

THERMODYNAMICS

DME-CO₂-CH₃OH和DME-CO₂-C₂H₅OH体系的高压汽液相平衡研究

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摘要 In this study, the Gibbs-Duhem equation was applied to make the thermodynamic consistency test and thermodynamic model estimation for systems of CO₂-DME (dimethyl ether), DME-CH₃OH, CO₂-CH₃OH and DME-C₂H₅OH systems on the basis of the vapor-liquid equilibrium (VLE) experimental data in published reports. And the NRTL binary interaction parameters of the systems mentioned above were regressed by the VLE data and were subjected to a thermodynamic consistency test because the study showed that PR-NRTL model combination was appropriate for the four systems mentioned above. The regressed binary interaction parameters were used to estimate the VLE for DME-CO₂-CH₃OH at temperatures of 313.15K and 333.15K, and the estimated result was coincident with the experimental data. On the basis of the predicted VLE data for systems of DME-CO₂-CH₃OH and DME-CO₂-C₂H₅OH, the VLE behaviors of the two systems were studied by the phase diagrams of these two ternary systems, with the forms of both the two dimensional and three dimensional phase diagrams, respectively.

关键词 [phase equilibria](#), [model reduction](#), [dimethyl ether](#), [phase diagram](#).

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High-pressure Vapor-Liquid Equilibrium Studies for DME-CO₂-CH₃OH and DME-CO₂-C₂H₅OH Systems

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Abstract In this study, the Gibbs-Duhem equation was applied to make the thermodynamic consistency test and thermodynamic model estimation for systems of CO₂-DME (dimethyl ether), DME-CH₃OH, CO₂-CH₃OH and DME-C₂H₅OH systems on the basis of the vapor-liquid equilibrium (VLE) experimental data in published reports. And the NRTL binary interaction parameters of the systems mentioned above were regressed by the VLE data and were subjected to a thermodynamic consistency test because the study showed that PR-NRTL model combination was appropriate for the four systems mentioned above. The regressed binary interaction parameters were used to estimate the VLE for DME-CO₂-CH₃OH at temperatures of 313.15K and 333.15K, and the estimated result was coincident with the experimental data. On the basis of the predicted VLE data for systems of DME-CO₂-CH₃OH and DME-CO₂-C₂H₅OH, the VLE behaviors of the two systems were studied by the phase diagrams of these two ternary systems, with the forms of both the two dimensional and three dimensional phase diagrams, respectively.

Key words [phase equilibria](#), [model reduction](#), [dimethyl ether](#), [phase diagram](#).

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