

Thermodynamical VLE modeling of water and methanol mixture using PRSV2 equation of state

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Abstract

Nowadays, researchers are trying to synthesis a hundreds of new material that acquiring their thermodynamical properties using experimental procedure is impossible. So by using modeling softwares and accessibility of thermodynamical equations, thermodynamic and equilibrium properties can be predicted accurately. PRSV2 equation of state is a modified form of Peng-Robinson EOS that is recently considered by researchers for prediction of multicomponent mixtures thermodynamic equilibrium behavior. In this study is tried to emphasize on advantages of VLE thermodynamic modeling using EOS for liquid and vapor phases rather than using EOS for vapor phase and activity coefficient method for liquid phase. Equilibrium calculations were performed using experimental data in two condition of isothermal and isobar. In two condition advantages of using EOS for vapor and EOS for liquid rather than using EOS for vapor and activity model for liquid has been demonstrated. A first order equation was obtained to show the dependence of k_{ij} to temperature that has shown good relation in the temperature range $TR < 0.7$.

KEYWORDS

Thermodynamic properties, prsv2 equation of state, VLE(vapor-liquid equilibrium), binary coefficient

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