Application of the cubic-plus-association equation of state to mixtures with polar chemicals and high pressures - DTU Orbit (07/02/2019)

**Application of the cubic-plus-association equation of state to mixtures with polar chemicals and high pressures**

The cubic-plus-association (CPA) equation of state has been previously applied to vapor-liquid, liquid-liquid, and solid-liquid equilibria of mixtures containing associating compounds (water, alcohols, glycols, acids, amines). Although some high-pressure applications have been presented, emphasis was given to low pressures and liquid-liquid equilibria. In this work, CPA is applied to two classes of mixtures containing polar chemicals for which high-pressure data are available: acetone-containing systems and dimethyl ether mixtures. They are of both scientific and industrial importance. Moreover, CPA is applied to high-pressure solid-liquid equilibria (SLE) for alcohol-alkane mixtures. In the case of acetone-hydrocarbon mixtures, satisfactory results are achieved if acetone is allowed to self-associate. Satisfactory high-pressure acetone-water vapor-liquid equilibrium (VLE) is obtained, comparable to conventional models such as MHV2. Very good results are also obtained for multicomponent vapor-liquid-liquid equilibria for mixtures containing gases, water, and dimethyl ether. Finally, it is shown that high-pressure SLE can be predicted based on interaction parameters obtained from low-pressure SLE data.

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