The Next Generation Reference Equations of State

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Thermodynamics, and in particular Equations of State (EoS) are the cornerstones of engineering simulations. The desire to represent the available experimental data in a compact and precise manner has motivated the development of state-of-the-art multiparameter EoS.[1] A drawback with multiparameter EoS is their computational demands with respect to time and numerical stability, for instance in phase equilibrium calculations.[1] This has restricted their popularity, in particular for mixtures.[1,2] One of the main reasons for these challenges is their behavior within the two-phase regions, where the pressure as function of density often has several artificial roots.[1] The motivation for removing these artificial roots and obtain a "van-der-Waals like" behavior in the two-phase region has so far been almost absent. One reason for this is the misconception that properties within this region have no physical significance.[1] Density functional theory relies on the properties of exactly this region to predict for instance surface tension, Tolman lengths, rigidity constants, nonequilibrium transfer properties, and much more.[3-5] The current formulations of the reference EoS restrict the possibility to apply them for this purpose, even if the benefits of doing so may be immense. We shall in this work explain how the properties in the strongly metastable regions of a fluid can be mapped using the concept of "superstabilization".[6] Then, we discuss how the next generation multiparameter EoS can be extended properly to the two-phase regions. We give important perspectives on the future development of reference EoS.

References

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