

Contribution to study the effect of exhaust gas recirculation EGR on HCCI combustion mode

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ABSTRACT

Nowadays, the exhaust emissions of vehicle become very dangerous. Low temperature combustion in automotive engines becomes more and more important and it is achieved by high rates of Exhaust Gas Recirculation (EGR). EGR gases are used to dilute the fuel/air mixture in the engine and to control ignition delay times. In this paper we will present a numerical study of the impact of various additives on the oxidation of a typical automotive surrogate fuel blend, i.e. n-heptane/toluene mixture. It examines the impact of EGR compounds on the operating parameters of homogeneous charge compression ignition (HCCI) engine combustion -fueled by a mixture of heptane and toluene- and on the formation of emissions pollutant and how to reduce it. We used the CHEMKIN software and the combined chemical kinetics mechanism of the heptane and toluene to determine the exhausts gases composition. The numerical simulation is based on the code PSR (perfectly-Stirred Reactor). The influence of various additives, namely nitric oxide (NO) and ethylene (C₂H₄) on the oxidation of n-heptane/toluene blend was studied with a different concentrations of NO and C₂H₄. First, the NO addition guided to an inhibition, more or less important with added quantities, of cool flame, but an important promotion of main combustion. Second, C₂H₄ had no impact on the cool flame ignition, but promoted the main combustion. Indeed, some components of the EGR gas species had a very significant effect on initiation of combustion, which gives a general idea about the control of combustion in HCCI mode.

Keywords: Combustion, Pollution, Kinetics mechanism, EGR, HCCI, Nitrogen oxides.

1. INTRODUCTION

Internal combustion engines are the primary power horses in the automotive industries. Engines develop power by consuming a huge amount of fuel by combustion, and emit harmful exhaust emissions such as unburned hydrocarbon (HC), carbon monoxide (CO), carbon dioxide (CO₂), oxides of nitrogen (NO_x), and particulate matter (PM) [1,2]. To better respect the exhaust emission regulations, new Low Temperature Combustion (LTC) processes such as HCCI engine (Homogeneous Charge Compression Ignition) are currently studied. HCCI process is based on the auto-ignition of a highly diluted air/fuel mixture. The ignition occurs at several locations in the whole combustion chamber. It can reduce significantly NO_x and particulate exhaust emissions.

The HCCI mode is known for longer, and these applications are more difficult until now. Onishi presented homogeneous mode in 1979 and he applied on two stroke engine [3]. The application on four-stroke engine is made by Najt in 1983[4].

The HCCI engine has a high efficiency like the efficiency of a diesel engine but with a low formation of NO_x and a little formation of particulate emissions [5].

Maurya investigated the effects of intake air temperature and air/fuel ratio on the combustion and emission characteristics of HCCI combustion in a four stroke diesel engine fueled with ethanol, methanol and gasoline. The test results showed that the in-cylinder peak pressure increased with the increase of intake air temperature. They have also concluded that CO and HC emissions decreased but NO_x emissions slightly increased, with the increase of intake air temperature with gasoline fuel [6].

The simultaneous combustion of gasoline and natural gas, called Double Fuel (DF) [7] combustion, with the Homogeneous Charge Compression Ignition has a strong reduction of pollutant emissions were found in comparison to SI operation [8], above all in terms of NO_x, which was reduced by tow order of magnitude [7].

The major problem of HCCI engine is the control of start ignition and burning rate. The SI combustion is controlled by

the start of sparks and the CI combustion is controlled by the injection time, but in the HCCI engine there isn't a mechanism to control the combustion timing [9].

Controlling of HCCI combustion is very difficult, but there are possibilities to control from the temperature, pressure, chemical composition of the mixture and thus by the use of exhaust gas recirculation.

The introduction of fuel into the combustion chamber of an HCCI engine occurs very early. This leads to a relative homogeneity of the mixture between the fuel and the oxidant at the time of combustion and therefore to a substantially pre mixed combustion. This type of combustion results in a significant reduction of particulate matter and NOx. It is mainly controlled by chemical kinetics [10, 11, and 12].

NOx emission is reduced greatly with low level of EGR than that of without EGR, but smoke opacity emission increases. NOx emission and smoke emission are limited below 120 ppm which is thought to achieve low NOx and smoke emission combustion [13].

Several studies show that there is a progress of the combustion during the addition of NOx [14, 15, and 16].

Amneus had shown that there are no flame zones in HCCI mode [17]. He therefore followed that the formation of NOx is low. This result is justified by Christensen and Johansson [10].

Moreac had shown experimentally the effect of CO (carbon monoxide) on the oxidation of hydrocarbons such as methanol, n-heptanes, iso-octane and toluene [18].

The addition of small amounts of NO (nitric oxide) has an effect of accelerating the oxidation of hydrocarbons such as heptanes (Dubreuil and al.2006, Moreac and al. 2003 and Glaude and al.2005,) [15, 118, and 19].

Increasing EGR dilutes the intake charge and reduces the amount of oxygen. This dilution also decreases combustion temperature and leads to incomplete HCCI combustion and therefore increases CO emission and the amount of unburned fuel thus (HC emission) [20].

The presence of NO lowers the overall fuel reactivity at low temperatures and increases it at high temperatures. Therefore, the content of recycled NO might impact strongly the ignition delay in an HCCI-engine. The addition of NO reduces considerably the formation of ethylene, ethane, CO and H₂ above 900K [21].

Lower NOx emission is observed for all the HCCI modes of operation as compared to that of the conventional mode with different fuel. This study shows that the CO₂ emission from the HCCI mode is lower than that of the conventional mode [22].

Two experimental setups were used: HCCI engine and jet-stirred reactor (JSR) used to study the influence of EGR on the fuel oxidation, especially the effects of NO and ethylene. NO and ethylene were selected because NO is known for its high reactivity and ethylene has a high concentration in the EGR gases. A complex impact of NO and little influence of C₂H₄ on the fuel oxidation kinetics was observed. For the fuel oxidation, a considerable inhibition at low temperatures and a significant promotion at high temperatures were observed [23].

EGR has been investigated in many previous works to reduce the pressure gradient and control combustion initiation at appropriate period [24, 25].

Dubreuil and Moréac had studied the importance of the impact of NO on the oxidation of hydrocarbons and thy result. Generally, the presence of NO lowers the overall fuel

reactivity at low temperatures and increases it at high temperatures [15, 18].

The subject of this work is in a first step to examine the impact of EGR compounds on the operating parameters of HCCI engine, for in a second step to see the influence of various additives (NO and C₂H₄) on the oxidation of heptanes/toluene mixture.

2. THE CALCULATION TOOLS

2.1 Software Chemkin

The modeling allows understanding the fuel combustion chemistry, reaction mechanism and treats pollutant emissions from an internal combustion type HCCI engine. It also allows knowing the validation of the experimental results conducted and to limit experiences which are generally very expensive.

We used the package "CHEMKIN" [26, 27] to model the HCCI combustion. In doing this, the modeling is done by computer codes, such as computes code which called HCCI and auto-stirred reactor. The latter was achieved through the PSR program (Perfect Stirred Reactor) [28] which contained in the library of CHEMKIN software. This software allows to interpret the reaction mechanism developed from reaction mechanism existed in the literature which is formed of two files. The first file which called (chem.inp), we introduce all chemical reactions. The second one file (therm.dat) contains thermodynamic data for all species declared in the reaction mechanism.

The CHEMKIN interpreter reads these two files and checks the atomic scale chemical reactions. After a calculation which is done by the software, a binary link file is generated.

PSR and HCCI calculation codes solve the conservation equations (the conservation of mass and conservation of energy). This application of CHEMKIN will therefore use binary file generated by the interpreter to create the output text files containing the modeling results requested by the user (mole fractions, speed of consumption, formation rate and sensitivity analysis).

The following diagram (FIG.1) represents the necessary elements to use the CHEMKIN code and presents the links between files.

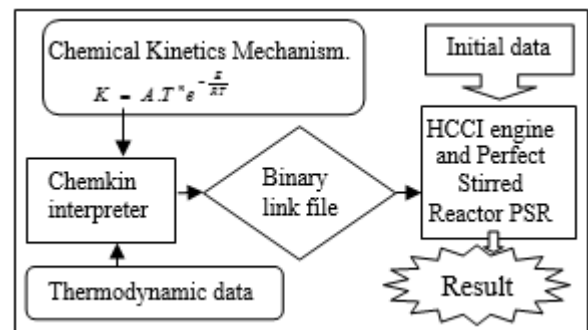


Figure 1. Schematic represents the structure of Chemkin software

2.2 The calculation code HCCI

The HCCI combustion mode is a new combustion process of the internal combustion engine which uses to reduce

pollutant emissions and to save fuel consumption. By using the CHEMKIN software and computer code HCCI, we can study the effect of certain species resulting of exhaust gas on the combustion process and more accurately on the pressure and temperature in the engine cylinder.

2.3 The computer code PSR (Perfect Stirred Reactor)

The computer code PSR solves the conservation of mass and energy equations. It helps us to study the impact of certain species of exhaust gas on fuel oxidation and on the formation of pollutants. The reactor is characterized by a volume V , a time of passage τ , a mass flow \dot{m} and a mass fraction Y_k . The mass flow rate is considered as constant. The transit time τ is written as follows.

$$\tau = \rho \left(\frac{V}{\dot{m}} \right) \quad (1)$$

$$\rho = \frac{P\bar{M}}{RT} \quad (2)$$

with:

T : temperature [K].

R : ideal gas constant [cal.K-1.mol-1].

M : molecular weight [g.mol-1].

ρ : density [g.cm-3].

The conservation of mass is written as follows:

$$\dot{m}(Y_{k,o} - Y_{k,i}) - \omega_k M_k V = 0 \quad (3)$$

Conservation of energy is expressed by:

$$\dot{m} \sum_{k=1}^k (Y_{k,o} h_{k,o} - Y_{k,i} h_{k,i}) + Q = 0 \quad (4)$$

with:

$Y_{k,i}$: Mass fraction of k species at the input of the PSR.

$Y_{k,o}$: Mass fraction of k species at the output of the PSR.

ω_k : Net production rate of the k species.

M_k : Molar mass of the k species.

Q : Thermal loss of PSR.

$h_{k,i}$: Specific enthalpy of k species at the input of the PSR.

$h_{k,o}$: Specific enthalpy of k species at the output of the PSR.

2.4 Equivalence of reactor-engine results

We can realize the simulation using two processing tools (the perfect stirred reactor and the HCCI engine) and it is possible to make comparison of interpretation of the results obtained from the two numerical codes. The following table describes comparison existed in the literature [29].

Table 1. The equivalence of the results obtained from tests on PSR and HCCI engine [29]

Results in PSR reactor	↔	HCCI engine results
Promotion of the hydrocarbon oxidation at low temperature	↔	Decreasing the initiation period of the Cold Flame
Inhibition of hydro-carbons oxidation at low temperature	↔	Increasing the initiation period of the Cold Flame
Promoting the hydro-carbons oxidation at high temperature	↔	Decreasing the degree of initiation main combustion period
Inhibition of the hydrocarbons oxidation at high temperature	↔	increase the period of initiation for the main combustion

3. RESULTS AND DISCUSSIONS

3.1 HCCI engine

The following results are obtained from the numerical simulation and from use of HCCI computer code existed in the CHEMKIN software. In this case, we used different concentrations of NO (50,100 and 200ppm) to see its effect on the initiation and conduct of the HCCI combustion.

The following table summarizes the engine parameters used and thus the initial conditions of temperature and pressure.

Table 2. Parameters and initial conditions used in our HCCI engine

Parameter	Setting
Compression ratio	15
Engine cylinder displacement volume	416 cm ³
Diameter of piston	78,3 mm
Stroke	86,4 mm
Connecting road length	158 mm
initial Pressure	3 bar
initial Temperature	423 k°

3.1.1 Influence of the addition of the NO on the combustion in HCCI mode

In Fig.2, we represented the pressure and the temperature vs. degree crankshaft for different added of NO (50,100 and 200 ppm). For this operating conditions of HCCI engine and the three NO mole fractions (Fig.2), NO led to decrease the burning time by little degrees (CAD) at the Low-Temperature region. However, the impact on the burning time depends on the added quantities of NO. In reality, the addition of 50 and 100 ppm led an important increase of the burning time, but the addition of 200 ppm of NO did not modify the delay times (see Fig.2).

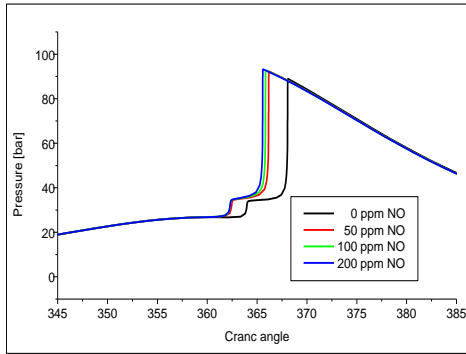
This inhibition of the cool flame could be explained by reactions (R1-R3) and especially the reaction (R3) [15], with R° representing all kinds of organic radicals issued from hydrocarbon oxidation. At high temperature a new reaction could be competitive, and could promote hydrocarbon oxidation by the OH formation (reaction R4).



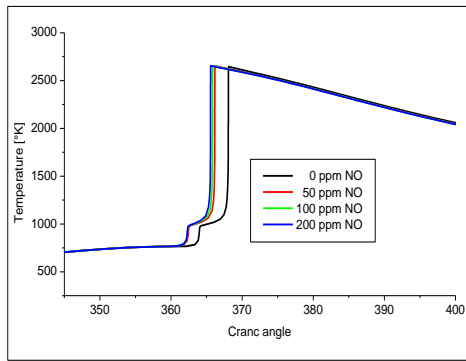


Therefore, NO addition led to an inhibition of the cool flame at low quantities, and to a promotion of the main flame. This addition led to a better combustion with lower concentrations.

The addition of NO has a very important effect on the initiation and period of the HCCI combustion and we notice that small concentrations of nitric oxide can be changing pre-ignition oxidation.



(a) Pressure



(b) Temperature

Figure 2. Impact of NO addition on the process and the initiation of combustion

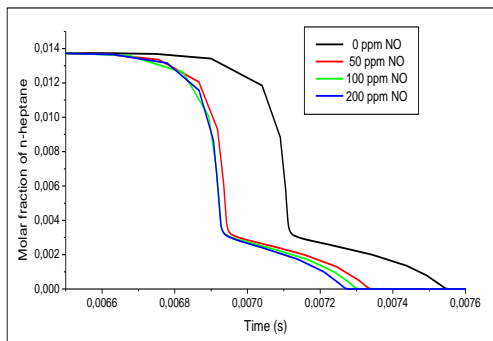


Figure 3. Impact of NO addition on the process and the initiation of combustion

3.1.2 Influence of the addition of C₂H₄ in the HCCI combustion mode

The following figure shows the consumption of the fuel (n-heptane) as function of the time for different addition of ethylene (C₂H₄) (0, 200, 400 and 2000 ppm).

We notice that the added ethylene generates a slightly late inflammation and a little fuel consumption (n-heptane). Indeed, there was no impact on the cool flame ignition, but the NTC domain was shorter, leading to a promotion of the high temperature flame. This result shows that the actual chemical effect of ethylene is low.

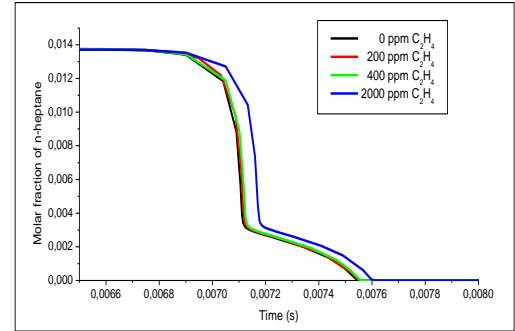
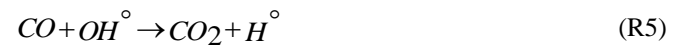


Figure 4. Impact of C₂H₄ addition on the course and the initiation of combustion

3.1.3 Influence of the addition of NO on the formation of CO and HC

The figure below illustrates the formation of CO discharged to the exhaust of the engine for the added NO, and it shows that the increase of added NO causes a reduction of a CO production at the end of combustion. CO emissions decreased with the increase of combustion temperature (higher gas temperature accelerates CO oxidation reaction, which promotes the conversion reaction from CO to CO₂ via reaction R5), and HC emissions decreased with the increase of mole fraction of n-heptane (lean mixture). This decrease is due to the advance of initiation and also the decrease of the ignition.



We know that the delay is longer, the peak temperature is low, and thus an increase in the formation of HC and CO [30 and 31]. Therefore the presence of NO accompanies a decrease the formation of HC and CO.

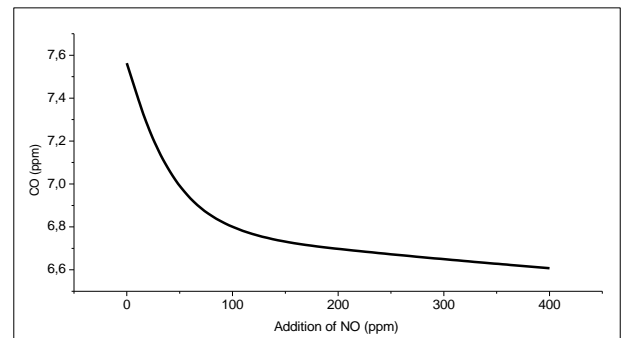


Figure 5. Impact of NO addition on the formation of CO

3.2 PSR operating conditions

We use the PSR calculation code to see the impact of certain species of exhaust gas on the fuel oxidation (heptane). Oxidation kinetics of heptanes were studied under fuel lean conditions ($\phi=0.75$), at 10 bars and for a mean residence time of 0.7s. A wide temperature range, from 560 to 1160 K, was investigated, including cool-flame, NTC effect and high temperature regimes.

3.2.1 Influence of added NO

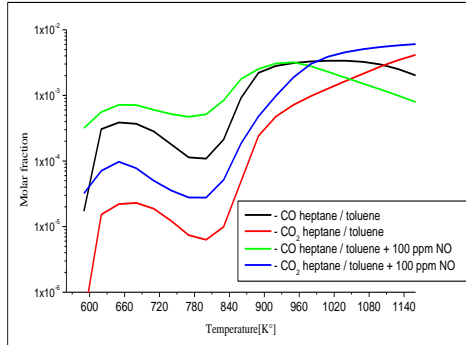


Figure 6. Simulated concentrations of CO and CO₂ (Impact of NO on n-heptane/toluene oxidation)

The concentration profiles of the fuel, heptane, are shown in Fig.7, the concentration profiles of combustion product (CO₂) and intermediate (CO) are indicators in Fig.6.

The oxidation of heptane could be divided into three domains:

-560- 650 K: Low temperature range where increasing temperature leads an increased reactivity.

-650-800 K: the NTC domain where increasing temperature leads decreased reactivity.

-Above 800 K: High temperature range where increasing temperature leads an increased reactivity.

The addition of NO inhibits the fuel oxidation, reduces the NTC effect at low temperature and it accelerates the heptane oxidation at high temperature (Fig.6 and Fig.7). This inhibition of heptane oxidation at low temperature is noticeable through the decrease in the fuel consumption (Fig.7). Therefore, the fuel conversion is delayed and this leads to an inhibition in the production of combustion intermediate (CO) and product (CO₂) (Fig.6).

NO also influences fuel oxidation in the NTC temperature range. The reduction of the NTC importance is probably caused by the conversion of HO₂ into OH via:



At high temperature the oxidation is promoted by NO, where the production of CO₂ is high with NO than in the base case (no addition of NO). Reaction (R6) and reaction (R7) becoming important at high temperatures could explain the increasing of reactivity [29].

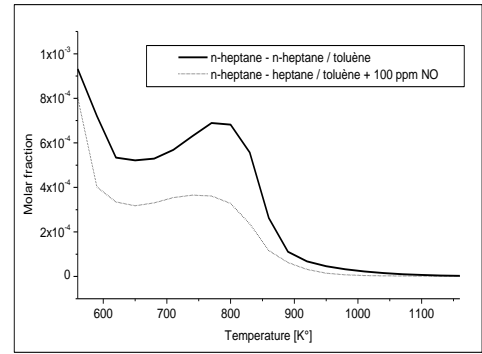


Figure 7. Simulated mole fractions for n-heptanes/toluene oxidation (Impact of NO on n-heptane/toluene oxidation)

3.2.2 Influence of the addition of C₂H₄

The unburned hydrocarbons HC are numerous in the EGR gas. The study of the impact of its species on the combustion is very important.

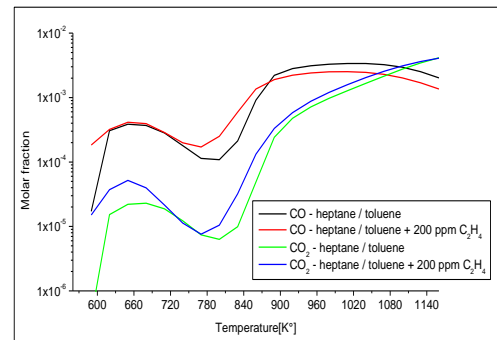


Figure 8. Simulated concentrations of CO and CO₂ (Impact of the addition of 200ppm C₂H₄)

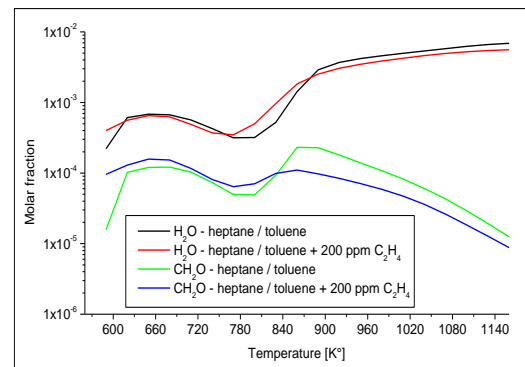


Figure 9. Simulated concentrations of H₂O and CH₂O (Impact of the addition of 200ppm C₂H₄)

Figure 8 and 9 show the influence of the addition of 200ppm of C₂H₄ (ethylene) on the formation of (CO and CO₂) and (CH₂O and H₂O), respectively. With the addition of ethylene, all the concentration plots for CO, CO₂ and CH₂O to allow comparison with to base case. The addition of C₂H₄ slightly reduces the importance of NTC region. This can be also seen from the higher concentrations of combustion products and intermediate products when ethylene is added (Fig.8 and Fig.9).

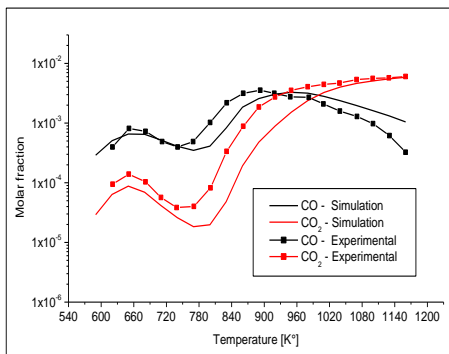
Note that the presence of C_2H_4 acts very low in the production of CO , CO_2 and H_2O in the field of NTC temperature which results in a decrease in responsiveness.

3.3 Comparison of results

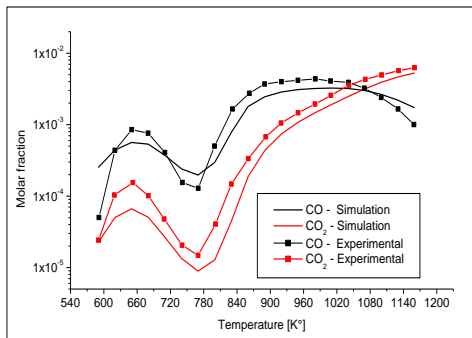
We chose results which obtained by the simulation and compare them with the experimental results performed under the same conditions.

3.3.1 The addition of NO

It is possible to see from figure 10 and 11 that the formation of combustion products (CO_2 and H_2O) and intermediate particulate (CO) model is in a good agreement with the experimental data of [29], although we see some differences but it are small.



(a) Addition of 100ppm NO



(b) No addition of NO.

Figure 10. Impact of the addition of NO on the formation of CO and CO_2 : simulation and experimental results (experimental result [29]).

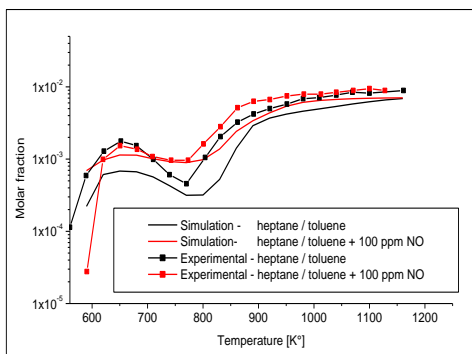


Figure 11. Impact of the addition of 100ppm NO on the formation of H_2O : simulation and experimental results (experimental result [29]).

It is possible to see from figure 10 and 11 that the formation of combustion products (CO_2 and H_2O) and intermediate particulate (CO), our simulation is in a good agreement with the experimental data, although we see some differences but it are small.

3.3.2 The addition of C_2H_4

The Comparison of numerical simulation and experimental results of [29] are shown in Figure 12 and 13. The comparison results show a good agreement between simulations and experiments (see Fig.12). The good agreement between the measured and calculated results for this study gives confidence in the simulation predictions, and suggests that the simulation can be used for parametric investigations.

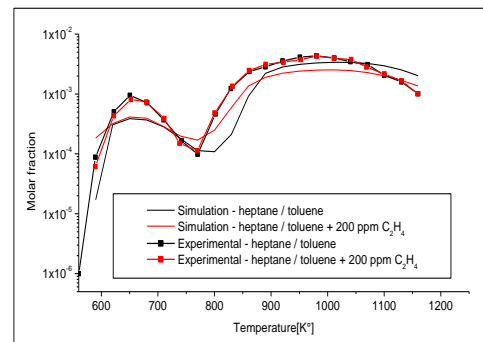


Figure 12. Impact of the addition of C_2H_4 on the formation of CO_2 : simulation and experimental results (experimental result [29]).

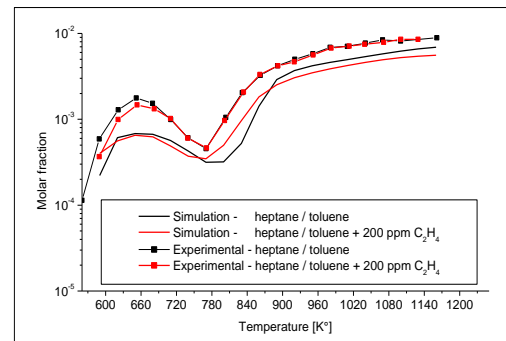


Figure 13. Impact of the addition of C_2H_4 on the formation of H_2O : simulation and experimental results (experimental result [29]).

4. CONCLUSION

We studied the effect of certain species of exhaust gas on the progress of combustion in HCCI engine and so on reducing pollutant emissions rejected by this type of engine. The conclusions of this study are as follow.

- Overall the addition of NO leads to inhibition of the cool flame that is explained by a reduction of the NTC effect and effective promotion for the oxidation of hydrocarbons at high temperature.
- There is a decrease in the formation of the contents of unburned hydrocarbons HC and a carbon monoxide CO due to the increase of the added NO.

- The unburned hydrocarbons are in several quantities in the EGR gases and in our work we tested a few species and we found that some species can increase the efficiency of initiation and conduct of the main combustion and others allow delaying the combustion.

- Some components of the EGR gas species had a very significant effect on initiation of combustion, which gives a general idea about the control of combustion in HCCI mode.

- The influence of the EGR gas on the initiation and the period of the combustion depend on his compositions.

Following this study, several studies can accomplish this study to get good control of the HCCI mode such as better management of used fuel chemistry, the study of the composition of the soot and reaction mechanisms in the circuit EGR and the use of post-treatment of exhaust gas systems to achieve a burnt gas composition nearer to the perfect combustion.

Finally, this work contains an important data base but it needs improvement to achieve the best results.

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NOMENCLATURE

A	pre-exponential factor
E	activation energy for [cal.mol ⁻¹]
h _k	specific enthalpy of k species
K	Arrhenius rate coefficients
\dot{m}	mass flow [kg/s]
M	molar mass [g mol ⁻¹]
\bar{M}	the mean molar mass [g mol ⁻¹]
n	corrective coefficient
P	pressure [bar]
Q	thermal loss
R	ideal gas constant [cal.K ⁻¹ .mol ⁻¹]
T	temperature [K]
V	volume [m ³]
Y _k	mass fraction of k species

Greek letters

ρ	density [kg/m ³]
τ	time [s]
φ	equivalence ratio
ω	net production rate

Abbreviations

CI	compression ignition
CH ₂ O	formaldehyde
C ₂ H ₄	ethylene
CO	carbon monoxide
CO ₂	carbon dioxide
EGR	exhaust gas recirculation
HCCI	homogenous charge compression ignition
HC	hydrocarbon
H ₂ O	water
JSR	jet-stirred reactor
LTC	low temperature combustion
NO	nitrogen oxide
NO _x	nitrogen oxides
NTC	negative Temperature Coefficient
PSR	perfectly-Stirred Reactor
SI	spark ignition