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Numerical Investigation of Steam Methane Reforming over Ni- and Rh-based Catalysts to Produce Hydrogen, Syngas and Reduce Surface Coverage

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ABSTRACT: Steam methane reforming has the highest efficiency compared with other hydrogen production ways. Temperature, pressure, steam to methane ratio, and catalyst play essential roles in the Steam methane reforming process. In this paper, a numerical simulation method is performed using Cantera software in Python programming language to produce syngas and hydrogen in the Steam methane reforming process over Nickel- and Rhodium-based catalysts. The simulation is done in 600-1300K, steam to methane ratio of 2-4, and pressure of 0.25-4 bars to determine a suitable catalyst and the best range to produce hydrogen and syngas and to reduce Carbone surface coverage. The results demonstrate that the preferred ranges for hydrogen production over Nickel and Rhodium are temperature between 1000 to 1100K, pressure 1 to 2 bars, and steam to methane ratio 2.5 to 3 and 3 to 3.5 for each, respectively. The appropriate ranges to produce syngas over Nickel and Rhodium are temperature 1200-1300K and 1100-1300K, steam to methane ratio 2.5-3 and 3-3.5, respectively, and the pressure is suggested between 1-2 bars. However, Rhodium in the same condition is more active than Nickel, while the surface coverage formation is lower over Nickel than Rhodium. Therefore, Nickel is proposed to produce hydrogen via Steam Methane Reforming.

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1- Introduction

Hydrogen is a clean energy resource that is suggested instead of fossil fuels. At present, steam methane reforming is one of the most developed and cost-effective methods of hydrogen production from fossil fuels on an industrial scale [1]. The steam methane reforming process includes a set of methane reforming reactions (1), (2) and water gas shift (3) as follows [2]:

$$CH_4 + H_2O \rightleftarrows CO + 3H_2 \qquad H_{298} = 206.1 \text{ kJ / mol} \tag{1}$$

$$CH_4 + 2H_2O \rightleftarrows CO_2 + 4H_2 \qquad H_{298} = 165.0 \text{ kJ / mol} \tag{2}$$

$$CO + H_2O \rightleftarrows CO_2 + H_2 \qquad H_{298} = -41.15 \text{ kJ / mol} \tag{3}$$

Abbas et al. [3] studied the kinetic data of the steam methane reforming process over Nickel catalyst numerically and experimentally at the pressure of 1 bar and a temperature range of 300-700°C. The results showed that at high temperature, low pressure, and high steam to carbon (*S/C*) ratio, the system has high performance for methane conversion and the purity of hydrogen produced. Castillo et al. [4] investigate the steam methane reforming process over Ru/Al_2O_3 catalyst numerically and experimentally at low temperature (573-723 K), high steam to carbon ratio (2.5), and low pressure (0.1-0.2 MPa) conditions. According to their results, the steam methane reforming process is highly active in a temperature range of 573-723 K over the reactor bed, and increasing the steam to carbon ratio causes the reactor bed to be cleaner. Therefore, it improves the reaction at low pressure.

2- Methodology

A numerical solution is performed using Cantera software in the Python programming environment. A plug flow reactor, a series of volumes with axial distribution, can be modeled under steady-state conditions using Cantera. The output state of each reactor will be the input boundary condition of the next well-stirred reactor.

2- 1- Equations

The dynamics of local change of surface coverage of adsorbed species on the surface are expressed by Eq. (4).

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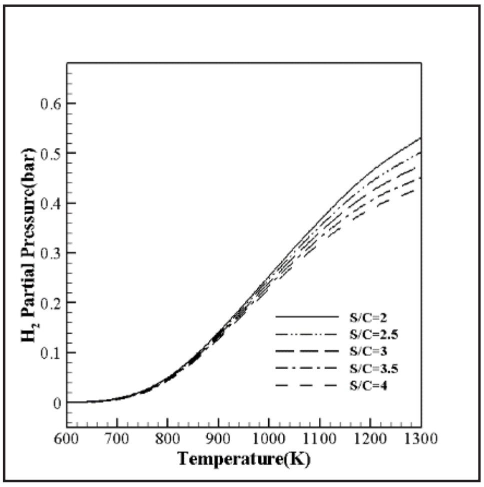

Fig. 1. Hydrogen production in the temperature range of 600-1300 K and steam to carbon ratio of 2-4 over Nickel-based catalyst

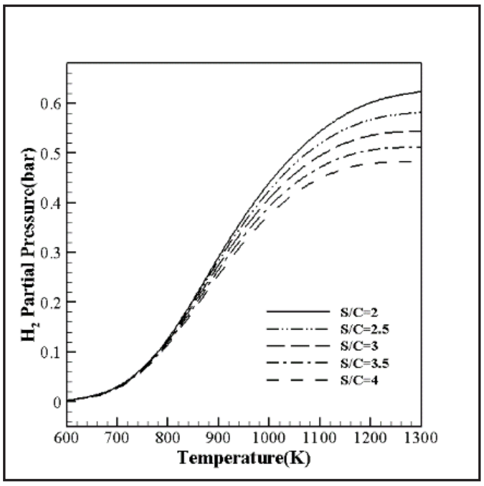

Fig. 2. Hydrogen production in the temperature range of 600-1300 K and steam to carbon ratio of 2-4 over Rhodium-based catalyst

$$\frac{d\theta_k}{dt}=\frac{s_k\,\sigma_k}{\Gamma} \tag{4}$$

Arrhenius function is a general form that shows reaction constant is temperature-dependent and can be calculated according to Eq. (5).

$$k_{f,i}=A_iT^{\beta i}\exp\left(-\frac{E_i}{RT}\right) \tag{5}$$

In most cases, the reaction constant is calculated according to Eq. (5); but sometimes, the Arrhenius function change by some surface species. So we have Eq. (6) [5]:

$$k_{f,i}=A_iT^{\beta i}\exp\left(-\frac{E_i}{RT}\right)\prod_{k_s}10^{a_{ki}\theta_{ki}}\,\theta_{ki}{}^{m_{ki}}\exp\left(-\frac{\epsilon_{ki}\theta_{ki}}{RT}\right) \tag{6}$$

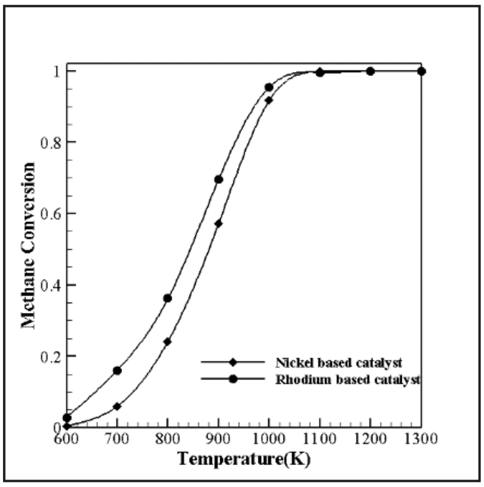

Fig. 3. Comparison of methane conversion over Nickel and Rhodium based catalysts in the temperature range of 600-1300 K and steam to carbon ratio of 3

3- Results and Discussion

Fig. 1 shows the hydrogen mole fraction at the reactor outlet in the temperature range of 600-1300 K for different steam to carbon ratios of 2-4 at atmospheric pressure over the Nickel catalyst. The highest amount of hydrogen production is related to steam to carbon ratio equal to 2, and the lowest occurs in steam to carbon ratio of 4; the appropriate range for hydrogen production is more than 1000 K.

Fig. 2 shows the hydrogen mole fraction at the reactor outlet in the temperature range of 600-1300 K for different steam to carbon ratios of 2-4 at atmospheric pressure over the Rhodium catalyst. The highest amount of hydrogen production is related to steam to carbon ratio equal to 2, and the lowest occurs in steam to carbon ratio of 4. The appropriate range for hydrogen production is more than 900 K.

Fig. 3 shows methane conversion over Nickel and Rhodium catalysts in a temperature range of 600-1300 K and steam to carbon ratio equal to 3 at atmospheric pressure. The activity of the Rhodium catalyst in comparison with the Nickel catalyst is considerable in a temperature range of 600-800 K, but at 800-1300 K, they behave similarly and closely. Therefore, if it is desirable to carry out the process at a low temperature of 600-800 K, a Rhodium catalyst is recommended. In a temperature range of 800-1300 K, a Nickel catalyst is a good option.

4- Conclusions

The Steam Methane Reforming process over Nickel and Rhodium catalysts was simulated to produce hydrogen and syngas. The important results of this modeling are:

- a preferred range for hydrogen production over Nickel and Rhodium catalysts are 1000-1100 K, steam to carbon ratio of 2.5-3 and 3-3.5, and pressure 1-2 bar, respectively.
- appropriate range for syngas production over Nickel and Rhodium catalysts is in the range of 1200-1300 and 1100-1300 K, steam to carbon ratio of 2.5-3 and 3-3.5 and pressure 1-2 bar, respectively.
- The performance of the steam methane reforming process under suitable conditions for both Nickel and Rhodium catalysts are similar; however, the Nickel catalyst is recommended due to its cost-effectiveness and availability.
- Based on methane conversion, Rhodium catalyst is recommended for processing at low temperatures of 600 to 800 K.

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