Prediction of Vapour-Liquid, Liquid-Liquid, and Solid-Liquid Equilibria in Aqueous Solution with the SAFT-Gamma Group Contribution Approach

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In the scope of group contribution methods derived entirely within an equation of state, the SAFT-gamma EOS[1] has recently been developed to describe fluids of heteronuclear molecules which are formed from fused square-well segments of different types. The different groups are then defined by one or multiple[2] spherical segments characterized by size and attractive energy (well-depth and range) parameters, and shape factor parameter which describes the contribution that each segment makes to the overall molecular properties. For associating groups a number of bonding sites are also included on the segment introducing two additional energy and range parameters. The formulation of SAFT-gamma as a continuum fluid theory offers the key advantage that the binary interaction parameters between groups can be obtained directly from an examination of pure component properties alone. This is particular useful in describing the properties of fluid mixture (vapour-liquid and liquid-liquid equilibria, VLE and LLE) when no experimental data on the mixture are available. In this work the parameter table of this new group contribution approach is extended to include water and predictions for the VLE and LLE of a number of aqueous solutions are presented. Some preliminary calculations with SAFT-gamma of the solid-liquid equilibria (solubility) will also be discussed. Furthermore, we will present the extension of the theory to deal with heteronuclear molecules formed from Mie segments of different type. This more realistic potential as an elementary brick of an homonuclear SAFT-like EOS[3] has proven previously to be highly accurate in predicting second-order derivative properties (isobaric heat capacity, isobaric thermal expansivity, speed of sound etc.) of complex fluids. We will show that the use of this generalized Lennard-Jones potential in the context of the SAFT-gamma group contribution approach allows for the simultaneous description of both VLE and second-derivative properties of pure fluids and their mixtures.

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