

Development of Equation of State based on NIST-modified UNIFAC

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New group-contribution interaction parameters for equation of state based on NIST-modified UNIFAC were reported. The proposed model is combination of Peng-Robinson equation state and Universal Mixing Rule (UMR) proposed by Voutsas and co-workers. Interaction parameters were regressed using critically evaluated vapour-liquid equilibrium (VLE), liquid-liquid equilibrium (LLE) solid-liquid equilibrium (SLE), excess enthalpy (HE), infinite dilution activity coefficient (AINF) and excess heat capacity (CPE) data. This work is a further extension of NIST-modified UNIFAC to high pressure application and consistent with previous publication on low-pressure phase equilibria. The algorithmic framework for quality assessment of phase equilibrium data was applied for qualifying the consistency of data and screening of possible erroneous data. Parameters matrix involves 14 gaseous components and 96 main groups for NIST-modified UNIFAC.