The role of monomer fraction data in association theories—Can we improve the performance for phase equilibrium calculations? - DTU Orbit (06/12/2018)

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Monomer fraction (fraction of non-hydrogen bonded molecules) data obtained from spectroscopy are available for a few associating compounds. Such data can be used for testing the performance of association models like CPA and SAFT or alternatively be employed in the model development. But how accurate and how useful are such data today and how successful is their use in the context of association models? In this work we attempt to answer these questions in the case of the CPA model and for ethanol. CPA has been already successfully used to describe thermodynamic properties of many ethanol containing mixtures, using an ethanol parameter set that was adjusted to experimental vapor pressure and liquid density data. We present in this work a new parameter set for ethanol which is estimated using experimental vapor pressure, liquid density data as well as the experimental monomer fractions for liquid ethanol. Using both the existing ("old") and the new parameter sets, we perform an extensive comparison of CPA results for a wide range of ethanol-containing systems, with water and alkanes as well as multicomponent water–ethanol–hydrocarbon liquid–liquid equilibria and hydrate curves with different ethanol content as inhibitor. There are some differences in the performance of CPA with the two sets but on average the results are similar. This may indicate that monomer fraction data are not very useful in this case or that ethanol monomer fraction data are not accurate and both possibilities are discussed.

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