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Comparison of production costs and degree of pollution by emissions in the industrial sector of Ecuador using natural gas as fuel by means of process simulation

Comparación de los costos de producción y grado de contaminación por emisiones en el sector industrial del ecuador usando como combustible gas natural mediante la simulación de procesos.

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Abstract
In this investigation, the comparison of industrial costs and the degree of pollution due to emissions generated using traditional fuels, especially diesel, which is the most used in the Ecuadorian industry against natural gas through a program of Open source chemical engineering called DWSIM for the simulation of the chemical combustion reactions of diesel and natural gas as energy generators in the production processes of the Industries, in which it was evidenced that getting the same amount of energy can be obtained reduce up to 22.46% of carbon dioxide emissions to the environment using natural gas, a variation in production costs was also determined, which is a function of indirect manufacturing costs since in this element of costs Total production of fuels is found thus saving 3.9296% per month used natural gas as a fuel generator against diesel as traditional fuel

key words
Pollution, Carbon dioxide, Fuel, Natural gas

Resumen
En la presente investigación se realizó la comparación de los costos industriales y el grado de contaminación por emisiones que se genera utilizando los combustibles tradicionales en especial el diésel el cual es el más usado en la industria ecuatoriana frente al gas natural por medio de un programa de Ingeniería química de código abierto denominado DWSIM para la simulación de las reacciones químicas de combustión del diésel y el gas natural como generadores de energía en los procesos productivos de las Industrias, en el cual se demostró que llegando a obtener la misma cantidad de energía se pueden reducir hasta en un 22,46% de emisiones de dióxido de carbono al ambiente utilizando gas natural , también se determinó una variación de los costos de producción , el cual está en función de los costos indirectos de fabricación ya que en este elemento de los costos totales de producción se encuentran los combustibles teniendo así un ahorro de un 3,9296% al mes usado gas natural como combustible generador de energía frente al diésel como combustible tradicional.

Palabras clave
Contaminación, Dióxido de carbono, Combustible, Gas natural

1. Introduction

Energy has become a significant factor in the development of the industrial sector, which in turn promotes the economic and sustainable growth of a nation by generating jobs and competitiveness. However, the fuels used to generate this energy are largely associated with harmful environmental effects due to the release of greenhouse gases that contaminate the ozone layer [1]. Currently, the reduction of harmful emissions to the environment is a challenge that developed and developing countries must face, which has led to various environmental agreements such as the Kyoto Protocol, the United Nations Convention, among other

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treaties, with the aim of controlling greenhouse gas emissions, including carbon dioxide and nitrogen compounds [2].

According to a study conducted by the Natural Resources Defense Council, large amounts of greenhouse gases are released in Latin America, with black carbon being one of the main pollutants after carbon dioxide. This is mainly due to the productive and transportation sectors that operate on diesel engines, which have adverse effects on public health, food security, and the environment [3].

In Ecuador, natural gas is not widely implemented in industrial production, with the exception of certain ceramics industries. According to a study by the Ibero-American Network of Ecology, approximately 82% of Ecuador's energy matrix is generated from hydrocarbons such as diesel, bunker, and fuel oil. These not only cause significant environmental pollution but are also heavily subsidized, leading to substantial costs for the Ecuadorian economy, with diesel being the most demanded fuel [4].

However, this research will focus on the indirect manufacturing costs, specifically in the supplies, including the fuel used for transforming raw materials in the industrial sector, which directly affects energy efficiency. An example is the textile industry, where savings of 20 to 30 percent are achieved by using heat transfer through conduction, unlike liquid fuels or medium fluids that generate residues in access pipelines. This highlights the need to evaluate production costs and emissions generated by the combustion of natural gas compared to traditional fuels [1].

Currently, the Ecuadorian government has repealed Executive Decree 883, which eliminated subsidies for fossil fuels such as extra gasoline, ethanol-blended extra gasoline, and diesel, which were priced at international market rates considering the fluctuation of the WTI crude barrel, which serves as the benchmark value [5].

Considering that Ecuador is committed, ratified, and accepted in an agreement of the United Nations Convention on Climate Change held in Paris, France, known as the Paris Agreement, which aims to reduce greenhouse gas emissions to prevent a temperature increase of approximately 2 degrees Celsius by the end of this century [6].

For this reason, the use of cleaner energy in the country's productive sector is proposed. Although fuels such as diesel, which is the most subsidized and therefore the cheapest in the country, generate high carbon dioxide emissions, in contrast, natural gas, due to its molecular structure, is very ideal, as will be seen in this research and analysis of the energy generated by natural gas compared to other fuels. This offers a better alternative for the industrial sector and the country, thus complying not only with the Paris Agreement but also reducing the amount of carbon dioxide generated, which is approximately 1.9 metric tons, representing 0.1% globally [7].

The industrialization of natural gas has become a topic of interest in recent years due to environmental pollution and the use of natural resources that can be sustainable and profitable for a country's growth. The development of the Canadian industry using natural gas has been very beneficial for the country, generating high revenues not only from exporting the fuel to other regions but mainly from using natural gas in industries and the formation of technology companies that use this raw material. Their per capita GDP growth reached $26,764, doubling the previous decade's value of $14,000 per citizen [8].

According to studies by the Latin American Energy Organization, natural gas is one of the most produced resources, with a 20% share since 2011, occupying the second place and achieving a growth rate of 4.68%. A clear example of this industrial development of natural gas in Latin America is the Democratic Republic of Peru due to its proven reserves. Additionally, it has great potential as, in the last 5 years, the country has had an excellent growth rate and low inflation rate, making it attractive for investments. Currently, there are 4 major projects to industrialize the country using natural gas, including the production of ammonia and urea, ammonia and nitrates, ammonium nitrate, and ethylene and polyethylene [8].

Similarly, Bolivia is a country proposing the industrialization of natural gas, albeit with a different methodology, where the state is the sole investor to establish plans or projects. Currently, Bolivia has two projects: ammonia and urea plants, and the production of ethylene and polyethylene [8].

In Ecuador, there is currently no proposal for the industrialization of natural gas like in other countries, although it has a natural gas liquefaction plant (Amistad field) located in the province of El Oro, and another project in Bajo Alto, also located in the same province [9].

According to a study conducted by the Natural Resources Defense Council, large amounts of greenhouse gases are released in Latin America, with black carbon being one of the main pollutants after carbon dioxide. This is mainly due to the productive and transportation sectors that operate on diesel engines, which have adverse effects on public health, food security, and the environment [3].

Currently, in Ecuador's productive and energy matrix, 82% of the energy generated comes from fuels such as diesel, bunker, or fuel oil, and especially in the city of Guayaquil, diesel is the most demanded fuel. It is not only a major environmental pollutant but also imposes a significant cost on Ecuador's economy due to its subsidy [4].

For this reason, the prompt adoption of cleaner energy sources for the industrial development of a country is necessary, considering the costs generated by extraction, production, and the pollution resulting from their use.

2. Materials and methods

A Chemical Engineering Software called DWSIM (Open Source Chemical Process Simulator) is included for the simulation of chemical reactions, such as the combustion of different hydrocarbons used in the industrial sector of Ecuador, including natural gas, to resolve the investigation [10].

In particular, the heats of combustion and the emissions generated by the various hydrocarbons used in industrial boilers for energy generation will be evaluated through process simulation using the DWSIM software. Following the simulation, the analysis and comparison of production costs and emissions resulting from combustion will be conducted, compared to natural gas, to determine the best energy and environmental solution for industries [11]

2.1. Diesel combustion simulation: entering components into the simulator

The first step to begin the simulation is entering the components, both reactants and products. In the combustion process, n-hexadecane (diesel), oxygen, and nitrogen (air) are entered as reactants, and water and carbon dioxide as resulting products.

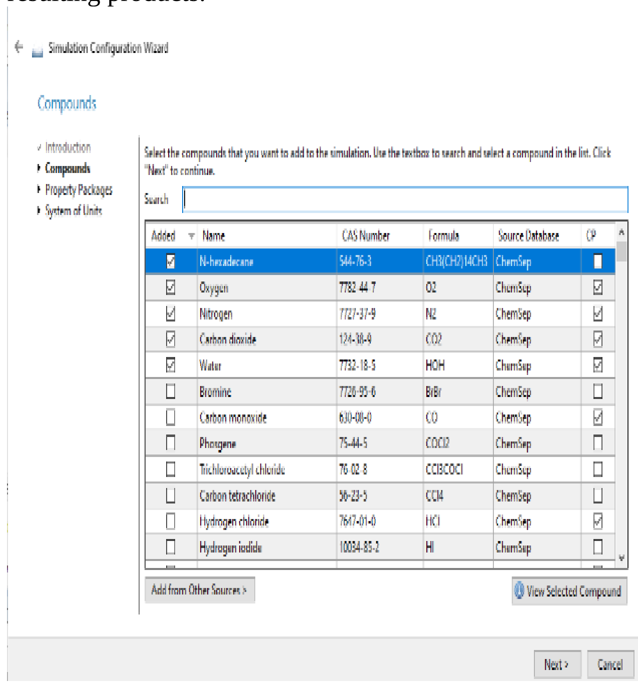

Figure. 1. Input of main components into the simulator
Source: (Lopez, 2020)

Next, we select the thermodynamic model to be used in the reaction. Since our process involves hydrocarbons and non-polar compounds, we select the Peng-Robinson model, as it best fits our process.

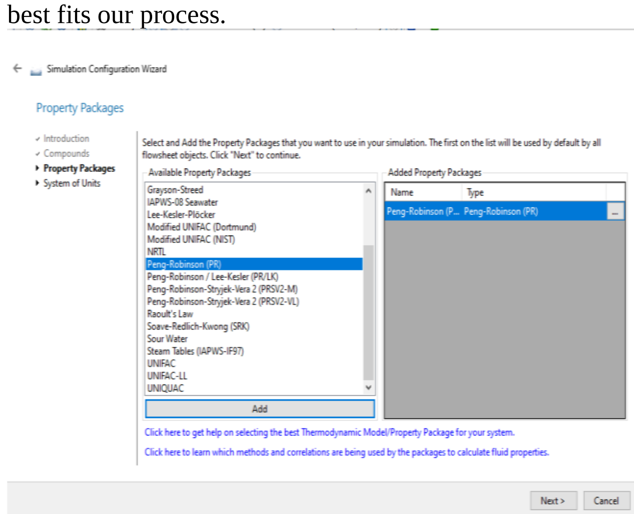

Figure. 2. Selection of the thermodynamic model in the simulator

Source: (Lopez, 2020)

2.2. Entering unit operations in the simulation window

We now proceed to enter unit operations such as the reactor, mixer, and flow lines in the simulation window.

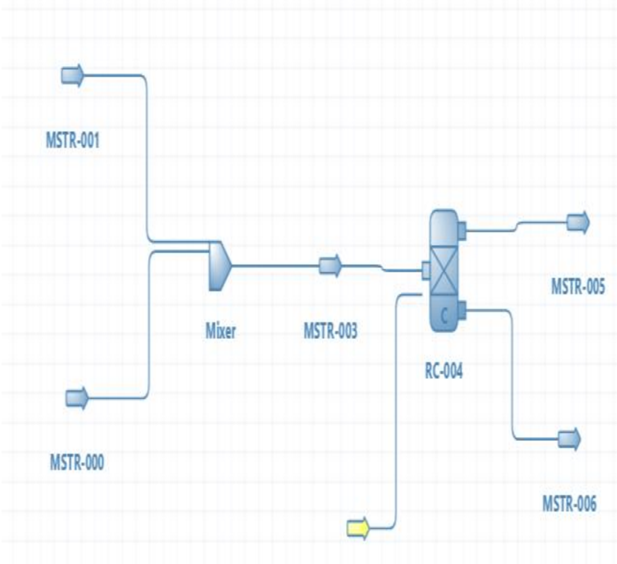

Figure. 3. Entry of Unit Operations into the Simulato
Source: (Lopez, 2020)

We then begin labeling the flow lines appropriately.

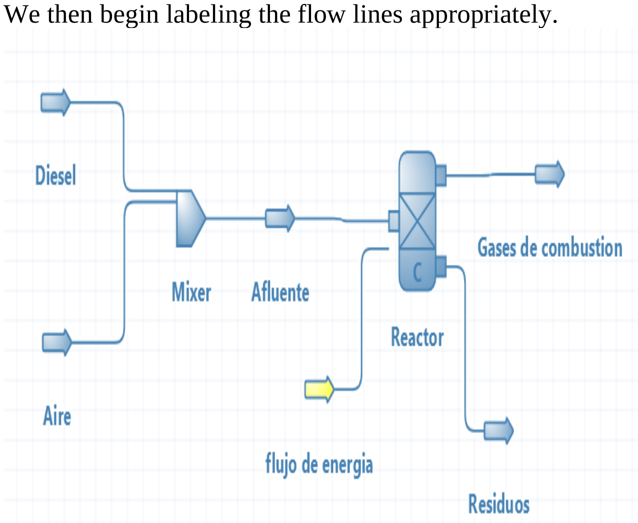

Figure. 4. Labeling of unit operations and flow lines in the diesel combustion process
Source: (Lopez, 2020)

2.3. Entering thermodynamic variables into the simulator

To enter the variables into the simulator, we position ourselves on the diesel flow line and double-click to edit and input the corresponding information.

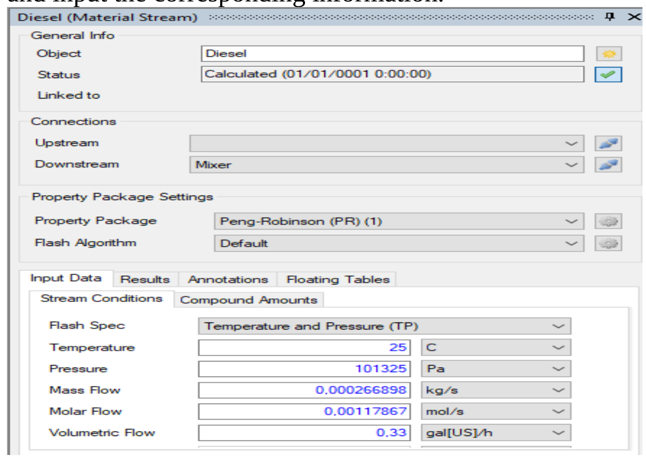

Figure. 5. Entry of thermodynamic variables into the process simulator
Source: (Lopez, 2020)

Next, in the composition section of each compound, we enter the corresponding mole fractions. Since we are dealing with diesel, the mole fraction will be 1.

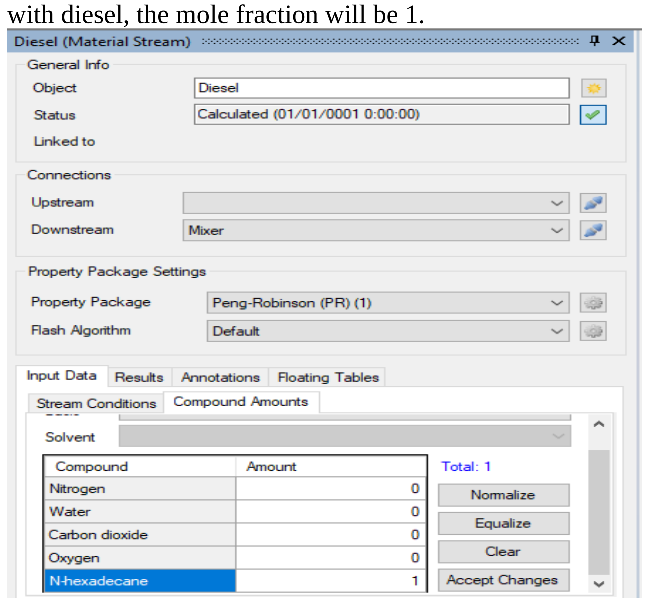

Figure. 6. Input of the corresponding mole fraction for diesel in the simulator

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Source: (Lopez, 2020)

To enter the corresponding values for the air, we need to perform a small material balance, using the volumetric flow of the fuel as the primary data point, which is 240 gallons/month.

$$240\frac{gallons}{month}*\frac{1month}{30day}*\frac{1day}{24hours} = 0.33\frac{gallons}{hours}C_{16}H_{34} = 0.00117867\frac{mol}{second}\ C_{16}H_{34}\ (value\ obtained\ in\ the\ simulator\ ) \quad (1)$$

Using the molar flow obtained in the simulator and the combustion equation, we will calculate how many moles of theoretical oxygen are needed for combustion.

$$2C_{16}H_{34} + 49O_2 \rightarrow 34H_2O + 32CO_2 \quad (2)$$

$$O_2Theoretical = 0.00117867\frac{mol\ C_{16}H_{34}}{second} * \frac{49mol\ O_2}{2mol\ C_{16}H_{34}} = 0.02888\frac{molO_2}{second} \quad (3)$$

Since we know that in our process the air flow corresponds to 21% oxygen, with 79% being nitrogen, we convert to moles of theoretical air.

$$Air\ theoretical = 0.02888\frac{molO_2}{second} * \frac{100moles\ Air}{21mol\ O_2} = 0.13752\frac{mol\ Air}{second} \quad (4)$$

Finally, we must consider that for complete combustion, an excess air percentage is needed. This percentage is determined based on the fuel used; in our case, diesel requires a 20% excess air for combustion [12]

$$Excess\ Air = 0.13752\frac{mol\ Air}{second} * 1.20 = 0.165\frac{mol\ Air}{second} \quad (5)$$

2.4. Natural gas combustion simulation: entering components into the simulator

The same procedure as in the previous simulation is followed: components of both reactants and products are entered. In the natural gas combustion process, methane, oxygen, and nitrogen (air) are entered, along with water and carbon dioxide as products.

Next, we select the thermodynamic model to be used in the reaction. Since our process involves hydrocarbons and non-polar compounds, we select the Peng-Robinson model, as it best fits the process.

3. Results

Results of Diesel Fuel Simulation (240 gal/month)

Table 1. Results of diesel combustion for a flow of 240 gal/month in the DWSIM simulator

Object	Combustion gases	Residues	Unit
Temperature	1856,5	1856,5	C
Pressure	101325	101325	Pa
Mass Flow	18,0979	-4,02E-15	kg/h
Molar Flow	0,175019	0	mol/s
Molar Fraction (Mixture) / Water	0,114487	0	
Mass Fraction (Mixture) / Water	0,0718049	0	
Mass Flow (Mixture) / Water	1,29952	0	kg/h
Molar Fraction (Mixture) / Carbon Dioxide	0,107752	0	
Mass Fraction (Mixture) / Carbon Dioxide	0,165094	0	
Mass Flow (Mixture) / Carbon Dioxide	**2,98785**	**0**	**kg/h**
Molar Fraction (Mixture) / Oxygen	0,0329834	0	
Mass Fraction (Mixture) / Oxygen	0,036744	0	
Mass Flow (Mixture) / Oxygen	0,664991	0	kg/h
Molar Fraction (Mixture) / N-hexadecane	0	0	

Mass Fraction (Mixture) / N-hexadecane	0	0	
Mass Flow (Mixture) / N-hexadecane	0	0	kg/h
Energy Flow	**40043,2**	**0**	**BTU/h**

Source: (Lopez, 2020)

Table 2. Results of natural gas combustion in the DWSIM simulator for a volumetric flow of 1m³/h

Object	Combustion gases	Residues	Unit
Temperature	1923,59	1923,59	C
Pressure	101325	101325	Pa
Mass Flow	13,0374	0	kg/h
Molar Flow	0,130578	0	mol/s
Molar Fraction (Mixture) / Carbon Dioxide	0,0871365	0	
Mass Fraction (Mixture) / Carbon Dioxide	0,13827	0	
Mass Flow (Mixture) / Carbon Dioxide	1,80268	0	kg/h
Molar Fraction (Mixture) / Methane	0	0	
Mass Fraction (Mixture) / Methane	0	0	
Mass Flow (Mixture) / Methane	0	0	kg/h
Molar Fraction (Mixture) / Oxygen	0,0174284	0	
Mass Fraction (Mixture) / Oxygen	0,0201082	0	
Mass Flow (Mixture) / Oxygen	0,262158	0	kg/h
Molar Fraction (Mixture) / Water	0,174273	0	
Mass Fraction (Mixture) / Water	0,113202	0	
Mass Flow (Mixture) / Water	1,47586	0	kg/h
Energy Flow	31156,6	0	BTU/h

Source: (Lopez, 2020)

Now, after obtaining the energy results for natural gas and diesel, we can perform a quick calculation to determine how many cubic meters of natural gas will be required to generate the same amount of energy as diesel fuel.

$$x = \frac{1\frac{m3}{h} * 40043{,}2\frac{Btu}{h}}{31156{,}6\frac{Btu}{h}} \quad (6)$$

$$x = 1{,}2852\, m3/h \quad (7)$$

With the result we have just obtained, we re-enter the data into the simulator and repeat the same process carried out with a flow of 1m3/h, observing that the energy flow is equivalent to that of diesel.

Table 3. Results of natural gas combustion for a volumetric flow of 1.2852 m3/h in the DWSIM simulator

Object	Combustion gases	Residues	Unit
Temperature	1923,6	1923,6	C
Pressure	101325	101325	Pa
Mass Flow	16,7555	-3,72E-15	kg/h
Molar Flow	0,167818	0	mol/s
Molar Fraction (Mixture) / Carbon Dioxide	0,0871369	0	
Mass Fraction (Mixture) / Carbon Dioxide	0,138271	0	
Mass Flow (Mixture) / Carbon Dioxide	**2,31681**	**0**	**kg/h**
Molar Fraction (Mixture) / Methane	0	0	
Mass Fraction (Mixture) / Methane	0	0	
Mass Flow (Mixture) / Methane	0	0	kg/h

Source: (Lopez, 2020)

3.1. Comparison of production costs for diesel and natural gas

After obtaining the amount of energy generated by the fuels used in the simulation, it is necessary to perform a comparison of production costs. To do this, we need to conduct an individual analysis of the monetary cost of each fuel, taking into account the official fuel prices established by the Hydrocarbon Regulation and Control Agency [13]

3.2. Monetary cost of diesel fuel based on its volume

To calculate the monetary cost of diesel, we will perform a quick calculation based on the 240 gallons/month used in the process in relation to the official price, which is \$2.03758 per gallon of diesel. This value corresponds to Type 2 diesel, which is used industrially for energy generation processes [13]

$$x = \frac{240\,\frac{gallons}{month} * 2{,}03758\ dollars}{1\ gallon} \tag{8}$$

$$x = 489{,}0192\ \frac{dollars}{month} \tag{9}$$

3.3. Monetary cost of natural gas based on its energy

In the case of natural gas, the calculation is based on the energy generated in the simulation, in relation to the official fuel price, which is \$2.00 per million BTU [13]

$$x = \frac{40042{,}3\,\frac{BTU}{hour} * 2{,}00\ dollars}{1000000\ BTU} \tag{10}$$

$$x = 0{,}08\ \frac{dollars}{hour} = 57{,}66\,\frac{dollars}{month} \tag{11}$$

After performing the corresponding calculations for the monetary cost of the fuels used, we proceed to estimate the monthly savings that would be obtained in the combustion process.

$$x = 489{,}0192\,\frac{dollars}{month} - 57{,}66\,\frac{dollars}{month} \tag{12}$$

$$x = 431{,}3592\,\frac{dollars}{month} \tag{13}$$

In percentage terms, this would be as follows.

$$x = \frac{431{,}3592\,\frac{dollars}{month}}{489{,}0192\,\frac{dollars}{month}} * 100\% = 88{,}21\% \tag{14}$$

$$x = 100\% - 88{,}21\% = 11{,}79\% \tag{15}$$

We now proceed to calculate how the cost of fuels influences production costs, taking into account that production costs consist of three key elements: direct materials, direct labor, and manufacturing overhead, with the latter being the central focus of the investigation [14].

$$Production\ costs\ = D.L + D.M + M.O.H \tag{16}$$

To represent how a change in fuels would affect manufacturing overhead, it is considered that this element of the total production cost accounts for 33.33%. Using the percentage savings from natural gas and the equivalent percentage of manufacturing overhead in total production costs, the following calculation is made.

$$x = \frac{33{,}33\% * 11{,}79\%}{100\%} \tag{17}$$

$$x = 3{,}9296\% \tag{18}$$

3.4. Degree of contamination of the fuels used in the energy generation process (40043 BTU/h)

As with any combustion process, products such as water and carbon dioxide are generated, with the latter being a greenhouse gas that contributes to global warming. The following shows the results of natural gas and diesel combustion based on an energy generation of 40043BTU/h .

$$Diesel\ = 2{,}98785\,\frac{Kg\ CO2}{hour} \tag{19}$$

$$Natural\ Gas = 2{,}31681\,\frac{Kg\ CO2}{hour} \tag{20}$$

$$Mass\ flow\ difference = 2{,}98785 - 2{,}31681 = 0{,}6702\,\frac{Kg\ CO2}{hour} \tag{21}$$

$$Percentage\ variation = \frac{0{,}6702\,\frac{Kg\ CO2}{hour}}{2{,}98785\,\frac{Kg\ CO2}{hour}} * 100 = 22{,}46\% \tag{22}$$

In the simulation developed in the DWSIM program for the combustion of diesel and natural gas, Tables 1 and 3 show that the same amount of energy was generated with different volumetric flows, which affects the monetary cost due to the price established by the fuel regulatory authority [13]. For diesel, a monetary cost of \$489/month was obtained, while for natural gas, the cost was \$57.66/month. This means that generating the same amount of energy using natural gas saves about \$431/month compared to using diesel.

It is evident that production costs, particularly manufacturing overhead, which involves fuels, will have to change. A simple calculation was made to observe the percentage variation of these costs, using the natural gas savings percentage and the equivalent percentage of manufacturing overhead in total production costs. The result was a 3.9296% savings in manufacturing overhead using natural gas as fuel in the production process.

On the other hand, Table 1 shows the mass flow of 2.98785 kg CO2/h for diesel for the generation of the same amount of energy, corresponding to the level of contamination produced by combustion. A 22.46% reduction in carbon dioxide emissions was obtained by using natural gas in the process, which is of great importance in reducing greenhouse gases in the atmosphere. This calculated percentage is in line with research conducted in Spain, where the CO2 emissions per gigajoule of energy produced were analyzed, and the variation in emissions between diesel and natural gas was found to be 23.8% [15].

4. Conclusions

The main fuels used in the industries of Ecuador are non-renewable fossil fuels, with Type 2 diesel being the most used, followed by fuel oil and natural gas, with a contamination level of 30% of carbon dioxide emissions into the environment from the burning of these fuels.

A combustion energy of approximately 40043 BTU/h was determined for diesel, with an emission factor of 2.98785 kg CO2/h for a volumetric flow of 240 gallons/month. For natural gas, an energy output of 40042 BTU/h with an emission factor of 2.31168 kg CO2/h was obtained for a volumetric flow of 1.2852 m^3/h using the open-source DWSIM chemical process simulator.

Total production costs were evaluated based on manufacturing overhead, resulting in a monthly percentage savings of 3.9296% when using natural gas as fuel in the process.

Natural gas was identified as the most efficient fuel due to the economic savings it generates and the 22.46% reduction in CO2 emissions into the environment compared to diesel as the traditional fuel.

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