

Estimation of Interfacial Tension and Density Profiles from an Equation of State

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Interfacial properties, such as surface or interfacial tension, have recently acquired a renewed interest, particularly for multicomponent mixtures, as they are relevant for a wide variety of applications: from oil and gas production to emulsions and detergents. The density profiles of the species across coexisting phases may show preferential accumulation (adsorption), and this is directly related to the interfacial profiles and tension. Among other approaches, the gradient theory is one of the most widely accepted approaches, provided the interface density profiles, as well as the influence parameters, are known or can be estimated in a robust manner. From a calculation perspective, it is in the estimation of the density profiles where the application of the method may run into several obstacles that are not always easy to overcome, such as numerical convergence problems. In a recent related work, we have already proposed an alternative theory for the calculation of multicomponent interfacial profiles. In our approach, the interfacial integration must follow a minimum-effort path that is well-defined by any rational EoS, such as the cubic EoS. This has resulted in a procedure that independently solves the interfacial density profiles of the species in a robust and efficient way. We are now presenting the application of the approach for the actual direct calculation of the interfacial tension in any general multicomponent fluid system. The approach is demonstrated with cubic and SAFT type EoS on a purely predictive mode. The ideas explored in this work are further illustrated and also confirmed by molecular simulation results. In addition, we show how different types of phase behavior, as described by the EoS, affect the interfacial tension and the corresponding density profiles.