



National Iranian Oil Refining and Distribution Company (NIORDC)

Research/ Review Paper

Comparison of DRM22 and GRI3.0 Combustion Mechanisms in Creating Flameless Combustion in a Lab-Scale Furnace

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1. ABSTRACT

Progressing of science and technology were created new processes in combustion that the most important goal was optimizing the fuel consumption, increasing efficiency, and specifically reducing the amounts of gaseous pollutants (such as nitrogen oxides and carbon monoxide). One of these new technologies is flameless combustion, which is based on the preheating of fuel and air and the dilution of oxygen in the air to create a proper mixing of the reactants. In the present study, the flameless combustion of methane gas is simulated in a laboratory combustion chamber. Its results are compared in two modes of using DRM22 (as a reduced mechanism) and GRI3.0 (as a complete mechanism). The results show that both mechanisms correctly predict the occurrence of flameless combustion and temperature distribution curves, the concentration of chemical species, and gaseous pollutants, and on average, the DRM22 mechanism is closer to the experimental results. Also, it takes less time to solve.

Keywords: Flameless Combustion, Fuel Consumption, Gaseous Pollutants, Combustion Mechanisms.

2. INTRODUCTION

Emission of large amounts of gaseous pollutants such as nitrogen oxides (NOX), carbon monoxide (CO), unburned hydrocarbons (HC) and climate changes, such as excessive warming of the earth with the emission of carbon dioxide (CO₂) as a greenhouse gas, are the negative effects of fossil fuel combustion. Therefore, it is necessary to develop new methods to increase the efficiency and quality of the combustion processes. One of the new combustion methods is flameless combustion technology. This phenomenon was observed for the first time in Wünning's experiments [1]. To achieve flameless combustion, the fuel and air must be preheated to a temperature higher than the auto-ignition temperature of the fuel; such a way that combustion temperature (difference between reactants and products) to be lower than the auto-ignition temperature of the fuel, and the oxygen in the air must be diluted to below 10% of its initial value, Due to the proper mixing of fuel and air in this regime, it is possible to create a homogeneous combustion zone with uniform temperature, in which the fuel consumption, the rate of production of gas pollutants, specifically NOx and CO, are reduced and the efficiency of the system is increased. The recirculation of hot gases of combustion is a key issue in the flameless combustion process.

In the present work, flameless combustion in a laboratory combustion chamber is numerically simulated and the main goal is to compare the results of two different mechanisms, namely GRI3.0 as complete mechanism and DRM19 as a reduced mechanism in the accuracy of predicting temperature distribution, pollutants, and chemical species. Complete mechanisms have a more species and reactions which increases the run time. On the other hand, reduced mechanisms, which are obtained from the elimination of less important species in complete mechanisms, increase the rate of solution due to the small number of species and chemical reactions. However, reduced mechanisms are not able to predict some chemical species such as NOX. To calculate these species, chemical equilibrium can be used.

3. MATERIALS AND METHODS

The present research is carried out based on Dally furnace [2] with dimensions of 250mm * 250mm * 550mm. The input values of the above geometry for validation and simulation are given in Table 1.

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Table 1. I del alle all'intake settings for simulation [2]		
Parameters	Fuel	Air
Chemical compounds	CH_4	$\%79N_2 + \%21O_2$
Temperature(K)	306	306
Mass flow rate (kg/h)	0.68	13.62
Velocity (m/s)	9.32	22.38
Excess air	λ =1.25	

Table 1 Fuel and air intake settings for simulation [2]



Figure 1. Geometry of the inves combustion chamber [2]

RANS model (k- ε two-equation model) was used for the turbulent flow. To calculate the radiation intensity and formation and consumption rate of species ($\dot{\omega}_k$), discrete ordinates model (DO) in different wavelengths and angles with threepartition and 72 beams and EDC are used. SIMPLE model is used for the coupling of velocity and pressure equations.

4. RESULTS AND DISCUSSION

To validate the numerical solution, the results of the simulation model are compared with the experimental results of He et.al [3]. The error between experimental and numerical results in DRM19 and GRI3.0 is 3.21% and 1.66%, respectively, and also between the two mechanisms is 1.7%. Therefore, it can be said that the numerical simulation performed in the temperature field has a good and appropriate accuracy. The DRM19 mechanism shows more temperature than the GRI3.0 mechanism. As can be seen in Figure 2, the temperature in all sections, especially at higher altitudes, reaches about 1500 K, and by removing the temperature gradient, the temperature in the entire chamber is uniform and there are not hot spots that disturb the rate of chemical reactions.



Figure 2. Comparison between the temperatures obtained from the numerical simulation and the experimental data [3]

In Figure 3, in the case of carbon monoxide, at some locations, especially at lower altitudes and near the entrance, there is a difference between the numerical and the experimental results. For the means of justification, it can be said that at lower altitudes, carbon monoxide formation dominates oxidation, as moving along the chamber, the temperature decreases, oxidation overcomes the formation and the carbon monoxide species turns into carbon dioxide; therefore, according to Figure 3, the amount of CO decreases along the length of the chamber and reaches approximately below 5 ppm. The performance of two combustion mechanisms, DRM19 and GRI3.0, are very close. On average, the error between the experimental and numerical results in DRM19 and GRI3.0 are 36.6% and 45.6%, respectively, and the difference between the two mechanisms is 25%, and the DRM19 mechanism predicts carbon monoxide concentration less than the GRI3.0 mechanism.

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Figure 3. Comparison between the CO values obtained from the numerical simulation and the experimental data [3]

In Figure 4, NOX values obtained from simulation and experimental values are given. According to this figure, there is a good consistency between the results of DRM19 mechanism and experimental results, but GRI3.0 shows more value than DRM19. The average error between the experimental and numerical results in DRM19 and GRI3.0 are 14.3% and 57.8%, respectively, and the difference between the two mechanisms is 26%, and the DRM19 mechanism predicts the equilibrium nitrogen oxide concentration lower than the GRI3.0 mechanism. However, the maximum value of NOX reaches approximately below 10 ppm, which, as expected, has a significant reduction compared to traditional combustion.



Figure 4. Comparison between the NOX values obtained from the numerical simulation and the experimental data [3]

5. CONCLUSION

In this article, the effectiveness and accuracy of combustion mechanisms of complete and reduced ones in the simulation of flameless combustion were investigated. For this purpose, two mechanisms, namely DRM19 (with 19 species and 84 reactions) and GRI3.0 (with 53 species and 325 reactions) were used. The results indicate that the mentioned mechanisms are able to calculate the distribution of temperature, chemical species with good accuracy in relation to each other and the experimental results (errors are respectively 1.66%, 4.7% and 36.6%). In the case of NOX, despite the small percentage difference, the GRI3.0 mechanism calculated its concentration as slightly higher than expected (nearly 26%). Generally, in this particular case, the results of the reduced mechanism of DRM19 were closer to the experimental results than GRI3.0.

6. **REFERENCES**

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