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Measurement of the Density of Carbon Dioxide/Methanol and Dioxide/Ethanol Homogeneous Mixtures and Correlation with Equations of State

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Abstract (less than 300 words)

Equations of state (EoS) can be used to estimate a wide variety of physical properties. They are mainly of the van der Waals-type, the lattice-fluid type (the Flory-Huggins theory), and the SAFT type (the perturbation theory). They should be used according to the target system and property. However, the relationship between the physical properties and the validity of the EoS have not been studied much. The densities of homogeneous phase fluid mixtures of the carbon dioxide (CO_2)/Methanol (MeOH) and CO_2/Ethanol (EtOH) binary systems were measured and correlated to three equations of state. The density measurements were performed using a high-pressure vibration-type density meter equipped with a circulation pump and variable-volume viewing cell, which guaranteed the homogeneity of the mixtures. The densities were measured at temperatures ranging from 313 to 353 K, pressures up to 20 MPa, and CO_2 concentrations from 0 to 80 mol%.

The experimental data obtained were correlated to three typical EoS, namely Peng–Robinson (PR), Sanchez–Lacombe (SL), and Perturbed Chain statistical associating fluid theory (PC-SAFT) EoS. As the result, it was not possible to correlate the density of binary systems using the three EoS, presumably due to heterodimers were formed [1,2] when CO_2 and alcohol are mixed. Of the three, PC-SAFT gave the best correlation of densities, because it had the advantage of considering the association of alcohols compared to the other two equations. Similarly, the vapor liquid equilibrium (VLE) of the CO_2/MeOH and CO_2/EtOH mixtures was correlated but the accuracy of them were not sufficient for the same reason. These results suggest that it was difficult to correlate the density and VLE in the CO_2/MeOH and CO_2/EtOH systems using the equation of state, and that an approach using heterodimers of CO_2 and alcohols was necessary for accurate property correlation.

References

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