Predicting Interfacial Properties using iSAFT Classical Density Functional Theory for Associative and Non-Associative Fluid Mixtures of Industrial Interest

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Knowledge regarding fluid properties in the interfacial regions is needed for better design of many industrial processes. However, compared with approaches available to handle homogeneous/bulk fluids, the modeling of inhomogeneous fluids is still challenging. To bridge the gap between the knowledge of bulk regions and interfacial regions, a new version of classical density functional theory (DFT) based on interfacial Statistical Associating Fluid Theory (iSAFT) was developed. The new iSAFT DFT formalism reduces to Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) in the bulk region and does not need additional model parameters. With already developed PC-SAFT parameters, this theoretical framework allows convenient and accurate predictions of fluid properties in both inhomogeneous and bulk regions. The approach has been applied to predict the interfacial properties of systems of great interest to natural gas industries, involving non-associative species (i.e., carbon dioxide, hydrocarbons, etc.) and associative species (i.e., water, alcohol, etc.). Good agreement with experimental data can be achieved.