



The combustion and emissions characteristics of gasoline engines with the use of LPG: A numerical study

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ABSTRACT

The invention of the spark ignition engine was an important step in the history of internal combustion engines. In recent years, gasoline engines have undergone undeniable development thanks to their exceptional efficiency. However, they emit pollutants such as HC and CO emissions. The application of pollutant emission standards is becoming more and more rigorous. In this context, this work presents a numerical study of the effect of using liquefied petroleum gas (LPG) in place of gasoline on spark-ignition direct injection engine characteristics, including combustion and emissions characteristics. In this study, we have based our work on the CONVERGE code 2.4 to study the phenomena that appear in the cylinder during the combustion phase in particular. The RANS approach is used. The combustion is described by the SAGE model, the spray by the KH-RT model, and turbulence, ignition, and the formation of NO_x and soot by the RNG models k- ϵ , Hiroyasu, and Zeldovich, respectively. The numerical results compared to the situation of gasoline fuel showed that the peak pressure and heat release increased. An earlier combustion starting occurrence and closer to the top dead center (TDC) is noticed compared to gasoline. The cylinder temperature increased by 6%, and heat release decreased by 3%. For the emissions pollution, the NO_x, soot, CO, and CO₂ emissions decreased when using LPG by 16.5%, 59%, 75%, and 20%, respectively, compared to gasoline.

Keywords: Spark ignition engine, Liquefied Petroleum Gas, direct injection, combustion, CONVERGE V2.4.

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1. INTRODUCTION

Because of the growth of the population, there has been an increase in the use of machines and energy in various industries like transportation, agriculture, electricity production, and heavy industry. Diesel engines have become widely used in these fields because they offer power output at a low cost compared to other engines of similar size. As a result, important areas of research related to diesel engines include enhancing performance, reducing emissions, and minimizing fuel consumption. This is considering that traditional fuels are limited and there are increasingly strict emissions standards worldwide. Therefore, there is a growing focus on developing fuels and fuel systems for diesel engines as well as exploring alternative fuels to improve engine performance and decrease emissions [1].

The researchers have put forward a method to transform diesel engines into dual-fuel engines. This conversion allows the use of fuels like gas, biogas, and LPG, which can effectively reduce both fuel expenses and emissions. This technique holds potential for Algeria, a country that plays a role in LPG and natural gas production as it aligns with their energy transition policies. As a pilot project towards the adoption of engines, Algeria has already introduced the first two vehicles powered by LPG in 2021. Elnajjar et al. [2] examined the performance of various LPG compositions and propane and butane ratios using a four-stroke, single-cylinder engine. It has been discovered that combining the two gases improves engine performance. Additionally, whereas differing LPG compositions have a considerable impact on combustion noise, they have a minimal effect on engine efficiency. Seeking to understand how well a small-scale SI engine running on 100% LPG performs. Baris Erkus et al [3] conducted an experimental investigation into the impact of injection and carburetion fuel delivery methods on the performance of spark ignition engines in terms of indicated and volumetric efficiency. The findings showed that the researchers' prototype LPG injection control unit outperformed both the original LPG carburetion system and regular gasoline in terms of engine performance. When compared to pure LPG carburetion, volumetric efficiency was consistently higher with gasoline carburetion and LPG injection, with the LPG injection approach exhibiting the highest volumetric efficiency. J. Kim et al. [4] look into the impact of injector liquefied petroleum gas position. The experimental work for the direct-injection engine was conducted using a four-cylinder SI engine. The results show that the BSFC decreased marginally in the range of 0–9% for braking torque between 0 and 20 N·m. However, increased emissions of particulate matter (PM). The impact of employing an LPG-fueled direct injection spark ignition engine on the combustion properties obtained through experimentation by K. Kim et al. [5]. The findings demonstrated that because LPG has lower carbon content than other fuels, its CO and CO₂ emissions would be reduced. However, LPG's NO_x emissions were either comparable to or somewhat lower than those of gasoline. The load state had the best effect on BSFC; under high load conditions, a wide-open throttle was used to reduce pumping losses and maximize engine efficiency. E. Saleh [6] investigated the effects of LPG composition variation on emissions and performance in a dual-fuel engine that ran on diesel fuel and five different LPG gaseous fuel compositions. The researchers employed a two-cylinder, four-stroke, water-cooled diesel engine with a compression ratio of 16.4 to determine the optimal LPG composition for dual fuel operation. Exhaust emissions and the dual-fuel engine's fuel conversion efficiency were shown to be impacted by changes in LPG component compounds. While a larger percentage of propane results in lower CO levels, higher butane content lowers NO_x levels. Fuel (30% butane, 70% propane) with a mass fraction of 40% substitution of the diesel fuel was the better

LPG composition in the dual fuel operation, except that at part loads. Additionally, experiments were conducted on diesel mix fuel in dual fuel operation at partial loads to enhance engine performance and exhaust emissions through the use of the exhaust gas recirculation as great as anticipated for dual-fuel gasoline and LPG cars that run on LPG. T. W. Adam et al. [7] conducted a thorough analysis of ten vehicles from various manufacturers that ran on both gasoline and LPG. The researchers show that using LPG can result in lower emissions. However, the benefit is not as great as anticipated for dual-fuel gasoline and LPG cars that run on LPG. The primary reason is because even when LPG fuel is selected, dual-fuel vehicles typically start their engines on gasoline. The impact of the emissions depends on this cold-start phase. Additionally, they show an impact on the chemical makeup of pollutants and vehicle performance. This study simulate spark-ignition engine DI fuelled with gasoline and LPG to assess combustion and pollutant emissions. The analysis was conducted using CONVERGE Computational Fluid Dynamics (CFD) software, with the combustion process and emission behavior of the LPG engine thoroughly examined and discussed.

2. PHYSICAL MODELING

2.1. Engine specifications

The engine studied in the present work is a single cylinder engine fueled with a gasoline. A 3D view in Figure 1 illustrates the combustion chamber, while the operating specifications of the motor used are presented below in table (1), which shows the position of the intake and exhaust ports, intake and exhaust valves, direct injector, spark plug and combustion chamber with the shape of piston bowl.

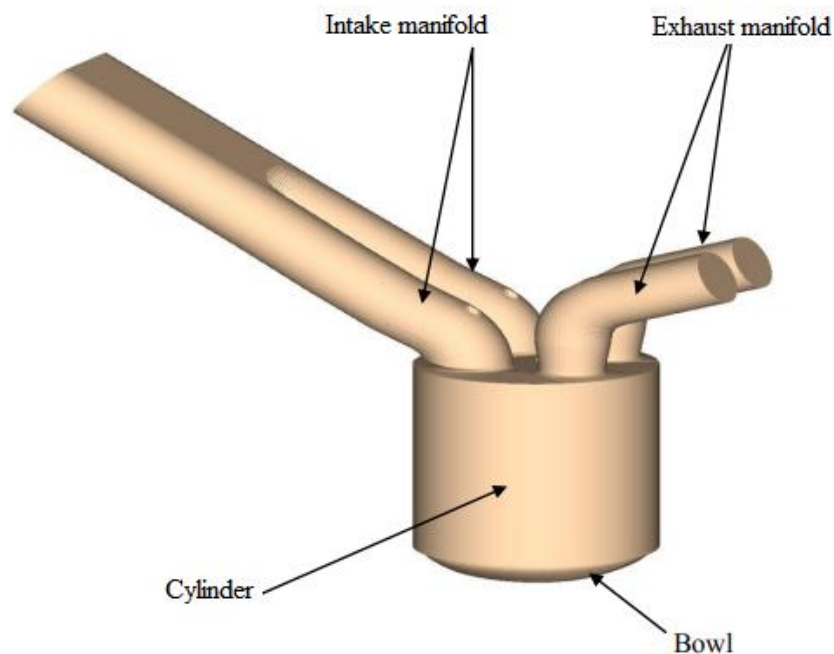


Fig.1. 3D view of the engine

Table 1. Description of the geometric features of the engine under study

Basic Geometry	
Engine bore	8.6 cm
Engine stroke	9.8 cm
Connecting rod length	14.37 cm
Squish	0.01 cm
Valve number	4 Valve
Rotation speed	3000 tr/min

2.2 Injection specifications

The specifications of injection in SI engine are listed in Table 2. In order to perform modeling, single injector for cylinder type of four-hole have been used.

Table 2. Description of the injection system characteristics of the engine studied [8-9]

Fuel injection system		
Fuel	C ₈ H ₁₈	LPG
Fuel temperature [K]	338	335
Start of injection [Deg]	-170	-220
Injection duration	50	50
Fuel mass [kg]	3x10 ⁻⁵	3,47 x10 ⁻⁵
Number of nozzles	4	4
Nozzle diameter [m]	0.0002	0.0002
Nozzle length [m]	0.0012	0.0012

3. NUMERICAL METHOD

3.1. Governing equations

Numerical simulation of a combustion problem aims to solve the aerothermochemical equations. These are the equations of conservation of mass, conservation of momentum, conservation of chemical species and conservation of energy [8-9].

○ *Continuity equation for chemical species m*

The mass fraction (m) of each species may be found by solving the transport equation for the first species, which takes the following form [1]:

$$\frac{\partial \rho_m}{\partial t} + \nabla(\rho_m u) = \nabla \left[\rho D \nabla \left(\frac{\rho_m}{\rho} \right) \right] + \dot{\rho}_m^c + \dot{\rho}_m^s \delta_{m1} \quad (9)$$

Where :

ρ_m : is the density of species m ,

- ρ : is the density of the mixture,
- u : is the velocity of the mixture,
- D : is the diffusion coefficient,
- $\dot{\rho}_m^c$: Includes source terms of chemical origin,
- $\dot{\rho}^s$: groups the source terms from the spray.

It is assumed that all species have identical diffusivities, represented by $D = \frac{\mu}{\rho S_c}$, where μ denotes the dynamic viscosity, and S_c stands for the Schmidt number, which compares the influence of fluid viscosity to that of diffusion, $S_c = \frac{\nu}{D}$.

- **Mass conservation equation**

By adding equation (9) for all species, we derive the equation that describes the conservation of the fluid's total mass [8-9].

$$\frac{\partial \rho}{\partial t} + \nabla(\rho u) = \dot{\rho}^s \quad (10)$$

- **Conservation of moment equation**

The mean equations for the conservation of momentum are derived from the second fundamental law of dynamics and given by [1]:

$$\frac{\partial \rho u}{\partial t} + \nabla(\rho u_i u_j) = -\frac{1}{\alpha^2} \nabla p - A_0 \nabla \left(\frac{2}{3} \rho k \right) + \nabla \sigma + F^s + \rho g \quad (11)$$

Where p represents the fluid pressure. The parameter α is applied alongside the Pressure Gradient Scaling (PGS) technique, which has proven to be efficient for low Mach number conditions.

In equation (11), the quantity A_0 is equal to zero for laminar flows and unity if a turbulence model is used. The viscous stress tensor is of Newtonian form [8-9]:

$$\sigma = \mu [\nabla u + (\nabla u)^T] + \lambda \nabla \cdot u I \quad (12)$$

The following defines the two viscosity coefficients, μ and λ . I stands for the unit matrix, whereas the superscript T indicates the transpose of a matrix. The momentum rate gain per unit volume resulting from spraying is called FS. The inertial force g is considered constant [8-9].

- **Energy conservation equation**

The equation for internal energy E is exclusive to chemical energy [8-9]:

$$\frac{\partial \rho E}{\partial t} + \nabla(\rho u E) = -p \nabla \cdot u - \nabla J + (1 - A_0) \sigma : \nabla u + A_0 \rho \varepsilon + \dot{Q}^c + \dot{Q}^s \quad (13)$$

The heat flow vector J is the sum of the contributions due to thermal conduction and enthalpy diffusion:

$$J = -K \nabla T - \rho D \sum_m h_m \nabla \left(\frac{\rho_m}{\rho} \right) \quad (14)$$

In this context, T represents the fluid temperature, while h_m denotes the specific enthalpy of species m . The thermal conductivity, K , is determined based on the Prandtl number and the specific heat capacity at constant pressure, C_p .

The species-specific heat capacity C_{pm} and specific enthalpies h_m in equation (14) are determined from the JANAF tables, which provide values based on temperature. The term $\rho \varepsilon$ in equation (13) corresponds to viscous dissipation, with ε being the rate at which turbulent kinetic energy dissipates. In equation (13), two source terms arise in equation (13): $\dot{Q}^c$ due to chemistry and $\dot{Q}^s$ due to spray [8-9].

3.1. Simulation Mesh

We meticulously generated the computational mesh here using CONVERGE V2.4 [8-9]. This mesh, comprising 1081764 cells at -296CA and 11467 cells at 21CA, is specifically designed for the combustion chamber of the DI gasoline engine, leveraging CONVERGE's advanced features such as adaptive mesh refinement (AMR) and automated meshing algorithms.



Fig.2. Three dimensional mesh in the simulation.

3.2 Initial conditions

The initial conditions introduced are: Pressure "pres_init", chamber temperature "temp_init", kinetic energy "tke_init", and dissipation rate "eps_init". The data are shown in Table (3).

Table 3. Initial conditions

pres_init [MPa]	0.101325
temp_init [K]	363
tke_init [m^2/s^2]	5
eps_ini [m^2/s^3]	120

3.3 Boundary conditions

Tcu, Tcy, and Tp, the temperatures of the cylinder head, cylinder, and piston crown respectively, indicate the boundary conditions. The table (4) displays the data.

Table 4. Boundary condition

Cylinder head temperature (Tcu) [K]	450
Cylinder temperature (Tcy) [K]	450
Piston temperature (Tp) [K]	450
Valve temperature (Tv) [K]	480
Spark plug temperature (T _b) [K]	550

3.4 Simulation models

In this work, we used the models shown in Table (5) to simulate combustion in the combustion chamber of a direct-injection gasoline engine.

Table 5. Choice of models [8-12]

Process	Model
Combustion	SAGE
Turbulence	RNG $k-\varepsilon$
Atomization	KH-RT
Heat transfer	Loi de paroi
NO _x	Zeldovich
Soot	Hiroyasu

- **Detailed reaction mechanisms SAGE [8-9]**

A reaction mechanism consists of a series of elementary reactions. These elementary reactions happen precisely as outlined in the corresponding equation. Unlike complex or overall reactions, they cannot be further divided into simpler steps. Reaction mechanisms explain the molecular-level process of a reaction, detailing which bonds are formed or broken, the sequence of events, and the speed at which each step occurs. Consequently, knowledge of

knowledge of the properties of the reactants and products is required. Each step of the mechanism involves a combination of species. The dependence of these steps leads to the stoichiometric equilibrium of the overall chemical reaction equation. For a mechanism to be considered valid, it must satisfy the previous requirement, and its intermediate that its intermediate predictions (species and rates of progression of the elementary and rates of progression of the elementary reactions) do not contradict experimental observations. In general a reaction can be represented with [8-9]:

$$\sum_{m=1}^M v'_{m,r} X_m \Leftrightarrow \sum_{m=1}^M v''_{m,r} X_m, \text{ Pour } r = 1, 2, \dots, R \quad (1)$$

$$\dot{\rho}_m^c = M_{max} \sum (v''_{m,r} - v'_{m,r}) \omega_m \quad (2)$$

$$\dot{Q}^c = \sum Q_r \cdot \omega_m \quad (3)$$

Where X_m denotes one mole of species m , and $v'_{m,r}$ and $v''_{m,r}$ correspond to the integral stoichiometric coefficients for reaction r , M_{max} refers to the molecular mass.

Reaction r has a reaction rate given by:

$$\dot{\omega}_m = \sum_{r=1}^R v_{m,r} q_r \quad \text{pour } m = 1, 2, \dots, M \quad (4)$$

Where M is the total number of species

With:

$$v_{m,r} = v''_{m,r} - v'_{m,r} \quad (5)$$

And q_r the variable reaction rate is:

$$q_r = k_{fr} \prod_{m=1}^M [X_m]^{v'_{m,r}} - k_{rr} \prod_{m=1}^M [X_m]^{v''_{m,r}} \quad (6)$$

$[X_m]$ is the molar concentration of species m , k_{rr} and k_{fr} are the forward and reverse reaction rates respectively, and are of the generalized Arrhenius form.

$$K_{fr} = A_r T^{b_r} e^{\left(-\frac{E_r}{R_u T}\right)} \quad (7)$$

$$K_{rr} = \frac{k_{fr}}{K_{cr}} \quad (8)$$

The variables A_r , b_r , E_r , and R_u represent the temperature exponent, activation energy, and universal gas constant, respectively.

4. RESULTS AND DISCUSSIONS

4.1. Evolution of pressure

The combustion characteristics are determined by analyzing the variation in cylinder pressure relative to crank angle. Fig. 4 illustrates the comparison of cylinder pressure between gasoline fuel and LPG. The pressure difference is of the order of 0.1MPa, on the other hand the ignition delay; the LPG ignites 5 Deg before the gasoline. The numerical simulation of pressure demonstrates clearly that the SAGE model is highly capable of predicting the combustion phenomenon within the combustion chamber in engine fuelled with gasoline or LPG.

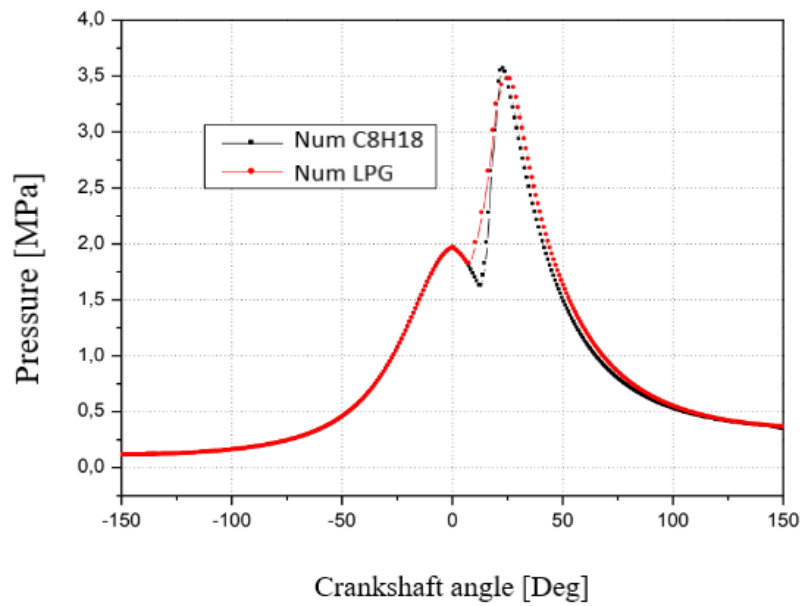


Fig.3. Evolution of pressure as a function of crankshaft angle

4.2 Evolution of heat release rate

Figure (4) shows the evolution of the heat release rate as a function of crankshaft angle during a cycle. For LPG, there is no heat release up to the eighth crankshaft angle, then a rapid increase up to 200 J/Deg. In the case of petrol, there is no heat release up to crankshaft angle 14. From this angle onwards, the rate of heat release increases rapidly, reaching a value of 250 J/Deg. The difference between C_8H_{18} and LPG is 50 J/Deg, due to the higher net calorific value of gasoline (32.25 MJ/l) and LPG (23.64 MJ/l).

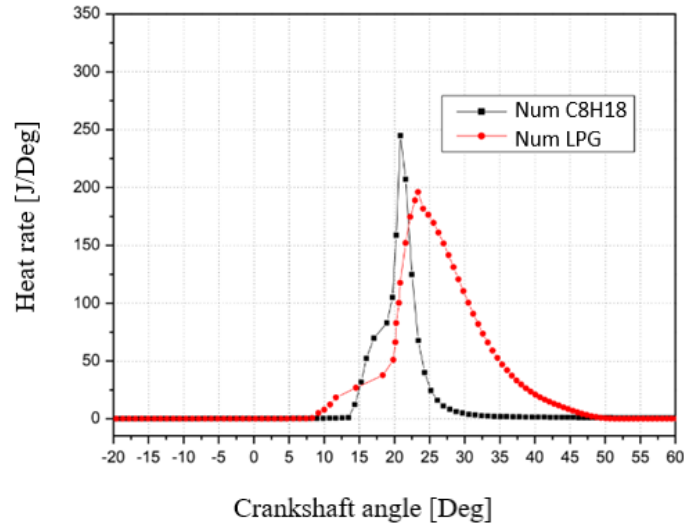


Fig .4. Heat rate evolution as a function of crankshaft angle

4.3 Evolution of temperature

This figure shows the temperature variation inside the cylinder as a function of crankshaft angle. For both profiles, for both fuels, we can see that they are almost identical, with a small difference in maximum temperature. We also note that this variation consists of 2 peaks:

- The first peak is 800K for C₈H₁₈ and LPG, at the moment of spark: this is the compressed air temperature of the compression phase.
- The temperature rises to a second peak of around 1900K for gasoline, and 1800K for LPG, when the combustion phase is triggered: this is the combustion temperature.

During expansion and exhaust, the temperature drops to an average value of around 1300K.

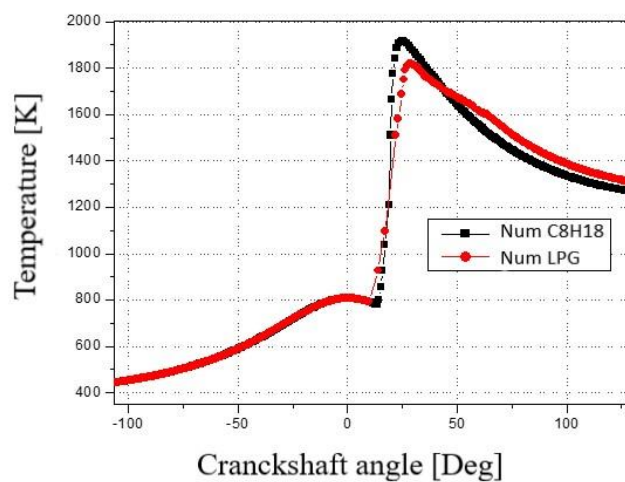


Fig .5. Temperature variation as a function of crankshaft angle

4.4 Evolution of fuel

Figure (6) shows the development of fuel quantity as a function of crankshaft angle in the combustion chamber.

- For LPG, the increase in fuel quantity starts at 220°V : beginning of injection, reaching a value of 2.8×10^{-5} , then decreases.

- For the second fuel, petrol, the injection start time differs, so we can see that the fuel quantity increases from -170°V to reach a maximum value of $2.3 \cdot 10^{-5}$ and then decreases.

Comparing the two curves, we can see that the quantity of LPG is higher than that of C_8H_{18} , because we injected 20% more LPG than petrol to obtain the same power in both cases.

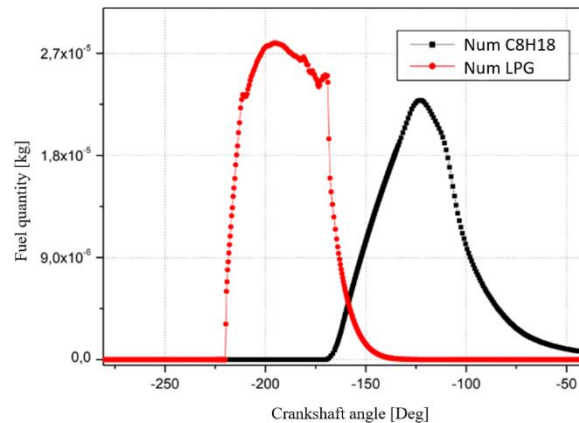


Fig .6. Evolution of fuel quantity as a function of crankshaft angle

4.5 Emissions pollutions evolution

4.5.1 NO_x emissions

Figure (7) shows the evolution of nitrogen oxide as a function of crankshaft angle for petrol and LPG. NO_x emissions take a zero value up to crankshaft angle 15 (start of combustion), at which point they develop rapidly due to the high temperatures reached during combustion.

We can also see that the petrol curve (black) takes on higher values than the LPG curve (red), with a percentage of 16.5%. The maximum values are 1.55×10^{-6} and 1×10^{-6} Kg respectively.

A decrease is then observed during the expansion phase (temperature drop).

Nitric oxide NO and nitrogen dioxide NO₂ are traditionally grouped together under the term NO_x. In an engine, however, NO is the most likely to be formed at the temperatures encountered during the combustion phase. Its formation is controlled by different mechanisms described in the literature:

- Thermal NO corresponds to an oxidation of atmospheric nitrogen described by the Zeldovitch mechanism. This mechanism represents the predominant pathway for NO formation during combustion.
- Fuel NO is linked to fuel decomposition, which can release NO_x compounds. The nitrogen content of today's fuels is so low that this NO formation pathway can be neglected.

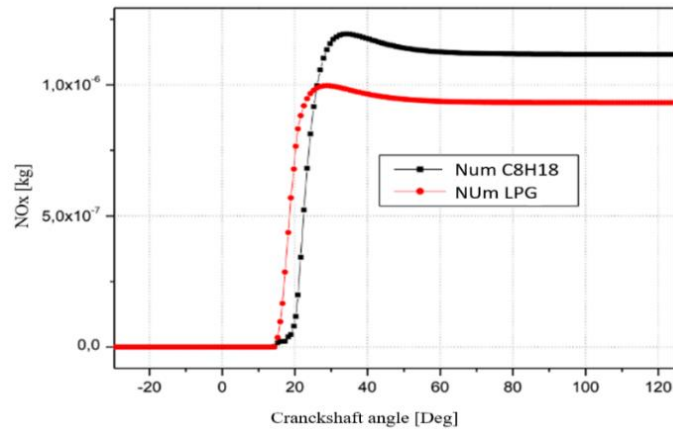


Fig .7. NOx evolution as a function of crankshaft angle

4.5.2 Soot emissions

The figure 8 shows the evolution of soot formation as a function of crankshaft angle. According to the profile, in the case of petrol, soot release takes a zero value up to crankshaft angle 15, when it begins to increase rapidly (this increase signifies the start of combustion) up to the peak at 30CA, with a maximum value of 6×10^{-8} Kg, after which it decreases. For LPG, the curve increases slightly at angle 10, reaching 0.8×10^{-8} Kg, then decreases and stabilizes at a value of 0.4×10^{-8} Kg. Soot emissions for petrol are eight times higher than for LPG.

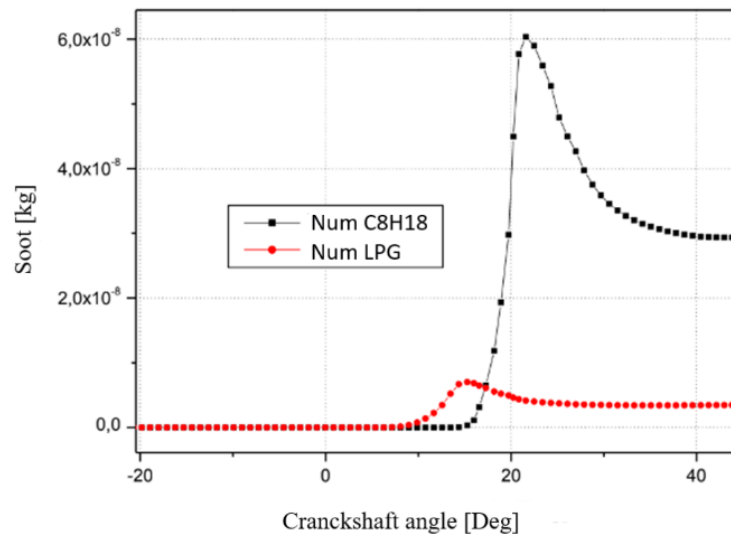


Fig .8. Soot evolution as a function of crankshaft angle

4.5.3 Carbon monoxide emissions

The figure 9 above shows the profile of carbon monoxide (CO) emissions as a function of crankshaft angle. The profile for C_8H_{18} shows that CO begins to rise with the onset of combustion ($15^\circ V$), reaching 2.7×10^{-6} Kg. This increase is caused by the richness of the fuel mixture (excess O_2). For LPG, the profile shows that the CO value in this case is 59.3% lower

than for petrol. At the end of combustion there is a decrease due to the poor quality of the mixture. CO emissions are formed at the heart of the flame with other intermediate combustion products. Most of these products are then converted to CO_2 , so the presence of CO when the exhaust valves open demonstrates the existence of an incomplete oxidation process.

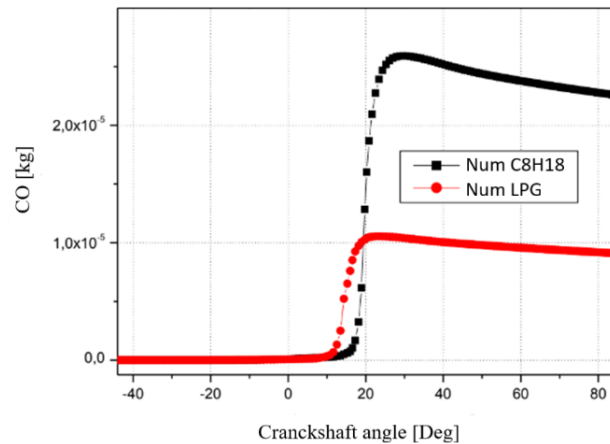


Fig.9. CO evolution as a function of crankshaft angle

4.5.4 CO_2 emissions

The figure 10 above illustrates the variation in carbon dioxide levels relative to the crankshaft angle. Due to the fuel mixture's richness, there is an initial increase at the onset of combustion for both types of fuel. The red curve (LPG) increases at 10CA and reaches a value of 4×10^{-5} Kg, while the black curve (petrol) starts to increase at 15CA and reaches $5 \cdot 10^{-5}$ Kg. The difference between the two curves is 20.2%. At the end of combustion, the CO_2 value remains stable, as CO_2 is a necessary constituent of chemical reaction products.

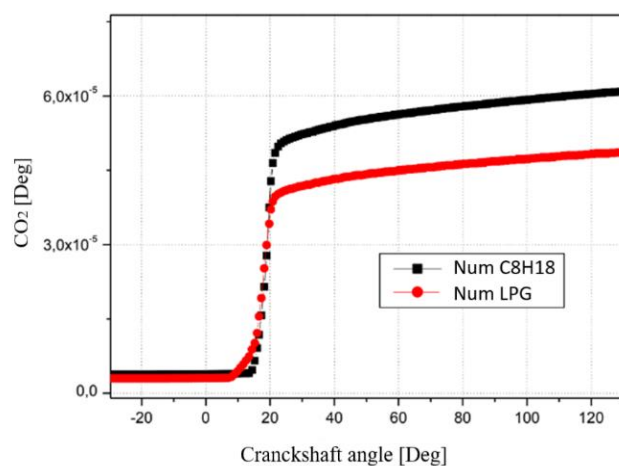


Fig.10. CO_2 evolution as a function of crankshaft angle.

4.6 Spray evolution

The figures 11-12 below show the mass progression of fuels (C_8H_{18} and LPG) at different crankshaft angles. Comparing the contours obtained using petrol and those using LPG, we notice a difference in the shape of the fuel when injected. This difference is due to density: LPG is less dense than gasoline, with values of 0.51 and 0.72 respectively, which is why gasoline takes on a well-defined shape and occupies more volume in the combustion chamber.

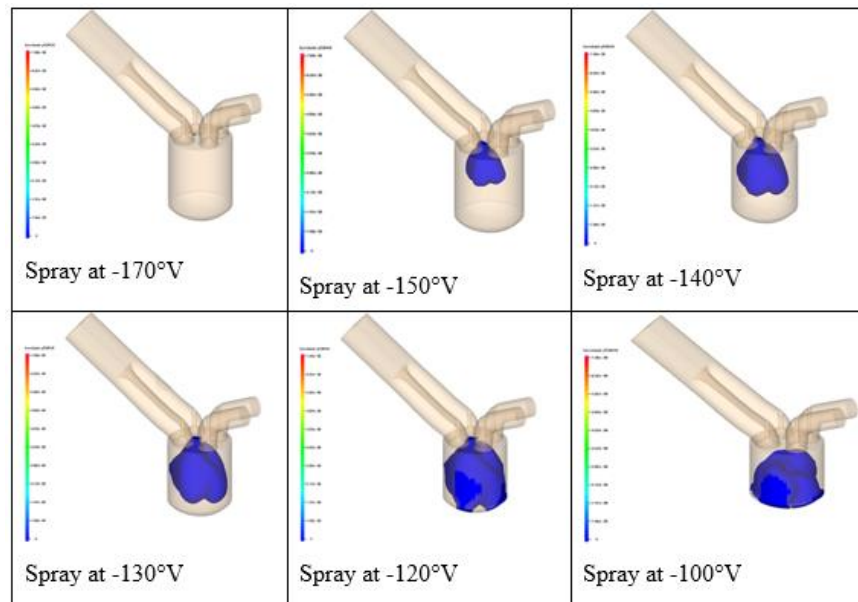


Fig .11. Contours of mass progression of C_8H_{18} at different crankshaft angles

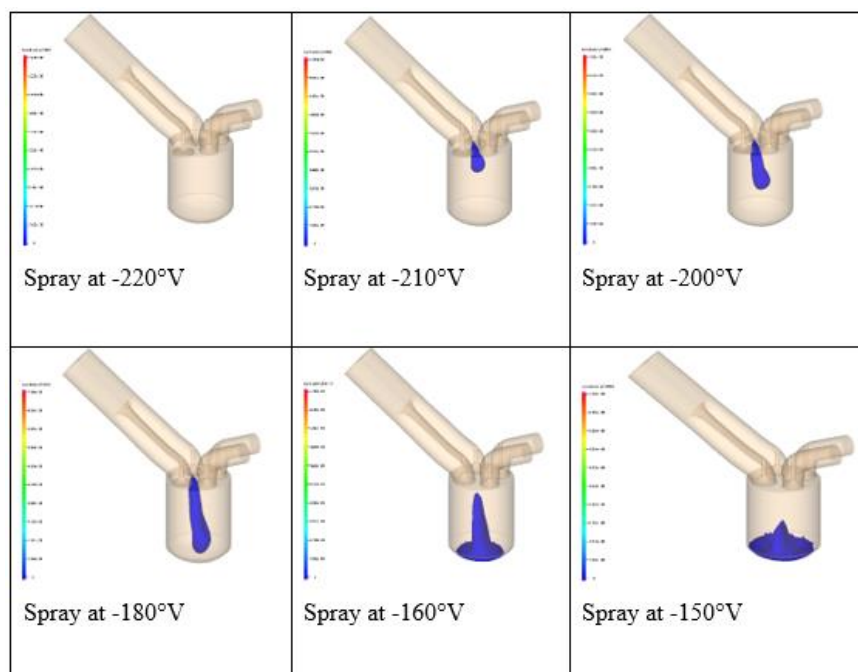


Fig.12. Contours of mass progression of LPG at different crankshaft angles

5. CONCLUSION

The study is purely numerical, based on the numerical simulation approach, which is a very important and less costly tool than experimental measurements, and which also allows us to visualize the results of a flow on a simple computer screen, recording variables such as velocity, pressure and temperature and many others. CFD validation is based on a comparison between the results of the spark-ignition engine and those of the LPG engine.

The reported results clearly show the combustion process and pollutant gas formation in a gasoline engine and a direct-injection LPG engine, as well as the evolution of temperature, pressure, heat release rate and pollutant gases during combustion. Taking this study into account, we can say that the results we have obtained are satisfactory, showing that LPG as an alternative solution, contributes to the reduction of atmospheric pollution which is becoming a major concern and issue worldwide thanks to its environmentally friendly characteristics, and relatively low pollutant emission levels compared to other fossil fuels such as gasoline. LPG consumption is around 20% higher; LPG produces 16.5%, 59%, 75%, and 20% less NO_x, soot, CO, and CO₂ respectively, compared to gasoline.

Despite the efforts and research made by all the worlds' engine manufacturers the world, there is still considerable scope for improving the use and production of production of biofuels from a variety of feedstocks.

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