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Numerical simulation of natural gas non-catalytic partial oxidation reformer

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ABSTRACT

A comprehensive 2D model of a natural gas (NG) non-catalytic partial oxidation (NC-POX) reformer is established in this study. The simplified mechanism (GRI-mech 3.0) is applied to calculate the reaction rates involved in the reformer process. Both the modified Eddy-Dissipation-Concept (EDC) model and the PDF model are applied to calculate the chemistry and turbulence interaction. The results of the EDC model agree well with the operating data of industrial reformer. The effects of operating pressure, the O_2/NG mole ratio and the steam/NG mole ratio on the performance of reformer are investigated by using the EDC model. The results indicate that the increase of pressure promotes the CH_4 conversion and a pressure higher than 3.0 MPa is suggested for industrial operation according to the conversion of the CH_4 in the range of this study. As the O_2/NG mole ratio increases, the temperature increases and the concentration of CH_4 in syngas decreases. The O_2/NG mole ratio range of 0.66–0.67 is optimal according to the yield of the effective syngas compositions (H_2 + CO) mole fraction in raw syngas and the consumption of oxygen. It is also confirmed that the decrease of highest temperature of flame in the reformer and the raise of the syngas H_2/CO mole ratio can be observed with the increase of the steam/NG mole ratio.

Introduction

With the successive development of shale gas, natural gas industry shows a sound prospect. The natural gas non-catalytic partial oxidation technology has drawn lots of attention due to the short supply of crude oil and the increasing requirement of liquid fuels. Compared with other natural gas to syngas technologies, such as steam reforming [1] and autothermal reforming [2–4], the most significant advantage of NC-POX process is that the syngas H_2/CO ratio is about 1.7–1.8 [5], which is exactly the desired ratio for both the Fischer–Tropsch synthesis and methanol synthesis.

The natural gas NC-POX process takes natural gas, oxygen and steam as raw materials to produce syngas without catalysts. These materials are injected into NC-POX reformer through corresponding channels of the industrial burner. Reactions take place with large amounts of heat released in the reformer. The temperature of outlet syngas is above

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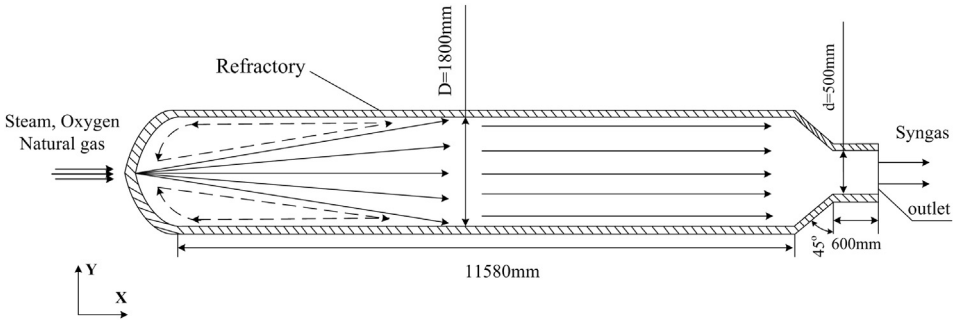

Fig. 1 – Structure diagram of natural gas NC-POX reformer.

1200 °C [6]. Because of the inherently high chemical stability of CH_4 [7], CH_4 is difficult to get complete conversion and the CH_4 concentration of outlet syngas is higher than the one of syngas in equilibrium state.

The research methods of NC-POX include equilibrium model, ideal reactor model, hot model experiment and computational fluid dynamics (CFD) simulation. Equilibrium model calculates very fast, but it is appropriate for the situation that the state of outlet gas from the reactor is close to equilibrium state. Zhu [8] discussed the effects of the initial O_2/CH_4 ratio and the pressure on the product composition with Gibbs free energy minimization method. The results illustrate that the yield of syngas effective compositions ($H_2 + CO$) reaches the peak when the initial O_2/CH_4 ratio is at 0.5. The ideal reactor model calculates the reactor with detailed kinetic data and ideal flow status. Rasmussen [9] simulated the fuel-rich oxidation process of methane using a laminar flow reactor. Albrecht [10] employed perfect stirred reactor (PSR) model to study the effects of equivalence ratio, pressure and residence time on syngas compositions. Lemke [11] studied the effects of inlet temperature, system pressure and equivalence ratio on reaction time and hydrogen yield in a PSR. Zhou studied the effects of O_2/CH_4 mole ratio and O_2/H_2O mole ratio on the methane conversion and the syngas H_2/CO ratio with premixed one-dimensional laminar flame model [12]. Hot model experiment is also adapted to research the natural gas NC-POX reformer. Brüggemann [6] discussed the deviation of main compositions between the results of NC-POX hot model experiment and outlet syngas of equilibrium model. Lemke [11] gave the temperature and species concentrations distribution at various locations in a hot model reactor. CFD model includes detailed information about flow and reaction in the reformer. With the enhancement of computer capability, CFD method is considered as one of reliable and affordable methods in the study of the reformer performance.

The CFD simulation of NC-POX reformer can be mainly divided into two different types of methods based on the calculation of chemical reaction rates. One of them calculates reaction rates based on turbulent mixing and considers the reactions reach chemical equilibrium state as soon as reaction species are mixing, such as the presumed PDF model. This method is suitable for calculation of quick reactions. Dai [13] discussed the velocity and temperature distribution in the NC-POX reformer with the PDF model. Guo [14] estimated the results of a NC-POX reformer with the presumed PDF model and considered the PDF model was sufficient for engineering level estimation. Zhou [15] also used the PDF model to assess the effects of O_2/CH_4 ratio, O_2/steam ratio and pressure on the performance of the NC-POX reformer.

The other method calculates reaction rates with consideration of both the detailed reaction kinetics and the turbulent mixing, such as the eddy dissipation concept (EDC) model and finite rate/eddy dissipation model. Those models can calculate all kinds of reactions with the sacrifice of calculation efficiency. Guo [14] simulated the NC-POX reformer with EDC model. Rehm [16] studied the effects of the modification of EDC model parameters on the syngas CH_4 concentration compared with experimental results.

This article aims at presenting the simulation of an industrial NC-POX reformer using detailed reaction kinetics and fluid dynamics. The effects of operating pressure, the O_2/NG mole ratio and the steam/NG mole ratio on the performance of the NC-POX reformer are investigated.

Industrial NC-POX reformer

The industrial NC-POX reformer

The structure of the industrial NC-POX reformer modeled in this study is shown in Fig. 1. The height and diameter of the reformer are 11.58 m and 1.8 m, respectively. Natural gas, oxygen and steam are injected into the reformer by a multi-channel burner. The operating pressure of the reformer is

Table 1 – Information of multi-channel burner and corresponding materials.

Channel	Radius mm	Material	Angle	Volume flowrate Nm^3/h	Temperature K
1	12.50	Oven material	0°	–	–
2	23.91	O_2	0°	17,188	516
3	31.18	Natural gas	12°	11,292	536
4	33.70	H_2O	15°	1841	594