Status of the Vapor-Liquid Equilibria Prediction using Temperature Dependent Interaction Parameters

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Based on our past results, use of temperature dependent interaction parameters (TDIP), instead of using temperature independent interaction parameters (TIIP), may lead to improvement in the prediction of the vapor-liquid coexistence curve. A survey of the results of the phase diagrams of simple fluids such as Ar, Kr, CH4 and globular UF6 is provided. The results using TDIP produce, in general, more accurate phase diagrams compared to the diagrams generated using TIIP. The root mean square deviation (RMSD) is reduced by 42.1% using TDIP for argon. Similar reductions in RMSD were observed for Kr, CH4, and UF6. The phase diagram in reduced units for temperature dependent interaction parameters is a family of curves rather than a universal curve such as the case with TIIP.