

STUDY ON THE DETERMINATION OF OPTIMIZED ADSORPTION ISOTHERM MODELS EMPLOYING ADVANCED STATISTICAL METHODS

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Name

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Title ISOTHERM MODELS EMPLOYING ADVANCED STATISTICAL
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論文内容の要旨

Thesis Summary

The prospect for adsorption technology over conventional systems is increasingly growing in different energy conversion applications. The main reasons are the suitability to utilize low-temperature heat sources (solar heat or waste heat) and environmentally benign working fluids (NH₃, H₂O, CO₂, and so on). Adsorption technology has a vast range of applications such as adsorption heat pump (AHP), water production & treatment, air conditioning & thermal comfort, thermal energy storage, gas separation, gas storage, desalination, heavy metal or liquid removal, CO₂ capture, recovery of chemicals from industrial and vent gases. In the case of AHP, it is strongly considered an alternative solution to the conventional mechanical vapor compression-based system regarding energy consumption and environmental concerns. The traditional vapor compression system uses an enormous amount of energy, and the refrigerants (HCFCs, HFCs) used in this system increase the risk for global warming and ozone depletion potential. However, AHP is powered by low-temperature waste heat and uses natural refrigerants such as water, ethanol, carbon dioxide, and ammonia as the working fluid. Additionally, the AHP has 80 to 90 percent lower energy consumption than the conventional cooling systems, and the lifespan is about twice as long. Another significant application of adsorption technology is the removal of hazardous materials from aqueous solutions. The massive earthquake and the subsequent tsunami in Japan on 11 March 2011 delivered substantial damage to the Fukushima Daiichi Nuclear Power Plant. As a result, large amounts of radioactive contaminants entered the groundwater, seawater, and the surrounding soil. These harmful compounds could be efficiently removed by employing adsorption-based removal technology. Therefore, the study of the adsorption process has attracted considerable attention from contemporary researchers.

The adsorption isotherm is the most significant aspect to describe the adsorption process. However, the experimental measurement of isotherms for all possible conditions is not feasible. Hence, researchers propose suitable mathematical models based on the available experimental data. An isotherm model provides a set of reliable fitting parameters, which can predict the accurate isotherm data for the conditions that were not experimentally measured. Over the years, numerous adsorption isotherm models are introduced in the literature. Hence, researchers encounter difficulties in selecting the appropriate isotherm model among the available models.

This thesis's main objective is to find out optimal models for adsorption isotherms based on advanced statistical analysis, which will help design efficient adsorption-based systems.

In the beginning, the two most popular adsorbent/adsorbate pairs, Maxsorb III/ethanol and silica gel/water, were considered. This research adopted five error evaluation functions in various study areas to find the optimum error function for a specific isotherm model. Six popular isotherm models, namely Freundlich, Langmuir, Dubinin-Astakhov (D-A), Tóth, Redlich-Peterson, and Hill, have been fitted with the experimental data of these two pairs using a generalized reduced gradient (GRG) non-linear optimization method. A Sum of normalized error (SNE) has been introduced for the first time in this study to find the optimum error evaluation function for each isotherm model. It is observed that the HYBRID error evaluation function is optimum for optimizing the parameters in the isotherm models. Statistical methods such as correlation coefficient (r), regression coefficient (R^2), two parametric tests (t -test and F -test), and two non-parametric tests (Mann-Whitney U -test, Kolmogorov-Smirnov (KS) test) identify that Tóth as an optimum model for both pairs. Finally, based on model selection criteria (AIC , BIC , AIC_c , $mAIC$, AIC_3 , $CAIC$, $ABIC$), the current study suggests that Tóth isotherm provides less information loss in both types of adsorption pairs.

There is an infinite number of adsorbent/adsorbate pairs. Hence, to generalize the proposed statistical approach for any pair, a new technique was adopted. Whatever the pair is, the isotherm shape is limited to eight types according to IUPAC. Hence, the optimum model for each IUPAC isotherm type was determined by considering fifteen extensively used adsorption isotherm models and thirteen relevant adsorption pairs. Several useful statistical approaches such as average error, confidence interval (CI), information criterion (ICs), and proportion tests using bootstrap sampling were employed. It is determined that the modified BET for Type-I(a) and Type-II, Tóth for Type-I(b), GAB for Type-III, Ng et al. for Type-IV(a) and Type IV(b), Sun and Chakraborty for Type-V and Yahia et al. for Type-VI are the optimum models from the perspective of information loss. The overall and pairwise proportion test ensured that the models suggested above are significantly optimum from a statistical point of view.

Specific cooling effect (SCE) is a significant parameter to determine the efficiency of the system. In this part, SCE was calculated for two pairs: Maxsorb III/ethanol and Silica gel/water for cooling applications using various isotherm models. Then, the impact of the optimum isotherm model is identified by comparing with Experimental SCE. Finally, as a removal application, cesium was selected to remove from its aqueous solutions. The 2^3 factorial experimental design was used. Two adsorbents, namely, nanoscale zero-valent iron-zeolite (nZVI-Z) and nano-Fe/Cu-zeolite (nFe/Cu-Z), have been considered for the removal process. Initial concentration was the most potential factor for this removal process, followed by contact time and the interaction between initial concentration and contact time for both adsorbents. Five widely used isotherm models were used to simulate the removal data for advanced analysis. The accuracy parameters such as RMSD, R^2 , and AIC have confirmed that the proposed optimum model is more efficient than other models.