Application of PC-SAFT to glycol containing systems - PC-SAFT towards a predictive approach

For equations of state of the SAFT type a major limitation is the procedure of obtaining pure compound parameters using saturated vapor pressure and liquid density data. However, for complex compounds such data are often not available. One solution is to develop a group contribution scheme for estimating pure compound parameters from low molecular weight data and extrapolate to complex compounds. For associating compounds this is not trivial since the two parameters for association (association energy and association volume) need to be fixed for a group. In this work, which focuses on glycols, new general pure compound parameters were obtained for PC-SAFT which are able to perform well for both vapor-liquid equilibria (VLE) and liquid-liquid equilibria (LLE). Linear trends of non-association parameters were obtained with respect to the molar mass. However, identical values for the association parameters were used for all glycol oligomers. This makes it possible to predict the pure compound parameters of other oligomers. With the new estimated parameters the simplified PC-SAFT equation of state has been applied for correlation and prediction of VLE and LLE in mixtures containing glycol oligomers + water, hydrocarbons, aromatic hydrocarbon, methane, N-2 and CO2. To improve correlations for mixtures containing glycol and aromatic hydrocarbons solvation was explicitly accounted for. (C) 2007 Elsevier B.V. All rights reserved.