Performance Assessment and Feed Optimization of a Multitubular Methanol Synthesis Reactor Under Variable Operating Conditions

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Methanol is increasingly regarded as a key molecule for the ecological transition due to its versatility as a fuel, hydrogen carrier, and chemical platform. Among the various emerging production pathways, the synthesis of methanol from syngas mixtures derived from renewable or low-carbon sources requires a deep understanding of reactor behavior under variable operating conditions. This study presents a detailed modeling and performance analysis of a boiling water-cooled multitubular fixed-bed reactor for methanol synthesis, based on the Vanden Bussche and Froment (VBF) kinetic model. The reactor is described using a one-dimensional pseudo-homogeneous model that incorporates mass and energy balances, pressure drop via the Ergun equation, and heat exchange with boiling water on the shell side. The quality of the syngas feed is characterized by two dimensionless parameters: the Stoichiometric Number (SN) and the Carbon Oxide Ratio (COR). The parameter used to measure the amount of feed related to the reactor's size is the Gas Hourly Space Velocity. Results show that reactor performance, quantified through methanol yield and overall carbon oxide conversion, is highly sensitive to the values of COR, SN, and GHSV. In this work, the COR parameter is defined as the ratio between CO and the total carbon oxides in the feed (COR = CO / (CO + CO_2)). This variable provides a compact and intuitive representation of syngas quality, allowing direct comparison between feedstocks derived from different sources. While thermodynamic equilibrium would suggest a preference for CO-rich feeds and stoichiometric H_2/C ratios, kinetic and heat transfer limitations shift the optimal operating conditions toward slightly higher SN and intermediate COx values, especially at high GHSV. To support feed design and reactor optimization, this study demonstrates how the COx parameter can be used as a guiding variable to tune the feed composition. A dedicated case study illustrates the impact of COx on reactor sizing and performance, showing that intermediate values (COx ≈ 0.1–0.2) often maximize methanol yield under realistic operating conditions. Furthermore, a dependence between COx and operating pressure is observed. Based on the results, we introduce the concept of COx, the ideal feed composition that maximizes reactor performance for a given set of operating conditions (SN, GHSV, and pressure). This value can serve as a practical target for feed adjustment in dynamic or partially constrained systems. Overall, the COx parameter emerges as a simple yet powerful tool to rationalize feed composition choices and improve the flexibility and performance of methanol synthesis reactors operating under varying process conditions. Its use supports the development of robust and adaptable methanol production units integrated with renewable and intermittent energy sources.

Keywords: *methanol synthesis, syngas composition, reactor modelling, process optimization, carbon oxide ratio*