172f Generalized Svrc-Qspr Predictions of Interfacial Tensions

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Accurate prediction of interfacial tensions (IFT) is important in many industrial applications, including enhanced oil recovery (EOR) processes where the relative magnitude of interfacial (capillary), gravitational and viscous forces considerably affects the recovery of oil. Current models for predicting the interfacial tensions have a limited range of applicability and poor suitability for generalization.

In this work, we develop non-linear Quantitative-Structure-Property Relationships (QSPR) for predicting the input parameters for the Scaled-Variable-Reduced-Coordinate (SVRC) framework, which provides reliable predictions for pure-fluid IFT over the entire saturation range (triple to critical point). Specifically, we (a) demonstrate the efficacy of the SVRC in providing accurate IFT predictions of diverse molecular species using QSPR parameter generalizations, and (b) explore significant molecular descriptors which are pertinent in modeling IFT of pure fluids.

In general, the SVRC-QSPR model is capable of predicting the pure-fluid saturation properties considered with average errors of less than 1%.