Water Solubility in N-Alkanes and Ethanol Mixtures for LLE Conditions Using the Polar GC-PC-SAFT EoS

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No consensus exists at this point on how to treat water with the polar GC-SAFT equation of state (Eos). Several authors have proposed methods for evaluating high pressure and high temperature phase envelopes of water containing mixtures [1-3]. Yet, none of them managed to determine correctly both solubilities (water in hydrocarbon and hydrocarbon in water). As a matter of fact, it has been shown that among the associating models, SAFT is not recommended for describing these two solubilities simulatenously [4, 5]. Recently, it has been shown how the number of parameters involved in the SAFT theories make it very difficult to identify unambiguously the parameters of a complex molecule such as water [6]. In this work, we have further investigated this issue, by including other type of data, as virial coefficients, or information concerning hydrogen bonding, and discussing the physical significance of the association parameters. This first investigation has led us to identify two sets of parameters that are further used for phase equilibrium calculations with alkanes, whose parameters are determined using Tamouza's group contribution method [7]. Both vapour-liquid as liquid-liquid equilibria are shown, and, using one set of parameters, can be predicted without binary interaction parameters. In mixture with ethanol, described according to NguyenHuynh et al. [8], cross-association is encountered. The cross-association combining rules are determined without interaction coefficients, and the ternary alkane-ethanol-water liquid-liquid system is predicted using an extrapolation for the ethanol-alkane binary interaction coefficient.

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