

Testing the Accuracy of the Soft-SAFT Parameterization: Simultaneous Description of Phase Equilibria and Derivative Properties

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Although it is of common practice to remark the theoretical background of statistical mechanics based equations of state (EoS), such as the family of SAFT EoSs, these approaches are not always used in a systematic and predictive manner becoming, in some occasions, to behave similarly to any correlation. The ability to describe polar and hydrogen bonding systems in wide ranges of thermodynamic conditions is undoubtedly a step forward in the thermodynamic modelling for industrial applications, but unfortunately most studies are limited to phase equilibria calculations. The so-called predictability and transferability of the SAFT molecular parameters should be given by the ability to describe other properties, such as heat capacity, isothermal compressibility and speed of sound. In some cases, different sets of molecular parameters offer a similar description of the phase envelope, while having a very different performance when studying derivative properties. In this work, we propose to test the soft-SAFT EoS to describe the phase equilibria and derivative properties of a series of systems, including alkanes, alcohols, carboxylic acids and ionic liquids. Apart from the classical parameters optimization method, where only density and vapor pressure data are used, a new method for determining the soft-SAFT compound parameters, including derivative properties data, is investigated and developed. A discussion about the most relevant thermodynamic properties to be included in the parameters fitting, their weight in the regression procedure and the influence of the association molecular parameters in the families where short-range interactions are present will be carried out. Since advanced association EoSs generally derive from the same theoretical background, the methods and conclusions developed can be easily transferred to other SAFT models.