

A Practical SAFT1 Model for Associating Fluids: Application to 1-Alkanols and Polymers (invited)

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In order to predict the physical properties and phase behavior of self- and cross-associating fluids, such as 1-alkanols, one needs predictive thermodynamic models that account for specific interactions that lead to molecular association. One approach to developing such models is on the basis of perturbation theory, such as Statistical Associating Fluid Theory (SAFT). This work builds on SAFT and on an engineering model called SAFT1 (Adidharma and Radosz, 1998), which treats molecules as chains of square-well segments. SAFT1 has been found to be effective for macromolecular systems, but it has not been extended to associating fluids yet.

The general form of the total potential of the associating fluids consists of a core potential and association site potentials:

$$\phi(12) = \phi_{core}(r) + \sum_{A \in \Gamma} \sum_{B \in \Gamma} \phi_{AB}(r_{AB}) \quad (1)$$

in which (12) designates the distance and orientation coordinates between molecules 1 and 2, r is the center-to-center distance between cores (segments), and r_{AB} is the center-to-center distance between association site A and B . For the core and for the association sites we postulate square-well potentials.

We find that, for small 1-alkanols, SAFT1 is more accurate than SAFT in correlating the vapor pressure and liquid density. Furthermore, the SAFT1 parameters are found to be well behaved and hence easy to estimate reliably for high-molecular-weight 1-alkanols and polymers.

[1] H. Adidharma and M. Radosz, *Ind. Eng. Chem. Res* **37**, 4453 (1998).