Phase Equilibrium Modeling of Intra- and Inter-molecular Hydrogen-Bonding Ethylene Glycols Mixed with Nonpolar Solvents

J.H. Lee[S] and C.S. Lee[C]
Department of Chemical and Biological Engineering, Korea University, Sungbuk-Ku, Seoul, Korea
cslee@korea.ac.kr

Vapor-liquid equilibrium properties of ethylene glycol oligomers and poly (ethyleneglycol) (PEG) mixed with nonpolar solvents, such as carbon dioxide, methane, propane, hexane, benzene, and cyclohexane, were modeled. Ethylene glycol and di-ethylene glycol are known to form ring-type intra-molecular hydrogen bonds, while other glycols form intra-bonds between hydroxyl end groups and internal ether groups. They also participate in inter-molecular hydrogen bonding. The recently developed hydrogen-bonding lattice fluid model with internal bonds was applied to model these mixtures. The pure component parameters segment number and segment interaction energy parameter were fitted to vapor pressure and saturated liquid density for sub-critical components, and to PV isotherms for super-critical components. Association parameters for intra- and inter-bonds were obtained from FTIR bonded fraction data of alkoxy alcohols, which share similar hydroxyl end groups and internal ether groups, in non-polar solvents. Inclusion of the intra bonding effect in the model was found to generally improve the agreement with data for PEG mixtures with one binary interaction parameter, compared to models without intra-bonding contributions. For ethylene glycol oligomer mixtures, a large change in the intra-bonding entropy was found to give better fitting without inducing liquid phase instability, which experimental data is expected to indicate.