Ammonia Decomposition for Hydrogen Production: Reactor design

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Abstract

The transition from fossil fuels to alternative energy sources is an important measure in reducing greenhouse gas emissions. Hydrogen (H_2) plays a significant role in this scenario. However, its low volumetric density and low boiling point (-252.87 °C) require extreme storage and transportation conditions. A promising alternative to handle these challenges is the chemical storage of hydrogen. Among the possible hydrogen vectors, ammonia is considered by the scientific community to be the most promising choice, due to its high hydrogen content, approximately 17.8% by mass, and high volumetric density (Lucentini et al., 2021). However, this alternative's viability depends directly on ammonia decomposition efficiency, which is an under-development process, with few studies addressing industrial-scale conditions.

In this context, this work aims to simulate and design an industrial reactor to produce hydrogen from ammonia decomposition. The simulations were carried out using the commercial simulator Aspen Plus® v.12. First, a thermodynamic study, based on Gibbs free energy minimization, was conducted to analyze the reaction limitations and to estimate operating conditions. This analysis allowed to conclude that the decomposition is favored at low pressures and high temperatures, reaching 99% of ammonia conversion at 1 bar and 389 °C. In contrast, at 40 bar, the same performance is obtained at 792 °C. In sequence, a kinetic model for an efficient catalyst was obtained (Sayas et al., 2020) and a multi-tubular fixed bed reactor was simulated. A sensitivity analysis was carried out to identify an adequate WHSV, pressure, and temperature, considering ammonia conversion and reactor pressure drop. For an industrial scale of 34 ton/h of H_2 production, the proposed reactor configuration achieved 81% ammonia conversion, operating at 550 °C and 40 bar. Comparison with the thermodynamic equilibrium revealed that the reactor operates at 86% of the maximum performance. Future work aims to refine the reactor model considering mass-transfer limitations. The results of this work will contribute to the industrial-scale implementation of ammonia decomposition units.

Keywords

Hydrogen, Ammonia decomposition, Reactor design, Process simulation.

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