Ten years with the CPA (Cubic-Plus-Association) equation of state. Part 1. Pure compounds and self-associating systems - DTU Orbit (01/12/2018)

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CPA (Cubic-Plus-Association) is an equation of state that is based on a combination of the Soave-Redlich-Kwong (SRK) equation with the association term of the Wertheim theory. The development of CPA started in 1995 as a research project funded by Shell (Amsterdam), and the model was first published in 1996. Since then, it has been successfully applied to a variety of complex phase equilibria, including mixtures containing alcohols, glycols, organic acids, water, and hydrocarbons. Focus has been placed on cases of industrial importance, e.g., systems with gas-hydrate inhibitors (methanol, glycols), glycol regeneration and gas dehydra-tion units, oxygenate additives in gasoline, alcohol separation, etc. This manuscript, which is the first of a series of two papers, offers a review of previous applications and illustrates current focus areas related to the estimation of pure compound parameters, alcohol-hydrocarbon vapor-liquid equilibria (VLE) and solid-liquid equilibria (SLE), as well as aqueous systems. The capabilities and limitations of CPA are discussed and suggestions for extension of the model to systems not covered in this work are provided.

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