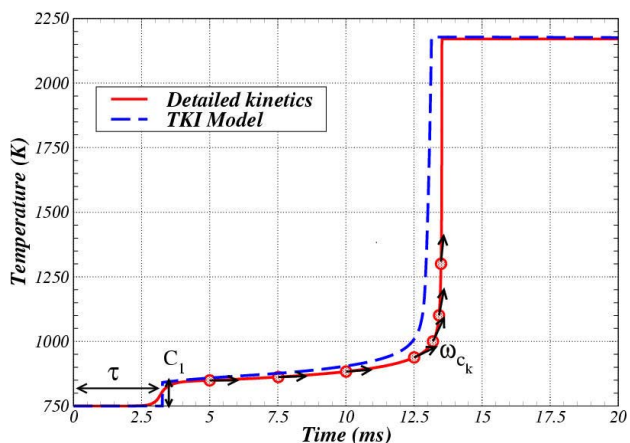


Figure 5 : Comparison of temperature evolution from detailed kinetics and the TKI model for a constant volume reactor

As in an internal combustion engine thermodynamic conditions evolve with the piston motion, all model variables (and among them the delay) extracted from the database vary on a per cell basis. To take this evolution into account, an intermediate species is considered for the in-cell auto-ignition delay whose concentration has a growth rate proportional to the local fuel tracer concentration and to the relevant auto-ignition delay. The actual auto-ignition occurs when the intermediate species concentration reaches that of the fuel tracer.

ENGINE CHARACTERISTICS

The modelled engine is a single-cylinder optical engine derived from a series Renault F7P engine. As mentioned in Table 1, its compression ratio has been increased to obtain a wider CAI™ operating range while maintaining its ability to be operated in conventional spark ignition mode for the higher loads without excessive knock propensity.

Table 1 : Main engine characteristics

Engine Type	Single-cylinder optical engine based on RENAULT F7P
Bore [mm]	82
Stroke [mm]	83.5
Compression ratio	12.3:1
Connecting Rod Length [mm]	144.0

VALVE LIFT STRATEGIES

The CAI™ combustion mode relies on the availability of a large rate of trapped burnt gases. These may basically be obtained with two different valve lift strategies:

- the Negative Valve Overlap (NVO) strategy, which aims to trap the needed amount of burnt gases based on a truncated exhaust stroke;
- the Exhaust Gas Re-Breathing (EGRB) strategy, which is based on a conventional exhaust stroke, followed by a re-aspiration of the needed amount of burnt gases during the intake stroke thanks to a re-opening of the exhaust valves.

These two strategies have different operating ranges because of their impact on mixture and thermodynamic conditions in the cylinder [8-9]. In the present study, they are compared from the mixture and the combustion points of view.

The valve lifts used in the present study are depicted on Figure 6. For the Negative Valve Overlap (NVO) strategy, all four engine valves open once in an engine cycle with low peak valve lift for both intake and exhaust. For the Exhaust Gas Re-Breathing (EGRB) strategy, only one intake and one exhaust valves open during an engine cycle and these are diametrically opposed to create a strong swirl motion in the cylinder. Furthermore, the exhaust valve lift has two opening phases, the first one being the conventional exhaust stroke and the second one allowing to rebreathe a part of the previously exhausted burnt gases.

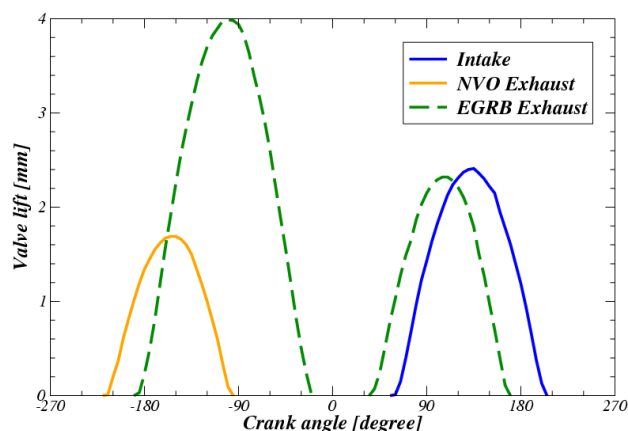


Figure 6 : Valve lift strategies

The NVO strategy is really efficient to trap burnt gases with the highest possible temperature. But during the NVO period, the trapped burnt gases are recompressed and re-expanded leading to a high in-cylinder temperature and consequently important heat losses. These heat losses are responsible for the existence of a non-negligible pumping work.

The EGRB strategy has therefore been designed to minimise these pumping losses by avoiding the recompression phase. With this strategy, the burnt gases are evacuated as in a conventional engine and then rebreathed during the intake stroke, simultaneously with the air. The pumping work is therefore largely reduced but the heat losses in the exhaust pipes cannot be avoided.

Table 2 : Operating conditions

	NVO	EGRB
Engine speed [rpm]	1200	1200
IMEP [bar]	2.9	4.8
Cylinder filling [-]	0.30	0.38
Air flow rate [kg/h]	5.70	7.27
Fuel mass [mg/st]	8.5	12.2
Fuel/Air eq. ratio [-]	0.83	0.95

The EGRB strategy can consequently limit the pumping losses with comparison to the NVO strategy but the burnt gas temperature is lower than that produced by the NVO strategy. As a consequence, the NVO strategy is the only one suitable for the lowest loads (where the burnt gas temperature is a critical parameter to sustain combustion) while the EGRB strategy allows higher loads

and better fuel economy at medium loads (in the CAI™ load range).

In the present study, for each valve lift strategy, a representative PFI operating point has been selected. Their operating conditions are summarised in Table 2.

MIXTURE FORMATION PROCESS

Thanks to the multicycle 1D CFD computations, there is no need to compute the entire engine cycle for any of the operating points. The 3D CFD computations are only performed for the mixture formation part of the cycle, the combustion process and the expansion stroke. For the NVO strategy, the calculation ranges from IVO to EVO. For the EGRB strategy, the calculation is started at exhaust valve re-opening and is ended at EVO.

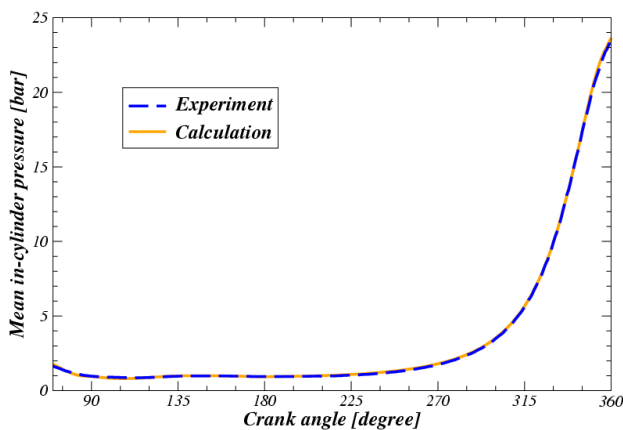


Figure 7 : Experimental and numerical pressure traces for the NVO strategy during mixture formation

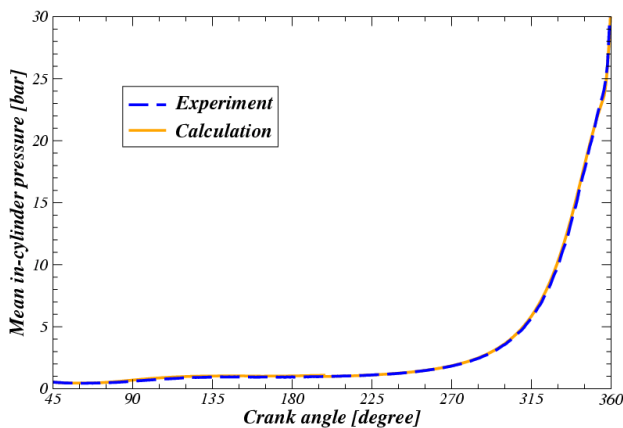


Figure 8 : Experimental and numerical pressure traces for the EGRB strategy during mixture formation

The mixture formation part of the cycle is validated based on the pressure traces (see Figure 7 and Figure 8) and the comparison of the experimental and numerical air flow rates (see Table 3) as well as the degree of mixture heterogeneity provided by the optical diagnostics and the CFD (see Figure 9 and Figure 10).

Table 3 : Mixture characteristics

		Experiment	Calculation
NVO	air flow rate [kg/h]	5.70	5.71
	burnt gas rate [%mas]	-	46.0
	inert gas rate [%vol]	-	39.6
EGRB	air flow rate [kg/h]	7.27	7.12
	burnt gas rate [%mas]	-	40.8
	inert gas rate [%vol]	-	40.2

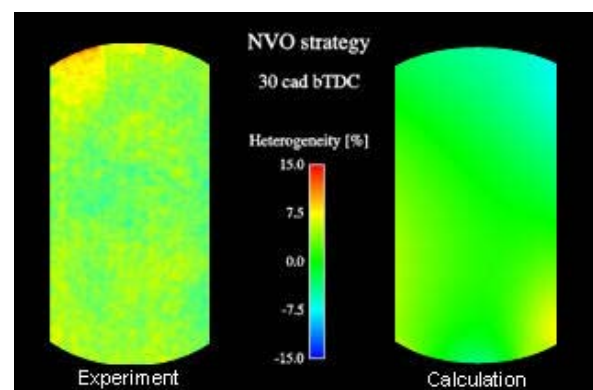


Figure 9 : Degree of mixture heterogeneity: experimental (left) and computed (right) dilution rate fields 30 cad bTDC for NVO strategy

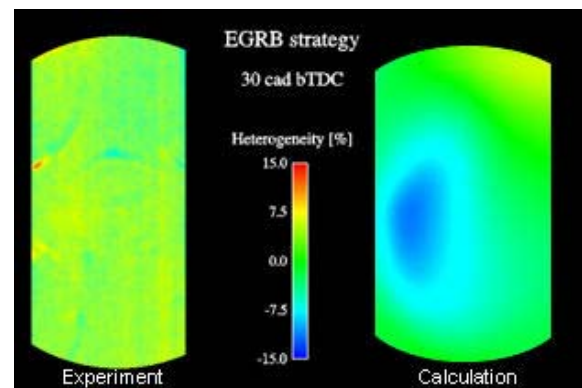


Figure 10 : Degree of mixture heterogeneity: experimental (left) and computed (right) dilution rate fields 30 cad bTDC for EGRB strategy

The agreement between experiment and calculation is good for the intake and compression strokes with small differences both for pressure evolutions and averaged air flow rates.

For the mixture heterogeneity characterisation, the comparison between optical diagnostics and CFD is