Estimation of Multicomponent Interfacial Density Profiles from a Direct Minimization of the Free Energy Surface

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The application of the gradient theory for the estimation of surface tension has recently acquired a renewed interest, particularly for multicomponent mixtures. The application of the gradient theory for the estimation of the surface tension of mixtures is perhaps the most powerful and straightforward method, provided the interface density profiles are known or can be estimated in a robust manner. It is precisely in the estimation of the density profiles, and the associated influence parameters, where the application of the method may run into several shortcomings that are not always easy to overcome, such as numerical convergence. In this work, an alternative theory is presented which allows for the accurate calculation the interfacial density profiles directly from the Helmholtz free energy surface, greatly simplifying the application of the gradient theory to just about all type of fluid mixtures. The theory presented in this work has also been confirmed by molecular simulation (MS) results. The analysis between the MS results and the theory is also presented and discussed in this work.