Advances in Exceptionally Reliable Mixture Calculations

Ian Bell [C, S] and Eric Lemmon
Applied Chemicals and Materials Division, NIST, Boulder, CO, U.S.A.
ian.bell@nist.gov

Andreas Jäger
TU Dresden, Dresden, Germany

Ulrich Deiters
University of Cologne, Köln, Germany

Flash calculations with the reference multi-fluid models implemented in REFPROP, CoolProp, and TREND are prone to failures, especially when it comes to calculations for mixture models for vapor-liquid equilibrium and all its other manifestations. The inversion of the equation of state to calculate the density given temperature, pressure, and composition is a particularly challenging calculation for which many heuristics have been used to arrive at the correct density root(s). Our goal is to develop algorithms that can forego many of the challenges of working with these highly-accurate multi-fluid models and allow for results that are as reliable as possible according to the pitfalls inherent in this modeling framework. In recent years we have made significant advances in three algorithm-related endeavors for thermodynamic modeling of mixtures: a) isochoric thermodynamics and its use to trace isolines of the phase boundary of binary mixtures b) calculation of the spinodal and critical points of binary mixtures c) the use of proxy Chebyshev expansions to yield quasi-guaranteed density roots from multi-fluid thermodynamic models. The goal of each of these research thrusts is to increase the reliability of calculations with the reference thermodynamic model formulations available in the literature. These algorithms will be implemented in an upcoming version of NIST REFPROP. and form the groundwork for the next generation of mixture model fitting work being carried out by the authors.