

Determination of Interfacial Properties using a PC-SAFT Based Classical Density Functional Theory for Fluid Mixtures of Industrial Interest

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A recent development of a PC-SAFT based classical density functional theory (DFT) is applied to the determination of interfacial properties of pure fluids and mixtures of industrial interest. Initially, the DFT formalism is described and the methodology for the property calculations explained. The consistency of this approach allows the determination of interfacial properties for fluids using the PC-SAFT equation of state parameters determined from bulk physical property data, such as vapor-liquid-equilibrium and densities. This methodology is an excellent alternative for the predictions of interfacial property of fluids and extrapolation to high pressure ranges where experimental measurements becomes challenging.