

CFD simulations using the TDAC method to model iso-octane combustion for a large range of ozone seeding and temperature conditions in a single cylinder HCCI engine

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1. Introduction

The HCCI engine presents several advantages compared to SI and CI engines: lower NO_x and PM emissions, and higher efficiency. Nevertheless, the control of the combustion process is still a challenge. One of the main parameters for ignition control is the initial temperature. Several options exist: exhaust gas trapping, compression ratio or external heating [1]. However, using the temperature as a control variable is generally difficult because of thermal inertia or unstable conditions [1].

More efficient strategies are based on dual fuel (reactivity controlled compression ignition) [2] or late injection (partially pre-mixed combustion) [3]. In these cases, ignition is mainly controlled by the fuel oxidation kinetics.

An alternative strategy is either the injection or in-cylinder production of oxidizing species such as nitric monoxide (NO) [4,5] or ozone (O₃) [6,7].

In this context, computational fluid dynamics (CFD) simulation is a very important tool to investigate these effects and to help the development of new control strategies. To accurately model fuel kinetics or predict the effect of a few ppm of active species, comprehensive chemical mechanisms are required. In particular, for HCCI engines, low temperature combustion and ignition may require hundreds to thousands of species according to the

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complexity of the fuel. There is generally a tradeoff between the size of the kinetic mechanism used and the complexity of the geometry investigated. In particular, heat transfer and crevices have an important impact on the onset of the combustion.

In a previous study, we showed that the Tabulation of Dynamic Adaptive Chemistry (TDAC) method can be used to predict the promoting effect of nitric monoxide on the auto-ignition of iso-octane [5]. That study used CFD simulations with a detailed mechanism of 1062 chemical species and 4494 elementary reactions on a mesh with around 20,000 cells. This promoting effect was significant above ten ppm of NO and well predicted by TDAC. In this paper, we are going a step further by analyzing the results obtained for ozone seeding where a significant effect is already observed with only one ppm [7]. Moreover, we also show that it is possible to investigate many case settings with CFD simulations while keeping a low computational cost.

Since only very small concentrations are needed, the long term objective is the production of these species on-board. Their concentrations could then be adjusted so that cycle-to-cycle control strategies are possible.

This article first describes the computational method. Then it presents the HCCI engine test bench with a detailed uncertainty analysis. Finally, it shows the validation of the TDAC method and it analyzes the effect of ozone seeding through simulation results.

2. Computational method

The following section briefly describes the settings of the simulations. More details are given in previous studies [8,9,5].

Simulations were carried out by using the Lib-ICE code [10], which is based on the OpenFOAM® technology [11]. Lib-ICE also includes the complete implementation of the TDAC technique.

TDAC consists of the coupling of a tabulation method and a mechanism reduction method [8]. The original implementation used the in situ adaptive tabulation technique [12] with the dynamic adaptive chemistry method [13].

The simulations cover the part of the cycle from -150 to 120 CAD. The initial conditions for temperature, pressure and chemical species are based on experimental measurements. The mesh is axisymmetric with $\sim 20,000$ cells at bottom dead center and includes a crevice region (see Fig. 1). We used the RNG $k-\varepsilon$ model to include the effect of turbulence [14], and a heat transfer model developed for engine simulations [15]. Boundary conditions were defined in previous studies.

A detailed kinetic scheme based on the mechanism of Curran et al. [16] coupled with the reactions involving ozone [17] has been used for the simulations presented in this paper. It includes 1063 chemical species and 4494 elementary reactions.

The mechanism reduction technique included in TDAC requires a search initiating set of species. Only the fuel, HO_2 and CO were specified as in previous studies [8,9,5]. Any other species is added to the mechanism through the strength of the link with these species. In the simulations below, O_3 was automatically included by the search algorithm in the first time-step. The link and effect of only 1 ppm of O_3 is therefore well captured by the method.

In previous studies, it was demonstrated that the TDAC methodology is approximately 1500 times faster than direct integration when applied to HCCI combustion simulations [5].

3. Experimental setup

We performed the experiments using a four-stroke diesel engine (PSA DW10) converted to single-cylinder HCCI operation. The engine was used to investigate the combustion of iso-octane

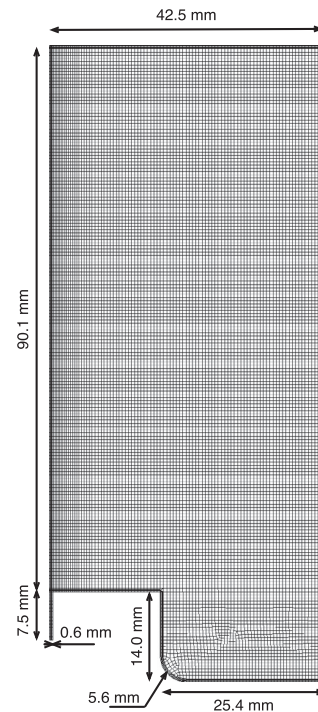


Fig. 1. The computational mesh is axisymmetric and counts $\sim 20,000$ cells at bottom dead center.

seeded with traces of ozone. The following subsections present the engine setup and the uncertainty analysis.

3.1. Engine settings

The engine settings have been presented in a previous study [7]. They are summarized in Table 1.

Equivalence ratio, inlet pressure and engine speed were kept constant at 0.3, 1.0 bar, and 1500 rpm, respectively. We have set the temperature measured at 10 cm before the inlet valve at six different levels: 100, 120, 140, 160, 180 and 200 °C. The concentration of O_3 obtained from a ANSEROS COM-AD-01 ozone generator was varied to keep the ignition timing near TDC. Ignition without ozone was only possible with an inlet temperature of 200 °C.

3.2. Uncertainty analysis

The pressure in the compression chamber was recorded for 100 consecutive cycles. This large number of recordings mitigates the impact of the variability of these cycles on the variance of the mean, which is an order of magnitude below the accuracy of the sensor. The overall uncertainty on the pressure measurement is below 2% of the measured value.

The heat release rate (HRR) is computed according to the pressure and the volume [18,19]. The uncertainty on the cumulative HRR is largely dominated by the accuracy of the pressure

Table 1
Engine characteristics.

Bore (mm)	85
Stroke (mm)	88
Connecting rod (mm)	145
Compression ratio	16 (Geometric) 15.5 (Effective)
Cylinder head	4 Valves

transducer and the crank angle encoder (measured with an accuracy of 0.1 CAD). For this engine setup, this uncertainty is below 5% of the total heat released. Yet when characterising the heat released in the negative temperature coefficient (NTC) region, it becomes significant. In this region, the uncertainty depends on the low temperature flame intensity, which decreases at higher temperature. The uncertainty is about 30% at 100 °C but rises up to 100% at 200 °C where the low temperature flame is barely observed. More details about the computation of the uncertainty are given in [20].

The uncertainty for the crank angle where $z\%$ of the heat has been released (CA_z) is determined by

$$U_{CA_z} = |\theta(Q_{z\%} + U_{Q_{z\%}}) - \theta_{Q_{z\%}}|,$$

where θ is the crank angle, $Q_{z\%}$ is $z\%$ of the total cumulative heat, and $U_{Q_{z\%}}$ is the uncertainty on the cumulative heat release rate mentioned hereinabove. The corresponding uncertainty on CA_{10} , CA_{50} and CA_{90} are similar and around 0.2 CAD. In addition to the precision of measurement, repeatability has also a strong impact on the uncertainty. In the results below, when ignition is late in the cycle (CA_{50} around 3 CAD ATDC), this uncertainty can go up to 1 CAD.

The uncertainty on the measurements of ozone is evaluated from the variance of repeated measurements and the error of the ozone analyzer. The uncertainty on the mean value is low due to the 40 measurements taken to determine this mean. The error of the ozone analyzer is ± 2 ppm (1% of the 200 ppm full scale output). Considering a constant distribution around the measured value for the error, the values reported below have an uncertainty of ± 1.5 ppm.

In addition to the accuracy of the mass flow rate controllers, two additional sources of uncertainty are related to the injection of O_3 and can affect the initial concentration of the species in the cylinder: the reactions involving O_3 (i.e. decomposition to O_2 and \dot{O} , and interactions with the fuel), and the catalytic conversion of O_3 at the walls of the inlet system.

The decomposition of O_3 into \dot{O} and O_2 and ultimately into O_2 depends on the temperature and the residence time from the injection in the plenum to the inlet port. The maximum temperature used is 200 °C. The average residence time is evaluated by taking the volume of the inlet piping and plenum and by dividing it by the volume flow rate. This leads to a conservative value around 4 s. The current setup is obviously not the design that would be used for the long term goal of cycle-to-cycle control. It is, however, a simplified setup that gives a very good accuracy on the ozone seeding.

To quantify the impact of the decomposition, we performed simulations of air seeded with ozone in a constant volume at 200 °C and 1.0 bar. The decomposition of ozone depends on the initial concentration. It ranges from a relative reduction of 5% when the initial value is 100 ppmv, to 0.01% when the initial value is 1 ppmv.

In presence of fuel, the decomposition of ozone is accelerated and its concentration significantly decreases. Table 2 shows a comparison between ozone measurements with and without fuel for

Table 2

The ozone concentration significantly decreases in presence of fuel for the same settings of the ozone generator.

	Measured value before inlet valve (ppm)
Air + ozone	18.8
Air + fuel	1.0
Air + fuel + ozone	11.6

the same settings of the ozone generator. Ozone measurements are based on UV absorption therefore the presence of fuel might modify the reading. However in this case it has a minor effect (1 ppm reading) on the measured value as shown in Table 2.

Even though ozone concentration significantly decreases before the engine inlet, the reactions are mainly due to the presence of fuel. Therefore, we considered that the equivalent effect of the initial ozone concentration is kept in the system albeit not completely in the form of O_3 .

To further test this hypothesis we have run a two-step 0D simulation. First, the inlet process is represented by a constant pressure vessel at 473 K and 1 bar during 4 s. Then the result of this simulation is used as the initial condition for a constant volume simulation at 1000 K and 30 bar which corresponds to the engine conditions at -10 CAD ATDC for an inlet temperature of 473 K. This two-step simulation where O_3 first decomposes in the admission is compared with the direct simulation of the constant volume vessel at 1000 K and 30 bar without the admission simulation. The difference of ignition timing is about 0.6 ms (see Fig. 2), which corresponds to 0.5 CAD for the chosen engine speed. This is considered as very small since this simulation does not take the delay provided by the compression stroke into account.

Finally, O_3 might also react with the walls. The decrease of ozone concentration due to reaction with stainless steel has been evaluated by Itoh et al. [21]. The effective lifetime of the ozone is in the order of tens of minutes which is significantly higher than the average residence time in the inlet system.

Accordingly, we considered that the O_3 concentration measured during the calibration with air is a good approximation of the initial concentration in the cylinder. This concentration was therefore used in the simulations below without any other species resulting from its decomposition.

The uncertainty on the inlet temperature measurement is around 2 K. However, many parameters affect the actual temperature in the cylinder at the beginning of the simulation: heat-transfer, mixing with residuals, gas dynamic effects and vaporization of directly injected liquid fuel [22]. Fuel is evaporated in an external fuel vaporizer, before the temperature measurement. Engine speed is kept constant among all experiments which keep the same gas dynamic effects in all cases. The initial temperatures are adjusted at each inlet temperature, which takes into account the different rate of heat transfer. At a same temperature level, the exhaust gas temperature was nearly constant, hence mixing with residuals is the same when ozone concentration varies.

To further improve the prediction of this model, a stratified temperature can be used as initial conditions [23]. This reduces the average temperature needed to meet a specific timing. However, no information is available on the profile nor on the amplitude of this stratification. Therefore, in the following simulations, only homogeneous initial conditions were considered.

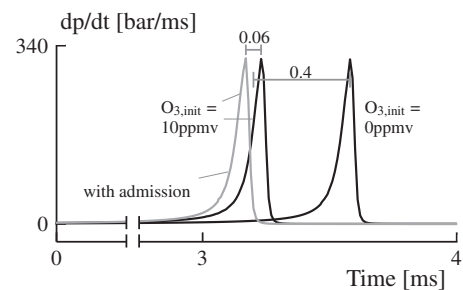


Fig. 2. The ignition delay predicted by the two-steps simulation (gray line) is slightly shorter when O_3 is included compared with the case where the constant volume simulation starts with the fresh gases (black lines).

4. Results and discussion

This section first presents the effect on ignition of seeding the air/iso-octane mixture with a few ppm of ozone. Then, it shows the combined effect of temperature and ozone on the onset of the combustion. Finally, it also describes the effect of ozone on the enhancement of the low temperature flame.

4.1. Effect of ozone on the ignition timing

The addition of a few ppm of O_3 in the initial iso-octane/air mixture significantly changes the ignition delay (see Fig. 3). As described above, the main role of O_3 is to decompose into \dot{O} , promoting in this way the production of the radical pool through reactions with the fuel. The TDAC method predicts very well the effect of a few ppm of O_3 and of the resulting radicals at very low concentration.

Moreover, Fig. 3 shows that, even though the ozone starts its decomposition in the inlet pipe, its main effect is kept in the system as described above.

Fig. 4 shows the average mass fraction in the simulation results of the main radicals OH and HO_2 with the seeding of 11 ppmv of O_3 . The concentration of HO_2 increases as the O_3 is consumed. This then leads to the main ignition which is accordingly sooner in the engine cycle:



Reactions of O_2 with the produced fuel radicals then lead to the accumulation of HO_2 due to its low reactivity (see Fig. 4)

The combustion timing, represented by the CA50, is very well predicted for different initial ozone concentrations (see Fig. 5). The sensitivity of the simulation results due to a 2.5 K variation of the inlet temperature is also included in Fig. 5.

In the experimental results, the combustion duration decreases when the ozone concentration increases, mainly due to the advance of ignition timing. Around 5 ppm there is a change of slope mainly because the effect of ozone on the combustion duration is reduced. In the simulations, the change of slope is well captured but there is some discrepancy for higher ozone concentration

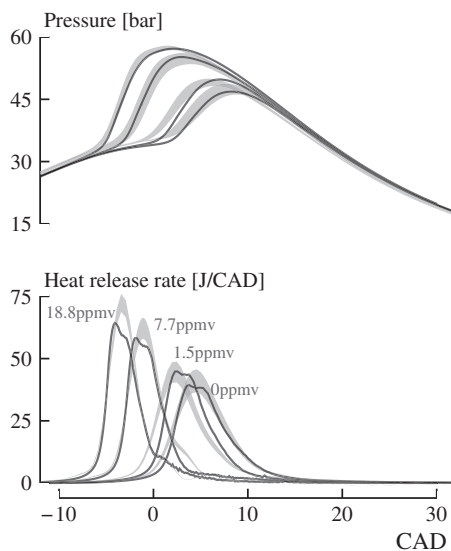


Fig. 3. Experimental (grey zones) and simulation results (black line) shows the significant effect of a few ppm of O_3 for the pressure (above) and the heat release rate (below).

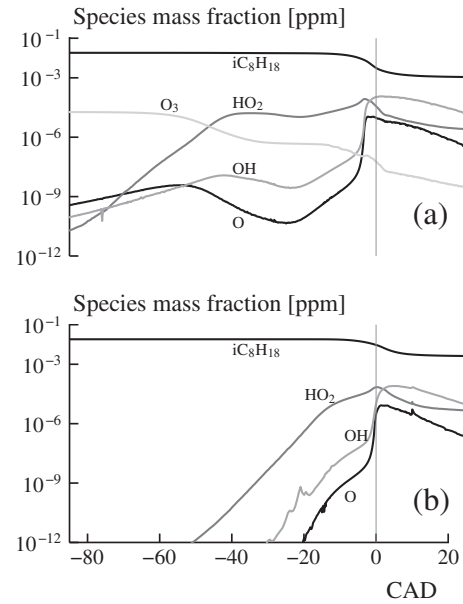


Fig. 4. Seeding the air/fuel mixture with O_3 (a) shifts the ignition timing compared to the case without O_3 (b).

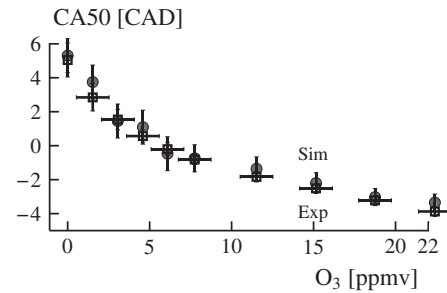


Fig. 5. CA50 decreases when the injection of O_3 increases. The combustion timing is well captured by the simulations (circles). The error bars for experiments (open squares) are due to uncertainty and repeatability while the bars for the simulations indicate the sensitivity due to a 2.5 K variation of the initial temperature.

(see Fig. 6). Since ignition timing, CA50 and pressure are well captured, this difference mainly comes from a lower predicted reactivity in the final part of the combustion. This can be due to uncertainty in the mechanism but also due to the inhomogeneity and the in-cylinder flow not completely taken into account.

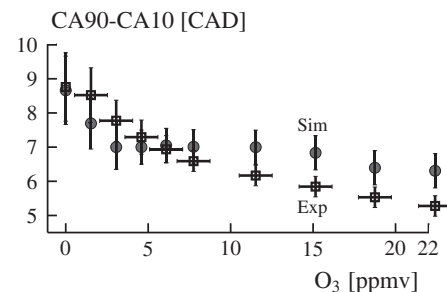


Fig. 6. The combustion duration (defined as CA90-CA10), decreases when the initial concentration of O_3 increases (experiments: squares). In the simulations (circles), it reaches a plateau around 7 CAD.

4.2. Combined effect of ozone and temperature

As mentioned above, the inlet temperature has a major impact on the onset of the combustion but is not a practical parameter for the cycle-to-cycle control of a HCCI engine. Since we have seen that the ozone can significantly modify the ignition delay, we present in this section the impact of both temperature and ozone and the link between both parameters.

The effect of ozone concentration difference on the ignition timing significantly changes according to the initial conditions. At high temperature, a small difference of ozone has a strong impact on the CA50, while the impact decreases at lower temperature. A temperature difference has however a similar impact on the combustion timing through the range of ozone concentrations tested (see Fig. 7).

As can be seen in Fig. 7, the effect of a 20 K difference on the CA50 is similar for different concentration of ozone and is around 3 CAD. When correcting the effect of temperature on the ignition timing, we can obtain CA50_{cor}:

$$CA50_{cor} = CA50 - (T_{ref} - T)\beta, \quad (3)$$

where T is the temperature, T_{ref} is the reference temperature (200 °C), and β is the effect of temperature on the CA50 (3.3 CAD per 20 K). The CA50_{cor} is shown in Fig. 8 and is in good agreement with the results from the simulations. CA50_{cor} decreases exponentially as the concentration of O₃ increases which indicates a saturation of the effect of O₃.

As already shown in Fig. 4, the decomposition of O₃ takes place well before the main combustion. This is also observed at different initial temperatures and ozone concentrations (see Fig. 9). The sensitivity of the ignition timing to the O₃ sub-mechanism is therefore not predominant.

4.3. Effect of the ozone on the low temperature flame

Modelling the low temperature flame generally requires a very detailed mechanism. Therefore, it is important to be able to include such a mechanism using the TDAC method. We further compare the simulation results with the experiments in this section.

Low temperature flame has been observed for iso-octane combustion in various experimental setups (jet stirred reactors [24,25], rapid compression machines [26], and shock tubes [27]). In the case of engine experiments, this is generally not observed because the required inlet temperature to ignite iso-octane leads to a temperature near TDC that is above the NTC region.

When injecting O₃, the production of the radical pool is promoted and this shifts the onset of the combustion earlier in the

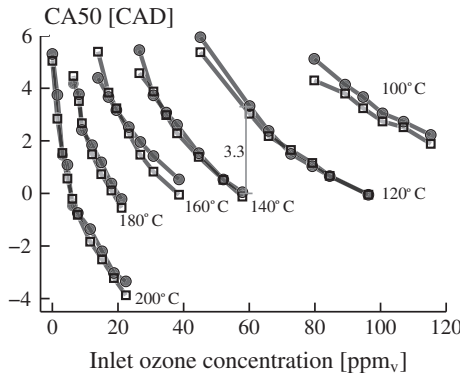


Fig. 7. The effect of ozone seeding on the CA50 depends on the initial temperature of the air/fuel mixture while the effect of a given difference of temperature is similar for different ozone seeding (open squares: experiments, circles: simulations).

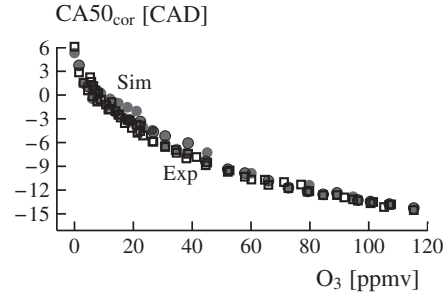


Fig. 8. The absolute effect of ozone (corrected for temperature) on CA50 decreases as the concentration increases (circles: simulations, squares: experiments).

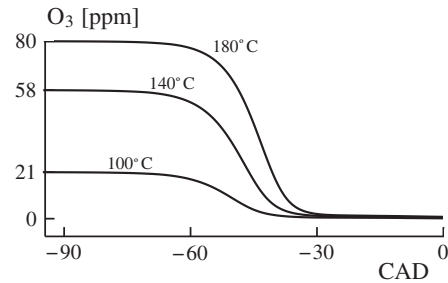


Fig. 9. The predicted ozone concentration decreases very early in the compression stroke (around 60 CAD BTDC) and is completely consumed at -30 CAD ATDC.

cycle. At lower inlet temperatures, the start of ignition thus falls in the NTC region. As can be seen from Fig. 10, the low temperature flame appears in the case of low initial temperature and high injection of O₃.

The ratio of the low temperature energy with the total fuel energy increases as the initial concentration of O₃ increases (see Fig. 11). As mentioned in Section 3.2, the uncertainty on the energy of the low temperature flame is very high. Therefore, the dataset for the inlet temperature of 200 °C was not added to Fig. 11. Even if there is a slight discrepancy with the experimental results, the simulation results fall in the error bars and predict the same trend.

The timing of the low temperature flame is defined as the maximum HRR observed in the NTC region. The simulation results have the same trends as the experimental results. The timing is mainly affected by temperature and to a lower extent by O₃. However the simulations are generally shifted 3–4 CAD sooner in the cycle (see Fig. 12). This might be due to a different temperature stratification or to some uncertainty in the kinetic mechanism for the NTC region.

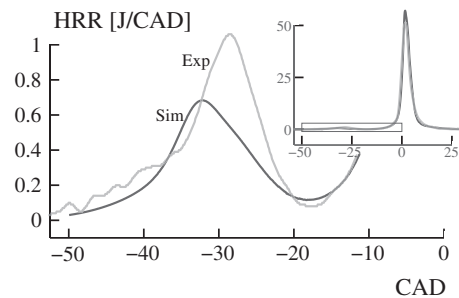


Fig. 10. Zoom in the low temperature region (the scale of y axis is around 1.5% of the maximum heat release during the complete cycle). At 100 °C and 115 ppmv initial O₃ concentration, the low temperature flame is observed and predicted by the simulation results.

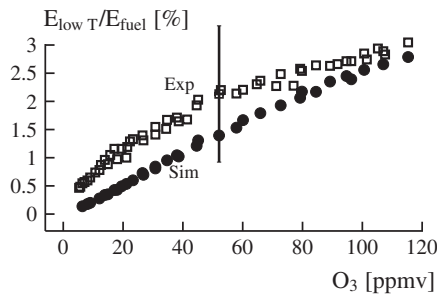


Fig. 11. The ratio between the energy of the low temperature flame and the total energy in the fuel increases as the O_3 seeding increases.

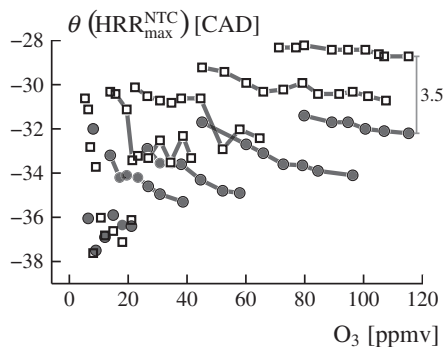


Fig. 12. The timing of the low temperature flame changes according to temperature and O_3 (experiments: open squares). The simulations (circles) predict the trends but are shifted 3–4 CAD sooner.

5. Conclusion

This paper demonstrates the significant effect of ozone seeding on the auto-ignition of iso-octane. A detailed analysis has been performed with the TDAC method which accurately predicts this effect.

Using a 20,000 cells mesh and including a mechanism of more than 1000 species, the TDAC method is able to predict the low temperature flame as well as the pressure gradient and the ignition timing. It also provides information about the combustion kinetics within the combustion chamber.

With the perspective of in situ production of ozone to control the HCCI engine on a cycle-to-cycle basis, but also the production of other active species such as NO or OH, advanced simulation tools are needed. This paper further shows that using CFD simulations to perform such an analysis does not involve extremely high computational time. Using the TDAC methodology, more than 50 case setups were simulated for the present work, each case requiring around 50 CPU hours.

Even though, the effect of ozone was well predicted, future studies will focus on the full cycle simulation and the inhomogeneity obtained when mixing with trapped EGR. As illustrated in other studies, this might lead to cycle-to-cycle variability [28]. Moreover, the reactive mixing of the in situ production of ozone will also represent a major step forward.

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