Phase Equilibrium and Interface Properties in Binary Mixtures: Molecular Dynamics and Density Gradient Theory Predictions

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In spite of the practical importance of precise knowledge of phase equilibria and interface properties for several applications, there are a limited number of techniques available to simultaneously describe both with the same level of accuracy.

We present here phase equilibria and interface properties as obtained by Molecular Dynamics (MD) simulations and predictions from the soft-SAFT equation combined with Density Gradient Theory (DGT) for the same systems. This is part of an on-going project aimed to advance in the understanding of the relationship between phase and interface properties [1]. For this purpose we use the Global Phase Diagram (GPD) of binary Lennard-Jones (LJ) mixtures, in conjunction with MD simulations and DGT. The principal advantage of MD versus other simulation and theoretical approaches is that it provides not only phase and interface behavior at equilibrium conditions, but also the dynamics of the phase separation. However, MD requires intensive computational efforts, precluding its use for systematic studies of global phase and interface behaviors.

We will discuss results for some particular cases: the liquid-vapor equilibria in Types I and V mixtures, as well as a heteroazeotropic state in Types II and V. A heteroazeotropic state is characterized by three-phase equilibrium, usually liquid-liquid-vapor equilibrium. Along a three-phase line, each phase has different density until it reaches a Critical End Point. The LJ-GPD has been used to define the molecular parameters of these mixtures to allow direct comparisons between MD and DGT results. Both approaches, MD and DGT, show excellent agreement with each other regarding both phase equilibrium and interface properties in the whole temperature, pressure and concentration range. Additionally, for the conditions explored in this work, neither Type II nor V show wetting transitions.

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