Design and Analysis of a CO_2 to Methanol Reactor

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ABSTRACT

Carbon capture and utilization (CCU) have emerged as a promising strategy to mitigate greenhouse gas emissions while enabling the production of value-added chemicals. Among the possible routes, the conversion of CO_2 into methanol has attracted increasing attention due to the growing global demand for this key chemical intermediate [1–2]. In this context, the catalytic hydrogenation of CO_2 represents a promising alternative route for sustainable methanol production. However, this process is strongly limited by thermodynamic constraints. This work presents a process simulation and reactor design study for CO_2 hydrogenation to methanol, integrating thermodynamic equilibrium analysis, kinetic modeling, and heat transfer effects. The process was modeled using Aspen Plus (V12) with the Peng–Robinson equation of state modified by the Boston–Mathias alpha function. The methanol synthesis reactor was represented as a plug flow reactor (PFR) using a Langmuir–Hinshelwood–Hougen–Watson (LHHW) kinetic approach based on the Vanden Bussche and Froment kinetic model [3]. Thermodynamic limitations were evaluated through Gibbs energy minimization, considering side reactions such as the reverse water-gas shift. The analysis revealed that CO_2 conversion is strongly limited by equilibrium, particularly at high temperatures, which favor CO formation, and reduces methanol selectivity. In contrast, high pressures (50–100 bar) and temperatures below 250 °C favor methanol formation, with selectivity values above 98% observed at approximately 50 bar. Regarding reactor modeling, both adiabatic and non-isothermal multitubular configurations were analyzed. The adiabatic reactor exhibited a higher temperature profile due to the absence of heat removal, whereas the non-isothermal configuration enabled partial control of the hotspot. In the latter case, a pronounced temperature peak was observed near the reactor inlet (approximately 270 °C), favoring CO formation and reducing methanol selectivity. The selected configuration was a non-isothermal multitubular reactor operated at 220 °C and 60 bar, with 6 m and a tube diameter of 0.058 m with 1300 tubes. Heat removal was modeled using an overall heat transfer coefficient of 600 $J/(s \cdot m^2 \cdot K)$, with a thermal fluid inlet temperature of 220 °C. The system processed 226 t/h, including a recycle (0.95 ratio). The reactor was designed to operate with a pressure drop below 10%, while the simulated process resulted in an estimated pressure drop of approximately 5%. At the reactor outlet, CO_2 conversion and methanol selectivity reached 29% and 98%, respectively. The results indicate that the system is primarily limited by thermodynamic equilibrium after the initial reaction zone. These findings highlight the critical role of thermodynamic, reaction kinetics, and heat management, providing insights into suitable operating ranges and scale-up considerations.

Keywords: CO_2 hydrogenation; Methanol synthesis; Reactor design.

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