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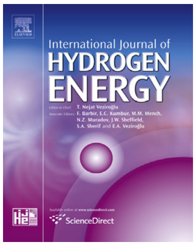

Inverse diffusion flame of CH_4–O_2 in hot syngas coflow

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ABSTRACT

The structure and combustion mode of inverse diffusion flame of CH_4 and O_2 in hot syngas coflow are numerically studied to gain a fundamental understanding of the flame in non-catalytic partial oxidation (NC-POX) reformer. The configuration is modified based on the burner system of Cabra et al. [*Combust. Flame* **2005**, 143 (4), 491–506] to make the flame representative of that in NC-POX reformer. The Eddy Dissipation Concept (EDC) model with the detailed GRI 3.0 mechanism is used to model the turbulence–reaction interactions. Results of the study show that the flame is stabilized by autoignition with a wide reaction zone located far away from the stoichiometric line. Analyses on combustion mode show that the flame is established in Moderate and Intense Low-oxygen Dilution (MILD) mode. The inverse diffusion flame configuration which ensures a fully dilution of oxygen plays a key role in achieving MILD combustion in fuel rich coflow. The Increase of coflow temperature or decrease of jet velocity within the range of this study can lead to an early autoignition, but doesn't change the combustion mode.

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Introduction

Non-catalytic partial oxidation (NC-POX) of natural gas is an important alternative technology used in the production of syngas ($CO + H_2$) for chemical and energetic use. Compared to other natural gas reforming technologies [1–3], the most significant advantage of NC-POX process is that the syngas H_2/CO ratio is about 1.7–1.8, which is close to the desired ratio for Fischer-Tropsch synthesis, methanol synthesis and glycol synthesis [4,5]. The natural gas and pure oxygen jet into natural gas NC-POX reformer with high speed (>80 m/s) from a coaxial nozzle mounted at top of the reformer. And therefore a jet zone, a recirculation zone and a reforming zone are formed in the reformer [6]. In most reported reformer designs [6,7], the oxygen stream jets from the central channel forming an inverse diffusion flame in jet zone. Slow reforming reactions between CH_4 and CO_2/H_2O occur in recirculation zone and reforming zone.

While commercial scale plants have been built using NC-POX technology, basic information of the NC-POX process still needs to be further studied. Experimental data available for reformers are mostly limited to outlet gas compositions. This is because measurement of the process in reformer is hard to conduct due to the high process temperature and pressure. Numerical study has been the main method in

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understanding the physical processes in such systems [7,8]. Both kinetic models [9–11] and multi-dimension CFD models [4,12–14] have been carried out in the modeling of partial oxidation reformer, but these previous work mostly focus on the syngas yields, the information on the combustion process is limited.

The characteristics of the combustion process and flame are important for the partial oxidation of natural gas, since the flame influences the temperature profile, oxidation zone volume and stability of the reformer, and therefore determines the overall natural gas conversion. This has attracted researcher's attention in recent years. Stelzner et al. [15] developed a laminar inverse diffusion flame model burner to study the rich inverse diffusion flame structure. They found that the use of pure O_2 as oxidizer leads to extremely high temperatures (~3000 K) and the flame structure is strongly influenced by radiation and diffusion effects. Time scale analysis [16], flamelet modeling [17] and radiation modeling [18] were also performed to study this rich inverse diffusion flame. Li et al. [19] studied the hysteresis of the CH_4–O_2 inverse diffusion flame in laminar conditions. Many other studies on inverse diffusion flame which were not originated from the reformer applications were also conducted to study the flame behavior and structure [20–22]. The studies on the rich inverse diffusion flame were all conducted in low velocity and room temperature environment. The effects of high jet velocity and hot syngas recirculating flow were not considered. The flame behavior and stabilization mechanism in hot recirculated gas may be totally different from those in normal temperature environment [23–25]. Recently, a series of tests were conducted on a semi-industrial scale NC-POX reformer to study the flame structure using optical measurements [7]. The measured peak temperatures were ~2000 K. The extremely high temperatures (>3500 K) reported in previous numerical studies [4,10,13,14,26] and laminar flame studies [15] were not observed. The authors owed this big deviation to the limitation of the measurements.

Although no study focused on the effect of hot syngas recirculating flow on flame in the research field of NC-POX, a good volume of work has been carried out in the fundamental study of turbulent flames with hot recirculating flow in the research field of combustion due to its wide application in many combustion systems. Because of the complex recirculation patterns within such systems, Jet-in-Hot-Coflow (JHC) flames have been developed to simulate recirculation. In such a simplified geometry, a fuel jet issues into a coflowing stream of hot combustion products, with a composition resembling that encountered in an actual recirculating system. Experiments using this configuration have been conducted by Cabra et al. [25,27] and Dally et al. [28] to investigate the autoignitive lifted flames and MILD combustion, respectively. Detailed information of temperature, velocity, and major species in these JHC flames had been measured to provide validation data for numerical study. Following these experimental studies, many numerical simulations had been conducted on JHC flames. Christo and Dally [29] studied the performance of various turbulence, combustion, and kinetic models in predicting the JHC flames, and found that the Eddy Dissipation Concept (EDC) model with a detailed kinetic scheme offers a practical and reasonably accurate tool for predicting the characteristics of JHC configurations. Results of a similar work [30] also shows that the EDC model with detailed mechanism can well predict the combustion characteristics. Effects of coflow temperature, coflow velocity, oxygen level and fuel type [27,31–33]were numerically studied based on the validation of model using data from JHC experiments. These data were also used for validation in the studying of oxy-fuel combustion of a methane jet in hot O_2/CO_2 coflow [34].

Considering the lack of studies on the effects of high jet velocity and hot recirculated syngas flow on reformer flames, this study attempts to study the inverse diffusion flame in such conditions. To avoid the complex recirculation patterns in reformer, this study uses an inverse diffusion flame of CH_4–O_2 in hot syngas coflow to represent the flame established in a NC-POX reformer with an inverse diffusion flame burner. The well-proved k-ε model and the EDC model with detailed chemical kinetics are used to study the flame in hot syngas coflow. The aim of this work is to investigate the characteristics of the inverse diffusion flame in hot syngas coflow and provide insight into the combustion process in natural gas NC-POX reformers.

Model description

Configuration of the burner system

In order to investigate the inverse diffusion flame in hot syngas coflow, the present study uses a modified configuration of the JHC burner used by Cabra et al. [27]. Fig. 1(a) and (b) show the structure of the original JHC burner and the present configuration, respectively. The original JHC burner had been well described in earlier work [25,27,35], so only the modified configuration will be described in detail here. The single fuel tube in the cabra burner is replaced by two coaxial tubes. The oxygen tube has an inner diameter of $D_o = 4$ mm and a wall thickness of 1 mm. The fuel tube has an inner diameter of $D_f = 8$ mm. The two tubes are located in the center of a hot syngas coflow. The area ratio of the two channels is 0.57 which is similar to that of the industrial burner in natural gas NC-POX reformer. This designed system provides conditions that can simulate the flame in the NC-POX reformer.

Turbulence models

According to the studies of Christo and Dally [29] on the performance of turbulence models in JHC flame modeling, the standard k-ε model with dissipation equation constant ($C_{\varepsilon 1}$) modified from 1.44 to 1.6 provided the best results. So the improved standard k-ε model with enhanced wall function is implemented to model the turbulent flow. The turbulence kinetic energy k and its dissipation rate ε are obtained from the following transport equations [36]:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon - Y_M + S_k \tag{1}$$

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