

Influence Factors Analysis for Gradient Theory of Surface Tension Calculation for Binary Mixtures

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The surface tension is a basic thermophysical property which plays an important role in many industrial processes. There are many methods for surface tension calculation, in which the gradient theory is now very popular especially for mixtures. And the only inputs to the gradient theory are the Helmholtz free energy density and the influence parameter. The liquid density and vapor liquid equilibrium (VLE) property are crucial basis for calculating these two input parameters. However, the contribution of accuracy improvement of the liquid density and VLE property to precise surface tension calculation is not fully investigated. This work studied the influence of the accuracy of liquid density and VLE property on surface tension calculation for polar binary mixtures. The Peng–Robinson (PR) equation of state (EOS) and the volume-translated Peng–Robinson (VTPR) EOS are two classical cubic EOSs. This work combined the gradient theory with the two cubic EOSs for surface tension calculation. By using the same mixing rule, the VTPR EOS can improve the accuracy of liquid density but does not change the accuracy of VLE property compared with the PR EOS. And by using the same cubic EOS, G^E -EOS mixing rule can improve the accuracy of VLE property but does not change the accuracy of liquid density compared with the van der Waals (vdW) mixing rule. Therefore, the calculation comparison of PR EOS and VTPR EOS with same mixing rule was made to investigate the accuracy contribution of the liquid density. And the calculation of VTPR EOS with G^E -EOS and vdW mixing rules was also compared for studying the accuracy contribution of the VLE property. And by using the VTPR EOS with G^E -EOS mixing rule, a high precision surface tension calculation for polar binary mixtures was obtained in this work.