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Multi-Scale, Gibbs-Helmholtz Constrained Cubic Equations of State

By

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Cubic equations of state (EOS) are often desirable when fast, reliable determination of physical properties is required. However, it is well known that they generally perform poorly at high pressure, especially in the compressed liquid regime. In this talk I will describe a radically new approach to the development of cubic equations of state. Specifically, I show how to develop a new thermodynamically rigorous framework for pure component parameters in cubic equations of state (EOS) based on using the Gibbs-Helmholtz equation as a constraint. I will present both closed-form and integral multi-scale expressions for pure component parameters that directly incorporate molecular level information obtained from Monte Carlo or molecular dynamics simulations. I will also present a new mixing rule based on the Gibbs-Helmholtz equation for mixtures. The resulting new family of multi-scale, thermodynamically constrained cubic EOS is truly predictive and has the capability of directly accounting for molecular interactions in non-electrolyte systems (e.g., van der Waals forces) as well as electrostatic effects in weak/strong electrolyte solutions (i.e., charge-charge, charge-dipole, quadrupole, etc.) through the use of an appropriate potential energy function.

High pressure behavior of many pure components and mixtures has been determined. Numerical results are compared with experimental data available in the literature for carbon dioxide, water, and carbon dioxide/water mixtures at high pressure and show excellent agreement. Numerical results are also compared to numerical results for other existing cubic EOS at high pressure and clearly show that the proposed Gibbs-Helmholtz constrained (GHC) cubic EOS is superior to all existing cubic EOS. Many geometric illustrations are used to elucidate key points.

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