Equation of State and Phase Separation in Binary Mixtures of Nonadditive Chains.

Abu-Sharkh, Basel F.

Department of Chemical Engineering, King Fahd University of Petroleum Minerals, Dhahran, Saudi Arabia.

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Abstract

Mol. dynamics simulations of equimolar mixts. of hard chains composed of equal size nonadditive segments were performed. Different ds.p., densities, and nonadditivities were used. Phase sepn. was investigated and visualized. The equation of state for these mixts. was investigated, and models based on the first order thermodn. perturbation theory (TPT1) and the polymeric analog of the Percus-Yevick approxn. (PPY) were developed to predict the compressibility factor of the polymer mixts. The TPT1 model was generally more accurate in predicting the compressibility factor than the PPY model for neg. and zero nonadditivity. Phase sepn. between polymers interacting with pos. nonadditivity was obsd. at high densities.