Separation of Carbon Dioxide from Sulfur Dioxide, Hydrogen Sulfide, and Nitrous Oxide using Room-Temperature Ionic Liquids

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A ternary equation of state (EOS) model has been developed in order to further our understanding of enhanced gas separation of industrial gases such as CO_2, SO_2, H_2S, and N_2O using room-temperature ionic liquids. The present model is based on a generic RK (Redlich-Kwong) EOS. The empirical binary interaction parameters have been determined using our measured VLE (vapor-liquid-equilibrium) data for CO_2, SO_2, H_2S, and N_2O in several ionic liquids ([bmim][PF_6], [bmim][$MeSO_4$], [bmim][Tf_2N], [hmim][Tf_2N], [bmim][BF_4], [bmim][$N(CN)_2$], [bmim][Ac], [eam][NO_3] and [bmim][SCN]).[1,2] The validity of the present EOS has been checked by conducting ternary VLE experiments for several systems (CO_2/SO_2/[hmim][Tf_2N][3], CO_2/SO_2/[bmim][$MeSO_4$][4], CO_2/H_2S/[bmim][PF_6][5], CO_2/H_2S/[bmim][$MeSO_4$][6], CO_2/N_2O/[bmim][BF_4][7] and CO_2/N_2O/[bmim][Ac][8]). With this EOS, an isothermal ternary phase diagram and solubility (VLE) behaviors have been calculated for various (*T*, *P*, and feed compositions) conditions. The addition of ionic liquids in CO_2/SO_2, CO_2/H_2S and CO_2/N_2O can significantly increase the selectivity and in some cases, the selectivity was high for even a small addition of ionic liquid due to preferential chemical absorption.

[1] M.B. Shiflett, A. Yokozeki, *Ind. Eng. Chem. Res. 49*, **2010**, 1370-1377.
[2] M.B. Shiflett, A.M.S. Niehaus, B.A. Elliott, A. Yokozeki, *Int. J. Thermophys*. **2011**, in press.
[3] A. Yokozeki, M.B. Shiflett, *Energy Fuels 23*, **2009**, 4701-4708.
[4] M.B. Shiflett, A. Yokozeki, *Energy Fuels 24*, **2010**, 1001-1008.
[5] M.B. Shiflett, A. Yokozeki, *Fluid Phase Equilibr*. *294*, **2010**, 105-113.
[6] M.B. Shiflett, A.M.S. Niehaus, A. Yokozeki, *J. Chem. Eng. Data 55*, **2010**, 4785-4793.
[7] M.B. Shiflett, A.M.S. Niehaus, A. Yokozeki, *J. Phys. Chem. B*. *115*, **2011**, 3478-3487.
[8] M.B. Shiflett, B.A. Elliott, A. Yokozeki, *J. Sep. Pur. Tech*. **2011**, DOI:10.1080/01496395.2011.627905.