

Equation of state for non-polar and associating fluids: An explanation of hydrogen bond with SAFT

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We proposed the new expression for dispersion and association contribution based on the original SAFT by Chapman et al.. We express the second order dispersion term with different potential range from relatively short to long range comparing with simulation result by Zhou and Solana. In addition, Helmholtz free energy of association contribution also modified by the temperature dependent correction function to represent not only thermodynamic vapor-liquid equilibrium properties of polar fluid but also degree of hydrogen bond of water, methanol and ethanol. To represent the wide applicability of our model, we examined the various model systems such as alkane, water, alkanol and polymer.