

A New Method for Evaluation of UNIFAC Interaction Parameters

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A new method for obtaining UNIFAC group–group interaction parameters is proposed using evaluated thermophysical property data generated at the Thermodynamics Research Center (TRC) of the National Institute of Standards and Technology (NIST). Using the proposed method, two sets of UNIFAC group–group interaction parameters (original UNIFAC and KT–UNFAC) for 52 main groups are produced based on vapor–liquid equilibrium (VLE), excess enthalpy, and infinite dilution activity coefficients data critically evaluated on–demand by the NIST ThermoData Engine (TDE) software. New regression analysis method includes the use of evaluated uncertainties in measured/calculated variables and assessment of quality factors evaluated on a basis of the variety of the consistency tests for VLE data. Validity and effectiveness of the proposed method are discussed.