Equilibrium and Interfacial Properties of Water + Alkanes: Measurements and Modeling

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Despite the considerable amount of data now available for the phase equilibria of systems containing water and organic phases, their liquid-liquid interfaces have received little quantitative attention. Most of the published results are related with the vapor-liquid interface and liquid-liquid interfacial tension data are particularly reduced.

An interesting approach for modeling interfacial tensions is the gradient theory of fluid interfaces. Due to some mathematical difficulties its application to real systems is particularly recent. This model is based on the correct description of the phase equilibria of the fluid phases separated by the interface. Since it incorporates an equation of state, that uses to calculate Helmholtz free energy densities, chemical potentials and equilibrium phase densities, it allows for the simultaneous modeling of phase equilibria and interfacial tensions of the system under study.

Recently a new equation of state (CPA – Cubic-plus-Association) that combines the characteristics of cubic equations of state with a Wertheim association term appeared in literature, thus allowing for the correct modeling of mixtures containing both associative and non-associative components distributed on different fluid phases. Results for water + n-alkanes have shown its good performance and opened its application for more complex systems such as water hydrocarbons.

This work aims at increasing the amount of available liquid-liquid interfacial tensions as well as their modeling. Interfacial tensions of water alkanes were measured in the temperature range 283.15 – 343.15 K using a NIMA DST 9005 tensiometer based on the Du Nouy ring method. A combination of the gradient theory of fluid interfaces with the CPA equation of state will be used for the simultaneous modeling of the phase equilibria and interfacial tensions of the reported measurements and other collected from the literature.

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