Natural Gas-Oxygen Combustion in a Super-Critical Carbon Dioxide Gas Turbine Combustor

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Abstract. The paper presents results for chemical kinetics of combustion process in the combustor of oxy-fuel cycle super-critical carbon dioxide gas turbine based on the Allam thermodynamic cycle. The work shows deviation of the normal flame propagation velocity for the case of transition from the traditional natural gas combustion in the N₂ diluent environment to the combustion at super-high pressure up to 300 bar in CO₂ diluent. The chemical kinetics parametric study involved the Chemkin code with the GRI-Mesh 3.0 kinetic mechanism. This mechanism provides good correspondence between calculation results and test data. The CO₂ and N₂ diluents temperature, pressure and contents influence the flame propagation velocity and the chemical kinetics parameters in the two gas turbine types. It is demonstrated that the CO₂ diluent slows down chemical reactions stronger than the N₂ one. The flame propagation velocity in carbon dioxide is four time smaller than in the N₂ one. In the oxy-fuel cycle combustor a pressure increase reduces the flame propagation velocity. Increase of the CO₂ content from 60 to 79% reduces the flame propagation velocity for 65% at atmospheric pressure and for 94% at super-critical pressure. An increase of the combustor inlet mixture temperature from 300 to 1100 K at super-critical pressure causes the flame propagation velocity increase for 94%. The flame propagation velocities compatible with the traditional gas turbines may be reached at the CO₂ diluent content of the O₂ + CO₂ mixture in the active combustion zone must be below 50%.

1 Introduction

Transition to the environmentally friendly, low toxic and greenhouse emissions cycles is one of the most prospective directions for the hydro-carbon power production industry. The closed gas turbine cycles on super-critical carbon dioxide with organic fuel combustion in pure oxygen seem very attractive. In these terms, the Allam cycle (Figure 1) promises maximal production efficiency and nearly zero emissions [1-5].

Introduction of the Allam cycle requires solutions of a range of research problems that includes development of the power equipment analysis to operate with new heat carriers at non-traditional thermodynamic parameters.

The Allam cycle parameters of oxy-fuel combustion differ from the traditional gas turbines by the following parameters:

- The oxy-fuel cycle combustor pressure of 300 bar instead of the traditional gas turbines values below 30 bar;
- Methane is burned in the carbon dioxide environment instead of the nitrogen diluent in traditional gas turbines.

The common combustor analysis is based on the detailed description of methane combustion in air

environment at pressures up to 30 bar. The analysis determines the complete fuel burnout conditions, oxygen-fuel mixture velocity at the combustor entry and the components residence time for the high temperature reaction zone. The oxy-fuel cycle combustor development involves methane oxygen combustion in the carbon dioxide environment at super-critical pressure up to 300 bar and investigation of the flow aerodynamic structure at the oxygen-fuel mixture formation and CH₄-O₂ combustion [6-9]. This paper discloses the chemical kinetics investigation that makes a base for further 3-D simulation of the CH₄-O₂-CO₂ combustion and the results that are adequate to the actual processes. Especially important is the transition from N₂ to CO₂ combined with the combustor inlet parameters increase that is related to the normal flame propagation velocity. This parameter depends upon temperature, pressure and the components contents but is not related to the combustor burner design, or the flame tube structures. The analysis results provide a conclusion on the necessity to change the combustor inlet oxygen-fuel mixture velocity and the diluent content ($\gamma = \text{CO}_2 / (\text{CO}_2 + \text{O}_2)$) that provide the flame stability and complete burn-out. The combustor envelope dimensions are similar to the traditional gas turbines [10-12].

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Fig. 1. Flow chart of Allam cycle on natural gas fuel.

2 Materials and Methods

The parametric study on influence of the diluent type and concentration upon the CH₄-O₂- CO₂ and CH₄-O₂-N₂ mixture combustion kinetic parameters was carried out with the Chemkin computer simulation code.

In the study were selected the following detailed kinetic mechanisms that allow calculations with numerous mixture contents and initial parameters. The following two kinetic mechanisms were considered [13-17]:

- Mechanism #1: GRI-Mesh 3.0 developed for the natural gas combustion including the chemical incomplete combustion. The mechanism basic kinetics

involves 53 intermediate reaction products and 325 convertible chemical reactions of the methane transformation into complete combustion products;

- Mechanism #2: USC II involves 325 components and 725 convertible reactions applied to a broad spectrum of combustion scripts. The USC II model was developed on the combustion mechanism GRI-Mesh 3.0, the hydrogen and carbon monoxide combustion, the fuel combustion model C3 and the complex model of ethylene and acetylene combustion. The both models include the reaction velocity data from the recent actual investigations.

The results were verified by comparison with the test data of the papers [18-20].

The results show that at atmospheric pressure the

Table 1. Summarizes input data for the chemical kinetics parametric studies on the N₂ and CO₂ diluents at different pressures, diluent contents and reactor inlet temperatures.

Analysis series	Pressure, bar	Diluent type and mass content, γ	Gas mixture temperature upstream combustion reactor, K	Oxidizer excess coefficient
Diluent CO ₂				
1	1	0.60	300	0.7-1.4
2	1	0.64	300	0.7-1.4
3	1	0.68	300	0.7-1.4
4	1	0.79	300	0.7-1.4
5	20-300	0.60	300	1.0
6	20-300	0.64	300	1.0
7	20-300	0.71	300	1.0
8	20-300	0.74	300	1.0
9	20-300	0.79	300-1200	1.0
Diluent N ₂				
10	1	0.79	300	0.7-1.4
11	20-300	0.79	300-1200	1.0

Fig. 2. Combustor structure comprised of the Chemkin reactors.

Fig. 3. Normal flame propagation velocity in the N2 and CO2 diluents ($\gamma = 0.79$) at atmospheric pressure and gas temperature 300 K.

both detailed mechanisms demonstrate moderate deviations from the test data. At high pressure the USC II shows overrated estimations of the flame propagation velocity and the GRI-Mesh 3.0 underrates it. The GRI-Mesh 3.0 calculation error is below 3.5% and the USC II One is above 6%. The further calculations were carried out with the GRI-Mesh 3.0.

Figure 2 shows the combustor structure model comprised of a set of elementary reactors. The model includes the staged supply of CO2 diluent into the combustor. The mixture is ignited at the CO2 volumetric content equal to the value γ . The second CO2 flow cools the combustor walls, the third flow supplied to the end of active combustion zone mixes with the main flow as to reach the target temperature.

3 Results

Figures 3-6 show the normal flame propagation velocities in the N2 and CO2 environments at different initial values of oxygen-fuel mixture temperature and

pressure, oxidizer excess and the diluent contents in diluent-oxygen mixture.

The calculation results show that the carbon dioxide is a stronger chemical reactions inhibitor than nitrogen. The maximal flame surface propagation velocity is 10 cm/s, and with the N2 diluent at other conditions being equal it is almost 40 cm/s. In average at the oxidizer excess coefficient from 0.7 to 1.4 the normal flame propagation velocity in the carbon dioxide environment is four times smaller.

Reduction of the CO2 content in its mixture with oxidizer at γ reduction for 0.1 increases the flame propagation velocity for 2 cm/s in average. The maximal increase occurs at the CO2 content reduction from 0.74 to 0.6. In the whole range of oxidizer excess coefficients the maximal flow propagation velocity occurs at $\alpha = 1$.

Pressure increase reduces the normal flame propagation velocity. The maximal reduction occurs at moderate pressure values below 70 bar. The further pressure increase also reduces U_n , but in a remarkably smaller degree.

Fig. 4. Normal flame propagation velocity at different γ (CO_2) and oxidizer excess values at atmospheric pressure and gas temperature 300 K.

Fig. 5. Normal flame propagation velocity at different pressure and γ (CO_2) values at gas temperature 300 K.

Fig. 6. Normal flame propagation velocity at in the CO_2 diluent at different combustor inlet gas pressure and temperature ($\gamma = 0.71$).

According to the **Ошибка! Источник ссылки не найден.** results increase of the gas mixture temperature is followed by the normal flame propagation velocity growth at all pressure values, and the growth rate is non-linear. The temperature increase from 900 to 1100°C increases the velocity for average 22 cm/s. At lower

mixture temperatures the similar 200°C temperature increase causes only a 8-10 cm/s increase. At the initial mixture temperature T_0 convection and radiation heat transfer heats the mixture up to the ignition temperature T_i that begins exothermal reactions and the mixture temperature grows. It is obvious that when the mixture

Fig. 7. Normal flame distribution velocity in the traditional and oxy-fuel cycle gas turbines.

temperature T_0 reaches the ignition border it causes a faster mixture ignition.

Ошибка! Источник ссылки не найден.a shows the normal flame propagation velocity for a traditional gas turbines combustor, pressure 30 atm and $T_{in} = 866$ K that corresponds to the compressor exit at compression up to 30 bar. **Ошибка! Источник ссылки не найден.**b demonstrates a similar velocity relation with the CO2 diluent rate γ in the oxy-fuel cycle combustor.

The **Ошибка! Источник ссылки не найден.**b results show that the flame propagation velocity in oxy-fuel cycle combustor is near to U_n of the traditional gas turbines if the CO2 diluent content in the mixture is below 0.5.

4 Discussion

The main research results are the following:

- The CO2 diluent is a stronger chemical reactions inhibitor than N2. At other conditions equal the normal flame propagation velocity in CO2 is four times smaller than the N2 diluent one, the 75% velocity reduction from 39 to 10 cm/s at the diluent content in oxidizer 79%;

- The combustor pressure increase reduces the flame propagation velocity, at the pressure increase from 20 atm up to super-critical pressure of 200 atm the reduction is 36%;

- A change in the CO2 concentration of the diluent in the mixture with the oxidizing agent in the range of the volume content from 60 to 79% leads to a decrease in the flame propagation rate by 65% (from 42.5 to 10 cm/s) at atmospheric pressure and by 94% at supercritical pressure (from 14.2 to 0.8 cm/s).

In relation with the ballasting gas content supplied together with oxidizer at CO2-O2 diluent mass contents from 0.945 to 0.460 the following parameters are determined:

- The normal flame propagation velocity verifies from 7 to 45 cm/s. A 1% reduction of the diluent content in CO2-O2 mixture increases the U_n velocity for 1.4%;

- The U_n amount for the natural gas combustion in the O2 and CO2 mixture is compatible with the traditional gas turbine combustors at the γ values from 0.47 to 0.65. This γ range corresponds to the CO2 content in the O2 + CO2 mixture in the active combustion zone below 15% of the total mass.

5 Conclusion

The investigation results show the problems concerned with transition to the new diluent and higher combustor pressure. In the oxy-fuel cycle conditions CO₂ remarkably slows the combustion process. Stable efficient methane combustion in the oxygen and carbon dioxide mixture may be reached under the following conditions:

- Carbon dioxide supply into the active combustion zone must be below 20% of its total mass flow. This flow must be split into two parts, one as a mixture with oxidizer with the γ of CO₂-O₂ mixture below 0.5, and second along the combustor walls for its cooling. This CO₂ flow split allows application of the traditional gas turbine combustor recommendations;

- The gas-fuel mixture velocity in the oxy-fuel cycle combustor must be below 20-25 m/s;

Further 3-D combustion simulation may employ the GRI-Mesh 3.0 kinetic mechanism, its calculation results fit test results with errors below 3.5%.

Acknowledgements

This study conducted by Moscow Power Engineering Institute was financially supported by the Ministry of Science and Higher Education of the Russian Federation (project No. FSWF-2020-0020).

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