Comparison of Surface Tension Predictions from Butler's Method and Classical Density Functional Theory Based on Statistical Associating Fluid Theory

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Gas-liquid surface tension modeling is essential to the efficient and reliable design of chemical processes. Accurate predictions of surface properties can be challenging, especially due to the presence of highly nonideal interactions (such as hydrogen bonding interactions) among molecules and nonuniform molecular distribution across the interface. In this work, we compare two of the theoretical methods, namely the Butler's method and classical density functional theory. Both models rely on Statistical Associating Fluid Theory (SAFT) in the homogenous bulk liquid and gas regions, allowing unbiased comparisons of prediction quality of surface properties.