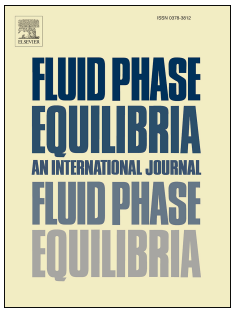

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Predicting phase equilibrium for polymer solutions using COSMO-SAC

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Abstract

With the aim of predicting mixture behavior based on information of pure components only, COSMO-based models have emerged as a promising alternative. Several works in the literature are available attesting the good performance of COSMO-RS variants in several different applications. However, the extension of COSMO calculations for polymers and other macromolecules was not extensively explored. In this work, a new procedure to evaluate the parameters of the polymers repeating unit for COSMO-based models is proposed. The idea of a large polymer molecule consisting of many repeating units is employed, however, a more comprehensive analysis using oligomers of different sizes is suggested. The COSMO-SAC model with parameters from the literature was used to test the new methodology. Infinite dilution activity coefficient (IDAC) and vapor-liquid equilibrium (VLE) calculations with homopolymer and copolymer systems were performed to verify the predictive capability of the approach. The good results obtained showed the adequacy of the proposed methodology to represent IDAC and VLE data of solvent-polymer and -copylymer systems.

Keywords: COSMO-based models, polymer solution, VLE equilibrium, IDAC data

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