Modelling of phase equilibria of glycol ethers mixtures using an association model

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Vapor-liquid and liquid-liquid equilibria of glycol ethers (surfactant) mixtures with hydrocarbons, polar compounds and water are calculated using an association model, the Cubic-Plus-Association Equation of State. Parameters are estimated for several non-ionic surfactants of the polyoxyethylene type but mixture calculations are mostly presented for three compounds for which many data are available (2-methoxyethanol, 2-ethoxyethanol and 2-butoxyethanol). The way pure compound vapor pressures and liquid densities are estimated, and the way parameter trends against the van der Waals volume, Kamlet-Taft parameters and, perhaps most importantly, mixture liquid-liquid equilibria data with alkanes are used for choosing optimum parameter sets is illustrated. Vapor-liquid, liquid-liquid equilibria and second virial coefficient data are used for model validation, including aqueous and other cross-associating mixtures. The influence on the results of the association schemes, type of data available, combining rules for cross-associating mixtures and interaction parameters are discussed also in connection to other cross-associating mixtures, previously studied with the model. Finally, the capabilities and limitations of the Cubic-Plus-Association Equation of State in representing this type of multi-functional chemicals, glycol ethers, are discussed. (C) 2008 Elsevier B.V. All rights reserved.

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