Modeling the Liquid-liquid Equilibria of Water + Perfluorocarbons with the Cubic-Plus-Association Equation of State

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Perfluorocarbons (PFCs) are non-polar, highly fluorinated molecules that due to their strong intramolecular and weak intermolecular forces possess chemical and biochemical inertness and atypical physico-chemical properties, leading to numerous applications.

PFCs, among other fluorocarbons, have shown to be attractive substitutes for chlorinated solvents, effective surfactants in supercritical extraction and found widespread use in biomedical applications such as tissue oxygenation fluids (blood substitutes), anti-tumural agents, perfusates for isolated organs, gas-carriers in eye surgery, diagnostic imaging agents and drug delivery systems.

Since a considerable number of PFCs applications involve the contact with aqueous solutions, mutual solubilities of water and PFCs are important. Namely, the solubilities of PFCs in water and aqueous salt solutions have a particular interest as these determine their fate in the body and the environment; help to understand the aging mechanisms of PFC emulsions used as blood substitutes and are involved in the technology of drug delivery systems and cell culture media.

Some recent measurements on the water solubility of PFC's are now available, but there is still a considerable lack of data for the solubility of PFC's in water.

Among the different models able to deal with the phase equilibria of aqueous systems, associating equations of state, such as the different versions of the statistical associating fluid theory (SAFT) and the cubic plus association equation of state (CPA) have provided interesting results.

In this work, the CPA equation of state is used for modeling the liquid-liquid equilibria of PFC's water. A discussion on the selection of pure component parameters is presented, as well as some pure component results for the vapor pressure and equilibrium densities are reported. Liquid-liquid equilibria results are reported for several linear, cyclic, aromatic and substituted PFC's.

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