An adsorption equilibria model for steady state analysis

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The investigation of adsorption isotherms is a prime factor in the ongoing development of adsorption cycles for a spectrum of advanced, thermally-driven engineering applications, including refrigeration, natural gas storage, and desalination processes. In this work, a novel semi-empirical mathematical model has been derived that significantly enhances the prediction of the steady state uptake in adsorbent surfaces. This model, a combination of classical Langmuir and a novel modern adsorption isotherm equation, allows for a higher degree of regression of both energetically homogenous and heterogeneous adsorbent surfaces compared to several isolated classical and modern isotherm models, and has the ability to regress isotherms for all six types under the IUPAC classification. Using a unified thermodynamic framework, a single asymmetrical energy distribution function (EDF) has also been proposed that directly relates the mathematical model to the adsorption isotherm types. This fits well with the statistical rate theory approach and offers mechanistic insights into adsorption isotherms.