Phase Behavior of Aromatic Molecules and their Mixtures Using the GC-SAFT-VR Equation of State

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The statistical associating fluid theory [1] is a commonly used molecular-based equation of state that has been successfully applied to study a wide range of fluid systems. In recent work, the GC-SAFT-VR equation was proposed which combines the SAFT equation for potentials of variable range (VR) [2] with a group contribution like approach [3]. Parameters for key functional groups (such as CH3, CH2, CH, CH2=CH, C=O, C6H5, ether and ester, OH, NH2, CH=O, COOH) were obtained by fitting to experimental vapor pressure and saturated liquid density data for selected low molecular weight fluids and then used to predict the phase behavior of pure non-associating fluids and their mixtures [3-5] without adjusting the group parameters to binary mixture data. Here we study benzene, alkylbenzenes and their mixtures with alkanes, ethers, alcohols and amides. In earlier work the benzene ring was modeled as a single group, however in common with other group-contribution based SAFT approaches, it failed to reproduce the correct curvature in the experimental liquid density data of alkylbenzenes. In this work we investigate modeling benzene as a ring composed of smaller groups to more accurately capture the interactions between rings.