A predictive group-contribution simplified PC-SAFT equation of state: Application to polymer systems

A group-contribution (GC) method is coupled with the molecular-based perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state (EoS) to predict its characteristic pure compound parameters. The estimation of group contributions for the parameters is based on a parameter database of 400 low-molecular-weight compounds estimated by fitting experimental vapor pressures and liquid densities. The method has been successfully used for estimating the PC-SAFT parameters for common polymers. Specifically, using the new polymer parameters as calculated from the proposed GC scheme, the simplified PC-SAFT yields rather good predictions of polymer densities and gives promising modeling results of various binary polymer mixtures exhibiting both vapor-liquid and liquid-liquid phase equilibria. In summary, the data required for calculating polymer phase equilibria with the proposed method are the molecular structure of the polymer of interest in terms of functional groups and a single binary interaction parameter for accurate mixture calculations.

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Contributors: Tihic, A., Kontogeorgis, G., von Solms, N., Michelsen, M. L., Constantinou, L.
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