Short Communication

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Catalytic hydrogenation of carbon dioxide for the production of methanol in a catalytic membrane reactor of fixed bed

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Introduction

It is known that fossil fuels pertain to hydrocarbons. Therefore, when they are burned for the purpose of getting heat and power, water and carbon dioxide (CO_2) are generated and liberated to the atmosphere. Global warming is largely attributed to an increase in the atmospheric level of greenhouse gases. CO_2 is considered as the most important greenhouse gas with the largest impact on climate change. Several preoccupations have been raised with respect to the impact in increasing concentrations of CO_2 in the atmosphere to the environment.[1] Catalytic hydrogenation of carbon dioxide (CHCD) in a catalytic membrane reactor of fixed bed is one of most important chemical processes for the production of methanol.[2,3]

Mathematical modelling

A schematic diagram of the membrane reactor (MR) is proposed in the present paper to carry out the CHCD. The MR consists of two concentric tubes, as shown in Figure 1. The proposed mathematical model was described by a partial differential equation system and it is restricted to the following assumptions:

i. Isothermal system;
ii. All flow rates are constant throughout the reactor;
iii. The intraparticle diffusion resistance was not considered;
iv. Radial concentration gradient was considered. Based on the above assumptions, mass balance equations in the reaction zones could be written as follows.

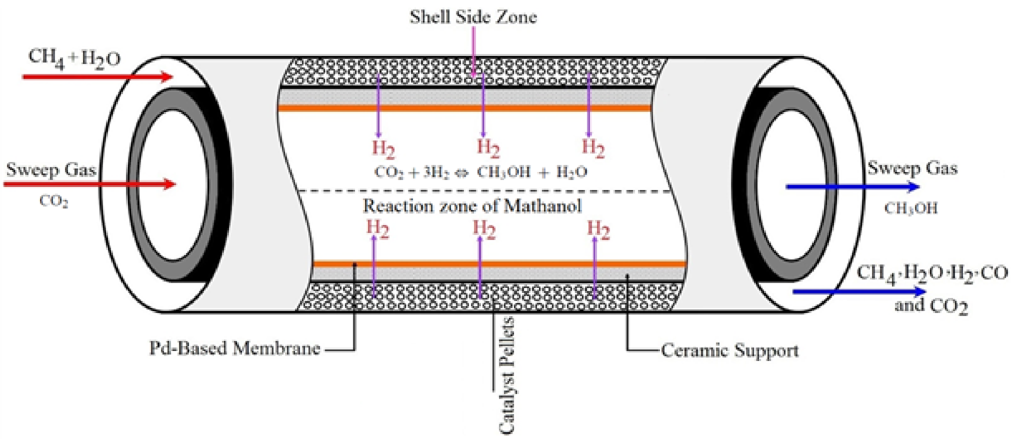

Figure 1 Scheme of the MR for the production of methanol.

Model of the shell side zone

The mass balance of chemical species i in the shell side is given as follows.

$$\frac{4Q_g}{\pi d_{shell}^2}\frac{\partial C_i}{\partial z}=\varepsilon D_{e,r}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right)+\rho_b\sum_{i=1}^{5}\sum_{j=1}^{3}\eta_j\sigma_{ij}R_j \quad (1)$$

Where, i = CH_4, H_2O, H_2, CO, CO_2

Model in the reaction zone of methanol

The mass balance of chemical species i in the reaction zone of methanol is given as follows.

$$\frac{4Q_g}{\pi d_{reac.Zone}^2}\frac{\partial C_i}{\partial z}=\varepsilon D_{e,r}\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial C_i}{\partial r}\right)+\rho_b\sum_{i=1}^{5}\sum_{j=1}^{3}\eta_j\sigma_{ij}R_j \quad (2)$$

Where, i = H_2, CO, CO_2, CH_3OH, H_2O

Results and discussion

The mathematical model was developed to analyze the behaviour of chemical species i (i = CH_4, H_2O, H_2, CO, CO_2) in the shell side of MR. Numerical experiments were performed using a computational code which was developed for catalytic hydrogenation of carbon dioxide. Figure 2 shows the predicted product distribution (concentrations i components) in wet basis (water vapour included in the product). It is noted that as the operation proceeds, methane is consumed by steam reforming reaction with water available in inlet gas mixture. Based on results from the mathematical modelling after that all curves describing the concentrations reach to stable levels, the following definition of the yield of methanol is used for describing the MR performance as follows:

$$Y_{MeOH} = \frac{C_{MeOH}}{C_{CH_4}^{in}} \tag{3}$$

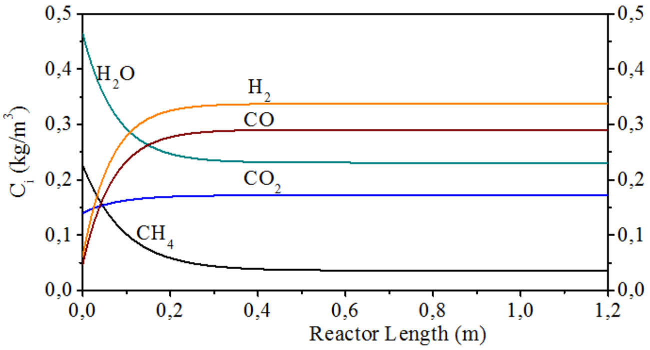

Figure 2 The concentrations profiles of i chemical species in the MR.

Figure 3 reports the effect of the operating temperature on the conversion of methane at reaction pressure (950kPa). As can be seen, the yield of methanol reaches to stable levels at operating temperatures from 200°C to 300°C, respectively.

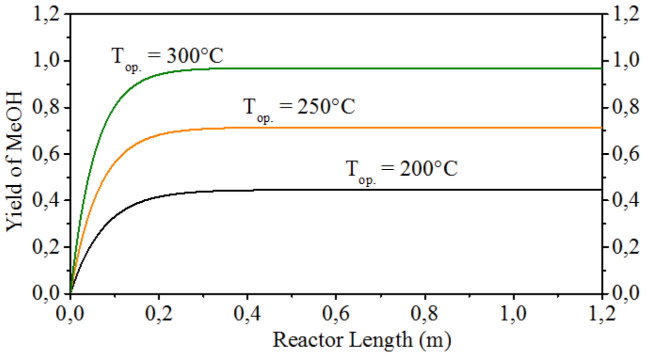

Figure 3 Yield of methanol versus reactor length.

Conclusion

A two-dimensional mathematical model along with a kinetic model was used to report predictions in the MR reactor. It can seen that the yield of methanol increase with increasing reaction temperature on the catalytic performance of Cu/ZrO_2 catalysts.

Acknowledgments

None.

Conflicts of interest

The author declares that there are no conflicts of interest.

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