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Numerical Simulation of Combustion Process of Fuel Gas Mixtures at Refining Industry

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At oil refinery is important evaluate efficiency of combustion process because variability of combustible gas composition, depending of characteristics and conditions at industry.
The combustion process assessment required thermodynamics properties and kinetics in order to know heating value, energy efficiency and emissions generated. These properties have been calculated with computational methods.
In this work has been used software PREMIX for evaluate combustion of representatives mixtures of refining industry; the simulation model used describes an isobaric system, in steady state and unidirectional, and reaction mechanics is carried out using GRI-MECH 3.0. Combustion products, temperature and rates of propagation flame were analyzed in the range of equivalence ratio from 0.8 to 1.8, for natural gas. Results were validated with experimental data carried out in a lab scale reactor. Combustion products show concordance with kinetic mechanism of reaction, adiabatic temperature maximum was 2040 K for stoichiometric equivalence ratio and maximum value for propagation flame rate was 0.007cm/s.
Results obtained by simulation and experimentally show agreement with data reported in the literature for combustion products, temperature and propagation flame rate, it showing that the model used describes combustion process and can be assessed reliably and economically.

Key words: combustion, simulation, equivalence radio,

1. Introduction

Combustion is a chemical reaction of fuel oxidation and rapid oxygen reduction accompanied by the release of a certain amount of heat (exothermic reaction) (United Nation, 2006) .In the actual conditions of the combustion process, it is not possible to achieve complete combustion supplying fuel air quantity theoretically necessary. This is due to the inability to achieve in real conditions perfect mixing fuel with air in the large volume of the furnace during the short residence time of the gases in furnace (1 - 2 s) (Mahallawy, 2002).
An analysis of the combustion process includes the thermodynamic properties to determine the quantity and quality of the transferred energy; complementing the energy aspects should be considered the study of chemical kinetics, reaction mechanisms and transport phenomena. In addition, process restriction must be considered, such as pressure, equivalence ratio and burners parameters.
Equivalence radio impacts in materials damages (Hsieh, 2007) for high temperature corrosion, energy efficiency and environmental emissions for increase greenhouse effect (Hsieh, 2009).
Energy efficiency was evaluated for fuel gas mixtures with different percentage of methane. Computational simulation and experimental test were carried out in order to validate combustion model and compare with industrial reports. The model presented by Miller et al. (Miller, 1990) describes light hydrocarbon combustion; this model permits simulate flame rate, temperature profile and products of combustion reaction on equilibrium conditions and it consider ideal gas (Toledo, 2009).

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2. Methodology

The fulfilment of the objectives included evaluation of energy efficiency and environmental emissions, this procedure start with definitions of variables and parameters for design experiments in order to develop computational simulation and experimental tests. Figure 1 shows stages of methodology. Table 1 shows variables and parameters for evaluation, this values were selected in agree with work by Kafarov and Saavedra (2013).

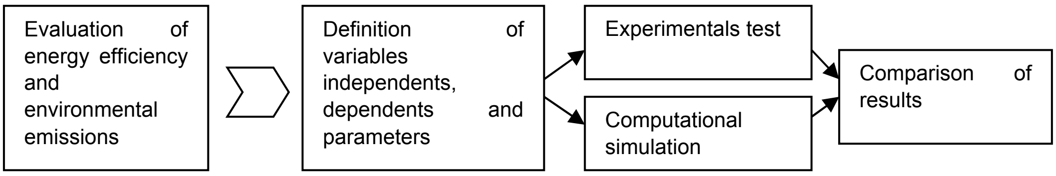

Figure 1: Stages of the methodology

Table 1: Variables and parameters

Variables independents	Variables dependents	Parameters
Composition of mixture	Temperature	Flow
Methane = 55, 70, 92.5 % mol	Wave propagation velocity	Pressure
Equivalence ratio (φ)	Composition of combustion products	Reactor
φ = 0.8, 1.0, 1.4, 1.8	(CO_2, CO, H_2, CH_4 y H_2O)	

2.1 Combustion Process Simulation

PREMIX was used, which is specialized software for simulation of combustion processes. Data on rate flame, temperature and flue gas compositions were obtained.

2.2 Experimental test

Experiments on combustion were conducted using the setup schematically show in Figure 2. The apparatus consisted of a quartz reactor filled with a porous medium, fuel and air supply system, temperature measurement system and gas emission analyzers. To prevent heat losses and achieve quasi-uniform temperature profiles, additional insulation was applied on the external diameter of the reactor.
The mixtures of fuel with air were prepared by a continuous flow method using a set of mass flow controller. To ensure uniform gas composition the reactants were premixed in a mixing chamber. The upstream propagating combustion wave was initiated at exit of reactor.

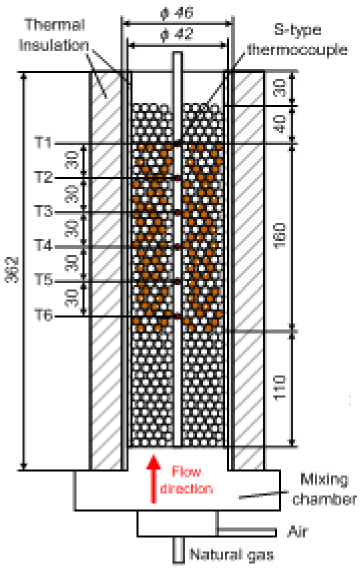

Figure 2: Experimental setup

3. Results

3.1 Combustion products

Combustion products were quantificated by gas chromatograph for a range of equivalence ratio from 0.8 to 1.8. Figure 3 shows composition of combustion products for mixture of natural gas and air; for φ < 1.0 combustion is complete, CO_2 percentage decrease when φ > 1.0. Numerical and experimental results show the same trend and they are in agree with reported by literature (Araya, 2014); For equivalence ratio between 0.8 y 1.8, CO_2 percentage is in range between 7.5 and 2.3 %.

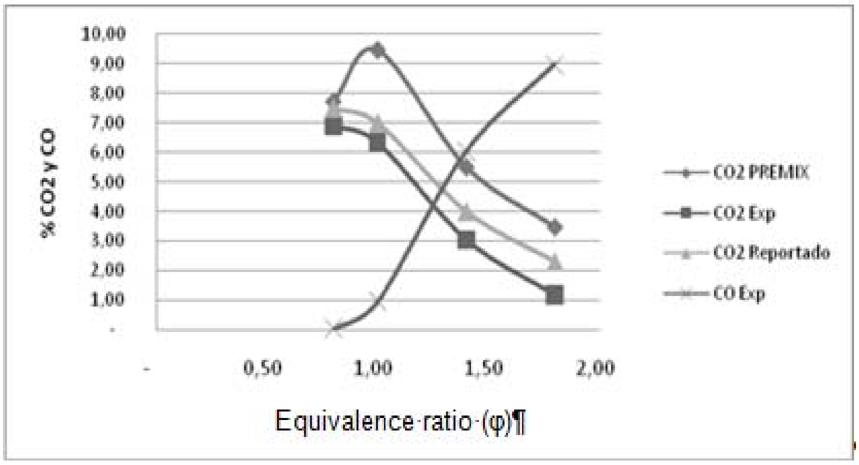

Figure 3: CO_2 and CO percentage for mixture of natural gas and air.

Table 2 shows experimental results of CO_2 percentage for mixtures with different compositions of methane; the higher percentage of CO_2 was founded for 1.8 equivalence ratio for mixture with 55 % of methane, the tendency is to increase CO_2 percentage when percentage of methane decrease in mixture. Numerical predictions are in concordance with experimental results (Araus, 2014).

Table 2: Experimental results for percentage of CO_2

Equivalence Ratio (ϕ) / Mixture % Methane	0.8	1	1.4	1.8
92.5	6.9274	6.345	3.05	1.17
70	8.304	6.98	3.3898	3.4307
55	7.8209	6.55	9.766	12.35

Factorial method of experiments design was applied for data analysis using Matlab ANOVA2 function. Figure 4 presents results

ANOVA Table

Source	SS	df	MS	F	Prob>F
Columns	9.731	3	3.2436	0.38	0.7684
Rows	49.076	2	24.5382	2.91	0.1309
Error	50.62	6	8.4367		
Total	109.427	11			

Figure 4. ANOVA table for CO_2 percentage.

The vector p shows the p-values for the three mixtures and the four equivalences ratio. Results demonstrate interaction between equivalence ratio and CO_2 generated (P-value > F); but synergy relationship between emissions and mixture type is not shown (P-value < F); ie, (0.1309 < 2.91).

Figure 5 shows percentage of hydrogen produced and methane consumed, results present higher percentage of hydrogen for φ = 1.8, values reported that percentage of hydrogen was increased in function of equivalence ratio (Araya 2014).

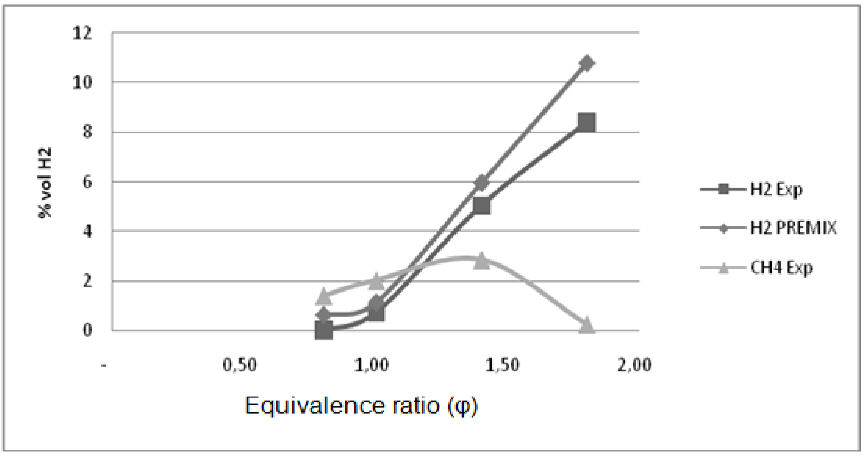

Figure 5: Percentage of Hydrogen.

3.2 Combustion wave temperature and propagation rate

Figure 6 shows results of combustion temperature for mixture methane-air in function of equivalence ratio. Analysis of the experimental data shows that the combustion temperature remains between 1343K and 1383K, 173K increase in φ = 1.8, these values agree with those reported by Araya (Araya, 2014) to the range of 0.5 <φ <3.0.

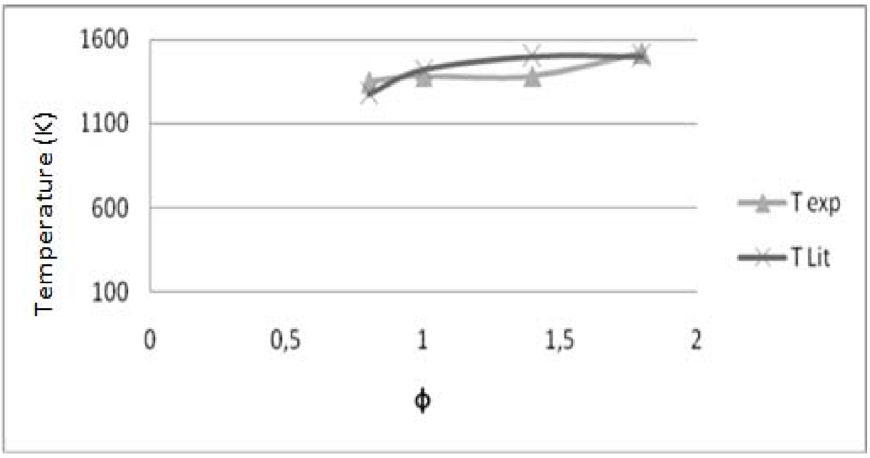

Figure 6: Combustion temperature.

Table 3 presents results for combustion temperature were register for mixtures with different percentage of methane.

Table 3: Experimental combustion temperature (K).

Relación de Equivalencia (ϕ) / Mixture % Methane	0.8	1	1.4	1.8
92.5	1348	1383	1383	1521
70	1252	1263	1396	1531
55	1302	1315	1336	1489

Figure 7 shows p-value and F for experimental data using Matlab ANOVA2 function.

ANOVA Table

Source	SS	df	MS	F	Prob>F
Columns	83230.3	3	27743.4	19.35	0.0017
Rows	6208.2	2	3104.1	2.17	0.1959
Error	8600.5	6	1433.4		
Total	98038.9	11			

Figure 7: ANOVA table for combustion temperature.

The vector p shows p-values for 4 equivalence ratios and 3 mixtures evaluated, results indicate that temperature is not depending of equivalence ratios (P-value < F); ie, 0.0017 < 19.35. p-values do not show interactions between temperature and mixtures type (p-value<F); ie, 0.1959 < 2.17.

Figure 8 shows the values obtained by simulation using PREMIX and experimentally compared with those reported by Araus (2014) and Vergara (2011) for methane combustion, found similar values.

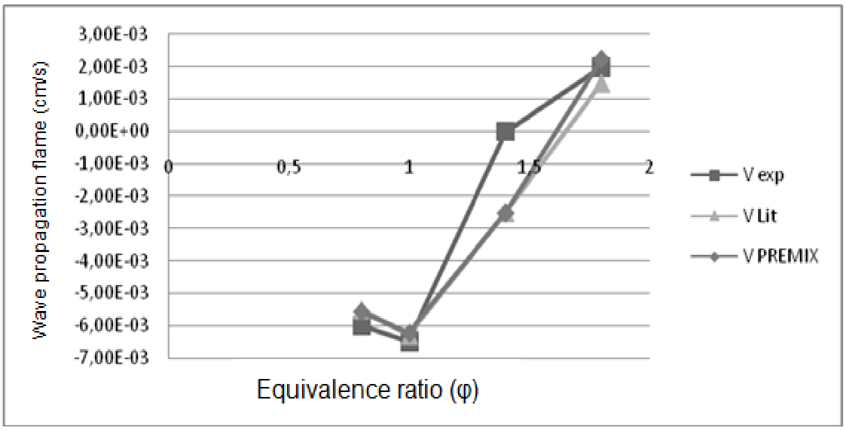

Figure 8: Wave propagation flame.

Wave propagation flame is shown as a function of equivalence ratio in figure 8, maximum absolute velocity value of 0.00615 cm/s is observed for φ = 1.0. Upstream underadiabatic regime of propagation is observed for equivalence ratios less than 1.4 (φ < 1.4), which corresponds to lean mixtures with high oxygen excess. Velocity for φ = 1.4 was approximately 0 cm/s, and downstream superadiabatic propagation occurs in ultrarich region, for mixtures with high content of methane (φ > 1.4).

4. Conclusions

The results obtained by simulation and experimentally show agreement with data reported in the literature for products of combustion temperature and flame front velocities, showing that the model used describes the process of combustion and combustion can be assessed reliably and economically.
Should take into account the constraints of the model in terms of equivalence ratio ranges, the combustion temperature was stable range evaluated for equivalence ratio between 0.8 and 1.8, being a temperature of about 1300 K to a mixture natural gas - air.
Combustion products evaluated in the range of equivalence ratio between 0.8 and 1.8 show agreement with complete oxidation reactions until φ ≤ 1.0, due to the excess air in the mixture and partial oxidation reactions for φ ≥ 1.0, leading the production of hydrogen and CO in the combustion products.

Acknowledgements

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References

Araus K., Reyes F., Toledo M., 2014, Syngas production from wood pellet using filtration combustion of lean natural gas - air mixtures. International Journal of Hydrogen Energy 39, 7819 – 7825.

Araya R., Araus K., Utria K., Toledo M., 2014, Optimization of hydrogen production by filtration combustion of natural gas by water addition, International Journal of Hydrogen Energy 39, 7338 -7345.

El-Mahallawy, F., El-Din Habik S., Fundamentals and Technology of Combustion. Elsevier 2002.

Hsieh Shih-Chieh and CHih-Ju G. Jou, 2009, Using Hydrogen-Rich Multifuel to Improve Energy Efficiency and Reduce CO_2 Emission for High-Energy Furnace. Environmental Progress & Sustainable Energy Vol.28, No.1.

Hsieh, S.C., Jou, C.J.G. 2007, Reduction of greenhouse gas emission on a medium-pressure boiler through hydrogen-rich fuel control, Applied Thermal Engineering, 27, 2924 – 2928.

Kafarov V., Merino L., Saavedra J., 2013, Computer aided evaluation of eco-efficiency of refinery combustion process, Chemical Engineering Transactions. 32, 217 – 222.

Miller J., Kee R., 1990, Chemical kinetics and combustion modeling, Combustion Research Facility, Sandia National Laboratories, California. Annu. Rev. Phys. Chem. 41: 345-87.

Saavedra J., Merino L., Kafarov V., 2013, Determination of the gas composition effect in carbon dioxide emission at refinery furnaces, Chemical Engineering Transactions, 35, 1357-1362.

Toledo M, Bubnovich V, Saveliev A, Kennedy L. 2009, Hydrogen production in ultrarich combustion of hydrocarbon fuels in porous media. International Journal of Hydrogen Energy 34:1818e27.

United Nations Environment Programme. 2006, Energy Efficiency Guide for Industry in Asia. Thermal Equipment: Fuels and Combustion. Asia. <www.energyefficiencyasia.org> access in: 24.02.2015 .

Vergara E., Saveliev A., Toledo M., 2011, Syngas production in hybrid filtration combustion. International Journal of Hydrogen Energy 36, 3907 – 3912.