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3D CFD Simulation of Combustion in Furnaces Using Mixture Gases with Variable Composition

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In the petroleum refining industry, furnaces are key equipment because they provide the necessary heat to carry out different processes. These furnaces are designed to use natural gas as fuel, but in most cases they use a mixture of waste gases known as refinery gases (RG), which molar composition varies depending on the process in which they are generated, in most cases with high content of propane, hydrogen, propylene, among others. This is done in most cases to save energy and reduce storage cost. However, this variation in molar composition also produces a change in calorific power that can be as high as 1,200 Btu/ft^3, producing alterations in the combustion process, affecting efficiency and increasing pollutant emissions. In this work, the Computational Fluid Dynamics (CFD) technique is used to simulate the combustion process in a representative segment of a typical refinery furnace using RG as fuel with 3 different molar compositions. Comparative CFD 3D simulation cases are performed to study the effect of molar composition variability in the temperature and chemical species profiles inside the furnace. The obtained results show that high contents of gases like propane, propylene or hydrogen increase the calorific power and peak temperature inside the furnace, but temperature profile distribution is less uniform. The chemical species profiles inside the furnace show that there is an increase in CO when using mixture gases with low CH_4 content, which indicates that a more detailed study regarding air excess and flow is needed. The results are very important because they can be used as a tool for decision-making regarding the convenience to use or not refinery waste gases as fuels in furnaces and to stablish a starting point for a detailed study about the improvement of furnaces operation and process safety.

1. Introduction

In the petrochemical industry, different refining processes are carried out in which waste gases are generated as by-products, called refinery gases, which are used as fuel in furnaces and boilers to avoid storage costs and save natural gas. However, these refinery gases have a wide variation in their molar composition depending on the unit in which they are produced, generating changes in the calorific power of these gases.

In the combustion process there are a set of strongly associated disciplines: thermodynamics, kinetics and transport phenomena. These phenomena can be represented mathematically using the fundamental equations of mass, momentum and energy conservation, (Gentile et al., 2016). However, these equations can only be solved analytically in very simplified cases, along with the additional equations when there is turbulent flow. In this sense, the implementation of the Computational Fluid Dynamics (CFD) technique has proved to be a very useful tool that can provide valuable information about the operating processes in furnaces, which can be evidenced in several studies published in the literature on modeling and simulation of combustion processes in typical industrial furnaces using CFD.

Stefanidis et al. (2006) performed the CFD simulation of the combustion process in a cracking furnace and studied the effects of the different combustion models. Flow, temperature and concentration profiles of chemical species were obtained in the combustion chamber of an industrial cracking furnace using two combustion models: The Eddy Dissipation Concept with detailed reaction kinetics and The Eddy Break Up Model with simplified reaction kinetics. At the end of their research they conclude that more sophisticated combustion models such as the Eddy Dissipation Concept with detailed reaction kinetics for combustion modeling should be used in cracking furnaces.

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Aminian et al. (2010) conducted an investigation on temperature and flow profiles in an alternative design of an industrial cracking furnace using CFD. In the study they used the RNG model k-ε to model the turbulence, the P1 and DO models to represent the radiation and the Eddy Dissipation Model for combustion. It was evidenced that the P1 and DO models are suitable as a solution method for the radiation transfer equation and the Eddy Dissipation Model for combustion in industrial cracking furnaces. Also, an alternative design was simulated to investigate the improvement of the recirculation of the combustion gas and the temperature distribution inside the furnace.

Many other researchers also used CFD to model and simulate combustion processes in furnaces obtaining flow profiles, temperature and concentration of species using fuels with defined composition. Li et al. (2015) used a fixed composition of methane as fuel for the CFD simulation of a refining vacuum furnace but in the literature there are very few studies that use fuels with variable calorific composition and power. The objective of this simulation is to evaluate the effect of using fuels with variable composition and calorific power in the combustion process in industrial furnaces by means of a three-dimensional simulation in CFD. This can be done by analyzing and comparing the temperature and CO mass fraction contours inside the furnace obtained from the different simulation cases. Cala et al. (2013) determined some chemical compositions of mixture gases and studied the effect of their composition variability on the characteristics of the combustion process like Wobbe Index, efficiency and adiabatic flame temperature. The results showed that it is possible to find a range of chemical compositions of refinery gases that can increase efficiency.

However, it is also important to study other aspects like temperature behavior inside the furnace in order to reduce or even avoid overheating and corrosion problems. The temperature profiles obtained from a CFD simulation can help to study this aspect as well as pollutant emissions. Thus, this work studies the effect of chemical composition variability on temperature and CO mass fraction profiles. The model is limited because in this stage of the research the idea is to use a simplified model (i.e, simplified geometry and burner) as a starting point for the whole investigation. In literature many authors use simplified geometry models in their investigations. An example of this is the paper of (Iancu et al., 2017), where they use a simplified 2D geometry and burner design for a CFD simulation of combustion process in a furnace. In the next stage of this work, a more complex geometry and burner will be analyzed. This is can be taken as a starting point for future studies regarding furnace efficiency improvement and reduction of pollutant emissions, so the purpose of this paper is to show preliminary interesting results.

2. Furnace characteristics

The configuration of the furnace object of the study is of non-premixed cylindrical type with burner in the floor, that is to say that the fuel and air have separated inlets and is considered to be adiabatic. Because the furnace is symmetrical only half of the total geometry needs to be modeled. The simulation was carried out in the commercial code ANSYS FLUENT and the dimensions of the geometry can be seen in Figure 1. In the boundary conditions the air and gas inlet flows are defined, which are 1.682 kg/s and 0.0974 kg/s, as well as the compositions of the gas mixtures shown in Table 1 among others. Since the furnace is cylindrical and symmetric, only half of the furnace needs to be simulated, which reduces computational costs considerably. The temperature of air and fuel at both inlets is 300 K, Fuel Stream Rich Flammability Limit is set to 0.06, and air excess is 10 % for all cases. The SIMPLE algorithm was used for the pressure-velocity coupling and the first-order UPWIND scheme for the discretization of the equations. The computational mesh used contains 800,000 elements.

Figure 2 shows zoom section of the burner, which has 2 circular inlets simple design, air inlet is 1.6 m diameter and gas 0.08 m diameter. The gas inlet is in the middle of the air inlet, which is larger in size due to requirement of air flow in this type of combustion.

3. Mathematical models

The mathematical models necessary to solve the simulation are based on the basic equations of conservation of mass, momentum, energy and chemical species. In combustion modeling with CFD this means that it is necessary to select a turbulence model, combustion model and radiation model in order to develop the simulation of a furnace. There are many CFD models available and the selection depends on the simulation case object of study. For more detailed information of mathematical models please refer to the work of (Díaz-Mateus and Castro-Gualdrón., 2011)

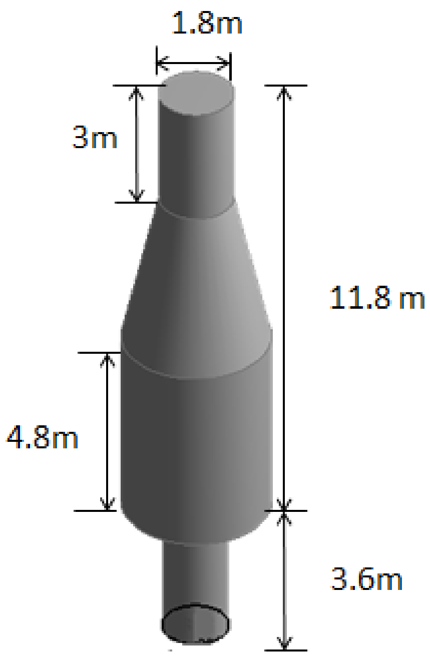

Figure 1: Geometry of the furnace object of study

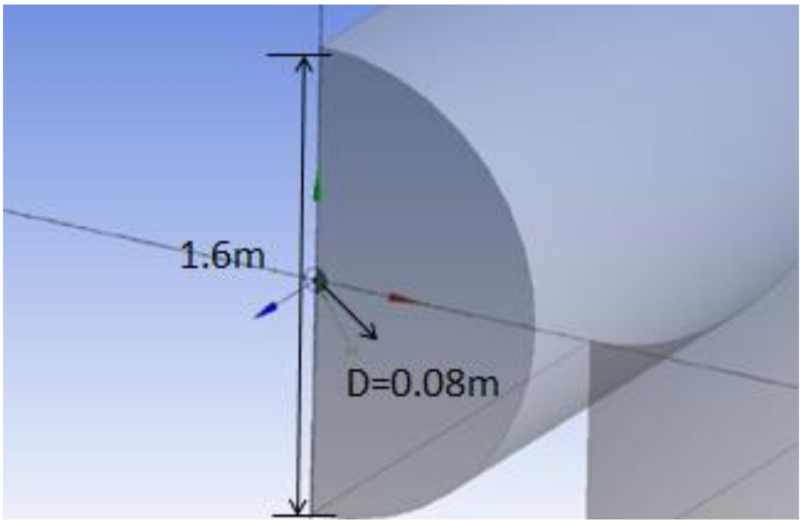

Figure 2: Burner zoom of the furnace object of study

3.1 Turbulence model

The turbulence model selected for this study is the standard k-ε model of two equations, one for k (kinetic energy) and one for ε (dissipation of kinetic-turbulent energy). This is the most used turbulence model because it suites a wide range of applications.

3.2 Combustion model

The most used model for this case is the "PDF Mixture Fraction" model. This model represents the transport of species by adding two equations, one of the average mixing fraction and another for the variance of the average mixture fraction.

3.3 Radiation model

Heat transfer inside the furnace occurs more than 80 % by radiation, in the radiant zone (Li et al., 2015). To represent this phenomenon, a radiation model must be selected. In this case the Discrete Ordinate Model (DOM) was chosen because it is the most robust model currently and the one that covers the widest range of optical thickness.

Additionally, it is important to take into account the influence of the flue gases in radiation, which are mainly water vapor and CO_2. The emissivity of these gases is calculated with the weighted sum of gray gases model (WSGGM).

4. Results

In this work the effect of the use of gases with variable composition for the combustion in industrial furnaces was evaluated by means of a three-dimensional simulation using CFD, for which three cases were simulated with gas mixtures of different composition that were taken from the work done by O. Cala et al, which are shown in Table 1.
The CFD simulation of the industrial furnace was carried out using the three gas mixtures shown in Table 1 to obtain temperature profiles and mass fraction of CO that can be analysed to know and conclude important aspects about the combustion process.

Table 1: Compositions of the mixture gases used in the 3 simulation cases

Component	Natural gas (%)	Mixture 1 (%)	Mixture 2 (%)
CH_4	100	55	25
C_2H_6	0	10	8
C_3H_8	0	0	25
C_4H_{10}	0	4	10
C_2H_4	0	5	10
C_3H_6	0	2	5
H_2S	0	4	2
H_2	0	20	15
Inferior Calorific Power (Btu/ft^3)	983	955	1530

Figure 3 shows the temperature profiles inside the furnace obtained from the 3 simulation cases using natural gas, mixture 1 and mixture 2. The simulation using natural gas is the base or ideal case that is taken as a reference to analyse the effect of the variation of the chemical composition. A uniform pattern of heat distribution from the middle to the chimney is observed. The second simulation using mixture 1 shows that the temperature profile changes with respect to the profile obtained with natural gas. In this case, greater uniformity of temperature is evidenced in the radiation zone (half) of the furnace, that is, the middle zone of the furnace heats up more than the chimney. This is due to the presence of other components in the gas mixture such as ethane, propane and hydrogen. The same happens in the third case with mixture 2, where more hot zones are observed. This means that when the methane content in the fuel decreases and the calorific value increases due to the presence of other components, more hot spots are observed inside the furnace.
Figure 4 shows the CO concentration profiles inside the furnace using natural gas, mixture 1 and mixture 2 respectively. According to this information, the molar concentration of CO inside the furnace is concentrated at the outlet of the burner and expands when the molar fraction of CH_4 decreases. This means that if the fuel has a higher concentration of CH_4, the molar fraction of CO decreases due to the fact that with natural gas the combustion process is more efficient, that is, the combustion is complete. The second and third cases simulations show a higher concentration of CO inside the furnace, which indicates that the combustion is incomplete and a detailed analysis must be done with adjustment of excess air and flow to improve the efficiency of the process. In the next stage of this study it is expected to perform a mesh analysis in order to find the optimal size and adjust the air excess so that combustion with gas mixtures is more efficient. It is also expected to analyze the effect of the use of these gases on the efficiency of the furnace.

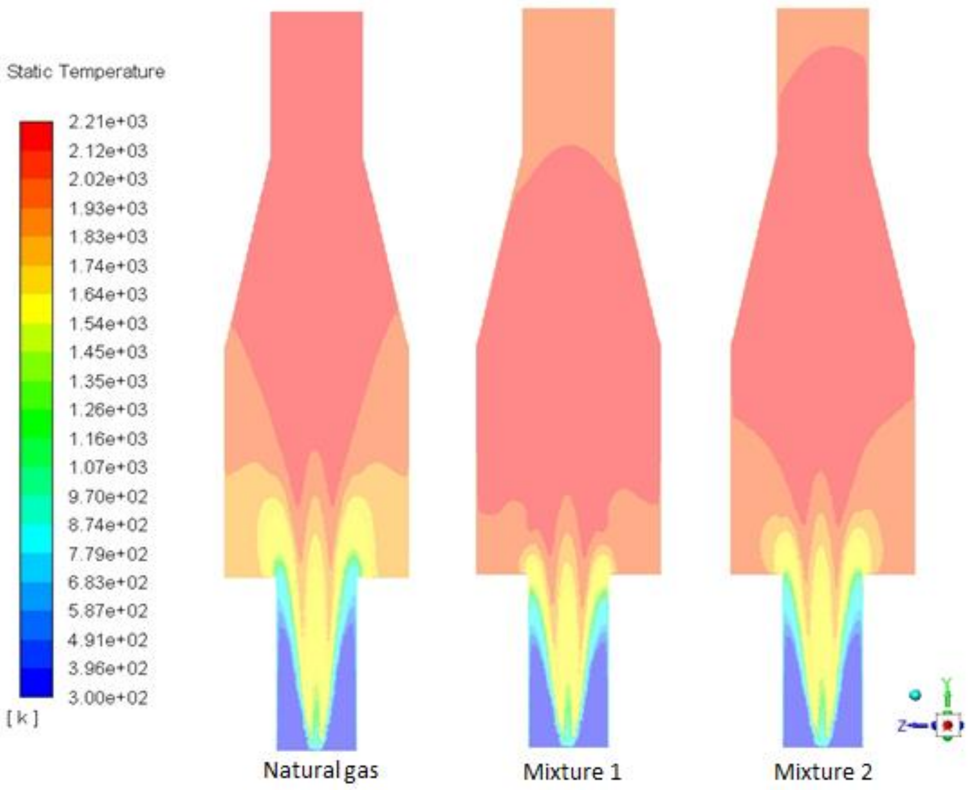

Figure 3: Temperature profiles inside the furnace obtained from 3 simulation cases

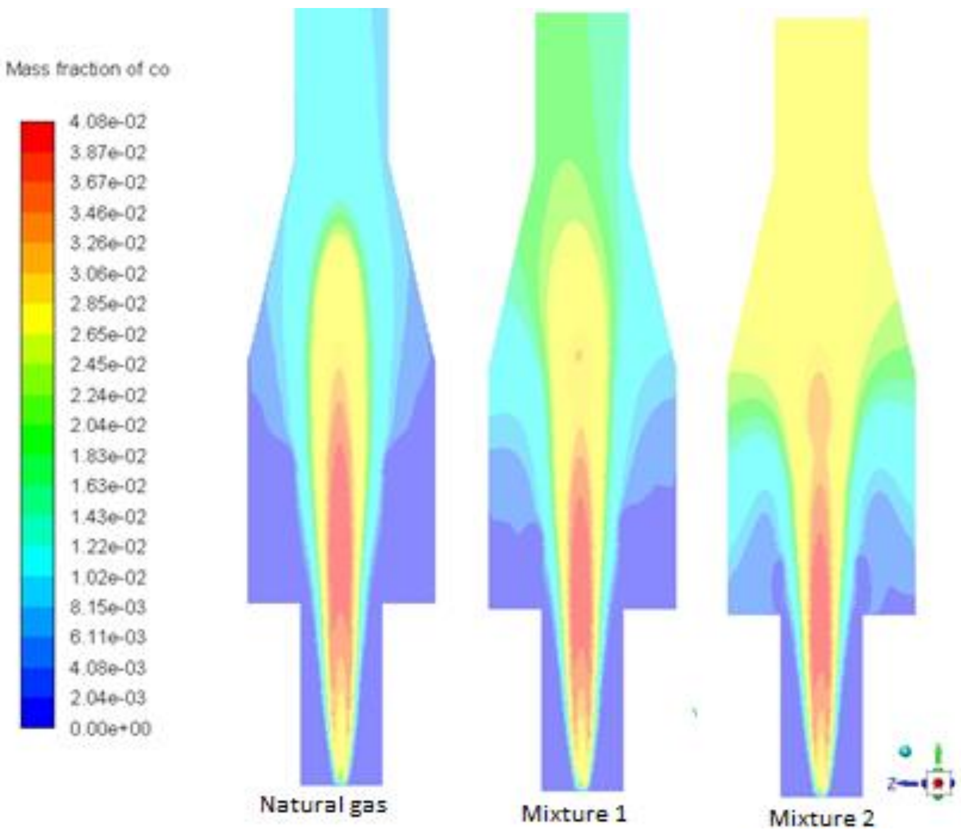

Figure 4: Profile of CO mass fraction inside the furnace obtained from 3 simulation cases

4. Conclusions

In this work, the effect of the use of a mixture of gases with variable composition in the combustion process of industrial furnaces by means of three-dimensional simulation in CFD was analyzed. The profiles of temperature and mass fraction CO inside the furnace were obtained. The simulation with less natural gas shows less heat distribution, that is to say less hot zones in the middle zone of the furnace and the distribution of the CO mass fraction also decreases, that is to say, that the combustion was complete. On the other hand, with the mixture 1 and the mixture 2 the combustion is incomplete and more CO is produced, the CO mass fraction increased from 1.02e-02 to 2.85e-02, which means that the combustion is not efficient and needs to be readjusted. Therefore, it is necessary to carry out a more detailed study of air excess and fuel flow when mixtures of gases of variable composition are used. The next stage of this investigation is to try a more complex geometry (cabin-type furnace), grid independency study, NOx emissions analysis (Post-process) and validation of obtained results to define which ranges of calorific power of refinery gases work best in furnaces.

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