Modeling VLE of H_2 + Hydrocarbon Mixtures Using a Group Contribution SAFT (GC -SAFT) with a K_{Ij} Correlation Method Based on London's Theory

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A group contribution PC-SAFT equation of state (GC-PC-SAFT) (Tamouza *et al.*, *Fluid Phase Equilibria*, 2004, *222-223*, 67-76)) combined with a recent method for correlating k_{ij} using only pure compound parameters (NguyenHuynh *et al.*, *Ind. Eng. Chem. Res.*, 2008. ***47****(22)*, 8847-8858), is extended here to model vapor-liquid phase equilibria of H_2 + alkanes and H_2 + aromatics mixtures. The correlation of k_{ij}s is inspired by the London's theory of dispersive interactions, and use 'pseudo-ionization energies' J_i and J_j of compounds i and j as adjustable parameters.
In order to make up for the lack of data, additional hydrogen + aromatic VLE data were calculated using a Monte Carlo Molecular Simulation. The GC-PC-SAFT parameters for alkanes and aromatics were re-used from previous works when available. Otherwise, the missing parameters were estimated by regression of corresponding pure VLE data. Those of H_2 were determined in this work by correlating some VLE data of H_2 + n-alkane systems. Using the parameters thus obtained, the phase envelopes of other H_2 + alkane and H_2 + aromatic systems were fully predicted. The prediction tests were as comprehensive as possible. Correlation and predictions are qualitatively and quantitatively satisfactory. The deviations are within 5-6 % i.e. comparable to those obtained on previously investigated systems. Mixtures containing H_2 are modeled here with deviations that compare well with those of the Grayson-Streed model.