POSTER SUMMARY

THERMODYNAMIC MODELLING OF CARBON DIOXIDE HYDRATES IN THE PRESENCE OF SYNTHESISED VINASSE MIXTURES

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Abstract

One of the challenges associated with treating or disposing of vinasse, the by-product of bioethanol production, is the high concentration of dissolved solids, largely in the form of K^+, SO_4^{2-}, Mg^{2+}, Ca^{2+} and Cl^-. While traditional desalination technologies such as evaporation and distillation are employed in the concentration of salts to recover purified or potable water, these methods are energy intensive. The application of a novel technology known as gas hydrate technology can make the process of desalination less energy intensive, since the latent heat of fusion is much less than the heat of vaporisation for water. Developing a reliable thermodynamic model plays an essential role in the design of a hydrate-based process to treat vinasse. In this study, a thermodynamic model based on the solid solution theory of van der Waals and Platteeuw and the UNIQUAC model along with a Debye-Hückel term were used to calculate the carbon dioxide hydrate dissociation conditions in the presence of mixed salt and synthesised vinasse mixtures. The investigated systems in this study were based on the results of an extensive literature review conducted on the characterisation of vinasse for which the composition of the synthesised mixture was 5 wt % KCl + 1 wt % Na_2SO_4 + 0.5 wt % $MgCl_2$ + 0.5 wt % $CaCl_2$ + 2.2 wt % ethanol + 0.5 wt % propionic acid + 0.3 wt % acetic acid. New UNIQUAC interaction parameters were optimised in this study, and good agreement between the experimental data and predictive model results was achieved.

Keywords: gas hydrate, inhibitor, vinasse, thermodynamic model