

## Predicting the Behavior of Interfacial Properties of Binary Mixtures by a Molecular Modeling Approach

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The prediction of bulk and interfacial fluid behavior (e.g. phase equilibrium and interface properties) is an important topic in diverse scientific areas and several industrial applications. Its relevance is due to the fact that phase equilibria and interfacial properties are the most appropriate way to describe the homogeneous and inhomogeneous behavior of fluid mixtures at equilibrium. Although phase and interface behavior can be predicted from theoretical[1,2] and simulation[3] approaches only few works are devoted to compare both approaches under similar conditions [4-6]. The work presented here is part of an on-going project [1-2],[4],[7-8] aimed to advance in the understanding of the relationship between phase and interface properties. The work has been done in a systematic manner: we first combined the density gradient theory with a molecular-based equation of state for calculating phase and interfacial properties of model systems. The accuracy of the theoretical approach is tested versus molecular dynamic simulations for the same systems. Finally the theoretical approach is used to predict the interfacial behavior of some experimental systems of special relevance. 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 a 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. Finally, the application of these techniques to some experimental systems will be presented and discussed here.

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