

Application of the SAFT-VR Equation of State to Vapor-Liquid Calculations for Pure Components and Binary Mixtures Using the Sutherland Potential

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An equation of state based on the statistical associating fluid theory for potentials of variable range (SAFT-VR) has been applied to model 35 pure associating and non-associating fluids and 30 binary mixtures. The pure components consist of alkanes, alcohols, water, aromatics and polar or multi-polar compounds like ammonia and H_2S . In contrast to other attempts which have used the SAFT-VR model for various thermodynamic calculations using the square-well or Yukawa potentials, the short-range dispersion interactions have been accounted for here using the Sutherland potential, while hydrogen bonding interactions are explicitly taken into account as in other versions of the SAFT approach. The Sutherland potential is particularly useful for modeling the interactions among multi-polar species. Model parameters for the pure components have been optimized by fitting available experimental data on vapor pressure, saturated vapor density and saturated liquid density for temperatures ranging from near the triple point up to reduced temperatures of 0.9. The effect of several simplifying assumptions aimed at reducing the number of model parameters has been investigated, and the resulting trends in parameters has been discussed. Binary interaction coefficients have been obtained for the binary systems by fitting experimental data on vapor-liquid equilibrium pressure and phase concentrations. Results have been compared to those obtained using other versions of the SAFT-VR model.