Application of the Group Contribution SAFT (GC-SAFT) equation of state to polyaromatic hydrocarbons

M. Benamira, J.P. Passarello,[C] and P. Tobaly
LIMHP, Université Paris Nord, Villetaneuse, France
Passarel@limhp.univ-paris13.fr

J.C. de Hemptinne[S]
Institut Francais du Petrole, Rueil Malmaison Cedex, France

The group contribution method for pure compound parameters proposed by S. Tamouza *et al.* is extended for the calculation of vapor pressures and saturated liquid volumes of polyaromatic hydrocarbons. It has been tested successfully with two versions of the statistical associating fluid theory (SAFT) equation of state: PC-SAFT and SAFT-VR.

The group contribution method consists of calculating the equation of state parameters (m, ε, σ, and λ) using group contribution rules. A quadrupolar contribution was found useful.

The method is used for the prediction of polyaromatic phase equilibrium properties, including that of branched components and mixtures containing such components. The tests were limited, due to a lack of experimental data.