A Crossover CPA Equation of State for Associating Fluids

XinHao Xu [S] and YuanYuan Duan [C]
Key Laboratory for Thermal Science and Power Engineering of Ministry of Education, Tsinghua University, Beijing, China

Fluids containing associating molecules are always of great interest from an industrial point and their thermophysical properties are needed for many practical applications. A very large number of association equations of state have been proposed in the literature. The Cubic-Plus-Association (CPA) equation of state is one of the successful examples. It is first proposed by Kontogeorgis *et al*. in 1996, based on a combination of the Soave-Redlich-Kwong (SRK) equation of state with the association term of the Wertheim theory. In the past twelve years, the CPA equation is widely applied to the systems that contain associating compounds, including alcohols, glycols, organic acids, water, and so on. However, as all other equations from mean field theories, this equation does not take into account the effect of long scale density fluctuations near the critical point, which makes it fail to reproduce the non-analytical, singular behavior in the critical region. To overcome this limitation, a crossover treatment is made to the CPA equation based on the renormalization group (RG) theory in this work. The results of the modified equation show good agreement with the experiment data. The crossover CPA equation is also compared with the original CPA equation and other crossover equations in this work.