Prediction of surface properties from the density gradient theory combined with equations of state

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The density gradient theory (DGT) is applied to calculate the surface properties of carbon dioxide and hydrocarbons. The only inputs of the theory are the Helmholtz energy density of the bulk homogeneous fluid and the influence parameters of the interfacial inhomogeneous fluid. Four thermodynamic models (volume-translated Peng-Robinson equation of state, the original Statistical Associating Fluid model, the Lattice Fluid model, and the Modified double lattice equation of state) are used to determine both the Helmholtz energy density and the bulk properties. The influence parameters are adjusted for each system by a linear temperature dependent function. The approach is able to accurately describe the surface tensions of pure systems as compared with available experimental data. The vapor-liquid equilibrium (VLE) phase behaviors of each fluid are also described in this work.