

## Modelling phase equilibria for acid gas mixtures using the CPA equation of state. Part VI. Multicomponent mixtures with glycols relevant to oil and gas and to liquid or supercritical CO<sub>2</sub> transport applications - DTU Orbit (08/11/2017)

### Modelling phase equilibria for acid gas mixtures using the CPA equation of state. Part VI. Multicomponent mixtures with glycols relevant to oil and gas and to liquid or supercritical CO<sub>2</sub> transport applications

In this work the Cubic Plus Association (CPA) equation of state is applied to multicomponent mixtures containing CO<sub>2</sub> with alkanes, water, and glycols. Various modelling approaches are used i.e. different association schemes for pure CO<sub>2</sub> (assuming that it is a non-associating compound, or that it is a self-associating fluid with two, three or four association sites) and different possibilities for modelling mixtures of CO<sub>2</sub> with other hydrogen bonding fluids (only use of one interaction parameter  $k_{ij}$  or assuming cross association interactions and obtaining the relevant parameters either via a combining rule or using an experimental value for the cross association energy). Initially, new binary interaction parameters were estimated for (CO<sub>2</sub> + glycol) binary mixtures. Having the binary parameters from the binary systems, the model was applied in a predictive way (i.e. no parameters were adjusted to data on ternary and multicomponent mixtures) to model the phase behaviour of ternary and quaternary systems with CO<sub>2</sub> and glycols. It is concluded that CPA performs satisfactorily for most multicomponent systems considered. Some differences between the various modelling approaches are observed. This work is the last part of a series of studies, which aim to arrive in a single "engineering approach" for applying CPA to acid gas mixtures, without introducing significant changes to the model. An overall assessment, based also on the obtained results of this series (Tsivintzelis et al., 2010, 2011, 2014, 2015, 2015), which is based on an investigation of about 30 multicomponent systems containing acid gases, water, alcohols, glycols and hydrocarbons, reveals that assuming cross association (solvation) of CO<sub>2</sub> with glycols, alcohols and water or alternatively considering CO<sub>2</sub> to be a self-associating molecule (with three or four sites) are the better approaches which perform similarly and quite satisfactorily. However, the use of the former one (solvation), using whenever possible experimental values for the cross association energy, in all cases is recommended.

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