# A Group Contribution SAFT-VR Equation of State to Predict the Fluid Phase Behavior of Complex Systems

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The statistical associating fluid theory for potentials of variable range (SAFT-VR) [1] is a widely used molecular-based equation of state that has been successfully applied to study a wide range of fluid systems. SAFT-VR provides a framework in which the effects of molecular shape and interactions on the thermodynamics and phase behavior of fluids can be separated and quantified. In the original approach, molecules were modeled as chains composed of identical segments, where the heterogeneity of molecules in terms of structure and functional groups was described implicitly through effective parameters. The GC-SAFT-VR [2] approach was developed to account explicitly for the effects of molecular structure and functionality. Parameters for a range of different functional groups have been determined by fitting to experimental vapor pressure and saturated liquid density data for a number of small molecules containing the functional groups of interest. Transferability of the parameters is tested by comparing the theoretical predictions with experimental data for pure fluids and binary mixtures not included in the fitting process, as well as by studying the VLE and LLE of small molecules in polymer systems [3]. Overall, the GC-SAFT-VR approach is found to accurately predict the phase behavior of a wide range of pure fluids and their mixtures, including alkanes, ketones, ethers, esters, alcohols and amines, as well as polymer systems.

[1] Gil-Villegas, A.; Galindo, A.; Whitehead, P. J.; Mills, S. J.; Jackson, G. and Burgess, A. N. *Journal Of Chemical Physics*, **1997**. 106, 4168-4186.
[2] Peng, Y.; Goff, K. D.; dos Ramos, M. C.; McCabe, C. Article in press *Fluid Phase Equilibria* **2008**.
[3] Peng, Y.; Goff, K. D.; dos Ramos, M. C.; McCabe, C. To be submitted to *Fluid Phase Equilibria* **2008.**