

Modelling the Liquid Phase Behaviour of Aqueous Non-Ionic Amphiphilic Mixtures in the Presence of Oil and Salt Modelled with SAFT-VRE

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The liquid phase behaviour of aqueous alkylpolyoxyethylene (CiEj) non-ionic amphiphilic mixtures is of great interest in many industrial processes. We propose a model for these mixtures with the SAFT-VR framework and study the coexistence properties of these systems in the presence of oil and salt. The surfactant is modelled with additional short-range attractive interaction sites which allow the explicit treatment of hydrogen bonding between the water and surfactant molecules. A transferable model for different sized CiEj amphiphiles is presented which reproduces the region of liquid-liquid immiscibility of the solutions. We introduce an n-alkane model to study the complex three component (water + amphiphile + oil) phase behaviour which under certain conditions can exhibit three coexisting liquid phases. We describe the liquid phase behaviour of these systems at ambient pressure and different temperatures where predictions for the high pressure regions are given. The influence of strong electrolytes on the phase behaviour of these systems is studied with the SAFT-VRE approach which incorporates additional terms for the long-range Coulombic interaction and the solvation energies of the ions. The Coulombic forces are modelled with the mean spherical approximation in the primitive model. The solvation energies of the ions are modelled with an expression derived by Born (1920) where the cavity formed by the ion rather than the ion size is treated. The dielectric constant of these systems which appears in the Coulombic and the Born terms has a crucial effect on the phase behaviour of electrolyte systems and we fit the dielectric to experimental data. We study the phase behaviour of water + amphiphile + salt where salting out is predicted in agreement with experimental data.