Introduction of New COSMO-SAC Parameters for Prediction of Solid-Liquid Equilibria Containing Carboxylic Acid

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Carboxylic acids are important chemical raw material used in the production of polymers, pharmaceuticals, food additives. Due to many carboxylic acids exist as a solid form in ambient condition, solid-liquid equilibria (SLE) of a solid carboxylic acid is one of the most important properties in the field of industry. Prediction of SLE of carboxylic acids is difficult because of the formation of dimer between acidic hydrogen and carbonyl oxygen in carboxylic acid and insufficient experimental data. COSMO-SAC is an interesting approach to predict thermodynamic properties without sufficient experimental data.   In this study, the new parameters of COSMO-SAC (2017) were introduced for describing the association of carboxylic acid. The molecular segments were categorized into four groups: NHB (non-hydrogen bonding group), COOH (carboxylic acid group), OH (hydroxyl group), OT (all other hydrogen bonding group). From the result, the prediction of VLE and LLE is similar and SLE is more accurate compared with original COSMO-SAC (2017). The result shows COSMO-SAC can be improved for prediction of VLE, LLE, and SLE containing carboxylic acid.