Vapor-Liquid and Liquid-Liquid Phase Equilibria and Interfacial Properties of Tetrahydrofuran + Methane Binary Mixtures from Experiments, Simulation, and Theory

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Tetrahydrofuran, or simply THF, is one of the most known and used thermodynamic hydrate promoters (THP) since many years. In particular, THF is able to reduce the equilibrium pressure dramatically and it makes it possible to treat gas hydrates under mild pressure conditions. From a theoretical modelling point of view, computer simulation offers insight into atomic level phenomena that are not observable from an experimental point of view. This provides unique and invaluable information about the underlying physicochemical principles governing hydrate behaviour, including thermodynamic properties, phase equilibria, and interfacial properties, among many others. This work is a preliminary study to predict the phase equilibrium of THF hydrates and hydrates of mixtures of THF with methane using molecular dynamics simulation and the SAFT formalism. In addition to that, experimental measurements are also made in order to validate our simulation results and theoretical predictions. Since fluid-fluid interfacial properties, and particularly surface tension, are particularly sensitive to subtle differences in molecular details, we studied the capability of two different molecular models of THF to predict the interfacial behaviour of the system. In this work, we determine the vapour-liquid and liquid-liquid phase equilibria and interfacial properties of the tetrahydrofuran + methane binary mixture at different thermodynamic conditions. THF is modelled following the united-atom approach. We use different models and perform molecular dynamics simulations in the canonical ensemble to determine the most representative vapour-liquid and liquid-liquid interfacial properties, including the interfacial tension, density profiles, coexistence phase diagrams, and interfacial thickness as functions of pressure. Theoretical predictions obtained from molecular dynamics simulation are compared with predictions from the Statistical Associating Theory for potentials of Variable Range (SAFT-VR) and experimental data.