Thermodynamic Modeling of CO2 Absorption in Aqueous Potassium Carbonate Solution with the Association eNRTL Model

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Aqueous potassium carbonate (K_2CO_3) solution is a common and environmentally benign chemical absorbent for CO_2 capture. To reduce energy requirements associated with CO_2 stripping and compression processes, the industry is interested in developing high-temperature and high-concentration K_2CO_3 -based CO_2 absorption processes. Previous thermodynamic modeling efforts for conventional K_2CO_3 -based CO_2 absorption processes focused on correlating and predicting the CO_2 partial pressure vs CO_2 loading [1] and paid little attention to other thermodynamic properties such as water partial pressure and enthalpy of absorption that are critically important for the development of high-temperature and high-concentration K_2CO_3 -based CO_2 absorption processes. This study presents a comprehensive thermodynamic modeling of the K_2CO_3 -H2O-CO2 ternary system and its binary systems with the recently developed association electrolyte nonrandom two-liquid (association eNRTL) model [2]. Taking into account the ion hydration and ion-pairing of carbonate ions in the aqueous solution, the association eNRTL model provides an accurate representation for various thermodynamic properties such as the CO_2 partial pressure, the water partial pressure, the enthalpy of absorption, and the K_2CO_3 solubility for the K_2CO_3 -H2O-CO2 system. The study covers temperature up to 473.15 K and K_2CO_3 concentration up to saturation.

References

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