Simultaneous predictions of phase and interface behavior of pure compounds and binary mixtures with the soft-SAFT + density gradient theory approach

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Although essential to the design of several processes, thermodynamics experimental data is not always available, and, in some cases, is difficult or expensive to achieve. Consequently great efforts have being made in the development of predictions tools. Of particular interest to the design, scale up and optimization of chemical processes, such as unit operations (e.g. distillation or extraction), need the knowledge of the phase and interfacial properties. Even though there are several accurate modeling methods for predicting phase behavior, the field of calculating phase and interfacial properties equally accurately remains a challenge.

In this work, we present the van der Waals Density Gradient Theory combined with a molecular-based Equation of State (soft-SAFT) in order to simultaneously predict the liquid-vapor phase behavior, interfacial tensions and interfacial profiles of some pure compounds and binary mixtures, including alkanes, alkanols, CO2 and other industrial relevant fluids. The equation can be applied to pure fluids as well as mixtures of them, with the same approach. The obtained predictions have been tested against the available experimental data and two correlations of the influence parameter as a function of the carbon number of the compounds have been proposed for the *n*-alkanes and 1-alkanols families. This empowers the method with predictive power, as the correlations allow the calculations of phase and interfacial properties of compounds belonging to these families for which no experimental data is available, in a confident manner.

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