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# Prediction of $CO_2$ solubility in ionic liquids and glymes with modified generalized BWR Eos

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Key Word (3 words)

Prediction, $CO_2$, Ionic liquid

Abstract (less than 300 words)

When the critical properties of a pure substance are known, it is possible to predict thermodynamic properties based on the corresponding states principle with an equation of state EoS. However, we can hardly find experimental values of critical properties of complex molecules such as ionic liquids. In this work, the extended Joback method is used to obtain the critical properties of ionic liquids or glymes.

To calculate a mixture property precisely, a binary interaction parameter, $m_{ij}$, should be determined. Based on other researcher's work and our own experimental data containing phosphorous ionic liquid, we determined optimal $m_{ij}$ values to fit $CO_2$ solubility in ionic liquids and glymes.

In 1977, using a modified generalized BWR EoS, one of author (Nishiumi) showed that $m_{ij}$ values for the system $CO_2$ + non-polar substances is expressed as a simple function of the ratio of critical volumes [1]. In this paper, we found that $m_{ij}$ values for these $CO_2$ + non-volatile mixtures could be useful for the prediction of $CO_2$ + ionic liquid mixture or glymes, although they are polar mixtures. The result in this work is expected that predictability of $CO_2$ solubility in ionic liquids will enable to give a prompt choice of a non-volatile solvent for $CO_2$ capture.

Reference

[1] H. Nishiumi, S. Saito, Correlation of the binary interaction parameter of the modified generalized BWR equation of state, J. Chem. Eng. Jpn. 10 (1977) 176-180.