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ORIGINAL PAPER

Control of emissions in an internal combustion engine: first approach for sustainable design

Andrés F. Duque Amaya[1,3] · **Adalberto Gabriel Díaz Torres**[1,3] · **Diego A. Acosta**[2,3]

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Abstract A mathematical model of emissions was developed in a Twingo D7F engine. The effects of variations in compression ratio, fuel/air equivalence ratio, spark advanced and combustion duration under pollutant emissions were studied. Analysis and data collection were performed in an engine bank using a data acquisition system integrated to an Interactive Engineering Environment. A control strategy was implemented to guarantee emissions reduction.

Keywords Internal combustion engine · Mathematical model · Control of emissions · Sustainable design · Interactive engineering environment

1 Introduction

Urban air pollution is a very complicated problem. Exhaust emissions from internal-combustion engines account for a major portion of this problem. Until the middle of the 20th century the number of internal combustion engines in the world was small enough that the pollution they emitted was tolerable, and the environment, with the help of sunlight, stayed relatively clean [5]. As world population grew, power plants, factories, and an ever-increasing number of automobiles, began to pollute the air to the extent that it was no longer acceptable. During the 1940s, air pollution as a problem was first recognized in the Los Angeles basin in California [17]. Two causes of this were the large population density and the natural weather conditions of the area. The large population created many factories and power plants, as well as one of the largest automobile densities in the world. Smoke and other pollutants from the many factories and automobiles, combined with fog that was common in this ocean area, led to generation of smog. During the 1950s, the smog problem increased along with the increase in population density and automobile density. It was recognized that the automobiles were the major contributors to the problem, and by the 1960s emission standards were enforced in California [17]. During the decades that followed, emission standards were adopted in the rest of the United States and in Europe and Japan. By making engines more fuel efficient, and with the use of after-exhaust treatment, emissions per vehicle of HC, CO, and NOx were reduced by about 95 % during the 1970s and 1980s [5]. Lead, one of the major air pollutants, was phased out as a fuel additive during the 1980s. More fuel-efficient engines were developed, and by the 1990s the average automobile consumed less than half the fuel used in 1970. However, during this time the number of automobiles greatly increased, resulting in no overall decrease in fuel usage. As world population grows, emission standards become more stringent out of necessity. The major causes of these emissions depend on various parameters (engine design parameters, operational parameters, exhaust gas after treatment, fuel types, fuel additives and lubricants). This work discusses and quantify the effect of some the parameters on the emissions to the environment in a Twingo D7F engine.

✉ Andrés F. Duque Amaya
aduquea1@eafit.edu.co

Adalberto Gabriel Díaz Torres
gdiaz@eafit.edu.co

Diego A. Acosta
dacostam@eafit.edu.co

1 Grupo de Ingeniería, Energía, Exergía y Sostenibilidad (IEXS), Cra 49 7sur 50, Medellín, Colombia

2 Grupo de Desarrollo y Diseño de Procesos, Cra 49 7sur 50, Medellín, Colombia

3 Universidad EAFIT, Medellín, Colombia

2 Undesirable emissions generated in the combustion process

Fuel combustion in internal combustion engines is almost always incomplete and generates emissions that pollute the environment and contribute to global warming, acid rain, smog, odors, and respiratory and other health problems. The major causes of these emissions are non-stoichiometric combustion conditions, dissociation of nitrogen, impurities in the fuel and air and other operational engine parameters [12]. The emissions of concern are hydrocarbons (HC), carbon monoxide (CO), nitrogen oxides (NOx), Sulphur, and solid carbon particulates. The characteristics and emission causes are presented below.

2.1 Hydrocarbons emissions

Exhaust gases leaving the combustion chamber of an internal combustion engine contain up to 6000 ppm of hydrocarbon components, the equivalent of 1–1.5 % of the fuel [11]. About 40 % of these gases are unburned gasoline fuel components. The other 60 % consists of partially reacted components that were not present in the original fuel. These consist of small non equilibrium molecules which are formed when large fuel molecules break up (thermal cracking) during the combustion reaction. It is often convenient to treat these molecules as if they contained one carbon atom. The makeup of HC emissions will be different for each gasoline blend, depending on the original fuel components. Combustion chamber geometry and engine operating parameters also influence the HC component production. When hydrocarbon emissions get into the atmosphere, they act as irritants and odorants; some are carcinogenic. All components except CH_4 react with atmospheric gases to form photochemical smog producing high atmospheric effects, making it necessary to control its generation. Main Causes of HC emissions are nonstoichiometric air–fuel ratio, incomplete combustion, crevice volumes, deposits and oil on combustion chamber walls.

2.1.1 Nonstoichiometric air–fuel ratio

Hydrocarbons (HC) emission levels are a strong function of air–fuel ratio (A_F). With a fuel-rich mixture there is not enough oxygen to react with all the carbon, resulting in high levels of HC and CO in the exhaust products. This is particularly true in engine start up, when the air–fuel mixture is purposely made very rich. It is also true to a lesser extent during rapid acceleration under load. HC emissions also increase at very lean mixtures due to poor combustion and misfires. Therefore, it is convenient to establish the optimal operation conditions for each engine to minimize HC generation.

2.1.2 Incomplete combustion

Even when the fuel and air entering an engine are at the ideal stoichiometric proportion, perfect combustion does not occur and some HC ends up in the exhaust. There are several causes for this: (1) Incomplete mixing of the air and fuel results in some fuel particles not finding oxygen to react with, (2) Flame quenching at the walls leaves a small volume of unreacted air-and-fuel mixture. The thickness of this unburned layer is on the order of tenths of a mm. Some of this mixture, near the wall that does not originally get burned as the flame front passes, will burn later in the combustion process as additional mixing occurs due to swirl and turbulence. Another cause of flame quenching is the expansion which occurs during combustion and power stroke. As the piston moves away from Top Death Center (TDC), expansion of the gases lowers both temperature and pressure within the cylinder. This slows down combustion and finally quenches the flame somewhere late in the power stroke. This leaves some fuel particles unreacted. High exhaust residual causes poor combustion and a greater likelihood of expansion quenching. This is experienced at low load and idle conditions. High levels of exhaust gas recirculation (EGR) will also cause this. It has been found that HC emissions can be reduced if a second spark plug is added to an engine combustion chamber. By starting combustion at two points, the flame travel distance and total reaction time are both reduced, and less expansion quenching results.

2.1.3 Crevice volumes

During the compression stroke and early part of the combustion process, air and fuel are compressed into the crevice volume of the combustion chamber at high pressure. As much as 3 % of the fuel in the chamber can be forced into this crevice volume. Later in the cycle during the expansion stroke, pressure in the cylinder is reduced below crevice volume pressure, and reverse blow by occurs. Fuel and air flow back into the combustion chamber, where most of the mixture is consumed in the flame reaction. However, by the time the last elements of reverse blow by flow occur, flame reaction has been quenched and unreacted fuel particles remain in the exhaust. Location of the spark plug relative to the top compression ring gap will affect the amount of HC in engine exhaust, the ring gap being a large percent of crevice volume. The farther the spark plug is from the ring gap, the greater is the HC in the exhaust. This is because more fuel will be forced into the gap before the flame front passes. Crevice volume around the piston rings is greatest when the engine is cold, due to the differences in thermal expansion of the various materials. Up to 80 % of all HC emissions can come from this source.

2.1.4 Deposits on combustion chamber walls

Gas particles, including those of fuel vapor, are absorbed by the deposits on the walls of the combustion chamber. The amount of absorption is a function of gas pressure, so that the maximum occurs during compression and combustion. Later in the cycle, when the exhaust valve opens and the cylinder pressure is reduced, absorption capacity of the deposit material is lowered and gas particles are desorbed back into the cylinder. These particles, including some HC, are then expelled from the cylinder during the exhaust stroke. This problem is greater in engines with higher compression ratios due to the higher pressure these engines generate. More gas absorption occurs as pressure goes up. Clean combustion chamber walls with minimum deposits will reduce HC emissions in the exhaust. Most gasoline blends include additives to reduce deposit build up in engines. Older engines will typically have a greater amount of wall deposit build up and a corresponding increase of HC emissions. This is due both to age and to less swirl that was generally found in earlier engine design. High swirl helps to keep wall deposits to a minimum. When lead was eliminated as a gasoline additive, HC emissions from wall deposits became more severe. When leaded gasoline is burned the lead treats the metal wall surfaces, making them harder and less porous to gas absorption.

2.1.5 Oil on combustion chamber walls

A very thin layer of oil is deposited on the cylinder walls of an engine to provide lubrication between them and the moving piston. During the intake and compression strokes, the incoming air and fuel comes in contact with this oil film. In much the same way, as wall deposits, this oil film absorbs and desorbs gas particles, depending on gas pressure. During compression and combustion, when the cylinder pressure is high, gas particles, including fuel vapor, are absorbed into the oil film. When pressure is later reduced during expansion and blow down, the absorption capability of the oil is reduced and fuel particles are desorbed back into the cylinder. Some of this fuel ends up in the exhaust. Propane is not soluble in oil, so in propane-fueled engines the absorption-desorption mechanism adds very little to HC emissions. As an engine ages, the clearance between piston rings and cylinder walls becomes greater, and a thicker film of oil is left on the walls. Some of this oil film is scraped off the walls during the compression stroke and ends up being burned during combustion. Oil is a high molecular weight hydrocarbon compound that does not burn as readily as gasoline. Some of it ends up as HC emissions. This happens at a very slow rate with a new engine but increases with engine age and wear. Oil consumption also increases as the piston rings and cylinder walls wear. In older engines, oil being burned in the combustion chamber is a major source of HC emissions. In addition to oil consumption going up as piston rings wear, blow by also increase. The increase in HC emissions is therefore both from combustion of oil and from the added crevice volume flow.

2.2 Carbon monoxide emissions

Carbon monoxide, a colorless, odorless, poisonous gas, is generated in an internal combustion engine when it's operated with a fuel-rich equivalence ratio. When there is not enough oxygen to convert all carbon to CO_2, fuel does not burn completely and some carbons ends up as Carbon Monoxide (CO). Typically, the exhaust of an SI engine contains about 0.2–0.5 % of carbon monoxide [11]. A well designed SI engine operating under ideal conditions can have an exhaust mole fraction of CO as low as 10^{-3} %. Since spark-ignition engines often operate close to stoichiometric conditions at part load and fuel rich at full load, CO emissions are significant and must be controlled. The levels of CO observed in spark-ignition engine exhaust gases are lower than the maximum values measured within the combustion chamber, but higher than equilibrium values for the exhaust conditions. Thus, the processes that govern CO exhaust levels are kinetically controlled. In premixed hydrocarbon-air flames, the CO concentration increases rapidly in the flame zone to a maximum value, which is larger than the equilibrium value for adiabatic of the fuel–air mixture. CO formation is one of the main reaction steps in the hydrocarbon combustion mechanism:

$$RH \rightarrow R \rightarrow RO_2 \rightarrow RCHO \rightarrow RCO \rightarrow CO \qquad \text{(R1)}$$

where R is a hydrocarbon radical. The CO formed by this combustion process path is then oxidized to CO_2, at a slower rate. The main CO oxidation reaction in hydrocarbon-air flames is:

$$CO + OH \rightleftarrows CO_2 + H \qquad \text{(R2)}$$

It is generally assumed that in the post flame combustion products in a spark ignition engine, at conditions close to peak cycle temperatures (2800 K) and pressures (15–40 atm-a), the carbon–oxygen–hydrogen system is equilibrated. Thus, CO concentrations in the immediate post flame burned gases are close to equilibrium. However, as the burned gases cool during the expansion and exhaust strokes, depending on the temperature and cooling rate, CO oxidation process [reaction (R2)] may not remain locally equilibrated. Other reactions important to CO chemistry are the recombination of three body radicals which are rate controlling.

$$H + H + M \rightleftarrows H_2 + M \qquad \text{(R3)}$$

$$H + OH + M \rightleftarrows H_2O + M \qquad \text{(R4)}$$

$$H + O_2 + M \rightleftarrows HO_2 + M \qquad \text{(R5)}$$

Studies using this simplified kinetic model have confirmed that at peak cylinder pressures and temperatures, equilibration times for CO are faster than those times characteristic of changes in burnt gas conditions due to compression or expansion. Thus the CO concentration rapidly equilibrates in the burnt gases just downstream of the reaction zone following combustion of the hydrocarbon fuel.

2.3 Oxides of nitrogen (NO_X)

Exhaust gases of an engine can have up to 2000 ppm of nitrogen oxides [11]. Most of this will be nitrogen monoxide (NO), with low amounts of nitrogen dioxide (NO_2), and traces of other nitrogen–oxygen combinations. These are all grouped together as NO_x, with x representing some suitable number. NO_x is a very undesirable emission, and regulations that restrict the allowable amount continue to become more stringent. Released NO_x reacts in the atmosphere to form ozone and is one of the major causes of photochemical smog. NO_x is created mostly from nitrogen present in air. Nitrogen can also be found in fuel blends, which may contain trace amounts of NH_3, NC, and HCN, but this would only contribute to a minor degree. There are a number of possible reactions that form NO (Zeldovich mechanism) [3], all of which are probably occurring during the combustion process and immediately after. Some of them are:

$$\mathrm{O} + \mathrm{N_2} \leftrightarrow \mathrm{N} + \mathrm{NO} \tag{R6}$$

$$\mathrm{O_2} + \mathrm{N} \leftrightarrow \mathrm{O} + \mathrm{NO} \tag{R7}$$

$$\mathrm{N} + \mathrm{OH} \leftrightarrow \mathrm{H} + \mathrm{NO} \tag{R8}$$

NO can react later with atmospheric oxygen to form NO_2 causing photochemical smog [11]:

$$\mathrm{NO} + \mathrm{H_2O} \leftrightarrow NO_2 + H_2 \tag{R9}$$

$$O_2 + N \leftrightarrow O + NO \tag{R10}$$

$$NO_X + sunlight \rightarrow NO + O + smog \tag{R11}$$

Monatomic oxygen is highly reactive and initiates a number of different reactions, one of which is the formation of ozone:

$$O + O_2 \rightarrow O_3 \tag{R12}$$

Ground level ozone is harmful to lungs and other biological tissues. It's harmful to trees and reacts with rubber, plastics, and other material producing noxious gases. The most important engine variables that affect NO emissions are the fuel/air equivalence ratio, the burned gas fraction and spark timing. The burned gas fraction depends on the amount of diluent such as recycled exhaust gas (EGR) used for NO_x emissions control, as well as the residual gas fraction [2]. Fuel properties also affect burned gas conditions; the effect of normal variations in gasoline properties is modest, however. The effect of variations in these parameters can be explained by the NO formation mechanism and changes in temperature profile and oxygen concentration in the burned gases during the combustion process and early stage of the expansion stroke, are the important factors.

2.3.1 air–fuel ratio

Large amounts of NO emissions occur when the gas cylinder temperature is at a maximum. Detailed predictions of NO concentrations in the burned gases suggest that the concentration versus time under fuel-lean conditions are different in character from those for fuel-rich conditions. In lean mixtures NO concentrations freeze early in the expansion process and little NO decomposition occurs. In rich mixtures, substantial NO decomposition occurs from the peak concentrations present when the cylinder pressure is at a maximum. Thus, in lean mixtures, gas conditions at the time of peak pressure are especially significant [13].

2.3.2 Burned gas fraction

The unburned mixture in the cylinder contains fuel vapor, air, and burned gases. The burned gases are residual gases from the previous cycle and any exhaust gases recycled to the intake for NO_x emissions control. The residual gas fraction is influenced by load, valve timing (especially the extent valve overlap), and, to a lesser degree, by speed, air–fuel ratio, and compression ratio. The burned gases act as a diluent in the unburned mixture; the temperature reached after combustion varies inversely with the burned gas mass fraction. Hence, increasing the burned gas fraction reduces NO emissions levels. However, it also reduces the combustion rate and, therefore, makes stable combustion more difficult to achieve. The main effect of the burned gases diluent in the unburned mixture on the NO formation is that it reduces flame temperatures by increasing the heat capacity of the cylinder charge, per unit mass of fuel.

2.3.3 Spark timing

Spark timing significantly affects NO emission levels. Advancing the timing so that combustion occurs earlier in the cycle increases the peak cylinder pressure (because more fuel is burned before TC and the peak pressure moves closer to TC where the cylinder volume is smaller); retarding the timing decreases the peak cylinder pressure (because more of the fuel burns after TC). Higher peak cylinder pressures result in higher peak burned gas temperatures, and hence higher NO formation rates. For lower peak cylinder pressures, lower NO formation rates result.

2.4 Other emissions

The exhaust of internal combustion engines contains solid carbon soot particles that are generated in the fuel-rich zones within the cylinder during combustion [5]. These are seen as exhaust smoke and are an undesirable odorous pollution. Maximum density of particulate emissions occurs when the engine is under maximum load fuel injection to supply maximum power. Soot particles are clusters of solid carbon spheres. These spheres have diameters from 10–80 nm with most within the range of 15–30 nm [19]. The spheres are solid carbon with *HC* and traces of other components absorbed on the surface. A single soot particle will contain up to 4000 carbon spheres. These carbon spheres are generated in the combustion chamber in the fuel-rich zones where there is not enough oxygen to convert all carbon to carbon dioxide (CO_2) [23]:

$$C_X H_Y + zO_2 \rightarrow CO_2 + bH_2O + cCO + dC \qquad \text{(R13)}$$

Particulate generation can be reduced by engine design and control of operating conditions, but quite often this will cause other adverse results [22]. If the combustion time is extended by combustion chamber design and timing control, particulate amounts in the exhaust can be reduced. Soot particles originally generated will have a greater time to be mixed with oxygen and combusted to CO_2. However, a longer combustion time means a high cylinder temperature and more NO_x generated. Dilution with EGR lowers NO_x emissions but increases particulates and *HC* emissions. Higher injection pressure gives a finer droplet size, which reduces *HC* and particulate emissions but increases cylinder temperature and NO_x emissions. Engine management systems are programmed to minimize NO_x, *HC*, *CO*, and particulate emissions, by controlling ignition timing, injection pressure, injection timing, and/or valve timing. Obviously, compromising is necessary. In most engines, exhaust particulate amounts cannot be reduced to acceptable levels solely by engine design and control.

2.5 Impact of control emissions in sustainable engines

The idea of sustainability goes beyond the engineering and science associated with green chemistry and engineering, to incorporate social/health and economic factors into the discussion of the most appropriate technologies to implement. Sustainability includes the concepts of ecosystems and human health. Incorporating these issues into engineering design creates new challenges in terms of valuation, thinking on a global scale. According to the Brundtland Commission (formerly known as the World Commission on Environment and Development), sustainable development is generally defined as "providing for human needs without compromising the ability of future generations to meet their needs" [17]. The U.S. Environmental Protection Agency describes sustainability from two perspectives [22]: a public policy perspective would define sustainability as the satisfaction of basic economic, social, and security needs now and in the future without undermining the natural resource base and environmental quality on which life depends. From a business perspective, the goal of sustainability is to increase long-term earnings and social value, while decreasing industry's use of materials and reducing negative impacts on the environment. Internal combustion engines play a dominant role in the fields of power, propulsion, energy and economy. Sustainable design is strongly linked to the fuels burnt and the overall efficiency, and reliable injection and ignition are required for relevant system performance. Ignition and combustion processes strongly affect the formation of pollutants and the extent of fuel conversion. Even a slight improvement contributes to considerable reduction of pollutant formation and emissions. Car usage has a significant impact on climate change, with about 12 % of the overall emissions of carbon dioxide (CO_2), the main greenhouse gas, coming from the fuel consumed by passenger cars. Regulations have been proposed to reduce the emission of this gas from the fuel consumed by combustion engine vehicles. This project aims to apply the principles of engineering sciences (thermodynamics, fluid mechanics, heat transfer, and chemistry) to the analysis and improvement of operation variables related to environmental performance of the machine. In the project, different technologies are used together to analyse and investigate the parameters and processes that controls ignitibility, mixture formation, combustion stability and pollutant emissions, proposing its control in order to allow that the engine be green and sustainable.

3 Mathematical model of emissions

3.1 Chemical kinetic model

The necessity to predict the main emissions of internal combustion engines have led to many researches to perform chemical kinetics models for the oxidation of primary reference fuels as gasoline and its surrogates. However, at first the reduced chemistry used includes only the low temperature reactions required to describe the ignition process and couldn't describe the complete combustion process responsible for the major energy release. The first generalized model developed was the shell model by Tanaka et al. [20], in which the two-stage ignition character of high carbon fuel is realized by an eight-step chain branching scheme including only five species. In order to avoid this drawback and make the fuel reaction kinetics closer to real process, many kinetic models have added additional information about high

hydrocarbon oxidation. Tanaka et al.[20] extended the Hu and Keck model including a two-stage ignition process and developed a reduced chemical kinetic model that included 32 species and 61 reactions taking into account the effects of wall heat transfer. Similar to Tanaka et al. [20], Jia and Xie [15], Machrafi and Cavadias [10] and Mehl et al. [14] developed reduced kinetic models for different fuel surrogates containing n-heptane, iso-octane and toluene and studied the effect of fuel composition in the auto ignition of gasoline. Those mechanisms were validated numerically against more detailed mechanisms models, and experimentally against experimental shock tube and rapid compression machine data varying input variables as inlet temperature and pressure, equivalence ratio, compression ratio and spark timing. Small differences in the air/fuel ratio significantly influenced the total ignition timing, while the low temperature step was scarcely affected. On the contrary, the effect of model parameters (e.g., temperature distribution profiles) resulted to be of less importance in the considered condition. Likewise, relatively high compression ratios were needed in order to auto-ignite the gasoline. Respect to the mixture fuel composition they found that the aromatics that are present in gasoline cause the so-called obstructed pre-ignition, followed by a delayed final ignition. This phenomenon can be explained by the competition generated between the consumption of fuel and the formation of stable benzyl radicals from toluene. These models helped Surushima [21] to developed a more complete model including high temperature mechanism reactions, intermediates as olefins and aldehydes, and the consideration of beta-scission of alkyl radicals in parallel with the low-temperature reactions taken from Ferguson [5], Georgious [6], Griffiths [8] and Halstead et al. [9]. High temperature reactions mechanisms performed by Surushima [21] were very simple and consist of the thermal decomposition of alkyl radicals to ethylene and the oxidation of ethylene and formaldehyde. The Beta-scission and thermal decomposition of alkyl radicals to ethylene consist of five elementary reactions and one global reaction, and oxidations of ethylene and formaldehyde consist of 10 elementary reactions and two additional global reactions. Shock tube ignition delay data and intermediate profiles from gas-sampling experiments in a homogeneous charge compression ignition engine (HCCI) were used to develop and validate the new model. Finally, lately multi-zone models have been developed to improve the fluid dynamics understanding and the emissions prediction. The principles of this type of models is the division of the combustion chamber into zones based on geometrical considerations. Heat and mass is exchanged between zones and the cylinder wall according to their spatial configuration, throughout the engine strokes operation. Kominos and Hountalas [16] and Gregory Chin and Chen [7] considered the piston crevice and the area of fluid close to the cylinder walls as responsible largely for emissions and improved numerical models dividing the combustion chamber into several areas. With the assumption of equal pressure for all zones, analytical models were developed for the mass transfer between the core fluids and those in the piston crevice. The numerical model was solved for the coupled mass, energy, and species equations simultaneously leading to consistent solutions at every time step. Comparisons of the calculated results were made between this multi-zone code, a 3D CFD model coupled with multiple zones, and experimental data showing good agreement.

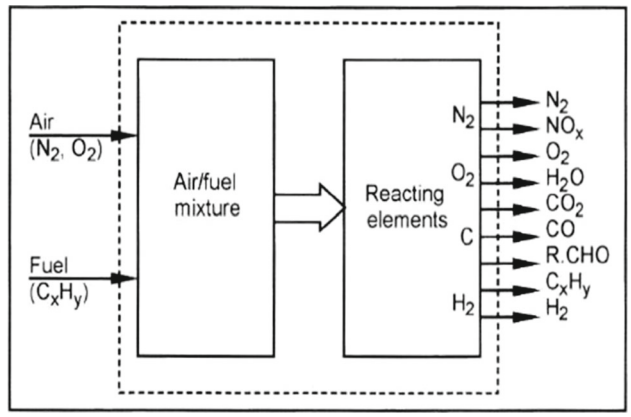

Fig. 1 Reaction mechanisms in the combustion Chamber

In this work, a Kinetic model of the isooctane combustion process was developed to quantify gas emissions and study greenhouse causes. A skeletal mechanism including 32 species and 61 reactions was developed, which could predict satisfactorily ignition timing, burn rate and the emissions of HC, CO, NO_x and the oxygen consumption. Figure 1 shows a schematic representation of the reaction mechanisms occurred in the engine.

The fuel kinetic oxidation model was constructed using a hierarchical approach, which establish sub-mechanisms for fuel molecules at high and lower temperatures. The low temperature mechanism was taken from the skeletal mechanism of Tanaka et al. [20], including the following reactions:

$$C_8H_{18} + O_2 \leftrightarrow C_8H_{17} + HO_2 \quad \text{(R14)}$$
$$C_8H_{17} + O_2 \leftrightarrow C_8H_{17}OO \quad \text{(R15)}$$
$$C_8H_{17}OO \leftrightarrow C_8H_{16}OOH \quad \text{(R16)}$$
$$C_8H_{16}OOH + O_2 \rightarrow \mathrm{OOC_8H_{16}OOH} \quad \text{(R17)}$$
$$OOC_8H_{16}OOH \rightarrow OC_8H_{15}OOH + OH \quad \text{(R18)}$$
$$C_8H_{18} + OH \rightarrow C_8H_{17} + H_2O \quad \text{(R19)}$$
$$OC_8H_{15}OOH \rightarrow OC_8H_{15}O + OH \quad \text{(R20)}$$
$$C_8H_{17} + O_2 \leftrightarrow C_8H_{16} + HO_2 \quad \text{(R21)}$$

This mechanism is followed by the reaction:

$$HO_2 + HO_2 \leftrightarrow H_2O_2 + O_2 \quad \text{(R22)}$$

Reactions (R21) and (R22) lower the reactivity of the system, causing the temperature of the system to rise slowly until the reaction (R23) becomes significant and the thermal explosion is initiated.

$$H_2O_2 + M \rightarrow OH + OH + M \tag{R23}$$

The main products of the reactions (R14)–(R21) were C_8H_{16} and $OC_8H_{15}O$. In order to describe the whole oxidation process, the Jia and Xie et al. [15] sub-model was taken to include three global reactions and directly decompose C_8H_{16} and $OC_8H_{15}O$ into CO and H_2O.

$$OC_8H_{15}O + O_2 \rightarrow C_2H_3 + 2CH_2O + C_3H_4 + CH_3 + HO_2 \tag{R24}$$

$$C_8H_{17} \rightarrow C_4H_8 + C_3H_6 + CH_3 \tag{R25}$$

$$C_8H_{16} \rightarrow C_4H_8 + C_3H_5 + CH_3 \tag{R26}$$

In these reactions large molecules formed during the low temperature stage break up into smaller molecules. After these three reactions isobutene (C_4H_8) was one of the major intermediates formed. Isobutene is further decomposed by the following reaction into smaller molecules [15].

$$C_4H_8 + O_2 \rightarrow C_2H_3 + C_2H_4 + HO_2 \tag{R27}$$

Tanaka et al. [20] ignore the process of the break fuel into low carbon hydrocarbons, therefore it is difficult for Tanaka mechanism predict HC and CO emissions. In order to take into account, a mechanism of 44 reactions of $C1-C3$ hydrocarbon oxidation developed by Patel et al. [18] was taken. This complete mechanism predicts no burned hydrocarbons as C_2H_3, C_2H_4, CH_4, CH_3 and CO. In the combustion of fuels that contain Nitrogen, NO_x can be formed by three chemical routes: the thermal or Zeldovivh mechanism, the Fennimore or prompt mechanism and the N_2O-intermediate mechanism. The thermal mechanism dominates in high temperature combustion over a fairly wide range of equivalence ratios, while the Fennimore mechanism is important in rich combustion. For the features of the system and high temperature chamber combustion the NO_x formation was modeled using the Zeldovich mechanism [4,10]. This mechanism consists of three reversible chain reactions:

$$O + N_2 \leftrightarrow N + NO \tag{R28}$$

$$O_2 + N \leftrightarrow O + NO \tag{R29}$$

$$N + OH \leftrightarrow H + NO \tag{R30}$$

For modelling combustion reactions, a mole balance for each component (i) is done into combustion chamber in temporal state. The general batch reactor equation design is:

$$\begin{aligned} &\{\text{Rate of Flow of i into the system}\} \\ &\quad - \{\text{Rate of Flow of i out the system}\} \\ &\quad + \{\text{Rate of generation of i by chemical reaction}\} \\ &\quad = \{\text{Rate of acumulation of i}\} \end{aligned} \tag{1}$$

As the mole balance is applied during combustion cycle we have a closed system, and only the term of reaction and accumulation are take into account. Applying this criterion, Eq. (1) gives:

$$\frac{dF_i}{d\theta} = \frac{(r_i.V)}{\omega} \tag{2}$$

where F_i is the molar accumulation and r_i represent the generation or consumption of each specie for the 61 combustion reactions. The molar accumulation has a strong dependence on the reactions kinetic and the angular velocity of the crankshaft ω.

$$r_i = \sum_{j=1}^{n} r_{ij} \tag{3}$$

The term r_{ij} represents the kinetic of each reaction and depends of the cylinder temperature and the concentration of the species. The expression for r_{ij} can be more simple for the elementary reactions since the concentration dependence is related to the stoichiometric coefficients of the reaction. The temperature dependence can be represented by the Arrhenius correlation.

$$k_{ij} = A_j T^b e^{\frac{-E_{aj}}{RT}} \tag{4}$$

Here A_j is a constant termed the pre-exponential factor or the frequency factor, E_a is the activation energy and b is an empirical parameter, all of them given for each combustion reaction. This kinetic model must be solved simultaneously using a thermodynamic cycle model from the energy conservation equations, positioning the model in a global engine engineering process. This interaction allows handle the kinetic model in order to support decision making that assure emissions reduction. The thermodynamic model used was the previously reported by Amaya et al. [1] for the isooctane oxidation process. The solution of this interactive model allows predict greenhouse emissions and analyze system responses to perturbation actions.

3.2 Engine cycle model

To simulation of emissions behavior face operational engines parameters is necessary propose a dynamic model of the engine, which allows handle the kinetic model to assure the reduction of greenhouse gases. The balances of inner energy

(U) and mass (m) into the cylinder yield the following equations:

$$\frac{dm}{d\theta} = \frac{dm_{c,in}}{d\theta} - \frac{dm_{c,out}}{d\theta} \tag{5}$$

$$\frac{dU}{d\theta} = m_\varphi H_l \frac{dx_b}{d\theta} - p\frac{dV}{d\theta} - \frac{dQ}{d\theta} + \frac{dH_{in}}{d\theta} - \frac{dH_{out}}{d\theta} \tag{6}$$

where m_φ is the mass of fuel evaporated during combustion, x_b is the mass fraction burned of fuel, V is the volume occupied by the gases mixture into cylinder, Q is the heat transfer toward cylinder walls and H is the enthalpy of the mixture. The mass fraction burned during combustion cycle can be calculated using a function call the Wiebe Function [11]. This function relates the mass fraction burned of the fuel with the angle when combustion start (spark timing), establishing a link between an action control and the engine model.

$$x_b = 1 - \exp\left[-\alpha\left(\frac{\theta - \theta_0}{\Delta\theta}\right)^{m+1}\right] \tag{7}$$

Here θ is the crank angle, θ_0 is the angle where the start of combustion occurs, $\Delta\theta$ is the total combustion duration and α and m are adjustable parameters.

To relate the air–fuel relation as an action control over the engine model, it was necessary develop a model for the admission mixture into the cylinders. Regarding the air system, the engine itself can be approximated as a volumetric pump, i.e., a device that enforces a volume flow approximately proportional to its speed. A typical formulation for such a model is:

$$\dot{m} = \rho_{in}\dot{V} = \rho_{in}(t) * \lambda_1(P_m, \omega_e) * \frac{V_d}{N} * \frac{\omega(t)}{2\pi} \tag{8}$$

Here ρ_{in} is the density of the gas at the engine's intake, λ_l is the volumetric efficiency; which describes how far the engine differs from a perfect volumetric device, V_d is the displaced volume of the mixture, N is the number of revolutions per cycle, and ω is the angular velocity of the engine. Respect with the air system the following equation can be used to calculate its mass flow:

$$\dot{m}_\beta = \rho_{in}\dot{V} = \rho_{in}(t) * \lambda_1(P_m, \omega_e) * \frac{V_d}{N} * \frac{\omega(t)}{2\pi} - \dot{m}_\varphi \tag{9}$$

The mechanical system of the engine also must be studied in order to relate the control variables with the production of mechanical power. The torque (T_e) is an adequately variable that represent the mechanical behavior of the system. It's a nonlinear function that depends of many variables, such as mass in cylinder, air/fuel ratio (λ), engine speed, ignition or injection timing, etc.

$$T_e = f(\dot{m}_\varphi, \lambda, \omega, \theta_0) \tag{10}$$

Since engine torque mainly depends on engine size, i.e., its displaced volume V_d, it is advantageous to use a normalized formulation introducing the brake mean effective pressure (p_{me}):

$$p_{me} = \frac{T_e.4\pi}{V_d} \tag{11}$$

And the mean effective pressure:

$$p_{m\varphi} = \frac{H_l.m_\varphi}{V_d} \tag{12}$$

where the mass of fuel, with lower heating value H_l, burnt per combustion cycle m_φ is related to the mean-value fuel mass flow by:

$$\dot{m}_\varphi(t) = m_\varphi(t) \cdot \frac{\omega(t)}{4\pi} \tag{13}$$

The brake mean effective pressure p_{me} is the pressure that has to act on the piston during one full expansion stroke to produce the same amount of work as the real engine does in two engine revolutions (assuming a four-stroke engine). The fuel mean effective pressure $p_{m\varphi}$ is that brake mean effective pressure that an engine with an efficiency of 1 would produce with the fuel mass m_φ burnt per engine cycle (with perfect conversion of the fuel's thermal energy into mechanical energy). Therefore, the engine's efficiency can be written as:

$$n_e = \frac{p_{me}}{p_{m\varphi}} = \frac{T_e.4\pi}{H_l.m_\varphi} \tag{14}$$

This thermodynamic efficiency depends of various operational parameters as engine speed, air fuel ratio, spark timing, and compression ratio.

$$n_e(\omega, \lambda, \zeta, R_c) = n_\omega(\omega)\, n_\lambda(\lambda)\, n_\zeta(\zeta)\, n_{R_c}(R_c) \tag{15}$$

The factor $n_\omega(\omega)$ has a parabolic form. At very low speeds, the relatively large heat losses through the wall reduce engine efficiency, while at very high speeds, the combustion times become unfavorably large compared to the available interval in the expansion stroke. The factor $n_\omega(\omega)$ has a magnitude substantially smaller than 1 since it incorporates the basic thermodynamic efficiency mechanisms, while the other factors by design are around 1.The factor $n_\lambda(\lambda)$ models the influence of the changing air/fuel ratio on the thermodynamic efficiency. In SI engines, rich to lean mixtures are possible. For rich mixtures, incomplete combustion and water/gas shift reactions substantially reduce the thermodynamic efficiency. For mixtures more than slightly lean, sufficient oxygen is

available for complete combustion such that efficiency is not affected by changing values of λ. For intermediate values, $\lambda_1 \leq \lambda \leq \lambda_2$ a smooth transition is observed. For $\lambda > \lambda_{max}$, finally, misfires start to interfere such that these operating points are not modeled. This behavior can be expressed quantitatively as:

$$n_\lambda(\lambda) = \left\{ \begin{array}{ll} \gamma_1 . \lambda - \gamma_0 & for\ \lambda_{min} < \lambda < \lambda_1 \\ n_{\lambda 1} + (1 - n_{\lambda 1}) . \sin \frac{\lambda - \lambda_1}{1 - \lambda_1} & for\ \lambda_1 < \lambda < \lambda_2 \\ 1 & for\ \lambda_2 < \lambda < \lambda_{max} \end{array} \right\} \tag{16}$$

The factor $n_\zeta(\zeta)$ models the influence of the spark timing on the thermodynamic efficiency. This behavior can be modeled as:

$$n_\zeta(\zeta) = 1 - k_\zeta . (\zeta - \zeta_0(\omega, p_{me}))^2 \tag{17}$$

where $\zeta_0(\omega, p_{me})$ is an optimal (maximum break torque, MBT) ignition angle and start of injection angle. This MBT angle varies strongly with engine operating conditions (especially speed and load). The constant k_ζ also depends of speed and load engine.

The factor n_{R_c} models the influence of the compression ratio. It is important to take into account the change of compression ratio, for instance when downsizing and supercharging an engine for fuel consumption reduction. Due to the higher cylinder pressures and cylinder temperatures the engine starts to show knocking already at part load because this load corresponds to the full-load of the identical engine without supercharger. Therefore, the compression ratio has to be reduced to avoid damage to pistons and other important engine parts. A straightforward approximation for this efficiency is given by:

$$n_{R_c} = \frac{1 - \frac{1}{R_c^{k_\varepsilon}}}{1 - \frac{1}{R_{c0}^{k_\varepsilon}}} \tag{18}$$

where k_ε is a constant estimated by the use of engine cycle calculations.

4 Implementation of emission control technologies in an interactive engineering environment

The need to control the emissions from automobiles gave rise to the computerization of the automobile. Hydrocarbons, carbon monoxide and oxides of nitrogen are created during the combustion process and are emitted into the atmosphere from the exhaust. The clean air law of 1977 set limits as to the amount of each of these pollutants that could be emitted from an automobile. The manufacturers answer was the addition of certain pollution control devices and the creation of a self-adjusting engine. In 1981 saw the first of these self-adjusting engines. They were called feedback fuel control systems. An oxygen sensor was installed in the exhaust system to measure the fuel content of the exhaust stream. It then sends a signal to a microprocessor, which analyses the reading and operate a proper air/fuel ratio. As computer systems progressed, they were able to adjust ignition spark timing as well as operate the other emission controls that were installed on the vehicle. In this work emissions were measured and controlled using a Matlab–LabVIEW interface that is suitable for interactive usage. One of the strengths of the interactive Matlab–LabVIEW interface resides in its seamless integration of data acquisition. The process was simplified by the use of National Instruments hardware, since they have absolutely superb drivers written for all of their equipment. When the National Instruments hardware was used, could utilize the DAQ Assistant (Fig. 2), which allowed to create virtual channels that serve as a handy, migratable way of handling data acquisition.

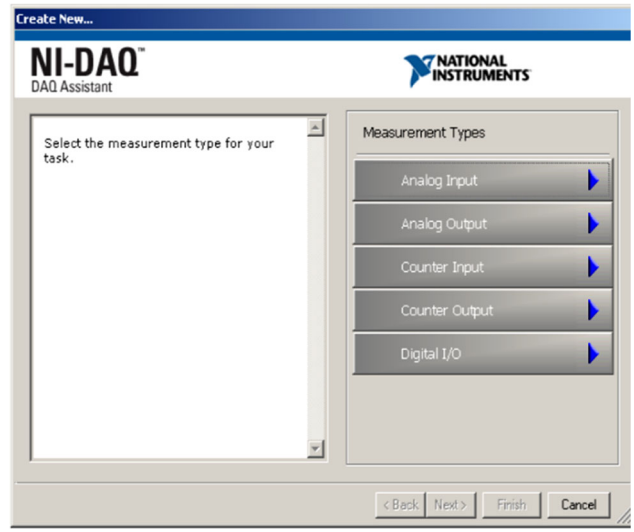

Fig. 2 DAQ assistant for interactive data acquisition development

Running the kinetic model in MATLAB and studying operational engines variables under pollutant emissions, requires importing real-world data (Fig. 3). LabVIEW is the most productive tools for acquiring data, and with the math interface toolkit (MIT), is ease import any LabVIEW data into MATLAB through an intuitive wizard. The MIT package converts the signals into a MEX function recognizable by MATLAB. After building the acquisition data, can be launched the MIT wizard from the Tools menu of LabVIEW. The wizard, displays the current inputs and outputs of the simulation, which will become the input and output parameters of the MEX function. The wizard allows customize the

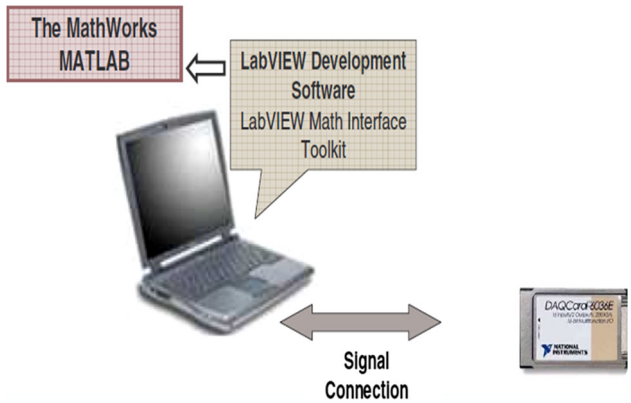

Fig. 3 Embedding LabVIEW into MATLAB

name of the MEX function, add or remove input and output parameters, and reorder the parameters and specifications.

The control and data acquisition system implemented with the Lab View software of National Instruments provide in an interface on a Windows based computer, output variables as crankshaft angular velocity, coolant temperature, intake air aspirated by the cylinders, stoichiometric air–fuel relation, crankshaft position, pressure and temperature in the chamber combustion, and emission concentrations. Some control devices installed on the automobile were: An EGR valve,an air pump and a PCV valve.

4.1 EGR valve

The purpose of the exhaust gas recirculation valve (EGR) is to intake a small amount of exhaust gases into the intake system, this dilutes the air/fuel mixture so as to lower the combustion chamber temperature. Excessive combustion chamber temperature creates oxides of nitrogen, which is a major pollutant. While the EGR valve is the most effective method of controlling oxides of nitrogen, in it's very design it adversely affects engine performance. The engine was not designed to run on exhaust gas. For this reason, the amount of exhaust entering the intake system has to be carefully monitored and controlled. This is accomplished through a series of electrical and vacuum switches and the vehicle computer. Since EGR action reduces performance by diluting the air/fuel mixture, the system does not allow EGR action when the engine is cold or when the engine needs full power.

4.2 PCV valve

The purpose of the positive crankcase ventilation (PCV) system, is to take the vapours produced in the crankcase during the normal combustion process, and redirecting them into the air/fuel intake system to be burned during combustion. These vapours dilute the air/fuel mixture so they have to be carefully controlled and metered in order to not affect the performance of the engine. This is the job of the positive crankcase ventilation (PCV) valve. At idle, when the air/fuel mixture is very critical, just a little of the vapours are allowed in to the intake system. At high speed when the mixture is less critical and the pressures in the engine are greater, more of the vapours are allowed in to the intake system. When the valve or the system is clogged, vapours will back up into the air filter housing or at worst, the excess pressure will push past seals and create engine oil leaks. If the wrong valve is used or the system has air leaks, the engine will idle rough, or at worst, engine oil will be sucked out of the engine.

4.3 Air injection

Since no internal combustion engine is 100 % efficient, there will always be some unburned fuel in the exhaust. This increases hydrocarbon emissions. To eliminate this source of emissions an air injection system was created. Combustion requires fuel, oxygen and heat. Without any one of the three, combustion cannot occur. Inside the exhaust manifold there is sufficient heat to support combustion, if we introduce some oxygen than any unburned fuel will ignite. This combustion will not produce any power, but it will reduce excessive hydrocarbon emissions. Unlike in the combustion chamber, this combustion is uncontrolled, so if the fuel content of the exhaust is excessive, explosions that sound like popping will occur. There are times when under normal conditions, such as deceleration, when the fuel content is excessive. Under these conditions we would want to shut off the air injection system. This is accomplished through the use of a diverter valve, which instead of shutting the air pump off, diverts the air away from the exhaust manifold. Since all of this is done after the combustion process is complete, this is one emission control that has no effect on engine performance. The only maintenance that is required is a careful inspection of the air pump drive belt.

4.4 Exhaust sensors and feedback control

In order to maintain the air–fuel ratio and spark timing in the optimum value to minimize emissions, a feedback system was required for their control. The air/fuel-ratio control-system is one of the most important control loops. Without an appropriate feedforward component, the performance of the air/fuel ratio control system would be much too slow. This slowness is due to the many delays and lags between the input (fuel injection) and the output (air/fuel ratio sensor) of this dynamic system. Under transient operating conditions, the correct amount of fuel to be injected must be determined as quickly as possible. This is only possible if the intake manifold dynamics are considered. The information available on either the throttle plate angle, the manifold pressure, or the

air mass flow into the intake manifold must be used to predict the air mass flow into the cylinder. This information is then used to estimate the amount of fuel to be injected in the next cycle. Exhaust oxygen sensors that are stabilized zirconium oxide detecting the oxygen partial pressure in the exhaust were used for providing direct feedback for the fuel injection process. Typically, the sensor output is converted to a binary signal, lean for sensor voltages U_λ smaller than 450 mV, rich for U_λ greater than 450 mV . Using this binary signal, a control structure similar to a PI control system is chosen.

Spark timing is maintaining in an optimum value using the spark plug as a "combustion chamber sensor". By measuring the ion flow at the electrodes during combustion, the start of ignition (misfiring diagnosis) and the progress of ignition can be measured, and knocking can be monitored. In conjunction with electronic combustion control, this permits effective diagnosis and, hence, lower emissions over long periods.

5 Analysis and results

5.1 Experimental engine and data acquisition system

Analysis and data collection of the Twingo D7F engine were performed at EAFIT University bank engines. As part of the bank were the Chassis, the engine and the data acquisition system with its sensors and actuators. Figure 4 shows the complete engine test bank used to validated the computer model and Table 1 the specifications of the engine. This structure gave maneuverability, interaction, stability and other characteristics necessary to have proficient and ease of system research study.

5.2 Parametric study

The effects of variations in compression ratio, fuel/air equivalence ratio and spark advanced under pollutant emissions were studied and determined from the kinetic and engine model. Optimal ranges of operation of these engine parameters were controlled to minimize the environmental impact. These parameters were selected as adequately operational variables in order to operate the engine under sustainable conditions. This study permits a first approach to design green engines, since combines the knowledge of the combustion chemistry with the engines theory in an interactive interface, which allows monitoring the engine operation variables.

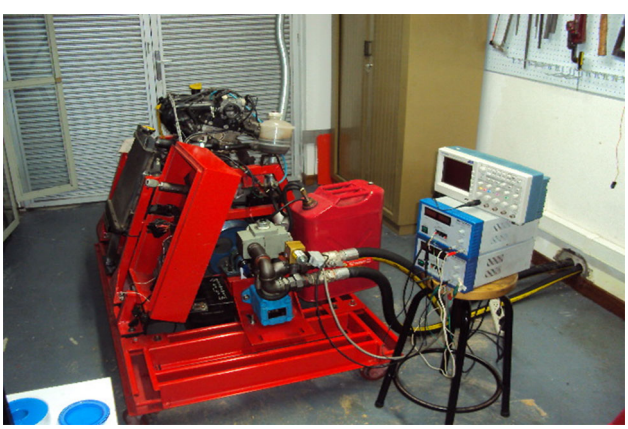

Fig. 4 Data acquisition system for a Twingo D7F engine

5.2.1 Effects of air–fuel ratio

The air–fuel ratio is the relation of the mass of air to fuel mass. When the amount of air is too large or small, fuel does not burn well causing incomplete combustion, generating undesirable residues. There is a minimum of 14.7 parts of air needed to completely burn 1-part of gasoline. This is called theoretical air–fuel ratio. However, in existing gasoline engines, even if the required fuel is injected at the theoretical air–fuel ratio, not all gasoline is vaporized and mixed with air. Therefore, under certain conditions, some motors operate with rich mixtures (above the stoichiometric ratio) or poor (below this), this being a parameter to be optimized for each type of engine. Figures 5, 6, 7, 8 allow us to analyze the effect of the air–fuel ratio on the generation of emissions and establish an optimum operation to minimize environmental effects of combustion. Figure 5 shows a relationship between the rate of oxygen consumption and the air–fuel ratio used. For very poor (above 14) mixtures there is a large amount of oxygen unreacted, whereas for relations of 12 and 14 the best oxygen consumption rate and oxygen utilization during combustion are found. In Fig. 6 the effect of the air–fuel ratio on the production of carbon monoxide (CO) is shown. CO production is increased dramatically for too rich mixtures due to the excess fuel, resulting in incomplete combustion of the hydrocarbon molecules. A considerable reduction in the amount of CO produced is obtained at values of AF slightly below the stoichiometric ratio. The production of unburned hydrocarbons during combustion (mainly C_2H_3) (Fig. 7) has a very similar behavior to the carbon monoxide (CO) production, increasing significantly to very rich mixtures and having a minimum optimum value for a relationship air–fuel of 14. Figure 8 shows the effect of the air–fuel ratio on the production of another highly undesirable byproduct of combustion, the Nitrogen oxides (NO_x). These compounds are produced when the nitrogen in the air reacts with the oxygen at high temperatures and pressures in the cylinder. In Fig. 8 it is showed that for rich mixtures the production of nitrogen monoxide (NO) is increased by the high heat transfer by excess fuel, and a considerable reduction is observed to poor mixtures or close to the stoichiometric relation. With respect to this parameter it is recommended for this engine working at an air–fuel ratio slightly below the stoichiomet-

Table 1 Twingo D7F engine specifications

Engine	Index	Vehicle	Volume ratio	Diameter (mm)	Sprint (mm)	Displacement (cm^3)
Twingo D7F	701	C076	9.65/1	69	76.8	1149

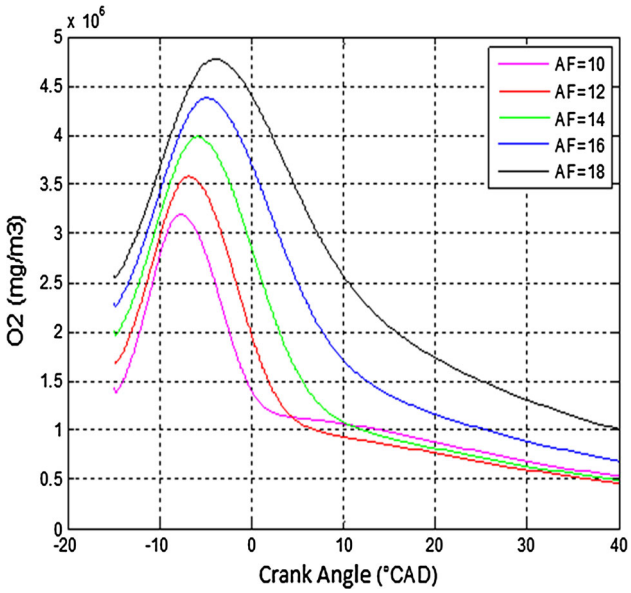

Fig. 5 Effect of air–fuel ratio on oxygen consumption

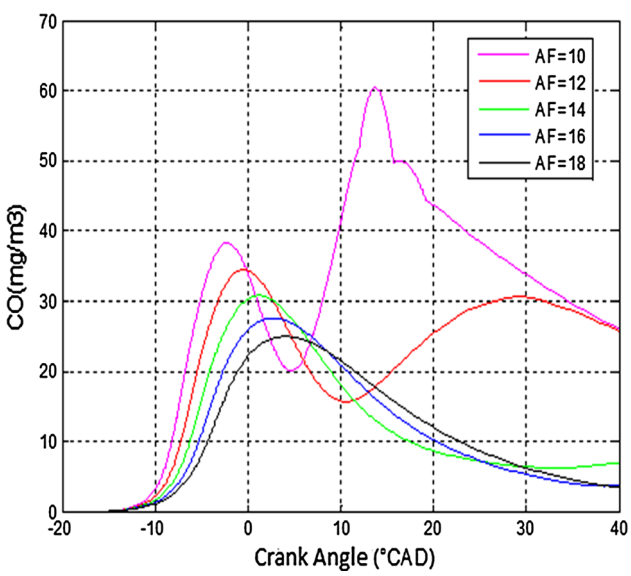

Fig. 6 Effect of air–fuel ratio on Carbon monoxide production

ric value (AF = 14), being the best use of oxygen during combustion and optimum reduction of polluting gases such as carbon monoxide (CO), unburned hydrocarbons (C_2H_3) and nitrogen monoxide (NO) production.

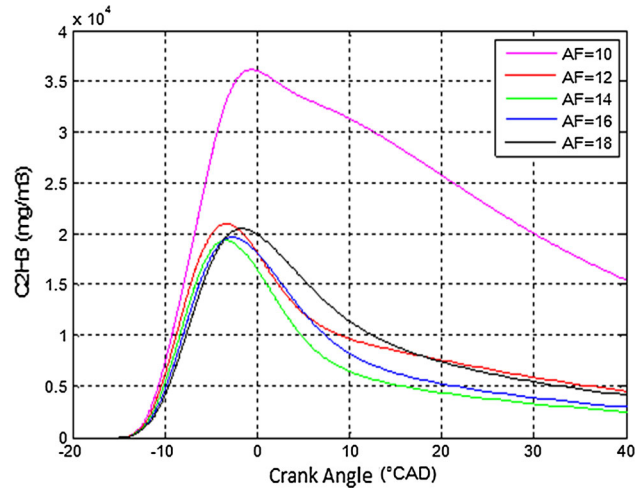

Fig. 7 Effects of air–fuel ratio over no burned hydrocarbons production

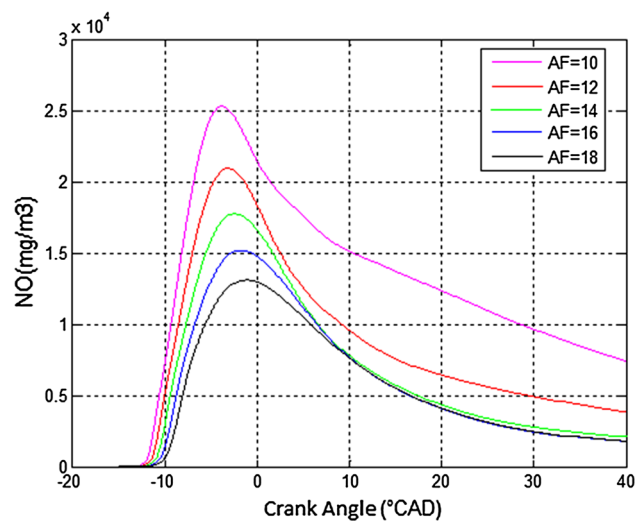

Fig. 8 Effect of air–fuel ratio on NO_x production

5.2.2 *Effects of spark timing*

The gasoline engine transforms the combustion of the air–fuel mixture in prime mover (power), energy and emissions. For the air–fuel mixture to burn correctly, it is important that the spark is powerful enough for the ignition timing to be adjusted. Likewise, the advance or retard of ignition is a critical operating parameter to be adjusted for each type of engine to achieve maximum mechanical energy and environmental efficiency. In Figs. 9, 10, 11, 12 the effects of spark

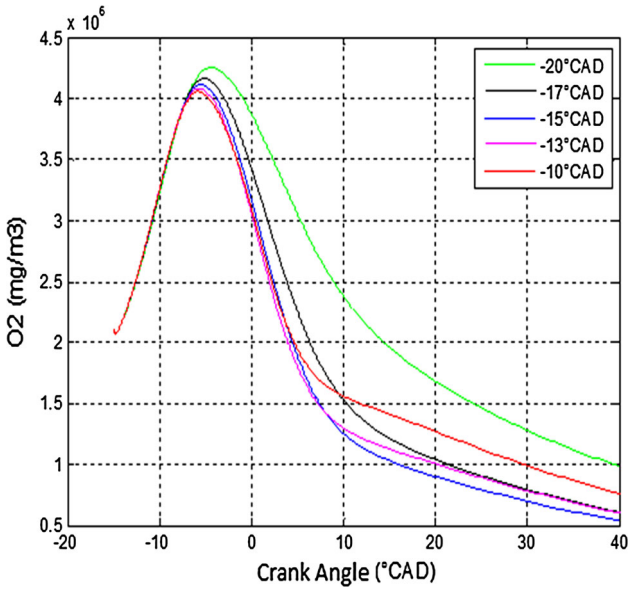

Fig. 9 Effect of spark timing on oxygen consumption

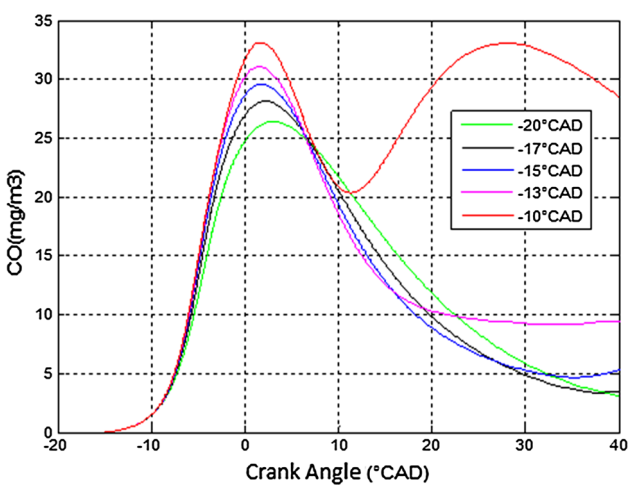

Fig. 10 Effect of spark timing on carbon monoxide production

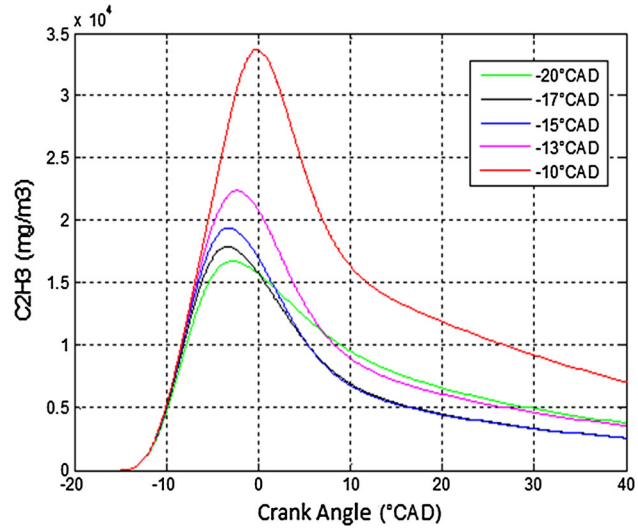

Fig. 11 Effect of spark timing on no burned hydrocarbons production

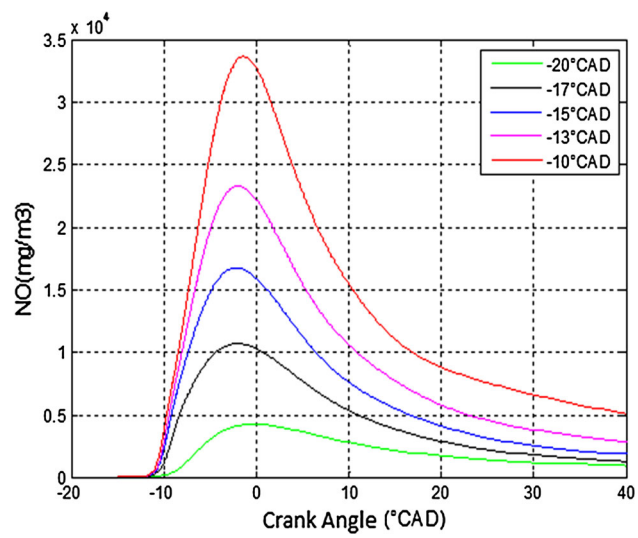

Fig. 12 Effect of spark timing on NO_x production

timing on engine emissions are shown. A preview of the spark high excessively (−20° CAD) produces a very poor use of oxygen in fuel combustion (Fig. 9), due to the premature start of combustion without proper initial thermodynamic conditions. Similarly, excessive delay of spark (−10° CAD) increases the production of carbon monoxide (Fig. 10) and unburned hydrocarbons (Fig. 11), due to the short period of combustion that causes a large amount of fuel which is not burned completely into CO_2 and H_2O remaining in the midway as CO and HC. Hence, a spark advance of −15° CAD is an optimum value of operation that allows the maximum rate of oxygen utilization, minimizes the production of unburned hydrocarbons (C_2H_3), carbon monoxide (CO) and Nitrogen oxides (NO_x).

5.2.3 Effects of compression ratio

The compression ratio is a design parameter of the engine. It indicates the number of times that is greater the volume occupied by the mixture at the end of admission (piston in the lower dead point LDP), regarding the final volume of compression (piston at top dead center PMS) which is the total volume of the combustion chamber. The volume of the combustion chamber is a design parameter that can be changed accordingly to optimize combustion efficiency. The definition of the compression ratio is summarized in the following formula:

$$R_C = \frac{V_u + V_c}{V_c} \tag{19}$$

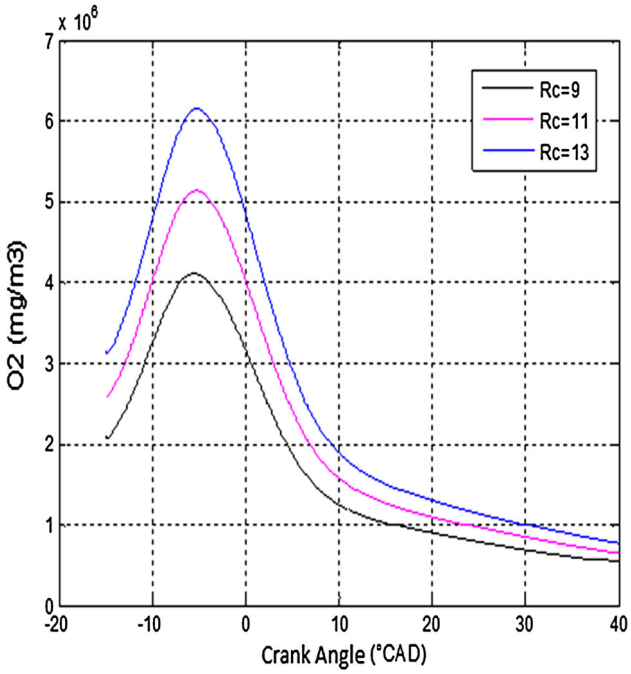

Fig. 13 Effect of compression ratio on oxygen consumption

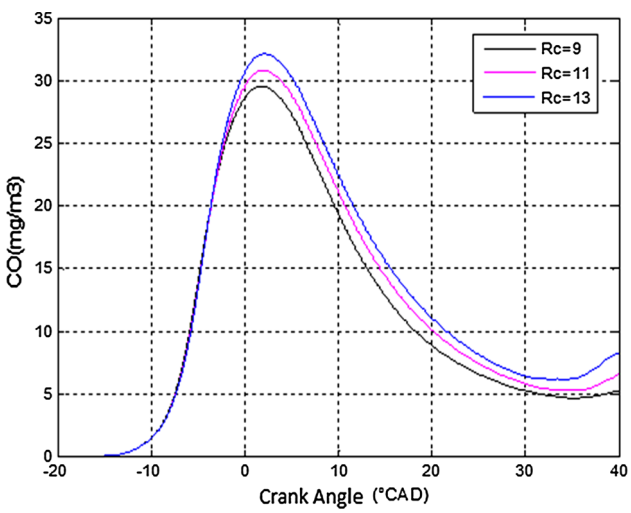

Fig. 14 Effect of compression ratio on carbon monoxide production

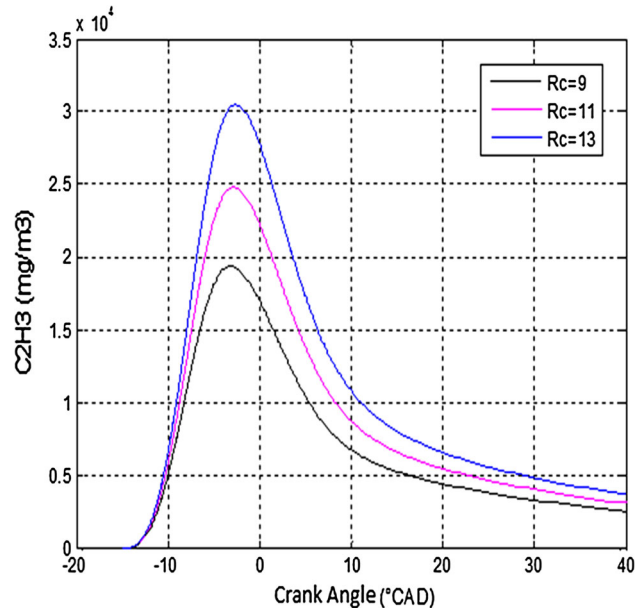

Fig. 15 Effect of compression ratio on no burned hydrocarbons production

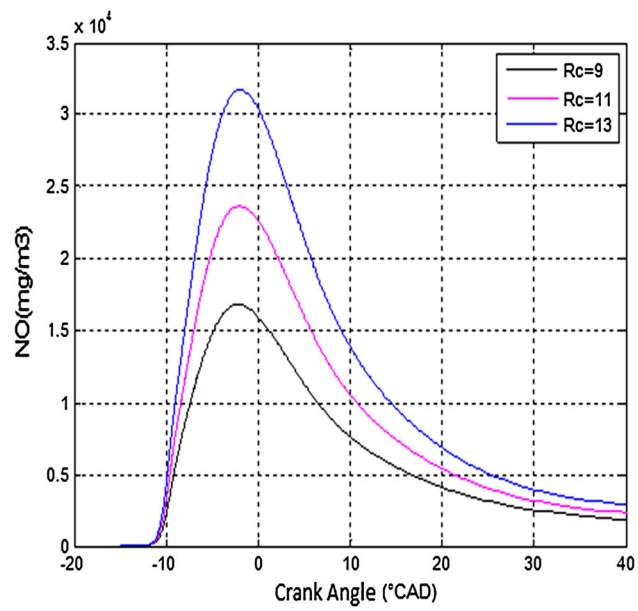

Fig. 16 Effect of compression ratio on NOx production

where V_u is the unit volume or engine capacity and V_c is the volume of the combustion chamber. If the volume of the cylinder increases, the compression ratio increases, but if the volume of the combustion chamber increases, the compression ratio decreases. Figures 13, 14, 15, 16 shows the effect of the compression ratio over engine emissions. For all critical components analyzed (oxygen consumption, carbon monoxide production, production of unburned hydrocarbons and nitrogen oxides production) it is always more profitable to work with an optimal compression ratio of 9. It results in an increase of size of the combustion chamber relative to the unit cylinder, creating more uniform mixing and less dead zones which increase the efficiency of combustion. As a result, greater amounts of desirable products (CO_2, H_2O, N_2) are obtained in comparison with unwanted products (CO, C_2H_3 and NO_x).

6 Conclusions

In this work was developed an environment model based on the explosion of isooctane fuel to quantify and reduce

the main emissions in a Twingo D7F engine. Analysis and data collection of the Twingo D7F engine were performed in the EAFIT University bank engines. Parametric study was performed to reduce HC, CO, NO_X emissions and improve oxygen consumption from variation of engine operation parameters. air–fuel ratio (A_F = 14), spark timing (−15° CAD) and compression ratio ($R_C = 9$) were optimum values to reduce emissions in this engine.

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