An Efficient Polar Cubic Equation of State for Predictive Modeling of Phase Behavior and Critical Phenomena of Mixtures

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Abstract

A polar cubic equation of state (EOS) is developed by incorporating the dipolar theory of Jog and Chapman into the Soave-Redlich-Kwong (SRK) EOS. We propose simplifying assumptions in the dipolar term of Jog and Chapman to reduce the double and triple sums in the theory to single sums. The simplified version of the dipolar theory can significantly improve computational speed and can be used with either Cubic EOS or SAFT-based EOS. The proposed model, which we here call polar-SRK (P-SRK), is parametrized in a similar fashion to classical cubic EOS to exactly reproduce T_ci,P_ci,ω_i, and will self-consistently reduce to the base SRK EOS in the absence of polar interactions. Binary VLE data with a non-polar reference hydrocarbon is used to extract the polarity of the respective functional group. The model shows superior performance in capturing the phase behavior of polar mixtures compared to the base SRK.

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