

## Computer Aided Evaluation of Eco-Efficiency of Refinery Combustion Process

Jaqueline Saavedra<sup>a</sup>, Lourdes Merino<sup>\*b</sup>, Viatcheslav Kafarov<sup>b</sup>

<sup>a</sup>Lider plantas piloto, Instituto Colombiano del Petróleo, Km 7 vía Piedecuesta, Piedecuesta - Santander.

<sup>b</sup>Universidad Industrial de Santander, Carrera 27 Calle 9, Bucaramanga - Santander

[loumerino2@gmail.com](mailto:loumerino2@gmail.com)

Combustion becomes the mechanism to generate energy in industrial equipment such as furnaces and boilers. In terms of trends, processes designed and implemented seek to increase energy efficiency, reduce pollution emissions, increase productivity and develop processes for burning gas of variable chemical composition. Recent research focuses on the implementation of operational control systems to minimize errors in operation and reducing the risks of industrial accidents. In this sense, the eco-efficiency contributes to sustainable development and competitiveness by adding more value to products and services, using fewer raw materials, producing less pollution through environmentally and economically efficient procedures and safety process.

This paper evaluates the eco-efficiency of combustion process using fuzzy logic, in order to find methods to achieve efficient processes that harmonize with the care of the environment and ensure process safety. The criteria used in the evaluation process were energy efficiency, the amount of CO<sub>2</sub> and stack temperature, to obtain indicators that allow the management of the process, using approximate reasoning based on fuzzy subsets. Comparing the simulation results with the process historical data, suggest that the calculated index of eco-efficiency describes the performance of the combustion process in furnaces of refinery.

### 1. Introduction

The refinery process of oil fractions faces major challenges due to the need to produce cleaner fuels that meet current environmental laws, especially those related to the increase of energy efficiency and emission reduction in the contaminants (Hsieh, 2009).

Combustion equipment in the oil refining industry in general and in the chemical industry can use mixtures of gases generated in the various plant processes. Heater fuels include refinery gas from the crude units and reformers as well as waste gases blended with natural gas. Fuel is regulated from exit feed temperature and firing rate is determined by the desired level of production and combustion air flow is regulated by positioning the stack damper (Showers, 2002).

Furnaces uses gas with widely varying caloric content as fuel, this can produce large variations in heat delivered in the radiant section, the temperature control of the process tubes and reactions is critical in reforming and cracking operations, so the challenge is to maximize heat delivery of the process-side feed while minimizing fuel consumption, maximize heat delivery with varying fuel quality, minimize heater structural wear, minimize stack emission and maximize safety levels (IEA, 2010). Unsafe operation of heaters or burner problems leads to premature failure, structural damages or tube leaks due to flame impingement, secondary combustion and flue gas leaks. Factors affecting safe and efficient process heater performance include safety, burner operation and environmental emissions (United Nation 2010).

According to this the environmental performance of a company shows the efficiency of the procees applied so, the environmental impact due to the generation of carbon dioxide emissions and its influence on greenhouse effect has given the impulse to the research in the efficient use of fuels and technology development in combustion associated with process eco-efficiency (Fonseca, 2010).

This paper presents the use of fuzzy logic as a tool to evaluate the performance of the combustion process taking into account energy efficiency, the amount of CO<sub>2</sub> emitted and the temperature as a parameter to determine the damage of equipment. In the following sections and subsections describe the concepts of fuzzy theory, fuzzy inference system, to evaluate the combustion of variable composition, the methodology followed, the proposed model, the results and conclusions of the study.

## 2. Theoretical bases

### 2.1 Combustion process

The combustion reaction study includes chemistry kinetics and gas theory, in this regard, in the area immediately after the flame, the combustion products are in chemical equilibrium or very close to equilibrium, so that it can develop methods for calculating the adiabatic flame temperature and the composition of the combustion products.

In order to perform the calculations of chemical equilibrium, thermodynamic properties and predict the conditions of combustion reactions for gas fuel, have been used equations of state in order to predict the behaviour of natural gas, as their experimental determination may be difficult and costly (Skander, 2007). Cubic equations of state are traditionally used for modelling in the oil industry because they offer good results and are mathematically simple (Valderrama, 2003). Numerous investigations have been raised in order to compare the quality of the predictions of the thermodynamic properties from these equations, the equation Peng and Robinson is the most widely used equation (Alfradique, 2007).

Gas fuel composition is usually specified in volumetric percentage of different gases that composes it, and the calorific value is a function of the composition and calorific value of each component. Program Aspen HYSYS allows the evaluation of the combustion process where it is provided the value of adiabatic temperature, efficiency and products of combustion for combustible gas mixtures.

### 2.2 Fuzzy logic

In 1965, based on the fundamental concept of temperature variation or multivalency, Professor Lotfi A. Zadeh in the Department of Electrical Engineering, University of California at Berkley, formalized fuzzy sets theory (Zadeh, 1965). An analysis tool fundamented on the observation that human decisions can be right even where despite the knowledge in different situations is imperfect and is associated with uncertainty. So, the problems solutions are solved with approximate data which indicates that precision is not always necessary (De Armas et al 2008).

The idea of fuzzy sets is that in common logic analysis, a point belongs (or not) to a single stage, but in real process, there are not only one belonging attached; an element can be 30% of a set X and 70% of the set X'. This explains the transition from a state set X to a set in state X' as a continuous process in the physical world and to describe as the boundaries tend to be subjective.

There are several defuzzification methods in the literature, the two most commonly used are the center of gravity and the maximum average. The average maximum, the output should be obtained from the average of the two extreme elements in the universe corresponding to the highest values of the consequent membership function. With the center of gravity, the output is the value in the universe that separates the area under the curve of the function in two equal parts. The applications are limitless, and adaptable to all areas.

### 2.3 Fuzzy Inference System

In the fuzzy inference is interpreted in the input values, and then based on some rules, values are assigned to the output.

The establishment of a fuzzy inference process is performed using a set of rules, which are phrases like structure with an IF / THEN that are interpreted by the system. It is noteworthy that there is a natural parallelism rule, as they are tested, this being one of the most important aspects of fuzzy logic systems. It provides a range of values for each variable analyzed case, as well as what is the meaning of each linguistic term. The fuzzy inference is the process of assigning a given input to an output using fuzzy logic. In this process, we have: membership functions, fuzzy logic operators and rules of the type IF / THEN. Type: [R] IF antecedent THEN consequent (weight).

Figure 1 represents a diagram containing a general scheme describing the fuzzy system.

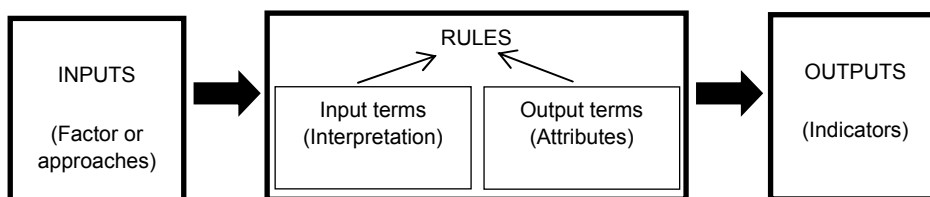


Figure 1: Fuzzy System scheme

### 3. Metodology

The fulfillment of the objectives included collecting historical data from refinery process furnaces and their statistical analysis, followed by computer simulation of the combustion process and development of the fuzzy inference process; these stages are illustrated in Figure 2.

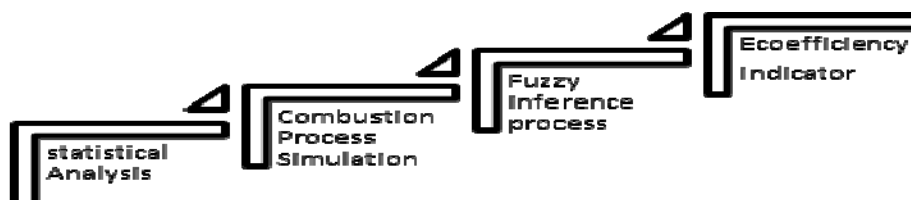


Figure 2: Stages of methodology

#### 3.1 Statistical analysis of historical data of combustion process at refinery furnaces

The review of historical production data includes measuring the flow or load, record input and output pressure, inlet temperature, outlet and wall tube and measuring the calorific value, were taken two years period of analysis of historical data.

Data chromatographies of streams identified as contributors to the combustible network were reviewed. Variability of the gas composition, the ranges of each of the identified compounds and analyzing the frequency deviation in the concentration was analyzed by StatGraphics program.

#### 3.2 Combustion Process Simulation

ASPEN HYSYS was used, which is specialized software for simulation of processes chemical and petrochemical industry. Data on energy efficiency, temperature and flue gas compositions were obtained.

#### 3.3 Fuzzy inference process

Data of energy efficiency, adiabatic temperature and amount of CO<sub>2</sub> were used as input in Mandani model, defined rules and defuzzyfication was performed by the centroid method.

#### 3.4 Eco-efficiency indicator

In the post-processing stage each sample by defuzzyfication corresponding to individual ratings between the composition of a position measurement as the mean or the median. In this particular case, the median was used for the characteristic of not being affected by extreme values. Importantly, the output value of the post-processing step can be again converted into the form of linguistic terms. Model results allow identifying the fuel mixtures that promote eco-efficiency in the combustion process.

#### 3.5 Equipment

In order to achieve the purpose of this research, a fired heater representative from a petroleum refining process was selected; This one consist on a heat exchanger where process fluid flows inside tubes and is heated by the radiation which comes from a combustion flame and convection coming from hot gas.

Fired heater consists in a closed steel array with an internal isolation of refractory bricks. The convective area is located in the upper side of the array and the stack. The radiation tubes are located over the walls and the flame is originated through the burners, the furnace analysed in this work has 37 tubes in the convective and 49 tubes in the radiation area. Figure 1 show an illustration of fired heater.

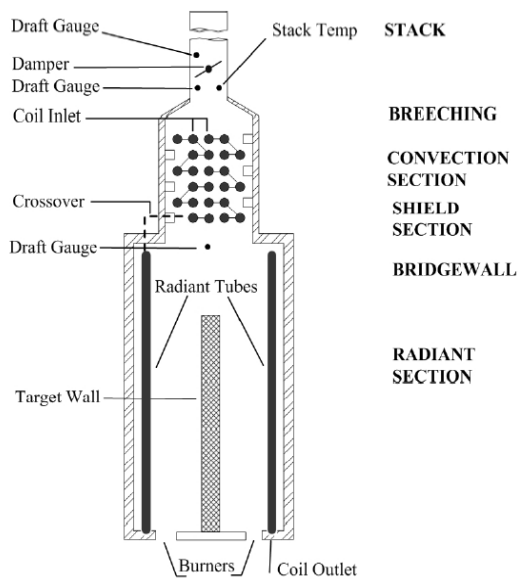


Figure 3. Illustration of fired heater.

#### 4. Results

##### 4.1 Statistical analysis of historical data of combustion process at refinery furnaces

The review of historical production data includes measuring the flow or load, record input and output pressure, inlet temperature, outlet and wall tube and measuring the calorific value, were taken two years period of analysis of historical data. Figure 2 show fuel gas network in a refinery.

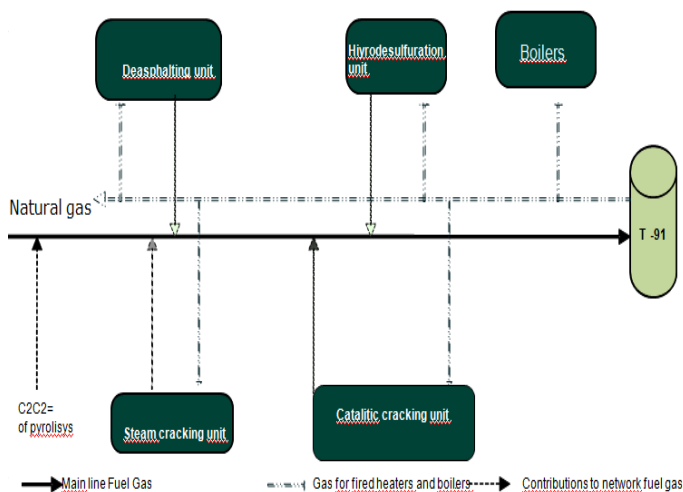


Figure 4. Fuel gas network.

Data chromatographies of streams identified as contributors to the combustible network were reviewed. 87 gas streams were evaluated in eight process areas, analysing the flows that were related with the fuel network and the incidence in the units. Each stream composition allowed to identify which ones have the potential to cause equipment failures and environmental emissions.

Variability of the gas composition, the ranges of each of the identified compounds and analyzing the frequency deviation in the concentration was analyzed by StatGraphics Centuriun XV.II program. Fuel gas composition in a refinery could be a mixture of compounds shown in table 1.

Table 1: Fuel gas composition

Compound	Natural gas	Stream 1	Stream 2	Stream 3	Stream 4	Stream 5
	Mol %					
Hydrogen	0,770	0	97,389	17,21	34,72	0
Carbon Monoxide	0	0	0,037	1,75	2,54	0
Methane	96,85	0	2,043	31,28	42,02	0,13
Ethane	0,375	0,001	0,036	13,34	3,50	0,40
Propane	0,051	25,490	0,033	1,94	1,22	8,48
n-Butane	0	0,005	0,028	0,21	0,37	59,85
i-Butane	0,014	0,253	0,011	0,55	0,62	30,30
n-Pentane	0	0	0	0	0	0,21
i-Pentane	0,074	0	0,038	1,46	0,01	0,51
Ethylene	0,069	0	0	12,20	0,96	0,02
Propylene	0	74,24	0	7,71	5,18	0,10
n-Butene	0,008	0	0	0	0	0
H2S	0	0,011	0,081	3,11	0	0
Carbon dioxide	0	0,0000	0,041	2,6	0	0
Nitrogen	1,764	0	0,263	6,64	8,86	0
Oxygen	0,025	0	0	0	0	0

#### 4.2 Simulation process

Aspen Hysys was used, which is specialized software for simulation of processes chemical and petrochemical industry. Data on energy efficiency, temperature and flue gas compositions were obtained. Based on the simulation scheme for the combustion process shown in Figure 3, fuel gas composition was changed according to boundary established by statistic analysis.

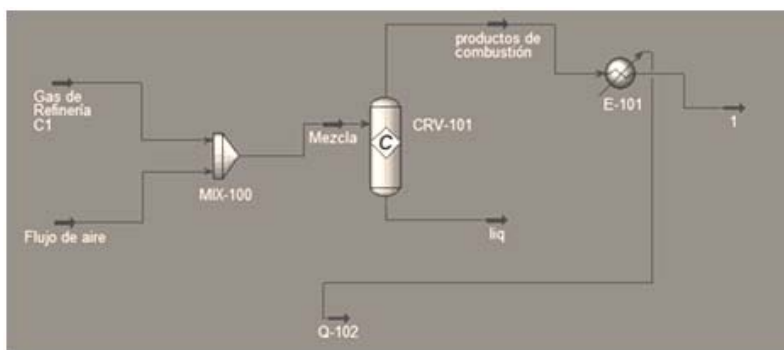


Figure 5: Simulation of combustion process in Aspen Hysys.

Combustible mixtures were simulated by varying the composition of gas components representative refinery fuels for furnaces, Figure 4 shows the input and output data of Hysys.

Simulation results allowed eliminating some components of the refinery gas (RG) (i-pentane, butylene, acetylene, carbon monoxide, carbon dioxide, nitrogen and oxygen) from the evaluated mixtures. The criteria used to dismiss these components were:

- ✓ Find those compounds whose contribution to the stream concentration is very low (<1%),
- ✓ Compounds which are not present in most of the streams,
- ✓ Compounds which do not contribute significantly to the heating value of the mixture.

In the case for n-butane and i-butane only one representative compound of this gas family was selected based on they represent the same lower heating value (LHV) and the same combustion reaction.

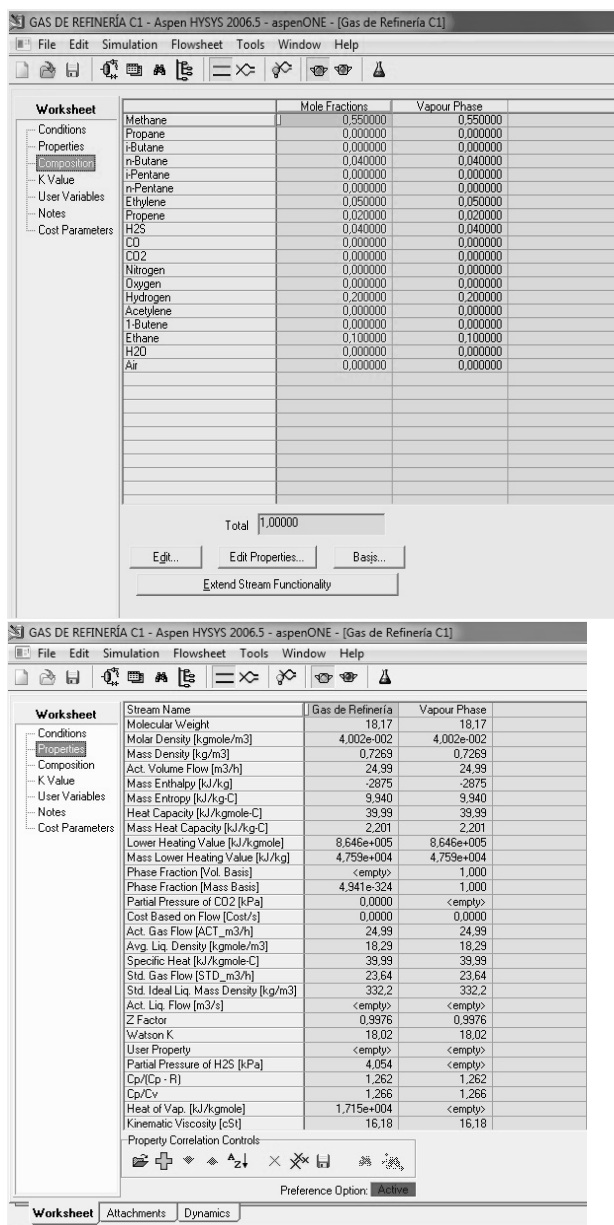


Figure 6: Input and output Hysys data.

Simulation results shows mixtures which are possible in the range of calorific value between  $7600$  and  $18800$   $\text{kCal/Nm}^3$ . Composition data, CO<sub>2</sub> emissions and energy potential of each stream were related. Factor emission method was applied to calculate CO<sub>2</sub> emissions and lower heating value was calculated, then the currents with the most environmental impact were determined. Based on these data it was possible to make a comprehensive analysis of energy and environmental aspects. Table 2 shows representative compositions of the possible mixtures and natural gas. Figure 7 shows the LHV values of the fuel mixtures and natural gas.

Table 2: Representative compositions of fuel gas

Compound	C1	C2	C3	C4	Natural Gas
CH <sub>4</sub>	55	70	25	35	97
C <sub>2</sub> H <sub>6</sub>	10	0	8	3	1
C <sub>3</sub> H <sub>8</sub>	0	16	25	35	1
C <sub>4</sub> H <sub>10</sub>	4	5	10	12	0
C <sub>2</sub> H <sub>4</sub>	5	3	10	7	0,5
C <sub>3</sub> H <sub>6</sub>	2	0	5	8	0,5
H <sub>2</sub> S	4	1	2	0	0
H <sub>2</sub>	20	5	15	0	0

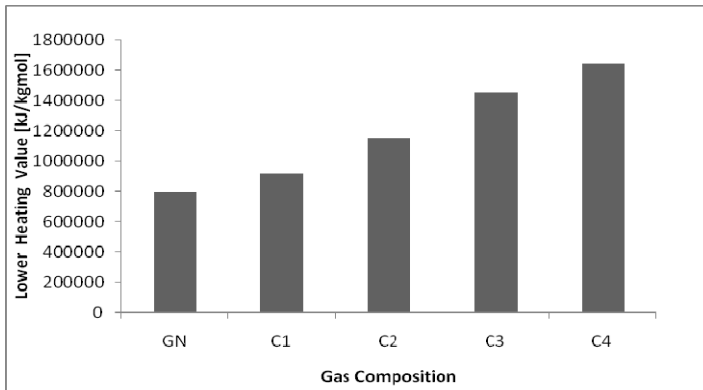


Figure 7. LHV values versus gas composition

Historical data process shows that combustion efficiency presented values between 60 and 90 %, but is affected for changes in gas fuel composition. Mixture C1 presents more difficult to control in operation, due hydrogen content, but it presents higher potential for use due to saving natural according to reported by Hsieh and Wildy (Wildy, 2002) for fired heater.

Fired heaters are designed to operate on natural gas, so the efficiency of these equipments is greater when using methane-rich fuel, but efficiency can be increased by using mixtures containing hydrogen, although this increases the risk of explosions.

#### 4.3 Model

A Mamdani type arrangement was chosen and to support the calculation we used the fuzzy logic toolbox under MATLAB environment. Figure 8 shows the outline of the model used.

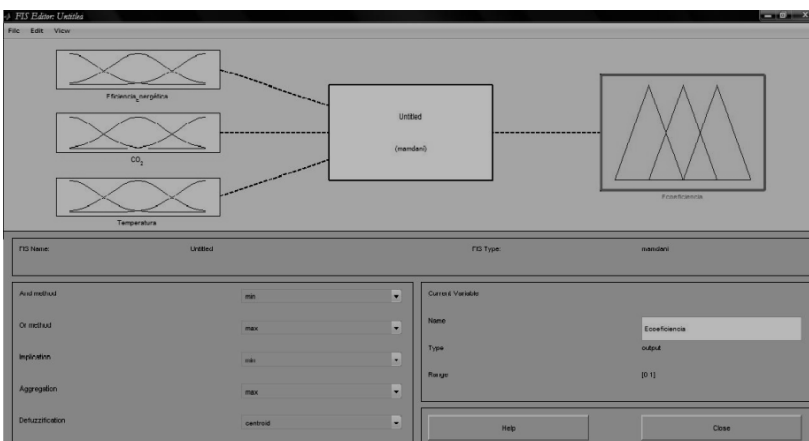


Figure 8: Fuzzy model designed.

#### 4.4 Membership functions

The input variables corresponding to the three components identified (energy efficiency, adiabatic temperature and CO<sub>2</sub> quantity). To define the membership functions has been established five levels that are shared by all components, defined levels are: very low, low, medium, high and very high, representing the state of each

component and their impact on the eco-efficiency of combustion. The rating of each component determines the values obtained above model input.

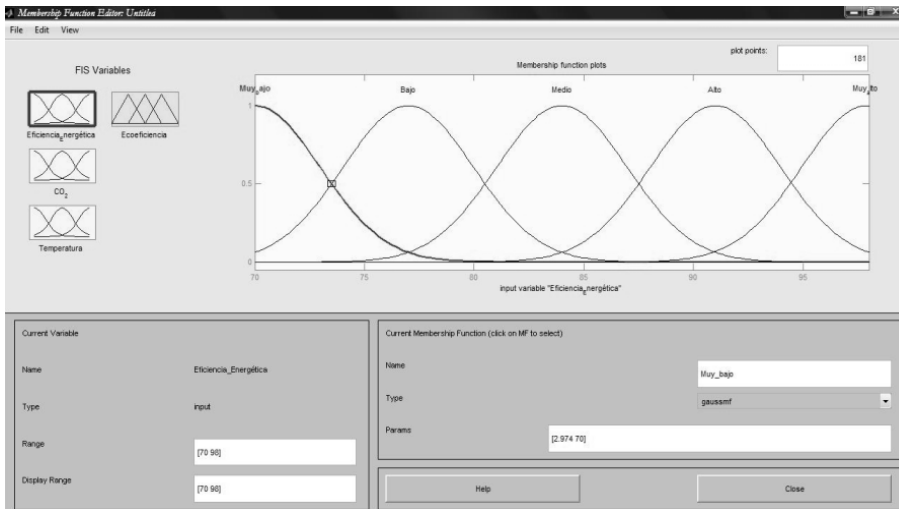


Figure 9: Membership functions.

The degree of membership was defined and used a Gauss membership function. Figure 9 shows the membership functions analyzed.

Later, 90 rules were identified with possible values of the variables. For this, it was used the format a set of rules (Del brío and Sanz, 2002):

$$R^{(i)} : \text{IF } X_1 \text{ is } F_1^1 \text{ and } \dots \text{ And } X_n \text{ is } F_n^1 \text{ THEN } y \text{ is } G^1 \quad (1)$$

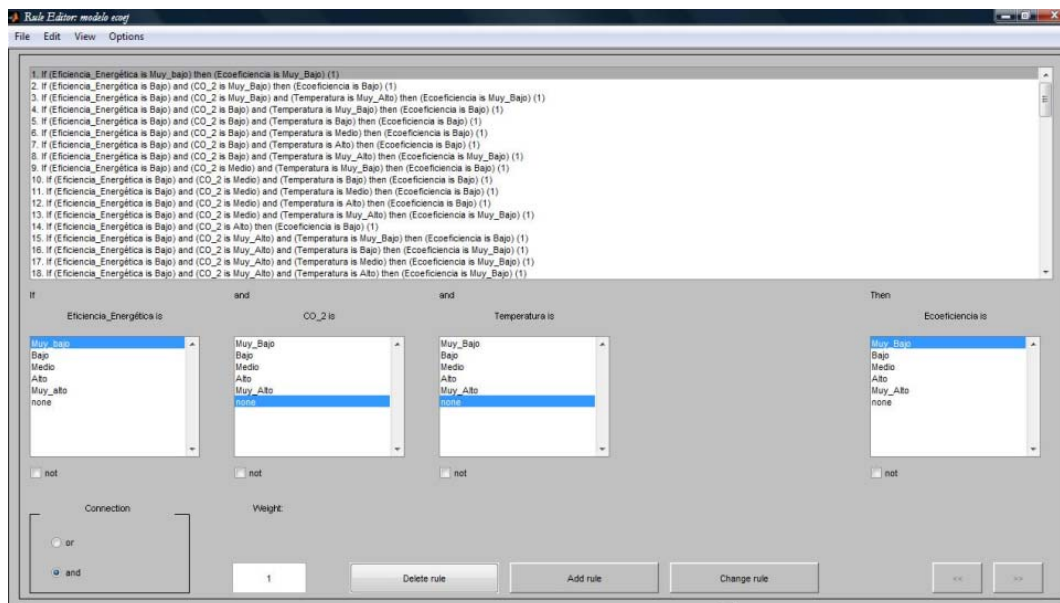


Figure 10: Rules.

Note that the rules are common sense and the system behaviour is written in terms of the labels of the membership functions. From this point, it is possible to use the screen and observe the behavior rules of the system to any changes in the parameters of the input variables. Figure 10 shows screen of rules identified.

Rules were validated by operators of refineries and the valuation was made according to the impact on the process of energy efficiency, CO<sub>2</sub> emissions and temperature and taking in count the interactions between them.



#### 4.5 Eco-efficiency indicator

Figure 11 shows an example of eco-efficiency indicator calculated consider high values for input variables.

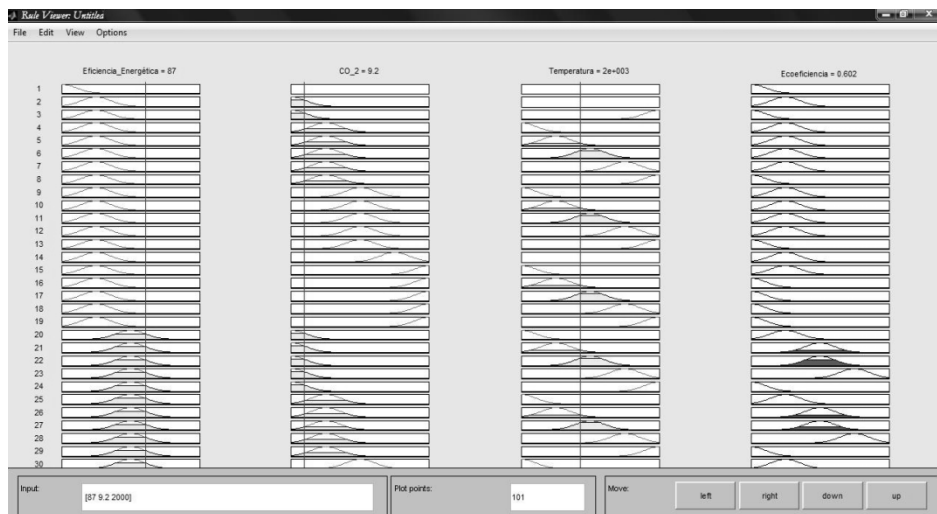


Figure 11: Eco-efficiency indicator

The procedure of this model is to calculate the fuzzy membership degree in fuzzy sets all of the dimensions of input from relevant evaluations for each fuel gas mixture. After this, the eco-efficiency level indicator is determined by fuzzy inference process, which uses a set of rules and then the fuzzy output defuzzification by means of centroid method.

Eco-efficiency indicator shows high values when the combustion process involving mixtures similar to natural gas composition, which is in accordance with the design of the furnaces; eco-efficiency indicator begins to present low values when the efficiency of the furnaces is low, which directly affects the heat supplied by the furnace to the refining process.

#### 5. Conclusions

The simulation of fuel mixtures in Hysys program helped assess the combustion characteristics by varying the fuel composition, allowing stable ranges for the percentage of energy efficiency, percentage of CO<sub>2</sub> and adiabatic temperature. The simulation data agree with the process data.

Mixture C1 presents 4 % of H<sub>2</sub>S and 20 % of Hydrogen has been an aggressive environment and increased risk for damages by high temperature and explosion, at this point it is necessary evaluate combustion efficiency to determine which mixtures generate less impacts.

A fuzzy model- based approach for calculated an eco-efficiency indicator was presented. The effectiveness of the model was verified through simulations with data obtained from historical data process at refinery industry. Rules identified for combustion process were easy attained with fuzzy sets, relating to the fundamental process knowledge.

The model outputs would be used to calculated real-time combustion quality measures, considering a measure for eco-efficiency that integrate safety, environmental emissions and efficiency energetic.

The eco-efficiency indicator allows identify which mixtures can achieve eco-efficiency of processes by integrating energy efficiency factors, the adiabatic temperature and CO<sub>2</sub> emissions. The results show that eco-efficiency indicator is strongly influenced by the energy efficiency of the combustion, presenting a high value when the energetic efficiency is high.

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