Liquid-Vapor Phase Equilibrium of a Simple Liquid Confined in a Random Porous Media: Second-Order Barker-Henderson Perturbation Theory and Scaled Particle Theory

A.K. Nelson [C, S]

Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN, U.S.A.
alyssa.k.nelson@vanderbilt.edu

Y.V. Kalyuzhnyi and T. Patsahan
Institute for Condensed Matter Physics NASU, Lviv, Ukraine

C.M. McCabe
Department of Chemical and Biomolecular Engineering, Vanderbilt University, Nashville, TN, U.S.A.

Confined fluid properties are notably different from bulk fluid properties. Therefore, a simple analytical theory for the thermodynamic properties of a multicomponent liquid mixture adsorbed in a random porous media is proposed.[1] The mixture is modeled by an n-component fluid of hard-sphere Morse (HSM) particles and the media is represented by the matrix of HSM obstacles randomly distributed in a configuration of HS fluid quenched at equilibrium. We combine scaled particle theory (SPT)[2] and the corresponding version of the second-order Barker-Henderson (BH2) perturbation theory[3] to describe the thermodynamics of the system. To assess the accuracy of the theory, Monte Carlo computer simulations are performed to determine the structure of the corresponding reference system and the chemical potential of the HSM liquid confined in a random HSM matrix. Based on agreement between the theoretical predictions and Monte Carlo simulation data, the structure of the reference system is shown to be accurately predicted using radial distribution functions of the n+1-component hard-sphere mixture with the n component representing the fluid and the one component representing the matrix obstacles. Theoretical predictions for the chemical potential are also in a very good agreement for the model for systems with weak fluid-matrix attractive interactions, though slight deviations are observed as the strength of the fluid-matrix attraction and/or matrix density is increased. With minimal adjustment of the HSM potential, the phase behavior of the Lennard-Jones and square-well fluids adsorbed in the matrix are also described. Due to its simplicity, the theory could be used in a number of applications to predict the properties of simple fluid mixtures with any number of components adsorbed in the porous media.

References:

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