Accounting for cross association in non-self-associating species using a physically consistent SAFT-VR Mie approach - DTU Orbit (30/01/2019)

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This work presents a formalised, physically consistent approach to account for cross association in the SAFT framework. The focus of the approach was to account for solvation of non-self-associating components, using members of the ketone and ether functional groups as model components. Physical consistency is captured by only considering a single negative site in these components, with the association mechanisms termed the "N scheme" as a result. An accurate polar parameter set is a prerequisite for the approach, where polar and dispersion interactions are already accounted for in pure component properties and those of mixtures where solvation is absent. Using SAFT-VR Mie-GV as the example framework, the approach considers the discretisation of the two association parameters, and it applies the resulting matrix of parameter sets to mixture VLE data for the ketone or ether with alcohols in the C₂ to C₄ range. Analysis of the resulting AAD contour plots demonstrate that the use of average solvation parameters for each functional groups are appropriate, rather than component-specific parameters, and they offer excellent pure predictions for alcohol mixtures and good predictions for aqueous mixtures. As a final test, the approach was applied to chloroform, considering a single positive site and using the proposed parameterisation method. The resulting "P scheme" for chloroform, in conjunction with the N scheme for acetone, yields excellent predictions for the quintessential chloroform/acetone mixture and emphasises the suitability and predictive strength of the approach.

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