Adsorption Model for Offset Data and Its Application Toward IAST

가성빈, 이재형†
KAIST
(jayhlee@kaist.ac.kr†)

Although many isotherm data have been reported, an isotherm model covering the S-shaped isotherm with offsets is yet to be available. The absence of such a model hinders the evaluation of many potentially promising adsorbents. Motivated by this, this work suggests a new model for S-shaped isotherm data with offset points for adsorbents. Furthermore, to resolve the problem that available isotherm information from experiments are mostly about pure components, this work extends pure isotherm information into that of mixtures by deriving the spreading pressure of the suggested isotherm model. This concept can be used with ideal adsorption solution theory (IAST) for mixture systems. By deriving the spreading pressure analytically, the computational cost reduction is also achieved. During this computation, moreover, the implicit structure of the IAST equations leads to a significant computational cost as well as divergence problems. To remove the implicit structure, a simple machine learning method is employed to create a neural network, which replaces some of the costly iterative computation paths.