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# COMBUSTION ANALYSIS OF PREMIXED NATURAL GAS - DIESEL-AIR MIXTURES

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***Abstract.*** *This work aims to develops a numerical simulation using the software Chemkin Pro 2017 to determine the laminar burning velocity of Natural Gas and Diesel in a reactor with a constant pressure of 0.1 MPa and different initial temperatures 358 K, 393 K, and 428 K. Natural Gas and Diesel were considered as methane and n-heptane respectively. The laminar burning velocity was carried out for the n-heptane-methane-air mixtures at different proportions of fuel compositions and equivalence ratios ranging from 0.7 to 1.5. As the methodology of analysis two kinetic reaction mechanisms were used, the reduced and the detailed n-heptane mechanisms, containing respectively, 160 species with 770 reactions, and 550 species with 2450 reactions. The simulations were validated comparing the results with some experimental results present in literature. The divergence of the results obtained for the simulations using the reduced and the detailed n-heptane mechanism diverged from the experimental results at around 20% and 5% respectively. Besides, it is simulated some compositions studied previously in an IC (internal combustion) engine module, in order to investigate the variation of species, pressure, temperature relating to the crank rotation angle. Beyond that, it is compared between the compositions and the equivalence ratio the temperature of burning, the power generated and specific fuel consumption of the samples.*

***Keywords:*** *Natural Gas, Diesel, Laminar burning velocities, n-heptane detailed mechanism, n-heptane reduced mechanism*

## 1. INTRODUCTION

The Emissions standards focus on regulating pollutants released from automobiles, industrial generators and any other specific source, in order to maintain the air quality standards and to protect human life. The industry is developing new technologies to research another's green combustibles to be used upon the petroleum-based ones. Natural gas (NG) is the cleanest burning petroleum-based fuel and therefore has a high potential to be used in industry and transportation systems, Demirbas (2006). The main component of NG is the methane, which does imply the potential to significantly reduce the $CO_2$ emission and to contribute to the reduction of Global warming, Tillmark (2006).

Natural gas is difficult to ignite in compression ignition engines and several studies have been extensively performed to find out a solution. Normally small amounts of diesel are injected directly into the cylinder while the NG is injected into the intake manifold, producing a premixed natural gas-diesel-air mixture. With this as the main objective of the study, Li *et al.* (2015) investigated the premixed combustion characteristics for natural gas-diesel-air mixtures for design and optimize the natural gas-diesel dual-fuel engines.

Natural gas and diesel are both complexes containing many species, diesel consists mainly by alkanes, cycloalkanes, and aromatics Edwards *et al.* (2007)-Leclerc (2008), and the composition of NG treated in literature depends upon origin, as studied by Tillmark (2006) the chemical kinetic combustion of three different natural gas compositions in a gas turbine. Since methane is the main component in NG, it was treated as NG by Li *et al.* (2015). Following some precedent cases present in literature, such as Leclerc (2008), Kumar and Sung (2007) and Wang *et al.* (2009), n-heptane was treated in Li *et al.* (2015) preliminary as representative of diesel for simplicity.

This study aims to generate some numerical simulations of the experimental results present on figure 7 of the work Li *et al.* (2015), related to the premixed laminar burning velocities of the methane-n-heptane-air mixtures in a cylindrical constant-volume combustion chamber. Moreover, the fuel mixtures regarded in the simulations of the premixed laminar burning velocities are burned inside an internal combustion engine module from Chemkin to compare the performance, specific fuel consumption and gases emissions of some natural gas-diesel-air mixtures.

## 2. METHODOLOGY OF SIMULATION

The numerical simulations were performed in the Chemkin Pro 2017 software from ANSYS Design (2011). The analysis was done using the model "flame speed" to determine the laminar burning velocity and the module "IC Engine" to determine the performance of a generic engine and the emissions of CO, $CO_2$, $CH_4$, and $H_2O$ during the engine operation with some natural gas-diesel-air mixtures. .

Firstly, it is determined the laminar burning velocity of a mixture varying the composition of natural gas and diesel, the equivalence ratio and the temperature of the unburned gases. These simulations are validated with the experimental results evaluated by Li *et al.* (2015). Secondly, will be assessed the combustion behavior of some mixtures evaluated in the first part and compare the results between the fuel samples relating the specific fuel consumption, the temperature of burning, pressure, and power generated. Regarding the first part of this work, the simulations on the module "flame speed" requires as boundary conditions the choice of the oxidant and the fuel, the equivalence ratio, pressure in the reactor, the temperature of the unburnt gases, etc.

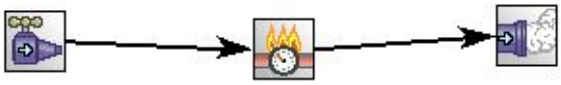

Figure 1. Diagram view of the Chemkin simulation regarding the laminar burning velocity.

A parametric study was performed relating the mass fraction of methane (0.00,0.25,0.50,1.00) in n-heptane fuel mixture and the equivalence ratio (0.7-1.5) related to the fuel to air ratio, resulting in 45 simulations to each case analyzed, of initial pressure of 1 bar and temperatures of 358K, 393K, and 428 K.

The ambient temperature was considered as 298 K, and the air with 79% N2 and 21% O2. The final grid of each simulation was at about 150-220 elements, with 90 cm reactor long. The GRAD and the CURV parameters were considered the default values of 0.1 and 0.5 respectively.

All simulations were executed using the reduced n-heptane mechanism obtained from LLNL n-heptane mechanism version 38 [9], and using the detailed n-heptane mechanism obtained as well from LLNL based on the previously developed mechanism of [10], the performance data from both mechanism are present in the following table 1.

Table 1. Mechanisms

| Mechanism | Number of Species | Number of Reaction | Reference |
|---|---|---|---|
| n-heptane reduced | 160 | 770 | (Seiser,H. et al., 2000) |
| n-heptane detailed | 550 | 2450 | (Curran *et al.*, 1998) |

The final analysis was carried out in the "IC Engine" module from Chemkin. This module simulates the combustion inside an internal combustion engine under auto-ignition conditions, and it is adequate to study of fuel auto-ignition behavior, engine knock, homogeneous charge compression ignition (HCCI) engines and gases emissions for given fuel mixtures, ANSYS (2017).

The detailed n-heptane reaction mechanism was considered for the simulations done in "IC Engine" chemkin module since it presents better results of laminar burning velocities presented in the next section. The engine configuration considered is a four-stroke oversquare engine with 1500 rpm, bore/stroke ratio of 2.13 and compression ratio of 15. The initial temperature and pressure considered for this engine are 358 K and 1 atm. It was not considered heat losses out of the system. As for laminar velocities simulation, methane is representing the natural gas and n-heptane the diesel. A parametric study was again considered for this simulation, mass fractions of (0, 0.25, 0.50 and 0.75) of methane in the mixture were burned in the internal combustion engine simulator without spark ignition. The mass fraction of 100% of methane did not burn because natural gas doesn't ignite alone with compression, it does require an amount of diesel in the mixture to be used in internal compression engines.

## 3. RESULTS

### 3.1 Laminar burning velocity

The experimental results in the article Li *et al.* (2015) were validated through the comparisons of the laminar burning velocity and Markstein length of methane and n-heptane separated with other studies successfully, implying that the results present in the article Li *et al.* (2015) were well executed and are correct. The figure 2 presents the results of the simulations carried out with the reduced and the detailed n-heptane mechanisms compared with the results present in figure 7 of the article Li *et al.* (2015). Before analyses the results, it is worth to mention the performance of the mechanism to execute the same simulations related to processing time.

The simulations using the reduced n-heptane mechanism took approximately one hour to run the 45 simulations related to any of the temperatures assessed (T= 358K, 393K, 428K), but couldn't solve all the cases requested, failing 2 cases for the temperature of 393K and 3 cases for the temperature of 428 K. On the other hand, the simulations using the detailed n-heptane mechanism took approximately 12 hours to solve each of the cases assessed (T= 358K, 393K, 428K) successfully.

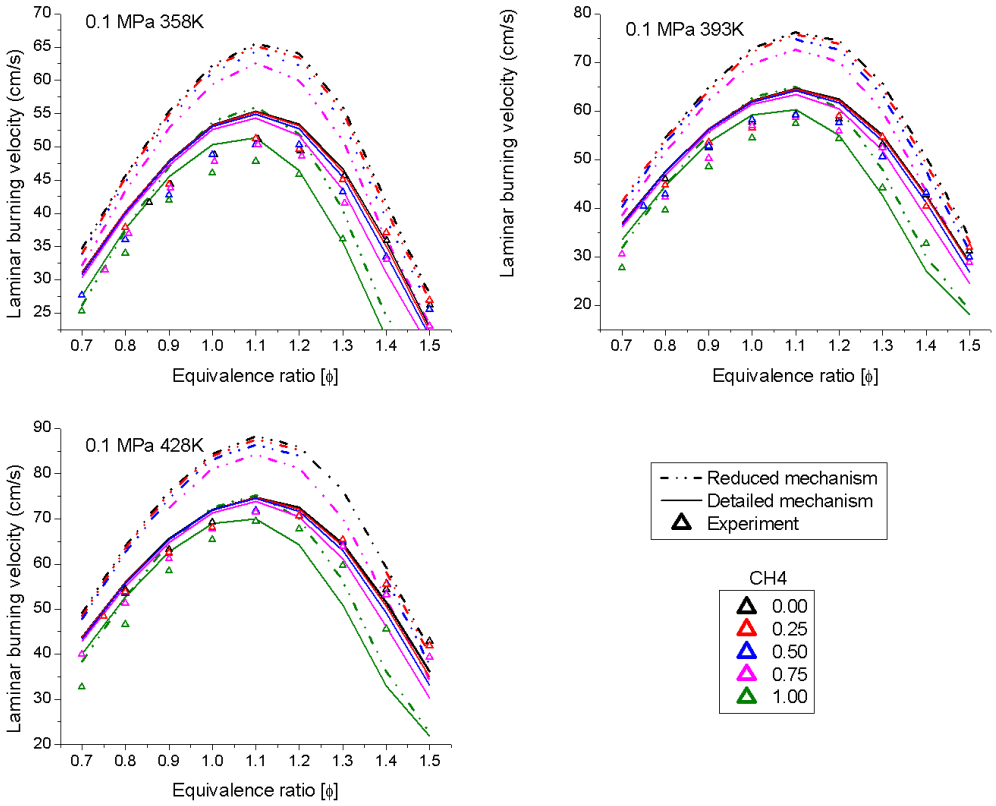


Figure 2. Compare between the experimental results of Li *et al.* and the numerical results related to the laminar burning velocities for methane n-heptane-air mixtures at various equivalence ratio and T = 358K, 393K and 428 K.

The laminar burning velocities of n-heptane-methane-air mixtures seem to not be affected at all with the increase of methane showing a slight decrease of the laminar burning velocities until it reaches 75% of methane in the mixture. The step between 75% of methane in the mixture and pure methane laminar burning velocities decreases with increase in initial temperature of the mixture, Li *et al.* (2015).

Looking to the figure 2, the simulations performed using the reduced mechanism showed major differences from the experimental results at the equivalence ratio of 1.1 for all the cases, while the simulations using the detailed n-heptane mechanism provided better accuracy in the results from 0.7 up to 1.3 of equivalence ratio.

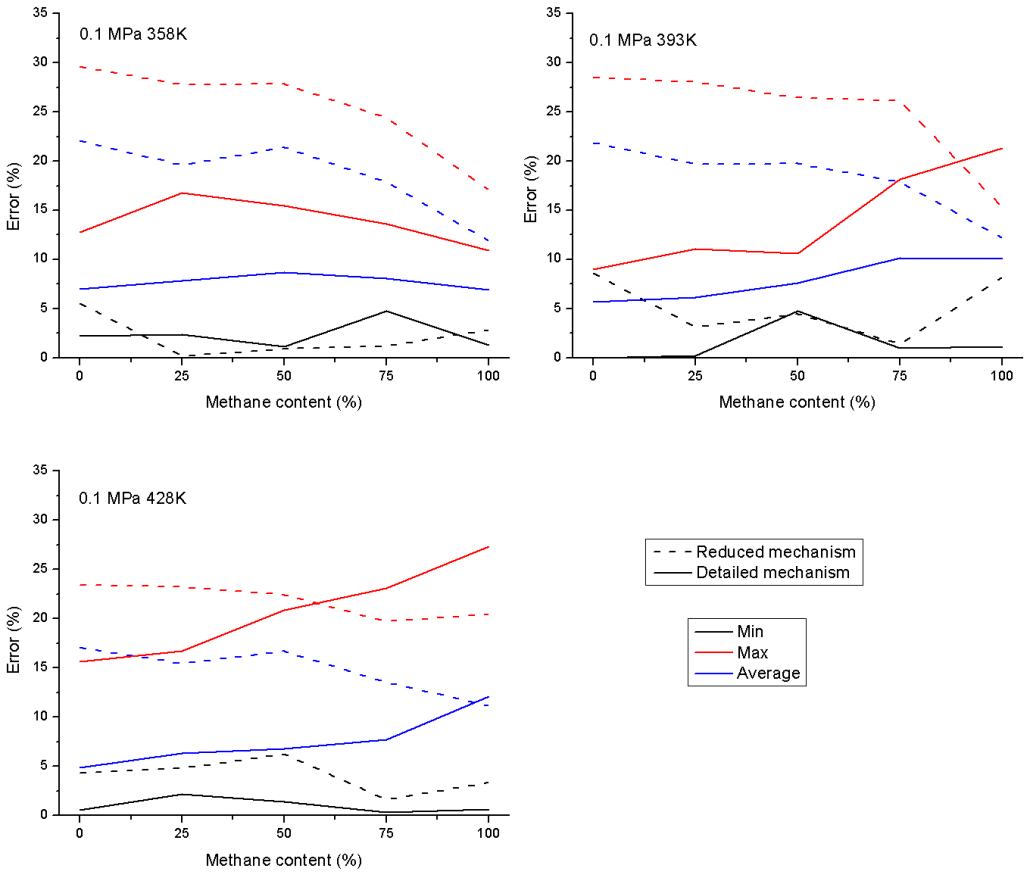


Figure 3. Error analysis of the simulations using the reduced and the detailed n-heptane kinetic mechanism for the various additions of methane in the fuel mixture.

The difference between results quality is well present in figure 3, that exhibits the residuals between simulation results and experimental results obtained by Li *et al.* (2015). The average residual between the experimental and the simulations for the reduced n-heptane mechanism float at around 20 % and the detailed n-heptane mechanism float at around 5%. A curious fact, the decrease of residuals for the reduced n-heptane mechanism at richer combustion regime, while the detailed n-heptane mechanism increases the error rapidly with the increase in temperature and in methane content.

### 3.2 Internal combustion engine

In order to show a comparison of natural gas-diesel-air mixtures inside a combustion engine, a simulation in module "IC Engine" from Chemkin was carried out. A parametric study relating equivalence ratio (0.7 to 1.5) and the mass fraction of natural gas in the fuel mixture of (0, 0.25, 0.5 and 0.75) were considered. The performance of this 4 stroke engine is presented in figure 4.

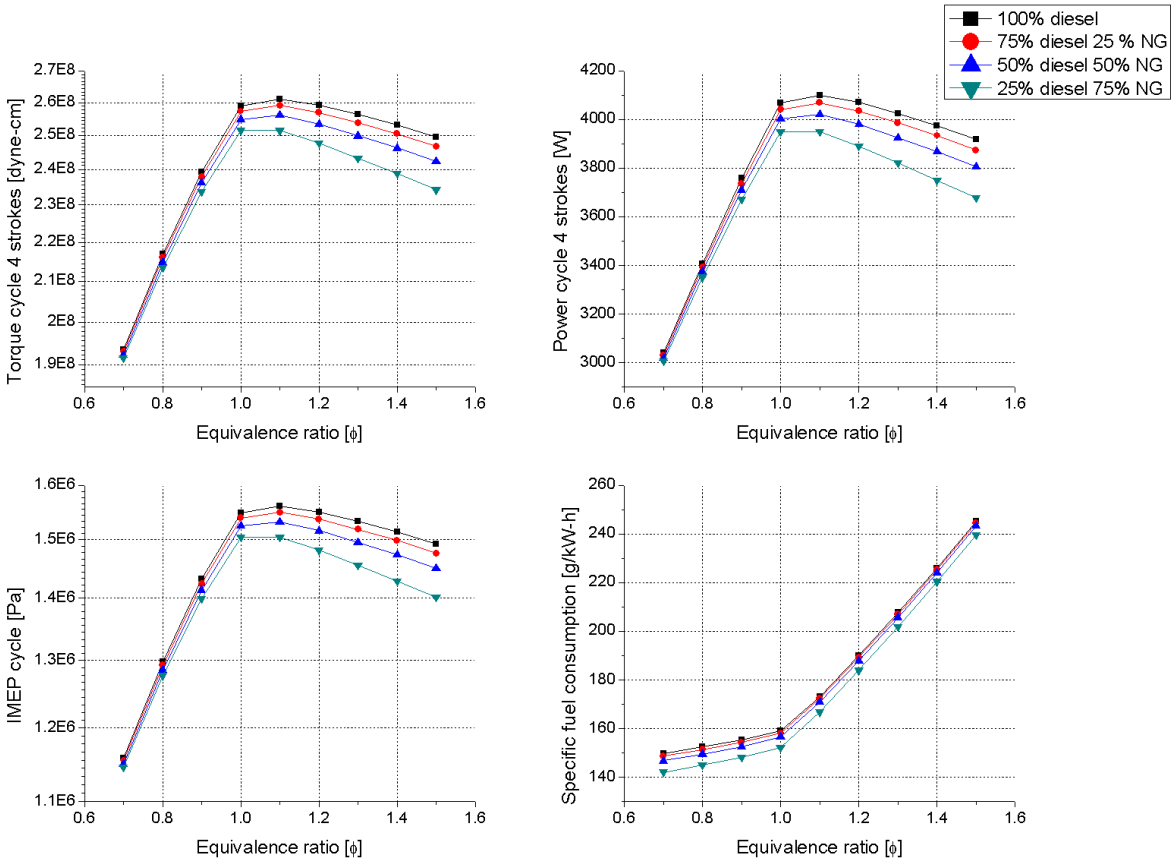


Figure 4. Torque, power, IMEP and specific fuel consumption of a 4 stroke engine relating to equivalence ratio and the amount of natural gas in the mixture.

Torque, power, and IMEP follow similar behavior between properties over equivalence ratio, distinguishing only the values and units. These properties are all superior to pure diesel and decreases as natural gas is added to the mixture, including specific fuel consumption. Analyzing the lean mixture of fuel where equivalence ratio is lower than 1, the properties between the fuel mixtures don't distinguish too much from each other.

The concentration of some species, such as CO, $CO_2$, $CH_4$ and $H_2O$, at the end of the combustion cycle were analyzed and are present in figure 5. These gases were chosen because it's importance in the global warming theme. $CO_2$, $CH_4$ and $H_2O$ in vapor phase are greenhouse gases, in other words, they warm the earth by slowing the heat transfer between Earth and space, they act like a blanket insulating earth, EPA (2017a), and EPA (2017b). $CO$ is not considered a greenhouse gas, but it acts indirectly creating or destroying greenhouse gases in the atmosphere through chemical reactions, ACS (2017).

Compression ignition engines normally works in lean mixture of fuel ($\phi < 1$). In this range $CO$ and $CH_4$ are null, $CO_2$ and $H_2O$ shows increasing values of concentration, with peak at $\phi = 1$ and $\phi = 0.9$ respectively, and all concentrations of these molecules presents lower values at $\phi = 0.7$.

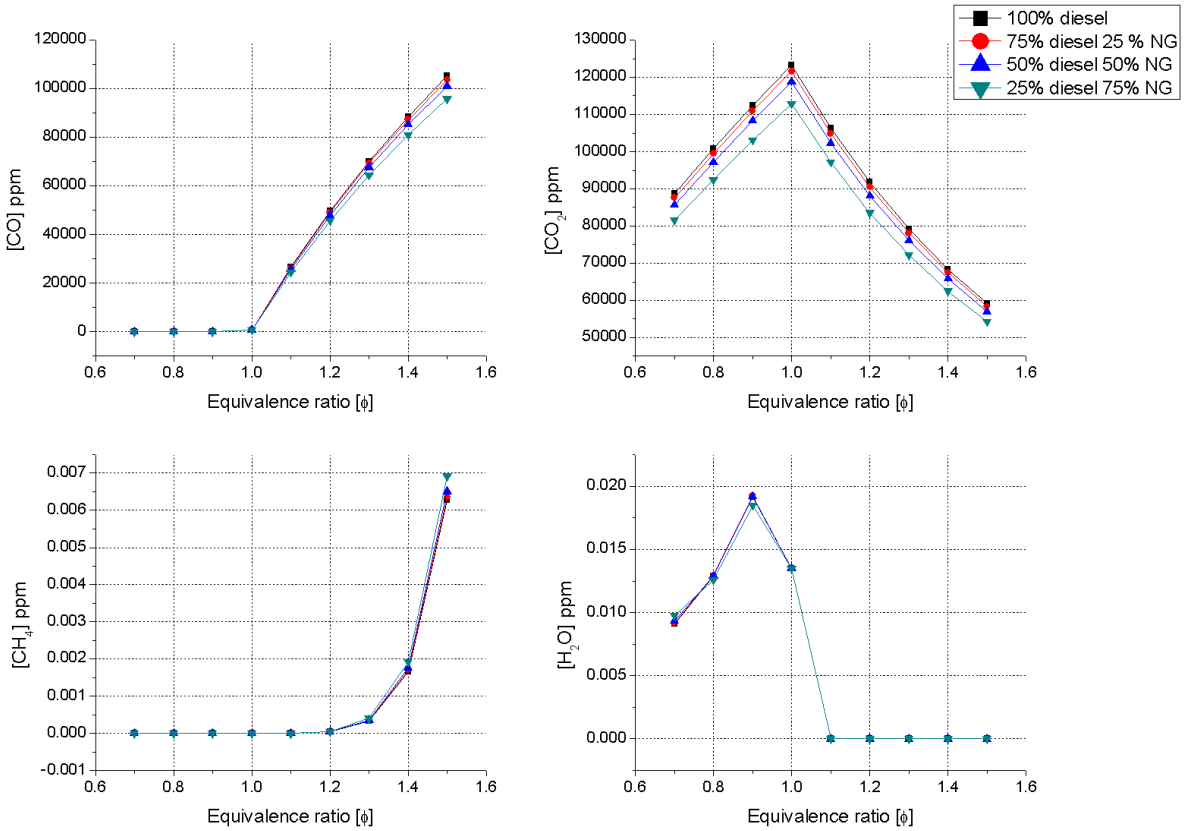


Figure 5. CO, $CO_2$, $CH_4$ and $H_2O$ concentrations relating to equivalence ratio and the amount of natural gas in the mixture at the final of the cycle.

To evaluate the species along the engine cycle, $CO$ and $CO_2$ were selected from the species available in the reaction mechanism and. The concentrations of these species were analyzed along with the crank angle rotation for equivalence ratios of 0.7, 1, 1.2 and 1.5 and they are present in the figures 6 and 7.

As shown in figure 5, $[CO]$ shows increasing values at the end of the engine cycle for values of $\phi > 1$, so does in figure 6. Richer mixtures lead to emission of $CO$ to the atmosphere, therefore it would be recommended to use this engine with $\phi < 1$. The ignition moment can be noted in figures 6 and 7, it is right before 0 ° where the maximum compression of the cylinders happens, leading to the peak in concentration of the molecules as well pressure and temperature. Change in molecules concentrations along the crank angle rotation is due to kinetic reactions between the gases that happen fast.

Figures 5 and 7 can also be compared for the concentrations of $[CO_2]$ at the end of engine cycle since the results present in figure 5 are obtained when the crank angle rotation is 180 °. Comparing figures 6 and 7, it is noted that $[CO]$ is always consumed for the equivalence ratios evaluated after ignition while $[CO_2]$ is produced.

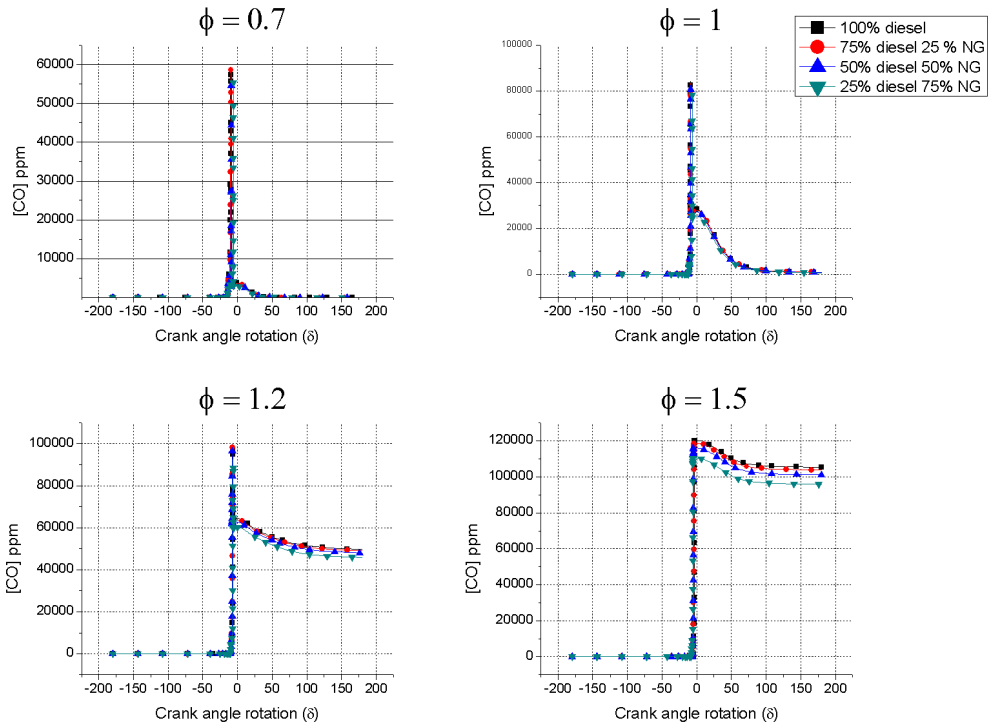


Figure 6. CO concentrations distributions over crank angle rotation for equivalence ratio of 0.7, 1, 1.2 and 1.5.

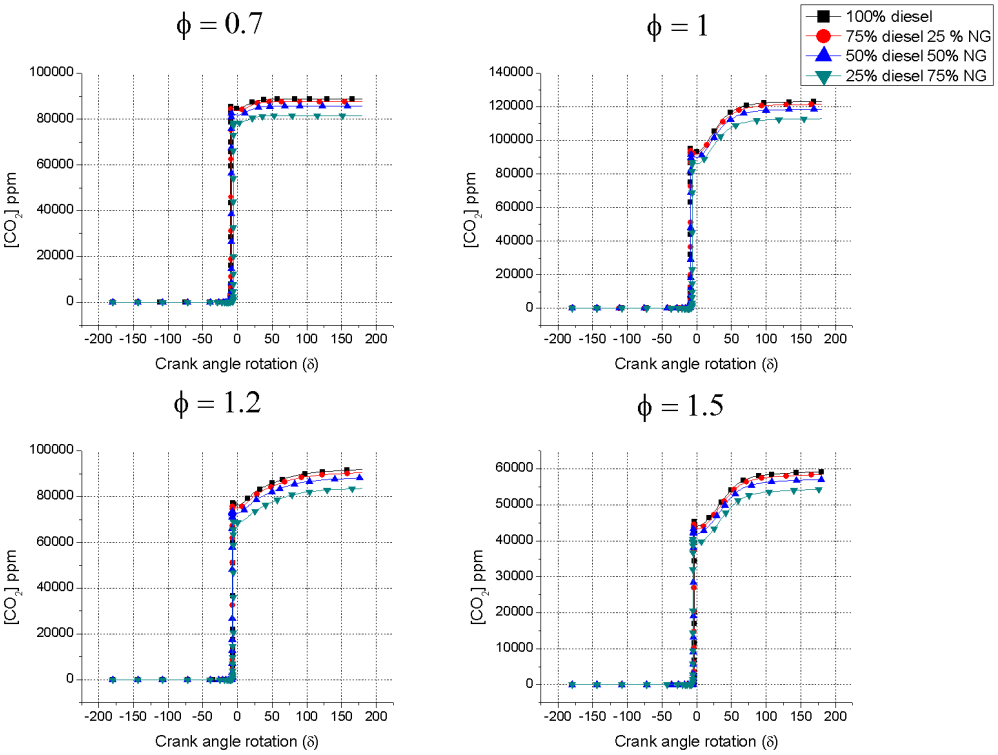


Figure 7. $CO_2$ concentrations distributions over crank angle rotation for equivalence ratio of 0.7, 1, 1.2 and 1.5.

## 4. CONCLUSIONS AND DISCUSSIONS

The numerical laminar burning velocity of n-heptane-methane-air mixtures at an initial pressure of 0.1 MPa and initial temperatures of 358K, 393K and 428 K using two kinetic reaction mechanisms (reduced n-heptane and detailed n-heptane) were determined using various methane content. Both reaction mechanisms were compared concerning the processing time and to the accuracy through error analysis to give a better interpretation and precision of data for both reaction mechanisms. As a conclusion for the first part, depending upon the state of the laminar burning velocity for n-heptane-methane-air mixtures, the reduced n-heptane mechanism may be precise enough to get satisfactory results in a faster way than the detailed n-heptane mechanism.

In the second part of the work, a simulation in "IC Engine" module from Chemkin was carried out. A generic diesel engine has been considered to analyze the performance, specific fuel consumption, IMEP and emissions of some gases through the burning of some fuels investigated previously in the first part of this work. With all the information generated in these simulations was concluded that the increase of natural gas in the diesel-natural gas mixture results in a loss of performance and a diminishing of specific fuel consumption, moreover it has been noted that for lean mixtures of fuel ($\phi < 1$) there are no emissions of $CO$ and $CH_4$.

## 5. ACKNOWLEDGEMENTS

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