

Comparison of SAFT-VR-Mie and CP-PC-SAFT in predicting phase behavior of associating systems

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Abstract

The experimentally measured thermodynamic properties of fluid systems are defined by various molecular phenomena, which currently cannot be precisely described even by the most advanced theories. Hence, the pure compound parameters of different variations of SAFT often do not have genuine values yielded by the micro-level molecular considerations but are evaluated by fitting vast and vague bases of the experimental macro-level data. This practice not only diminishes the theoretical backgrounds of these models, but also affects their transparencies and predictive values. Although the latter values can at times be recovered by implementing various methods, such as the CP-based numerical solution [1] or the corresponding-state correlation [2], in the cases of strongly associating compounds the data fitting still seems unavoidable. Such circumstances rise the following fundamental question: do the over-all robustness and reliability of SAFT models strictly dependent on the profundity of their molecular backgrounds, or they are rather defined by the parameterization strategies?

To provide some relevant observations, in this study we have compared the accuracy of two SAFT approaches having different degrees of complexity and the number of fitted parameters in modeling pure ammonia, water, methanol, ethanol, hydrazine, and the pertinent binary ammonia systems. This comparison has been performed in the entire thermodynamic phase space while considering not only the extreme pressure range, but also various thermodynamic properties.

References

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