Molecular Simulation of Thermodynamic and Transport Properties for the H_2O+CO_2+NaCl System

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Thermodynamic and transport properties of H_2O+NaCl, H_2O+CO_2, and H_2O+CO_2+NaCl mixtures were studied by Monte Carlo and molecular dynamics simulations. For the binary mixture H_2O+NaCl, the vapor pressure, liquid densities, viscosities and liquid-vapor interfacial tensions were obtained. For the binary mixture H_2O+CO_2 and the ternary mixture H_2O+CO_2+NaCl, the CO_2 solubilities in H_2O-rich and CO_2-rich phases as well as CO_2 and H_2O diffusivities were obtained. Two sets of recently proposed Drude oscillator based polarizable force field models were studied and compared with several fixed-point-charge non-polarizable models. [1, 2] These models use either Lennard-Jones 12-6 or Buckingham exponential-6 functional forms to describe the short range interactions, while the long-range Coulombic interactions were modeled by point charges or Gaussian charges. In particular, for polarizable models, the SWM4-NDP [3] and BK3[4] water models, and the AHNDP [5] and BK3 [6] ion models were studied. For fixed-point-charge non-polarizable models, several existing models for H2O (SPC, SPC/E, Exp-6 [7] and TIP4P/2005), CO_2 (EPM2 and TraPPE), and ions (Smith-Dang, Joung-Cheatham and Tosi-Fumi) were investigated. It was found that none of the non-polarizable models was able to produce simultaneously all properties of interest.

References

[1] Orozco, G. A.; Economou, I. G.; Panagiotopoulos, A. Z. *J. Phys. Chem. B*. **2014**, 118, 11504-11511.
[2] Moultos, O. A.; Tsimpanogiannis, I. N.; Panagiotopoulos, A. Z.; Economou, I. G. *J. Phys. Chem. B*. **2014**, 118, 5532-5541.
[3] Lamoureus, G.; Harder, E.; Vorobyov, I. V.; Roux, B.; MacKerell, A. D. *Chem. Phys. Lett*. **2006**, 418, 245-249.
[4] Kiss, P.; Baranyai, A. *J. Chem. Phys*. **2013**, 138, 204507.
[5] Yu, H.; Whitfield, T. W.; Harder, E.; Lamoureux, G.; Vorobyov, I.; Anisimov, V. M.; MacKerell, A. D.; Roux, B. *J. Chem. Theory. Comput*. **2010**, 6, 774-786.
[6] Kiss, P.; Baranyai, A. *J. Chem. Phys*. **2014**, 141, 114501.
[7] Errington, J. R.; Panagiotopoulos, A. Z. *J. Phys. Chem. B*. **1998**, 102, 7470-7475.