MODELING OF DRY REFORMING OF METHANE FOR H₂ PRODUCTION IN A CATALYTIC MEMBRANE REACTOR

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ABSTRACT

With the rapid growth of the population and development of the economy, the consumption of fossil fuels is continuously increasing to satisfy the growing energy demand. The emission of greenhouse gases (GHGs), mostly carbon dioxide (CO_2) and methane (CH_4), is detrimental to the environment with a subsequent change of climate, e.g. the global surface temperature increased by 0.8 °C in the 20th century^[1]. Therefore, there is an urgency to control and convert these GHGs with the most effective way in a useful product^[2]. In view of this, dry reforming of methane (DRM) is a highly regarded technological approach for not only converting these two GHGs simultaneously but also producing H₂, which is considered a promising renewable energy source^[3]. Typically, DRM reaction (CH₄ + CO₂ \leftrightarrow 2H₂ + 2CO, $\Delta H_R^0 = 247 \text{ kJ/mol}$) produces syngas with a low H₂/CO molar ratio (\leq 3), which can be preferentially used for the production of hydrocarbons via Fischer-Tropsch synthesis and oxygenated chemicals^[4]. It is an endothermic reversible reaction and is performed at high temperatures (700 – 900 °C) to achieve optimum reactants conversion and product selectivity. However, extreme operating temperatures result in a substantial energy expenditure and, consequently, a higher operational cost^[5]. During DRM, catalyst deactivation due to carbon formation and accumulation on the catalyst surface via the methane decomposition and Boudouard reactions poses a challenge to maintain the catalytic activity and conversion into syngas. In addition, reverse water gas shift (RWGS), which occurs in parallel with DRM, is undesirable since it consumes the produced H₂. To meet these challenges and improve reactor performance, Catalytic Membrane Reactor (CMR) can be considered. According to the Le Chatelier's principle, the removal of one of the species (i.e. H_2) from the reaction mixture shifts the reaction equilibrium of the DRM to the product side, achieving higher conversions at lower temperatures. Herein, in this study, a one-dimensional non-isothermal mathematical model will be developed for DRM reaction in a membrane reactor. Main objective of this study is to understand the effect of membrane permselectivity, reaction and permeation rate on the performance of the membrane reactor. In addition, the effect of RWGS reaction will be also examined.

KEYWORDS: Modeling, Simulation, Membrane reactor, DRM reaction, RWGS reaction

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