

Fluctuation Solution Theory Correlation Function Integrals for Strongly Nonideal Multiphase Systems

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Fluctuation Solution Theory (FST) provides relationships between integrals of the molecular pair total and direct correlation functions (TCFI and DCFI) and FST properties of the pressure derivative of solution density, partial molar volumes, and composition derivatives of activity coefficients (Smith, et al.). For dense fluids, these integrals follow a relatively simple corresponding-states behavior, even for complex systems with strong nonidealities. The approach has been applied to compressed liquid densities (Abildskov, et al, 2015, Diky, et al), to gas solubility in single and mixed solvents (Campanella, et al; Abildskov, et al, 2009), and to aqueous electrolytes (O'Connell, et al) . Their behavior provides insights about molecular interactions as well as rigorous tests for equations of state and their mixing rules (O'Connell and Clairmont). Some evaluations of TCFI and DCFI at constant temperature have been done for a variety of miscible binary liquid nonelectrolyte systems (Wooley). But there seems not to have been any systematic collecting of FST data and evaluation of correlation function integrals for mixtures over wide ranges of temperature, including those with multiple liquids and with solids. This paper describes such an analysis for solid/liquid/liquid (SLLE) systems. Literature data and suitable estimates for FST properties have been regressed to establish a database of TCFI and DCFI for a series of binary SLLE solutions containing water, solvents and ionic liquids over wide ranges of temperature. These values should be useful in developing models for complex multiphase systems.

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