Área: FIS

Green Methanol: Application of Thermodynamic Modeling to Describe the Flash Separation Process – Enabling Power-to-Methanol.

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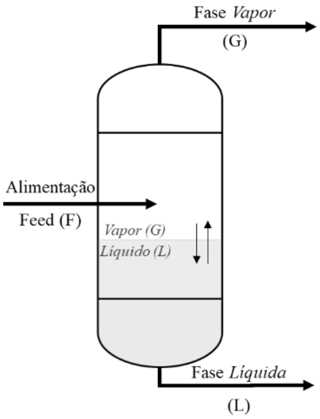
Highlights

This study compared thermodynamic modeling approaches for phase equilibrium in the industrial separation process involved in the green methanol synthesis via the hydrogenation of carbon dioxide.

Resumo/Abstract

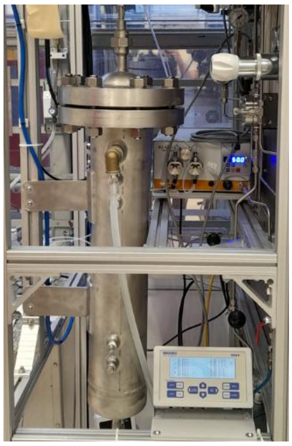
Figure 1. Flash Separation Vessel Diagram



One of the strategies to mitigate global warming and reduce CO_2 concentrations in the atmosphere is the sustainable conversion of this gas into value-added products. In this context, the green hydrogenation of CO_2 into methanol, known as Power-to-Methanol technology, emerges as a promising alternative. This process enables the storage of energy from renewable sources in the form of chemical bonds. However, for its scalability, it is essential to understand the thermodynamic modeling involved in the separation of products formed during the reaction.

The objective of this project was to compare different thermodynamic models, based on equations of state, group contribution, and mixing rules, to describe the gas-liquid separation process (Figure 1) of the $CO_2/H_2/H_2O/CH_3OH$ mixture. Different approaches, such as φ-φ and γ-φ, were implemented to calculate the phase concentrations and separation efficiency predicted by each model.

Figure 2. Flash Separation Vessel Built for Thermodynamic Study.



Theoretical results were obtained using commercial software, such as CoCo Café, as well as Python-based codes. These results were experimentally validated through tests in a pilot-scale flash separation unit (Figure 2). The determination of species concentrations in both gas and liquid phases was carried out through gas chromatography and mass balance analysis, based on samples collected every 30 minutes, until concentration equilibrium was reached under steady-state conditions. The operating conditions in the separator were 25 bar, 15°C, and a total volumetric flow rate of 1 m³/h.

Preliminary results indicate that thermodynamic models based on the PSRK equation show greater convergence between theoretical and experimental values, suggesting their suitability for modeling the separation process under study.

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