From Generalized Langmuir Isotherm to Mixed-gas Adsorption Equilibria

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This work presents a thermodynamically consistent modeling approach to estimate mixed-gas adsorption equilibria from pure gas adsorption isotherms. Incorporating the Adsorption Nonrandom Two-Liquid activity coefficient model for the adsorbate phase, the proposed generalized Langmuir model assumes constant adsorbent surface areas and considers adsorbate-adsorbent contact areas in the activity coefficient calculations for monolayer adsorption. The resulting model properly captures adsorbate composition dependency, temperature dependency, and surface loading dependency for mixed gas adsorption equilibria. The model is validated with an accurate representation of adsorption equilibrium data for multiple pure gas, binary, ternary, and quaternary mixed-gas systems. The model results are further compared with those calculated from Ideal Adsorbed Solution Theory and extended Langmuir model.