Modelling of associating mixtures for applications in the oil & gas and chemical industries - DTU Orbit (09/12/2018)

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Thermodynamic properties and phase equilibria of associating mixtures cannot often be satisfactorily modelled using conventional models such as cubic equations of state. CPA (cubic-plus-association) is an equation of state (EoS), which combines the SRK EoS with the association term of SAFT. For non-polar (non self-associating) compounds it reduces to SRK. The model was first published in 1996 and since then it has been developed and applied with success to binary systems containing water-alkanes and alcohol/glycol/acid-alkanes (both VLE and LLE) as well as ternary and multicomponent (V)LLE for water-alcohol (glycol)-alkanes and certain acid and amine-containing mixtures. Recent results include glycol-aromatic hydrocarbons including multiphase, multicomponent equilibria and gas hydrate calculations in combination with the van der Waals-Platteeuw model. This article will outline some new applications of the model of relevance to the petroleum and chemical industries: high pressure vapor-liquid and liquid-liquid equilibrium in alcohol-containing mixtures, mixtures with gas hydrate inhibitors and mixtures with polar and hydrogen bonding chemicals including organic acids. Some comparisons with conventional thermodynamic models especially those combining cubic EoS with local composition activity coefficient models are included. (C) 2007 Elsevier B.V. All rights reserved.