A New Analytical Formulation for the Generalized Corresponding States Model for Thermodynamic and Surface Properties of Pure Fluids

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In a previous study [1], we developed a formulation of the generalized corresponding-states (GCS) model which incorporated critical region nonanalytic behavior via a parametric crossover function. The parametric variable in that model was obtained from the crossover modification of the sine model originally proposed by Fisher and Zinn [2]. In this work, we have developed a new version of the GCS model that incorporates an analytical sine model (ANS) solution, which greatly simplifies the application of the resulting equation of state (EOS). Similar to the original GCS/CRS model, the new GCS/ANS model contains the critical point parameters and acentric factor as input, and yields a very accurate description of the PVT- and VLE-surfaces of one-component fluids in a wide range of thermodynamic states, including the nearest vicinity of the critical point. The GCS/ANS model reproduces the saturated pressure and liquid density data with an average absolute deviation (AAD) of about 1 % and the vapor density with an AAD of about 2 to 3 %. In the one phase region, for the densities d < 2dc, the model reproduces the PVT data with an AAD of less then 2 %, and for liquid densities where d > 2dc, with an AAD of about 1 to 2 %. In combination with the density functional theory (DFT), the GCS/ANS-DFT model is also capable of reproducing the surface tension of one-component fluids (polar and non-polar) with high accuracy.

[1] S.B. Kiselev[C,S] and J.F. Ely, *J. Chem. Phys.* **119(16)**, 8645 (2003).
[2] Fisher and Zinn, *Phys. Rev. B* **59(22)**, 14533 (1999)