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Ministère de l'enseignement supérieure et de la recherche scientifique

Ecole nationale polytechnique

Département de génie mécanique



End of studies project

To obtain the diploma of state engineer in mechanical engineering

# LPG-diesel dual fuel engine: literature review and CFD analysis

#### Done by: BENNOUR Mahmoud

Jury members:

Mr . Djamel BOUKHETALA Mr. Mohamed BEN BRAIKA Mr. Arezki SMAILI Mr. Abdelhamid BOUHELAL Professor, ENP MAA, ENP Professor, ENP MCB, ENP

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Projet de fin d'études

Pour l'obtention du diplôme d'ingénieur d'état en mécanqiue

## *Le moteur Dual Fuel LPG-Diesel:*

revue de littérature et simulation numérique

#### Realisé by: BENNOUR Mahmoud

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#### ملخص

الهدف من هذا المشروع هو دراسة تحويل محركات الديزل إلى محركات ثنائية الوقود. تستخدم المحركات ثنائية الوقود في وقت واحد وقوداً غازيًا أوليًا مع الحفاظ على كمية منخفضة من الديزل. تم تفصيل استخدام غاز البترول المسال كوقود أساسي وهذا للمحرك F4L912 في هذا العمل. الاشتغال بالنظام ثنائي الوقود يتطلب تعديلات على مستوى المحرك, حيث يعتمد المحرك ثنائي الوقود على مبدأي عمل كل من محركات الاشتعال بالضغط و محركات الاشتعال بالشرارة. و عليه, يجب دراسة العديد من عوامل التحويل مثل توقيت الحقن و كمية كل من الوقودين المستعملين.

يعتبر المحرك ثنائي الوقود تقنية فعالة في تقليل انبعاث الملوثات ، وقد تم التحقق من صحة ذلك من خلال محاكاة رقمية باستخدام برنامج CONVERGE الذي أظهر أهمية الميكانيك الرقمية في التنبؤ بأداء المحركات.

الكلمات المفتاحية: غاز البترول المسال, ديزل, ثنائي الوقود, تحويل, محاكاة رقمية

#### Résumé

L'objectif de ce projet est l'étude de la conversion des moteurs diesel en moteurs dual fuel. Les moteurs DF utilisent simultanément un carburant primaire gazeux et une quantité réduite de diesel comme carburant pilote. L'utilisation du GPL comme carburant primaire et ce, pour le moteur F4L912, a été détaillée dans ce travail. Le fonctionnement en mode DF nécessite une modification du moteur, car il est basé sur les principes des moteurs à allumage par étincelle et à allumage par compression. Par conséquent, de nombreux paramètres de conversion tels que l'avance à l'injection et la quantité de carburant primaire et pilote, doivent être étudiés.

La conversion en dual fuel est une technique efficace pour réduire les émissions polluantes, ceci a été validé par une simulation CFD utilisant le logiciel CONVERGE qui a montré l'importance de la mécanique computationnelle dans la prédiction des performances des moteurs.

Mots-clés : GPL, diesel, dual fuel, conversion, simulation CFD

#### Abstract

The objective of this project is the study of the conversion of diesel engines into dual fuel mode engines. DF engines use simultaneously a primary gaseous fuel with a reduced quantity of diesel as a pilot fuel. The use of LPG as a primary fuel and this, for the engine F4L912, has been detailed in this work. DF mode operation requires engine modification, as it is based on the principles of both spark ignition and compression ignition engines. Therefore, many conversion parameters such as injection timing and the quantity of primary and pilot fuels, need to be studied.

Dual fuel operation is an efficient technique in reducing pollutant emission, this has been validated with a CFD simulation using the software CONVERGE that showed the importance of computational mechanics in the prediction of engines performance.

Keywords : LPG, diesel, dual fuel, conversion, CFD simulation

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## **DEDICATION**

Praise to ALLAH Almighty who gave me the strength and patience to complete this work

I dedicate this modest work to those who gave me everything without hesitation, who made me the man I am today, the ones I will never thank enough: My dear parents.

My friends during my entire academic career.

To everyone who has ever supported me.

MAHMOUD

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## **Abbreviation List**

- WHO : World Health Organization
- TOE : Tonne of Oil Equivalent
- LPG : Liquefied petroleum gas
- ONS : L'office national des statistiques
- ppm : parts per million
- HC : Hydrocarbons
- CNG : Compressed natural gas
- LNG : Liquefied natural gas
- PM : Particulate matter
- IC : Internal combustion
- CI : Compression ignition
- SI : Spark ignition
- HPDI : High Pressure Direct Injection
- TDC : Top dead center
- BDC : Bottom dead center
- rpm : Revolutions per minute
- CFD : Computational fluid dynamics

## Nomenclature

$(kg/m^3)$
(m/s)
Pa
Pa.s
J/Kg.s
Pa
J/Kg
$m^3$
K
Pa
J
1
Kg
Kg/S
$\frac{Kg}{s}$
11101/ 111

$k_{Rr}$ : Reverse reaction rate coefficient of the reaction R	
$C_h$ : Hourly diesel consumption	g/h
$C_s$ : The specific consumption	g/kWh
$m_D$ : The mass of diesel consumed per cycle	g/cycle
N : Frequency of rotation	rpm
$L_{HVLPG}$ : The lower heating value of LPG	MJ/kg
$L_{HVDiesel}$ : The lower heating value of diesel	MJ/kg
$S_D$ : The substitution rate	%
$m_{LPG}$ : Mass of LPG injected per engine cycle	g/cycle

General introduction

#### **General introduction**

In the early years of automotive development, engine power and reliability were the major concerns of engine manufacturers. However, over the past three decades, emissions regulations and the depletion of oil resources have focused attention on the need to develop clean and efficient engine designs.

The difficulty lies in improving the efficiency of the engines while minimizing pollutant emissions. At present, the techniques that allow an improvement in efficiency unfortunately lead to high NOx emissions. On the other hand, there are processes that reduce this kind of emissions, like exhaust gas recirculation systems, but they are not beneficial because of the increase of HC and particulate emissions.

One of the techniques that the researchers presented was the conversion of the diesel engine into a dual-fuel engine. This conversion had for objective the reduction of fuel costs as well as the emissions. These converted engines use gaseous fuels such as natural gas, biogas and LPG.

Algeria, being an important producer of LPG and natural gas, and with the current energetic transition policy, can largely benefit from this technique. It has released the first two vehicles running on LPG this year (2021) as an initiative for further use of converted engines.

This study is divided into three main parts that aim to better understand the operation of LPG dual fuel engines and offer the base for further work of parts development and test bench realization.

- The first chapter represents a general review over energy and transport sectors in the world generally and in Algeria in particular, it shows numbers and statistics related to this study and describes the harmful effects of conventional diesel engines that pushed researchers to find alternative techniques.
- The second chapter defines the dual fuel mode, its operation and the main differences from the conventional diesel operation, it details the conversion process and indicates the main engine parts to be modified in order to run on dual fuel mode, at the end it shows the effect of these modifications on performance and combustion efficiency and also pollutant emissions from NOx, soot, HC, CO and CO2.

- The final chapter treats a CFD simulation performed to validate predicted performance and emissions. The software CONVERGE CFD is used and presented in this chapter, along with the different physical equations implemented. Results are presented, discussed and compared to literature.
- A general conclusion is given at the end resuming the work and making way for further development work.

## Chapter I

## Energy and transportation

#### I Energy and transportation

#### I.1 Introduction

In the automotive field, where a large percentage of the global energy is consumed, diesel engines are widely used due to their high combustion efficiency, reliability, adaptability and cost effectiveness [1]. However, diesel engines are among the major contributors to environmental pollution [2]. Main harmful pollutants from these engines are NOx and particulate matter. The latter are made up of various types of chemical compounds such as elemental carbon, organic carbon, inorganic ions, etc. [3]. These particles have extremely harmful effects on human health and deteriorate the environment. Numerous studies have proven that these particles are the cause of respiratory and cardiovascular problems [4]. In addition, diesel exhaust gases were identified as a carcinogenic by the World Health Organization (WHO) in June 2012 [5]. Since then, European directives have defined emission limit values for pollutants, aiming to reduce the rate of vehicle pollution. This has prompted the manufacturers to continue their research into the development of clean and efficient engines.

#### I.2 National energy consumption

With an estimated population of 43 million in 2019 [6], national energy needs have increased considerably in recent years. The latest balance sheet of the ministry of energy published in 2020, announced a final consumption of 50.4 million TOE during the year 2019 against 38.5 million for the year 2013 [7,8].

This energy is consumed in different forms, oil products, natural gas, electricity, LPG or coal. Figure 1 below represents the final national energy consumption in 2019 by type of energy.

This consumption is shared between the different sectors of activity: industry, transportation, the residential sector and the agricultural sector. Figure 2 below shows the energy consumption by sector of activity in 2019.



Total: 50,4 M TOE

Other: Wood, Petroleum coke

Figure 1 Final national energy consumption in 2019 [7]



Figure 2 Energy consumption by sector of activity in 2019 [7]

#### I.3 National vehicle fleet

With more than 6.4 million vehicles in 2018 according to the "ONS", Algeria has the largest fleet of cars in the Maghreb and the second largest in the continent after South Africa. However, the average age remains high, with 44.35% of vehicles aged over twenty years and only 20.15% less than five years (in 2018). [9]

Year of Release	Tourism Vehicle	Truck	Van	Coach/ Bus	Road tractor	Tractor	Special Vehicle	Trailer	Motorbik	e <i>TOTAL</i>	%
before 2008	2 314 287	350 705	781 273	66 460	60 885	131 312	4 634	112 052	12 222	3 833 830	59,73
2008	111 780	7 620	24 956	2 577	2 463	916	43	2 975	211	153 541	2,39
2009	131 237	11 248	31 519	2 761	3 186	1 368	96	3 862	544	185 821	2,90
2010	97 742	5 988	27 198	2 470	2 502	1 386	82	4 281	1 131	142 780	2,22
2011	165 386	7 063	51 130	2 275	2 059	2 454	215	2 770	1 531	234 883	3,66
2012	243 164	7 151	72 714	2 759	2 886	3 417	294	4 104	2 897	339 386	5,29
2013	167 984	5 342	50 204	2 650	1 598	2 930	268	2 553	1 431	234 960	3,66
2014	<b>214 674</b>	8 537	61 134	2 166	2 434	5 025	560	4 762	2 430	301 722	4,70
2015	177 500	5 917	56 579	1 308	2 079	5 495	498	5 183	3 039	257 598	4,01
2016	249 858	3 816	22 047	731	2 717	4 572	329	5 087	13 868	303 025	4,72
2017	111 347	4 054	11 919	585	2 699	3 052	145	3 912	38 649	176 362	2,75
2018	166 082	4 248	13 879	1 226	1 661	2 550	129	2 702	61 827	254 304	3,96
TOTAL	4 151 041	421 689	1 204 552	87 968	87 169	164 477	7 293	154 243	139 780	6 418 212	100

Table 1 The national vehicle fleet by age group 2018 (ONS) [9]

In the same year, the examination of the evolution of the national vehicle fleet by energy source, shows a trend towards gasoline for tourism vehicles.

On the other hand, utility vehicles (trucks, tractors) and collective transport vehicles (Coaches and Buses), which are characterized by large displacements (high consumption), are mostly diesel powered.

		τοται			
	Gasoline	%	Diesel	%	TOTAL
Tourism VEHICLES	3 229 336	77,80	921 705	22,20	4 151 041
TRUCK	25 098	5,95	396 591	94,05	421 689
VAN	669 845	55,61	534 707	44,39	1 204 552
COACH / BUS	4 865	5,53	83 103	94,47	87 968
ROAD TRACTOR	4 809	5,52	82 360	94,48	87 169
TRACTOR	8 048	4,89	156 429	95,11	164 477
SPECIAL VEHICLE	1 924	26,38	5 369	73,62	7 293
MOTORBIKE	130 243	93,18	9 537	6,82	139 780
TOTAL	4 074 168	65,04	2 189 801	34,96	6 263 969

(\*): Trailers and semi-trailers do not appear

Table 2 National vehicle fleet by fuel type in 2018 (ONS) [9]

This dominance of diesel in such active and vital categories of the national economy, have earned diesel the first place among the most consumed fuels in the transport and agriculture sectors.



Figure 3 Transportation Sector Consumption by Fuel Type (2013) [8]

Figure 3 above shows that diesel is the main consumed fuel, accounting for 62% of the energy balance of the transport sector in 2013.

#### I.4 Diesel engine pollution

The diesel engine is a thermal machine that converts chemical energy (i.e. fuel) into mechanical energy. Diesel fuel is a mixture of hydrocarbons which during an ideal combustion should produce only CO2 and H2O. However, during this combustion we observe the formation of other gaseous or solid products.

These formations are explained by the stoichiometry of the engines which is rarely perfect: on the one hand, modern engines are designed to work with a lean or rich mixtures (atmospheric or supercharged engines), on the other hand, the conditions of temperature and atmospheric pressure are constantly changing, as well as the engine speed and load, which vary according to the route and traffic conditions.

<i>CO</i> <sub>2</sub>	2 to 12 %
H <sub>2</sub> 0	2 to 12 %
02	3 to 17 %
NO <sub>x</sub>	50 to 1000 ppm
HC	20 to 300 ppm
СО	10 to 500 ppm
SO <sub>2</sub>	10 to 30 ppm
N <sub>2</sub> 0	≈ 3 ppm

The table below shows the typical composition of exhaust gases from a diesel engine:

 Table 3 Typical composition of diesel engine exhaust gases [11]

More details about these pollutants are given below.

#### I.4.1 Carbon dioxide (CO2)

Product of the complete oxidation of fuel, it is the main responsible for the increase of the greenhouse effect.

#### I.4.2 Carbon monoxide (CO):

Resulting from the incomplete combustion of fuel, it is combined in part with oxygen to form carbon dioxide and participates, with nitrogen oxides and volatile organic compounds, in the formation of tropospheric ozone.

#### I.4.3 Nitrogen oxides (NOx):

They include nitric oxide (NO) and nitrogen dioxide(NO<sub>2</sub>). They result from the combination of nitrogen and oxygen in the air at high temperatures. NO represents about 95% of these oxides and the rest is NO<sub>2</sub>.

They are involved in the formation of acids in the form of HNO3 and also contribute to the formation of tropospheric ozone

#### I.4.4 Sulfur dioxide (SO<sub>2</sub>):

It is formed from the sulfur found in fuels. It is the main component of acid pollution in the form of H<sub>2</sub>SO<sub>4</sub>.

Diesel engines have also the following emissions:

#### I.4.5 Solid particles:

They result from incomplete combustion of the fuel. They constitute the most visible fraction of air pollution (smoke). Those with a diameter of less than 10  $\mu$ m remain suspended in the air while those whose diameter is greater than 10  $\mu$ m are deposited by gravity in the vicinity of their emission sources.

#### I.4.6 Volatile organic compounds (VOC):

These are gases that group hydrocarbons (alkanes, alkenes, aromatics ...) and oxygenated compounds (aldehydes, ketones ...). With the nitrogen oxides and the carbon monoxide, they contribute to the formation of tropospheric ozone.

#### I.4.7 Polycyclic aromatic hydrocarbons (PAHs):

Such as benzoapyrene, they are known to be highly carcinogenic. The heaviest compounds are found on the surface of solid particles and the most volatile are in the gas phase. In cities, diesel engines are a major cause of PAH air pollution.

#### I.4.8 metals:

Initially present in oils and fuels, they are toxic for health and the environment. In the air, they are most often found trapped inside the fine particles.

These pollutants released into the atmosphere will induce a multitude of harmful effects for health and the environment. Some of them will play a role in the formation of urban smog and acid rain, such as SO2 and NOx. Moreover, NOx are at the origin of various reactions leading to the formation of ozone, a low altitude pollutant.

Ozone is the major secondary pollutant formed by the action of ultraviolet rays from the sun on primary pollutants, which are nitrogen oxides, volatile organic compounds and carbon monoxide. It is a chemical pollutant present at ground level: we speak of tropospheric ozone which is distinguished from stratospheric ozone (ozone layer).

Unburned hydrocarbons are carcinogenic, and solid particles are extremely dangerous to health because they are likely to penetrate the pulmonary alveoli.Parameters influencing pollutant formation in engines :

#### **I.5** Parameters influencing pollutant formation in engines:

There are several parameters according to which pollutants are formed:

- Engine construction parameters: volume ratio, type of cooling, supercharging...
- Engine operating parameters: injection law, advance, excess air, intake temperature and pressure...
- Physical characteristics of the fuel: density, surface tension, viscosity...
- Chemical composition of the fuel: aromatics, impurities.

#### I.6 Environmental aspect:

Nowadays, increasingly stringent air pollution regulations have pushed car manufacturers to reduce these emissions. However, while this reduction is observed on new engines, the old ones continue to release huge amounts of pollutants.

Stopping the growth of motor vehicle use is neither possible nor desirable, given the economic benefits and other advantages of increased mobility. The challenge, therefore, is to manage the growth of motorized transport in a way that maximizes its benefits while minimizing its negative environmental and social impacts.

In order to reduce pollutant gas emissions, two options are available:

- Filter the exhaust gases before releasing them to the atmosphere. This method is used in most of the recent engines, where a catalytic converter is installed on the exhaust line of a gasoline engine and a particle filter in the case of a diesel engine.
- Limit the formation of pollutants during combustion. This method consists of optimizing the injection systems but also using fuels that tend to generate less pollutants during combustion.

This second alternative remains the most interesting because it reduces the formation of pollutants at the source (during combustion). It requires the use of fuels that can ensure the conditions of low emissions, abundance, autonomy but also of cost.

At the moment, the only fuels that can satisfy these conditions are gaseous hydrocarbons.

#### I.7 Gaseous hydrocarbons:

Several works have been published on the use of gaseous fuels in diesel engines such as biogas, natural gas and liquefied petroleum gas.

These fuels have a different chemical composition from conventional fuels, which has a significant impact on the performance and emissions of the engines.

#### I.7.1 Biogas:

Biogas is produced from the fermentation of organic matter in the absence of air, this process is called anaerobic fermentation [12]. Biogas consists mainly of methane and carbon dioxide, and its high auto-ignition temperature and octane number make it suitable for use in spark ignition engines. Its use as a primary fuel in diesel engines contributes to the reduction of NOx and fine particle emissions on the one hand, but on the other hand to an increase in CO and HC emissions and a decrease in engine performance due to the long ignition time and the slow flame propagation of the air-fuel mixture.

The presence of CO2 in the biogas causes a decrease of the combustion speed and a reduction of the maximum pressure in the cylinder, which leads to a considerable decrease of the maximum power [13].

#### I.7.2 Natural gas

Natural gas is very interesting, it is colorless and odorless in its pure form. However, natural gas is combustible and has a high calorific value. it is cleaner because of its low emission of polluting gases into the air and this contrary to diesel or gasoline.

From a chemical point of view, the composition of natural gas depends on the factors involved in the gas field; production process, gathering, conditioning and transportation. Natural gas consists primarily of methane but also contains other hydrocarbons and non-hydrocarbons and exists as a gas under atmospheric conditions. It is used under two forms: Compressed natural gas (CNG) or Liquefied natural gas (LNG).

Natural gas is, however, a greenhouse gas. Its low energy content per unit volume remains a problem. At optimal storage pressure (200 bar), CNG occupies four times the volume of gasoline and five times that of diesel for the same energy content.

#### I.7.3 Liquefied petroleum gas

LPG is an excellent alternative fuel, a mixture of light hydrocarbons, stored in a liquid state and derived from oil refining and natural gas processing. The hydrocarbons that constitute LPG, in its official name, are primarily propane and butane; the mixture may contain up to 0.5% of other light

hydrocarbons such as butadiene. It can be used pure or in a mixture with other fuels for the propulsion of cars.

LPG is considered an alternative solution with a low environmental impact (its exhaust gases are less pollutant especially in terms of PM and NOx, with zero lead and Sulphur). [14]

#### I.7.3.1 Liquefied petroleum gas fuel

LPG fuel refers to LPG used as a motor fuel. From a legal point of view, the molar percentage of propane must be situated in the range of 50-96 % (50-80% in summer), while butane must represent a molar percentage of 2 to 45 % [15]. It is a fuel used in many regions around the world, mainly in America, Europe and South Asia.

The benefits of this fuel give it the properties of a clean fuel and less harmful to the environment than gasoline, the high octane number of LPG allows its substitution for gasoline without engine modification.

The following table represents the physical characteristics of butane and propane, the main gases constituting LPG.

	Propane	Butane
Chemical formula	C3H8	C4H10
Boiling point	- 42 °C	-0.5 °C
higher heating value	50 MJ/kg	49.5 MJ/kg
Density	2 kg/m <sup>3</sup> (0 °C, 1 bar)	2.7 kg/m <sup>3</sup> (0 °C, 1 bar)
saturation vapour pressure	8,327 bar at 20 °C	2,081 bar à 20 °C

#### Table 4 Physical characteristics of butane and propane

According to the data in Table 4, LPG fuel has a higher calorific value per unit mass than gasoline and diesel, but its gaseous heating value per unit volume is lower because its density is much lower.

By its combustion properties, the LPG fuel is, in most cases, in accordance with the operating principle of gasoline engines for its high octane number. In fact, LPG fuel cars are bi-fuel vehicles, meaning that they run on either gasoline or gas. This makes it possible to keep the possibility of running on gasoline if necessary. The original fuel tank is in most cases kept. Moreover, even in

LPG fuel mode, the vehicle is started with gasoline, while the engine warms up a bit (a few tens of seconds).

the low cetane number of LPG makes it difficult to be used in large proportions in compression ignition engines [14]. Hence it can be used in the CI engine in the dual fuel mode. A dual fuel engine is basically a modified diesel engine in which LPG fuel (primary fuel) is inducted along with air. This fuel is the main source of energy for the engine. The primary gaseous fuel is compressed with air, but does not auto ignite due to its high self-ignition temperature. A small amount of diesel, usually called the pilot, is injected as in a normal diesel engine near the end of compression of the primary fuel–air mixture. This pilot diesel fuel, auto ignites first and acts as a deliberate source of ignition for the combustion of the gaseous fuel–air mixture.

The LPG fuel is stored in a specific tank, usually toroidal (circular) to fit in the spare wheel space or cylindrical in the case of a tank placed in the trunk of the vehicle. This last solution allows the use of larger tanks and thus increases the autonomy. The pressure inside the tank is about 5 bar, which is still a modest value.

The tank is filled to about 80% (automatic stop) so that there is a so-called gas space, which is a part of the tank filled with LPG in the gaseous state. This space allows the fuel to occupy more volume when the temperature changes.

#### I.7.3.2 The demand for LPG

LPG has more than 1000 different uses, including applications in industry, civil engineering, agriculture, households and transport. Thanks to simplified transport logistics, diversification of supply, availability of sources and above all environmental aspects. LPG has a high production and consumption dynamic. The world production of this fuel is close to 280 million tons. [16]

The growing awareness of the benefits of using LPG as an alternative to fossil fuels and the increasing level of adoption of clean and green energy sources in developed and developing countries show its effectiveness. Figure 4 represents LPG demand by sector in 2018.



Figure 4 LPG global demand by sector in 2018 [16]

LPG also has many applications within these categories, in the transport sector it is the third most common fuel for road transport in the world, after gasoline and diesel.

#### I.7.3.3 The risk of explosion

Because LPG is denser than air, unlike natural gas, it can accumulate at ground level and in lowlying areas such as basements in the event of a leak. This may create an explosion when an LPG/air mixture accumulates in the presence of an ignition source. This also results in a danger of asphyxiation because the LPG replaces the air and therefore reduces the oxygen concentration. The regulations therefore require that any room in which a gas appliance (natural or LPG) is located be well ventilated. To facilitate the detection of leaks, an odorant gas is added to the gas (natural or LPG): this odor allows to detect the leak of this gas.

In 1999, a series of accidents involving LPG vehicles led to a change in regulations making it mandatory to install a safety valve and a non-return valve on LPG tanks to prevent them from exploding in the event of a fire. [16]

#### I.7.3.4 LPG in Algeria

Algeria is the largest producer of natural gas in the Mediterranean region, with a production of 0.284 million cubic meters, which represents about half of the total production in the region. Knowing that 60% of LPG is extracted from natural gas, we can estimate a very important quantity of LPG produced in Algeria. [16]

#### I.7.3.5 The promotion of LPG fuel in Algeria

Algeria has adopted an energy strategy based on the promotion of clean and renewable energies. LPG, often called "Sirghaz" fuel, is part of these energy sources because of its economic and environmental benefits. [16]



Figure 5 LPG filling station [17]

The figure below shows the first public transport bus operating in LPG-diesel dual fuel mode in Algeria that was launched along with the first truck of this kind in January 2021. [18]



Figure 6 The first public transport bus operating in LPG-diesel dual fuel mode in Algeria [18]I.7.3.6 Advantages of LPG

#### Clean

Today, LPG is the only clean conventional energy source, it does not emit any particles, lead, benzene or sulfur. 60% of LPG comes from natural gas fields, so it is non-toxic and has no effect on the land, sea and air. One of the most effective uses of LPG is as an automotive fuel. If it replaces traditional liquid fuels, it will effectively improve air quality.

#### Efficient

In terms of energy performance, LPG is more efficient than other energies, this is due to its high calorific value as well as the fact that the LPG flame gives off more heat and a combustion efficiency that can be up to five times higher than other energy sources, thus 1 kg of propane is thermally equivalent to 3-6 kg of wood, 1.5 to 2 kg of coal, 1.29L of fuel oil and 1.38 KWh of electricity.

Its energy performance reduces energy wastage rates. [16]

#### **Technically advantageous**

Technically speaking, LPG has a high octane number and a high calorific value, which ensures a higher energy efficiency, resulting in a much more complete combustion.

The gaseous nature of LPG fuel avoids the dilution of lubricants at the level of the walls of the cylinders thus ensuring a better lubrication which makes it possible to appreciably reduce the wear of the engine and in particular that of the liners, the cylinders, the pistons and the rings.

In its liquid state, LPG is about 270 times smaller than in its gaseous state, making it easier to store and bottle and making it available in the most remote areas.

#### **Economically advantageous**

The low prices of LPG allow to reduce the expenses, it is economically preferable and ecologically favorable. The widespread use of LPG reduces the dependence on oil as 60% of it is derived from natural gas. The local use of LPG instead of exporting it frees up large surpluses of other fossil fuels for export because the prices of the latter are higher on the international market, allowing for considerable gains. [16]

#### I.8 Conclusion

The worldwide use of conventional fossil fuels is dominant compared to other forms of energy, these fuels are favored for transportation as they do not require heavy infrastructure for distribution. Nevertheless, the engines and fuels used play a significant role in the evolution of this consumption and their effects on the environment, so the transition to less polluting alternative fuels (LPG fuel especially for its numerous advantages) will be mandatory.

## Chapter II Dual fuel mode

#### II Dual fuel mode

#### **II.1** LPG-diesel dual fuel operation

All internal combustion (IC) reciprocating engines operate by the same basic process. First, a combustible mixture is compressed in a small volume between the cylinder and the head of a piston. Then, the mixture is ignited and the resulting high-pressure products of combustion push the piston through the cylinder. Two ignition methods are used in reciprocating IC engines, spark ignition (SI) and compression ignition (CI). Diesel engines operate with compression ignition method, where the intake air alone is compressed and at the end of the compression stroke the diesel fuel is injected at high pressure over the compressed air inside the combustion chamber which leads to ignite easily by virtue of its ignition temperature. But the LPG–diesel dual fuel engine utilizes the concept of both compression ignition and spark ignition principles to burn the mixture of primary gaseous (LPG) fuel and liquid pilot fuel [14].

In case of LPG–diesel dual fuel engine, the air-to-LPG mixture from the intake is drawn into the cylinder, just as it would be in a spark-ignited engine and this mixture is compressed in order to increase the temperature and pressure. At the end of the compression stroke the mixture is ignited by the injection of small quantity of pilot diesel fuel as shown in Fig. 7. This pilot injection acts as a source of ignition. The LPG gas-air mixture in the vicinity of the injected diesel spray ignites at number of places establishing a number of flame-fronts. Thus the combustion starts smoothly and rapidly. It is interesting to note that in a dual-fuel engine the combustion starts in a fashion similar to the CI engine but it propagates by flame fronts, i.e. in a manner similar to the SI engine. The power output of the engine is normally controlled by changing the amount of primary LPG gaseous fuel added to inlet manifold. The quantity of diesel fuel used will be varied depending upon the engine operating conditions and its design parameters, and generally the amount of pilot diesel required for the ignition is between 10% and 20% of operation on the diesel fuel alone at normal working loads [14].



Figure 7 LPG diesel dual fuel engine

#### **II.2** Diesel engine modifications

Diesel engines can be configured to run on LPG-diesel dual fuel mode, where LPG is mixed into the air intake, while the normal diesel fuel injection system still supplies a certain amount of diesel fuel, but at a reduced rate. The engine has to be modified to work in the dual fuel mode by attaching an LPG line to the intake manifold (indirect injection or High Pressure Direct Injection "HPDI") along with an evaporator. In the first and most deployed case, gaseous fuel flows through the regulating valve into the gas mixer assembled on the intake manifold. Supply of the LPG into the engine is accompanied by mechanical or electronic control for various loads and speeds of the engine. Depending on the type of the engine and gaseous fuel supply system the combustion process and the engine output will be varied. The mass flow rate of LPG is in proportion to the pressure difference between the gas mixer and the evaporator where the pressure is maintained nearly same as atmospheric pressure. But controlling the flow rate of the primary LPG fuel and pilot diesel fuel at different engine operating conditions is very critical in the LPG dual fuel engines. Lower LPG content may have no effect on soot emission reduction and performance improvement, and at the same time much higher LPG content probably makes incylinder pressure increased rapidly and damages the engine.
#### **II.2.1** Gaseous fuel injection

There are two main methods of using a gaseous fuel in a diesel engine, depending on its introduction into the cylinder:

#### II.2.1.1 Indirect gas injection

Dual-fuel engines are basically diesel engines that have been converted to dual-fuel mode in order to use two fuels that burn simultaneously in the cylinder. These fuels are a pilot fuel and a primary fuel that is gaseous in nature and provides the majority of the energy introduced into the engine. This type of internal combustion engine operates by auto-ignition of the pilot fuel injected into a highly compressed primary fuel-air mixture.



Figure 8 Schematic of an engine in dual-fuel mode with indirect injection.

A small quantity of pilot fuel is injected shortly before top dead center (towards the end of compression) in order to ignite the gas mixture (primary fuel) introduced into the cylinder under thermodynamic conditions (pressure and temperature) corresponding to the self-ignition

conditions of this pilot fuel. The last two phases (expansion and exhaust) take place in the same way as in spark ignition or compression engines. Fig. 8 shows the schematic of the operating principle of the engine in dual-fuel mode with indirect injection.

#### II.2.1.2 High Pressure Direct Injection

In this mode, at the end of the compression phase (before TDC), a small amount of pilot fuel (diesel) is first injected, followed by direct injection of the primary fuel into the combustion chamber. At the beginning of the injection of the gaseous fuel, the diesel fuel self-ignites, and initiates the combustion of the primary fuel [19]. Figure 9 represents the schematic of the HPDI (High Pressure Direct Injection) system. As it can be visualized in Fig. 8 the gas presents a non-premixed combustion. This stratified combustion offers better fuel economy and more efficient combustion, maintaining power output and effective efficiency equivalent to those of the conventional diesel engine, especially at low and medium loads. However, the injector structure is more complicated and the cost is higher.



Figure 9 Schematic of the high pressure direct injection system

It has a special concentric-needle shape which is essential for the HPDI mode. Unlike the indirect injection mode, which requires the introduction of gaseous fuel into the combustion chamber at

low pressure, this indirect injection mode is easier to implement in the conventional diesel engine as well, without much engine modification. It should be noted that more than 80% of diesel fuel can be reduced in this mode. Studies have shown that the substitution of gaseous fuel in HPDI mode reached 95% [20]. However, it is clear that the indirect injection mode is more convenient compared to the HPDI mode, which makes it one of the most promising ways to use gaseous fuel in diesel engines.

#### **II.3** Characteristics and performance of a dual-fuel engine

#### **II.3.1** Cylinder pressure and total heat release rate

Among the parameters affecting the formation of pollutants, as well as engine performance, is the combustion of the gas mixture in the combustion chamber. Gaseous fuel and diesel fuel are two types of fuel with different physical and chemical properties. The combustion of diesel fuel in the cylinder is called diffusion-controlled combustion, while that of LPG is called premixed combustion [21].

Researchers in [22] have experimentally analyzed the effect of dual fuel mode on the combustion for three different rates of substitution. Results have shown that the pressure peak has been lower in dual fuel mode compared to this of conventional diesel mode, for the different cases studied.



Figure 10 Cylinder pressure and heat release rate in a dual-fuel engine in dual-fuel mode

They also found that increasing the intake temperature could lead to the engine knocking problem.

Researchers have opted for the injection advance of the pilot fuel in order to have a reduction of unburnt hydrocarbons and to see the possibility of improving the efficiency of this mode of operation. They found that by increasing the injection advance the temperatures rises and HC emissions decrease, on the other hand, this increase unfortunately leads to a high concentration of NOx emissions in the exhaust gas.

#### **II.3.2** Effect on performance

The effective efficiency  $\eta_{eff}$  is the ratio of the mechanical power of the engine to the fuel energy consumed by the engine. It indicates the efficiency with which the input energy is converted into useful energy. By studying the diesel engine operating in dual-fuel mode, researchers aim to improve its efficiency. Abd Alla et al [22] conducted tests to investigate the effect of pilot fuel quantity, and diesel fuel injection advance, on the effective efficiency of a dual-fuel diesel engine. Their results showed that with increasing the amount of diesel pilot fuel, and the injection timing, the thermal efficiency of the engine is improved at low loads, due to the high pressure and temperature. The decrease of  $\eta_{eff}$  in dual-fuel mode was more evident at low and intermediate loads. In addition, at high loads and with a high gas substitution rate, the efficiency is slightly improved.

#### **II.4** Effect on pollutant emissions

#### **II.4.1** Effect on $NO_x$

NOx is considered the most harmful of all engine emissions. It is mainly due to the emission of the compound nitric oxide NO and nitrogen dioxide NO2. However, NO is the main component, and often accounts for more than 90% of NOx emissions, inside the engine cylinder. The formation of NO in the combustion zone is chemically complex.

The comparison of NOx emissions between the diesel engine in conventional mode and in dualfuel mode has been carried out by several researchers, who noted that, under all engine loads, NOx emissions in dual-fuel mode were lower than those in normal mode. Furthermore, it was observed that NOx emissions decreased with increasing engine speed in both diesel and dual-fuel modes. The effects of pilot fuel quantity and injection timing on NOx emissions in a dual-fuel engine were analyzed [22]. It was found that NOx emissions increase with the amount of pilot fuel at low and high engine loads, and with the diesel injection advance.

#### II.4.2 Effect on CO

CO is also classified as one of the most harmful engine emissions. Its formation is due to the incomplete combustion of the fuel, and the temperature in the cylinder. These two parameters, control the rate of fuel decomposition as well as its oxidation. A significant amount of CO, is usually generated in the fuel richer regions, due to lack of oxygen. However, a large amount of CO, can also be produced in the fuel poor region, when the combustion temperature is below 1450 K [23].

Researchers have studied the effect of pilot fuel quantity and injection timing on CO emissions, a decrease in CO emissions, due to the increase in the quantity of pilot fuel and the injection advance, was observed [22]. According to these researchers, this decrease is generated by the improvement of the combustion process. However, at high load, CO emissions are considerably higher in dual-fuel mode compared to conventional diesel mode. This increase has been explained by the presence of certain flame extinction zones in the combustion chamber, and incomplete oxidation of the airfuel mixture [23]. It has been concluded that the increase in gas substitution rate, accompanied by a reduction in the air-fuel ratio, promoted the CO formation mechanism.

#### **II.4.3** Effect on unburned hydrocarbons

HC emission is one of the emissions due to incomplete combustion of hydrocarbons, despite the fact that complete oxidation of HC occurs at low temperature. The effect of operational parameters on HC emission in dual-fuel mode has been studied. It has been concluded that in order to eliminate HC emissions for low and intermediate loads, the injection quantity of the pilot fuel should be increased with an injection advance. However, in order to minimize HC emissions, it is recommended to avoid very lean gas-air mixtures.

At low loads, HC emissions increase rapidly as the gas substitution rate increases, while at high loads HC emissions increase more slowly. The increase of HC emissions can be produced also by the effect of the engine speed variation, for a constant substitution rate, HC emissions decrease with increasing engine load. Since HC emissions decrease with increasing amounts of pilot fuel at high loads, a trade-off relationship between NOx and HC emissions in engines operating in dual-fuel mode was concluded.

#### **II.4.4** Effect on carbon dioxide

Carbon dioxide CO<sub>2</sub>, is a product of hydrocarbon combustion. The hydrocarbon fuel is first oxidized to CO during the combustion process. At a sufficiently high temperature in the cylinder, and with the presence of oxygen, CO is oxidized to form CO<sub>2</sub>. Thus, the formation of CO<sub>2</sub> is highly dependent on the temperature and the concentration of oxygen in the cylinder.

Tests were performed on a single-cylinder diesel engine, converted to dual-fuel mode, to analyze the CO2 emissions at different engine loads [23]. The results show that at low load, the difference in CO2 emissions is not significant, but at high load, due to the increasing amount of gas intake, the difference is larger. The CO2 emissions in dual-fuel mode are lower than those of conventional diesel over the entire load range tested [23]. Other tests have been carried out on the same type of engine, where the effect of the addition of gas on the CO2 emission has been studied. The engine in dual-fuel mode produces less CO2 (a reduction of 23% and 30%).

#### **II.4.5** Effect on soot emission

Particulate matter (PM) emission is one of the main concerns attributed to diesel engines. PM consists primarily of some organic compounds, carbonaceous material and sulfates [23]. The formation and oxidation of soot particles, have an excellent relationship with the local temperature, and the oxygen concentration. Soot particles are formed very early in the process of diffusive combustion due to the dissociation of fuels at high temperature in the absence of oxygen. Therefore, most of them are oxidized at very high temperatures, in the presence of oxygen. The formation of a homogeneous mixture, is very important to reduce particulate matter.

Soot emissions for the engine operating in diesel and dual-fuel mode were compared at different speeds and engine loads [25]. In dual-fuel mode, the amount of pilot diesel fuel was kept constant, while the engine load was adjusted by increasing or decreasing the amount of gaseous fuel. The results showed that as the engine load increased, soot emissions increased in diesel mode. A reduction in soot was observed in dual-fuel mode with increasing load.

The dual-fuel mode is, then, a very efficient technique to reduce the soot emissions, especially at high loads, where soot emissions were largely produced. Soot emissions are significantly lower in dual-fuel mode, compared to conventional diesel, for all engine loads.

# II.5 Conclusion

Diesel engines can be modified to run in dual fuel mode, these modifications depend on the engine and the method in which gaseous fuel will be supplied.

The conversion of diesel engines into dual fuel mode shows an important influence on both performance and emissions of the engines, a lot of DF mode parameters, such as injection timing, substitution rate and pilot fuel quantity, affect the characteristics of the engines. A good combination of these parameters can reduce significantly HC, soot, and NOx emissions.

In the next chapter, a validation through CFD simulation will be performed in order to investigate and predict the characteristics of an engine to be converted into dual fuel mode operation.

# Chapter III

CFD Simulation analyzing performance and emissions of dual fuel mode

# **III** CFD Simulation analyzing performance and emissions of dual fuel mode

# **III.1** Introduction

Nowadays, numerical modeling is very popular because of the lower cost compared to the financial means involved in an experimental study. This modeling can be based on thermodynamic, theoretical models...etc.

This method allows to have a good appreciation of the evolution of the combustion, and vary its parameters in order to reach an optimal result before working on the prototype.

# **III.2** Description of FL419 engine

In order to correctly run the simulation, a description of the engine, its characteristics and its dimensions is made.

The F4L912 is a German-designed, direct mechanical injection diesel engine with a 4-stroke cycle. Equipped with four in-line pistons for a total displacement of 3.768 liters, an air cooling system and a mechanical timing chain, this engine combines reliability, robustness and performance.

With a power range of 15 kW to 88 kW, this engine offers flexibility of use. It can be found equipping agricultural tractors, generators, compressors, backhoe loaders as well as on SNVI K66 trucks.

#### **III.2.1** Characteristics of the engine FL419

Table 5 below shows the technical characteristics of the engine F4L912.

And the figure 11 Represents a schematic of the engine and its different components. While Fig. 12 shows the dimensions of the cylinder and the piston.

Number of cylinders	4
Maximum power	54 kW at 2800 rpm
Cooling	With air
Displacement ( $cm^3$ )	3768
Bore (mm)	100
Stroke (mm)	120
Engine torque at nominal operation	208.2 N.m / 1650 rpm
Weight (kg)	330
Specific fuel consumption	200 g/kWh
Ignition order	1-3-4-2
Engine idle speed	650-700
Compression ratio	19

**Table 5** Technical characteristics of the engine F4L912



Figure 11 Schematic of the engine F4L912

- 1- Nozzle holder.
- 3- Drips collection pipe
- 4- Extendable cylinder head bolt
- 5- Overflow pipe
- 6- Discharge line to the injector
- 7- Rocker cover
- 8- Oil bath air purifiers
- 9- Cooling turbine
- 10- Generator
- 11-V-belt (cooling turbine)
- 12-V-belt (generator)
- 13-Camshaft gear
- 14-Lubricant discharge pipe
- 15-Intermediate gear
- 16-Extendable screw
- 17- Crankshaft crown
- 18-Pulley

- 19-Vibration damper
- 20-lubricant pump
- 21-Injection timing device
- 22-Lubricant suction pipe
- 23-Fuel supply pump
- 24-Injection pump
- 25-Oil level gauge
- 26-Oil tank
- 27- Crankcase
- 28-Lubricant filter
- 29-Speed control lever
- 30-Feeder filter
- 31-Oil cooler
- 32-Cylinder
- 33- Upper part of the air guide
- 34-Cylinder head



Figure 12 Cylinder and piston dimensions

## **III.3** Simulation software description

CONVERGE CFD software has been used as the simulation tool in this study, because of its numerous numerical advantages in the simulation of flows in internal combustion engines. CONVERGE includes advanced numerical techniques but also physical models describing the processes of spraying, turbulence and combustion, and also the interactions of these processes. These models have been examined and validated on internal combustion engines.

The objective of the simulation of the combustion in the F4L912 engine, is to predict the evolution of combustion, which allows to compare between the characteristics, performance and pollutants emission in both diesel and dual fuel modes.

## **III.4** Simulation steps

The main steps applied in order to perform a simulation with CONVERGE are given below:

- Realization of the geometry to be studied on a compatible 3D design software, (SolidWorks in our case), then saving it in STL format.
- Import the geometry into CONVERGE, which will generate a mesh that will be rectified if necessary.
- Precise the application type: IC Engine
- Introduction of the parameters of matter: species, chemical reactions.
- Introduction of operation and geometry parameters
  - Piston diameter
  - Stroke
  - rpm
  - Compression ratio
- Boundary conditions specification
  - Walls temperature
  - Initial pressure
  - Mass fraction of the species present in the combustion chamber at the end of the admission
- Injection modeling and the selection of turbulence and combustion parameters

- Introduction of mesh parameters
- Specification of output parameters of the simulation: Pressure, temperature, combustion products, velocity, etc.
- Verification of inputs and running the calculation

#### **III.5** Equations and models used

Computational fluid dynamics (CFD) is a branch of fluid mechanics that uses numerical analysis and data structures to analyze and solve problems that involve fluid flows. CONVERGE, as all CFD tools, is governed by physical equations which describe the principle of conservation of mass, momentum and energy. There are also many models used in such codes that simplify the equations and describe different phenomena like turbulence, etc.

In this chapter, a simulation and a comparison between dual fuel and diesel modes are performed, based on the equations and models given below: [26]

#### **III.5.1** Conservation of mass equation

The mass transport or mass conservation equation for a fluid is expressed as follows:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = S \tag{1}$$

Where

 $\rho$  : is the density of the fluid

 $u_i$ : is the *i*<sup>th</sup> component of the instantaneous velocity

#### $S: Mass \ source$

This equation is used for both compressible and incompressible flows.

#### **III.5.2** Conservation of momentum equation

The continuity of the fluid in the direction i in an inertial reference frame is expressed by :

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + S_i$$
(2)

Where viscosity stress tensor is given by:

$$\sigma_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \left( \frac{\partial u_k}{\partial x_k} \delta_{ij} \right)$$
(3)

With

P : static pressure

 $\mu$ : dynamic viscosity

 $S_i$ : Source term

 $\delta_{ij}$  : the Kronecker delta notation

If a turbulence mode is adopted, then the viscosity is replaced by the turbulent viscosity given by:

$$\mu_t = \mu + C_\mu \rho \frac{k^2}{\varepsilon} \tag{4}$$

Where

 $\mathcal{C}_{\mu}$ : Constant of the chosen turbulence model

k : kinetic energy of turbulence

E: turbulent dissipation

#### **III.5.3** Equation of state

The conservation of mass and momentum equations mentioned above can be applied for both compressible and incompressible fluids. However, the realization of a study on a compressible fluid, will require another equation that will link density, temperature and pressure, it is the equation of state.

CONVERGE proposes four models, that of ideal gas, Redlich-Kwong, Redlich-Kwong Soave and Peng-Robinson. For the study of an engine, CONVERGE recommends the use of the Redlich-Kwong model given below:

$$P = \frac{RT}{\nu - \beta_{rk} \nu_c} - \frac{a}{\nu^2 + \beta_{rk} \nu_c \nu} \tag{5}$$

With:

$$v_{c} = \frac{RT_{c}}{P_{c}}$$
$$a = a_{rk} \frac{p_{c} {v_{c}}^{2}}{\sqrt{T_{r}}}$$

P : pressure; R : the ideal gas constant; v : volume ; T : temperature;  $v_c$ : critical volume;  $T_c$  : critical temperature;  $p_c$ : critical pressure;  $\beta_{rk} = 0.08664$ 

#### III.5.4 Energy equation

The expression of the energy conservation equation for a compressible fluid is given by :

$$\frac{\partial \rho e}{\partial t} + \frac{\partial u_j \rho e}{\partial x_j} = -P \frac{\partial u_j}{\partial x_j} + \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left( K \frac{\partial T}{\partial x_j} \right) + \frac{\partial}{\partial x_j} \left( \rho D \sum_m h_m \frac{\partial Y_m}{\partial x_j} \right) + S \quad (6)$$

With

e: The specific internal energy. K: The thermal conductivity.  $h_m$  and  $Y_m$  are respectively

The enthalpy and mass fraction of the species m.

If a turbulence model is adopted, the thermal conductivity K will be replaced by the turbulent thermal conductivity given by:

$$K_t = K + C_p \frac{\mu_t}{Pr_t} \qquad (7)$$

With

 $\mu_t$ : turbulent viscosity

 $Pr_t$ : the Prandtl number for the turbulence

#### **III.5.5** The conservation of species equation

This equation is used to calculate the mass fraction of each species m existing in the domain, the one used for the case of the flows. each species m existing in the domain, that used for the case of compressible flows is defined as follows:

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_m u_j}{\partial x_j} = \frac{\partial (\rho D \frac{\partial Y_m}{\partial x})}{\partial x_j} + S_m \qquad (8)$$

with

$$\rho_m = Y_m \rho$$

\_ \_

u : velocity;  $\rho$  : density ;  $\rho_m$  : density of the species m;  $Y_m$ : mass fraction of the species m; D: mass diffusivity;  $S_m$  : energy source

For a given turbulence mode, mass diffusivity is calculated as follows:

$$D = \frac{v}{Sc}$$

Where Sc is Schmidt number.

CONVERGE also uses some models describing different phenomena, the combustion for example is modeled with input files that include species, thermodynamic data, and the reactions with their properties. CONVERGE software allows, using to predefined models, to calculate the different emissions produced by combustion, such as NOx, unburned hydrocarbons and PM. In the following these models will be described.

#### III.5.6 PM Emission Model

The HIROYASU-NSC model proposed by HIROYASU and KADOTA is used in the case of particulate matter. This model determines the mass production of fine particles  $M_s$  as a function

of the difference between the mass formation rate of fine particles  $\dot{M}_{sf}$  and its mass oxidation rate  $\dot{M}_{so}$  by the following law:

$$\frac{dM_s}{dt} = \dot{M}_{sf} - \dot{M}_{so} \tag{9}$$

#### III.5.7 NOx formation model

CONVERGE adopts the Zeldovich model for the formation of NOx, this approach consists of calculating the formation rate based on the following chemical reactions:

$$0 + N_2 \leftrightarrow NO + N$$
$$N + O_2 \leftrightarrow NO + O$$
$$N + OH \leftrightarrow NO + H$$

From these equations, the NOx formation rate is given by the following formula:

$$\frac{d[NO]}{dt} = 2k_{R1,f}[O][N_2] \frac{1 - [NO]^2 / (K[O_2][N_2])}{1 + k_{R1,r}[NO] / (k_{R2,f}[O_2] + k_{R3,f}[OH])}$$
(10)

With

$$K = (k_{R1,f}/k_{R1,r})(k_{R2,f}/k_{R2,r})$$

The reactions constants:

$$k_{R1,f} = 7.6 \times 10^{13} \exp\left(-\frac{3800}{T}\right)$$
$$k_{R1,r} = 1.6 \times 10^{13}$$
$$k_{R2,f} = 6.4 \times 10^{9} T \exp\left(-\frac{3150}{T}\right)$$
$$k_{R2,r} = 1.5 \times 10^{9} T \exp\left(-\frac{19500}{T}\right)$$
$$k_{R3,f} = 4.1 \times 10^{13}$$

$$k_{R3,r} = 2 \times 10^{14} \exp\left(-\frac{23650}{T}\right)$$

The subscript "f" refers to a direct reaction, and the subscript "r" to a reverse reaction.

#### **III.5.8** Injection model

On a diesel engine, the jet of liquid diesel is injected into the combustion chamber near the end of the compression process. After injection, the fuel undergoes atomization and vaporization followed by mixing with air. Ignition and combustion occur due to thermodynamic conditions.

Thus to simulate the injection of diesel, CONVERGE initially introduces identical drops of diesel which are statistically represented in the spray domain. The atomization as well as the rupture of the droplets are described according to the hybrid Kevin-Helmholtz Rayleigh-Taylor model.

The CONVERGE software allows the user to enter the mass of diesel to be injected, the injection time, the injection duration and the injection pressure.



Figure 13 Injection model in CONVERGE

#### **III.5.9** Turbulence model

Turbulence is modeled by k- $\varepsilon$  model. This approach allows to take into account the compressibility of the spray as well as the effect of the interaction of the turbulences of the various physical phenomena that appear during the studied process.

This model is based on the two following equations:

• For turbulent kinetic energy k

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_i k}{\partial x_i} = \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ \frac{\mu}{P r_{tke}} \frac{\partial k}{\partial x_j} \right] - \rho \varepsilon + S \qquad (11)$$

With:

k the turbulent kinetic energy,  $\varepsilon$  turbulent dissipation and S the energy source.

Stress tensor is given by:

$$\sigma_{ij} = 2\mu_t S_{ij} - \frac{2}{3}\delta_{ij} \left(\rho k + \mu_t \frac{\partial u_i}{\partial x_i}\right)$$
(12)

And for the turbulent viscosity

$$\mu_t = C_{\mu} \rho \frac{k^2}{\varepsilon} \qquad (13)$$

For dissipation ε

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial (\rho u_i \varepsilon)}{\partial x_i} = \frac{\partial}{\partial x_j} \left( \frac{\mu}{P r_{tke}} \frac{\partial \varepsilon}{\partial x_j} \right) - c_{\varepsilon 3} \rho \varepsilon \frac{\partial u_i}{\partial x_j} + \left( c_{\varepsilon 1} \frac{\partial u_i}{\partial x_i} \sigma_{ij} - c_{\varepsilon 2} \rho \varepsilon + c_s s_s \right) - \rho R$$

R,  $c_{\varepsilon 1}$ ,  $c_{\varepsilon 2}$ ,  $c_{\varepsilon 3}$  are constants of the turbulence model.

#### **III.6** The geometry adopted for the simulation

In CONVERGE the geometric model represents the domain occupied by the fluid. In our case, it represents the volume delimited by the cylinder, the piston and the cylinder head. It is represented in the following figures.

In order reduce the simulation time, the computational domain is only a 1/5 of the cylinder with periodic limits. This reduced domain includes one of the 5 injection nozzles.



Figure 14 Combustion chamber geometry



Figure 15 Piston geometry

#### **III.7** Preliminary calculations

#### **III.7.1** Proportion of pilot and primary fuels consumed per cycle

#### **III.7.1.1** Diesel mass consumed per cycle (diesel mode)

The hourly diesel consumption in diesel mode operation is given by:

$$C_h = C_s P \quad [g/h] \qquad (13)$$

Where P is the power in kW and  $C_s$  is the specific consumption in g/kWh. (extracted from characteristic curves, for the K66 truck engine found in appendices)

Since one engine cycle corresponds to two crankshaft revolutions, the fuel consumption per cycle is given by:

$$m_D = \frac{2C_h}{60N} = \frac{2C_s P}{60N}$$
 [g/cycle] (14)

Where  $m_D$  is the mass of diesel consumed per cycle, and N the frequency of rotation in rpm.

#### **III.7.1.2** Calculation of the primary fuel mass (LPG)

Since the substitution of diesel in the dual-fuel mode is a calorific substitution (in a way that keeps the same energy content), the mass of LPG to be injected for a given substitution rate  $S_D$  is calculated as follows:

$$m_{LPG}L_{HVLPG} = \frac{S_D m_D L_{HVDiesel}}{100}$$
(15)

Which gives : 
$$m_{LPG} = \frac{S_D m_D L_{HVDiesel}}{100 L_{HVLPG}}$$
 (16)

With:

 $L_{HVLPG}$  is the lower heating value of LPG (50 MJ/kg)

 $L_{HVDiesel}$  is the lower heating value of diesel (42 MJ/kg)

55

 $S_D$  is the substitution rate in %

 $m_D$  Mass of diesel injected per engine cycle in kg

 $m_{LPG}$  is Mass of LPG injected per engine cycle in kg

The diesel consumption for dual-fuel operation is given by :

$$m_D' = m_D \left( 1 - \frac{S_D}{100} \right)$$

Which gives us the following table:

Substitution	Fuel consumption $\dot{m}[g/s]$ :						
rate $S_D[\%]$ :	0	25		50		80	
N[rpm]:	Diesel	LPG	Diesel	LPG	Diesel	LPG	Diesel
700	0.8278	0.17302	0.6209	0.34604	0.4139	0.5562	0.1655
800	0.9633	0.20133	0.7225	0.40266	0.4816	0.6473	0.1926
900	1.1488	0.24009	0.8616	0.48019	0.5744	0.7719	0.2297
1000	1.407	0.29407	1.0553	0.58814	0.7035	0.9455	0.2814
1100	1.7276	0.36106	1.2957	0.72212	0.8638	1.1609	0.3455
1200	1.9886	0.41562	1.4915	0.83124	0.9943	1.3363	0.3977
1300	2.2598	0.4723	1.6949	0.9446	1.1299	1.5185	0.4519
1400	2.3673	0.49478	1.7755	0.98955	1.1837	1.5908	0.4734
1500	2.4789	0.51809	1.8592	1.03617	1.2394	1.6658	0.4957

Table 6 LPG/diesel injection rate as a function of engine speed

The figure 16 below represents the consumption curves of diesel fuel as a function of engine speed (700 rpm to 1500 rpm) at different substitution rates.

For this simulation, the speed 1500 rpm with a substitution rate of 80% are adopted.



Figure 16 Consumption curves of diesel fuel as a function of engine speed at different substitution rates

#### III.7.2 Mass fractions in the cylinder

The dual fuel mode is implemented into the simulation by modifying the species present in the cylinder before combustion (the results of admission of the air/LPG mixture), initial conditions like admission pressure and temperature were studied by CHENDOUH and HAMMOUDI in [10], who analyzed the air/fuel mixer, and boundary conditions used in the simulation are presented in the following table:

Substitution rate	80 %
Diesel consumption	0.4957 [g/s]
LPG consumption	1.6658 [g/s]
Admission temperature	355 K
Admission pressure	91489 Pa
Cylinder temperature	410 K
Cylinder head temperature	484 K
Head of piston temperature	538 K

 Table 7 Initial conditions of the simulation

## **III.8** Dynamic mesh

One of the advantageous of the use of CONVERGE software is its adaptive mesh. CONVERGE automatically creates the mesh at runtime, and dynamically adapts it throughout the simulation, the figure below shows the difference in the mesh before and after compression.



Figure 17 Mesh in two different positions (a) before compression (b) near TDC

# **III.9** Presentation of results

#### **III.9.1** Evolution of the pressure in the cylinder

The superposition of the two diagrams of the two modes: diesel and 80% dual mode operation gives us:



**Figure 18** Evolution of the pressure in the cylinder for both modes (diesel and 80% dual fuel) The following results are found

Mode	Diesel	Dual fuel
Maximum pressure (MPa)	12.38	11.75

Table 8 Maximum pressures in diesel and dual fuel modes

#### **Discussion:**

A light diminution of the maximum pressure is observed in the dual fuel mode compared to pure diesel mode, which may explain the decrease in overall performance, a brutal augmentation of the pressure after injection is also observed, which can cause deterioration of engine components, this phenomenon can be controlled by adjusting injection timing, as discussed above. Different steps of the combustion that led to these observations is presented below:



(a) Compression stroke



(b) Combustion



(c) Expansion

Figure 19 Different steps of the combustion





Figure 20 Soot mass production

The results obtained clearly show that dual-fuel operation is a very effective technique for reducing soot emissions. In fact, soot emissions in dual fuel mode are much lower than diesel operation, (<5% in our case) and this for a substitution rate of 80%.

Thus, the dual-fuel operation allows a significant reduction of fine particle emissions. This is due to the fact that gaseous fuels have a very low tendency to produce particles.

#### III.9.3 NOx emissions

Fig. 19 below shows NOx emission for both modes, it can be seen that NOx emissions in dual fuel operation are lower (about 50 %) than conventional diesel mode.

Since NOx formation is directly related to high temperatures, this reduction is mainly due the relatively lower temperature in the cylinder during combustion.



Figure 21 NOx emission for both operation modes





Figure 22 Unburned hydrocarbons in diesel and DF modes

Before injection, diesel mode does not show HC while a constant value of HC is present for DF mode, this is explained by the fact that CONVERGE considers the primary fuel/air mixture of the admission stroke as unburned hydrocarbons.

In the other hand, after injection and combustion, HC increase significantly in diesel mode, while they become nearly absent in DF mode, which shows the efficiency of the combustion in this latter mode.





Figure 23 CO emission for the two operation modes

Since CO is a result of combustion, there is no trace for it before injection. CO emissions, however, increase rapidly after injection.

A large difference between the two modes is observed, dual fuel operation ensures much lower CO emissions in these particular conditions. Different loads or injection timings can change this improvement and diesel may perform better.

This reduction, like HC emissions, reflects the good and complete combustion of the fuel.



III.9.6 CO<sub>2</sub> emission

Figure 24 CO2 emission for both modes

In a way similar to CO, dual fuel mode shows a considerable reduction in CO<sub>2</sub> emissions.

This shows the effectiveness and the benefits of dual fuel operation in reducing the emissions of such a greenhouse gas.

#### III.10 Conclusion

Through this CFD simulation, we obtained a first overview of the combustion process in dual-fuel mode of the studied engine.

This analysis has shown, for a substitution rate of 80%, very good efficiency in reducing pollutant emissions, including NOx, HC, soot, CO and CO<sub>2</sub>. Many emissions depend on several functioning parameters like injection timing and the quantity of pilot fuel. Thus, other simulations with different parameters need to be performed to completely analyze this operation mode.

CONVERGE has proven itself to be an efficient tool in analyzing IC engines and predicting not only performance variations, but also emissions.

# General Conclusion

# **General conclusion**

Countries and major energy producers are confronted with an increasingly energy consuming world. The progressive depletion of fossil fuels and the resulting environmental degradation is becoming very worrying and is prompting an intensive search for a substitution process using alternative fuels in internal combustion engines.

Alternative gaseous fuels open up an interesting and promising new technique in terms of soot and NOx reduction compared to the conventional mode. However, hydrocarbon and carbon monoxide remain dependent to many operation conditions such as injection timing and primary fuel quantity emissions. Research laboratories are therefore developing new techniques to reduce these polluting emissions while trying to preserve engine performance.

Gaseous fuels, especially LPG, offer not only lower pollutant emissions, but also many technical and economical advantageous. With Algeria being one of the major producers of LPG and natural gas, it can profit from the conversion of engines into dual fuel mode at many levels.

CFD simulation using CONVERGE has shown a significant importance through this study, it allows to predict performance and emissions. With a smooth interface, precision and specialized IC engines applications, CONVERGE marks its efficiency performing such simulations.

This work offers a theoretical base that prompts further work that aims to improve the comprehension of LPG dual fuel engines through developing its different components (fuel mixer, injectors, etc.) and also realizing a test bench that offers the possibility of experimental tests with different conditions to validate the theoretical search.

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## Appendices

