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In this study, five error evaluation functions are used to calculate the error deviation between the experimental data and the predicted data for Maxsorb III/ethanol and RD silica gel/water pairs when the isotherm data fitted with six isotherm models. An error analysis based on the sum of normalized error (SNE) is performed to observe the effect of different error evaluation functions for the determination of isotherm parameters. On the basis of error values, Tòth isotherm provides less error compared to other models for both pairs. Error analysis using SNE advocates that HYBRID error evaluation function is suitable for D-A, Freundlich, and Hill models for both pairs whereas ARED error evaluation function is appropriate for Tòth and Langmuir models for Maxsorb III/ethanol pairs. However, RMSD for Redlich-Peterson and SSE for Tòth are appropriate for Maxsorb III/ethanol and silica gel/water pairs, respectively. Seven statistical tools are employed to predict the best isotherm model for the studied pairs. It is found that, except F-test, all other functions provide agreeable results for the better fitting of Tòth model for Maxsorb III/ethanol pair. More or less, similar findings are observed for the RD silica gel/water pair. Moreover, seven information criteria (IC's) are also performed in order to find the optimum isotherm model. On the basis of IC's, Tòth model provides less information loss compared to other models for the studied pairs.

Keywords: activated carbon; error analysis; isotherm model; silica gel; statistical tools

1. Introduction

Adsorption isotherms describe the equilibrium adsorption capacity at a given temperature and pressures. Accuracy of measuring these data are essential for the optimum design and development of adsorption heat pump (AHP) system. Generally, measured isotherm data are correlated applying various isotherm models where the best fitted model is used to analyze the system performance[1–6]. It always generates error when the experimental data are fitted with isotherm models. Therefore, it is necessary to find the appropriate isotherm models which produce minimum error.

Error evaluation function analysis is a mathematical tool to extract worthwhile information from the experimental data. Experimental data sometime deviates from its true value which subject to error. As the fitting of isotherm model with the experimental data creates error, statistical analysis in this case can help to summarize those observations by estimating the true mean of the data. Several error evaluation functions are used to estimate the error deviation when a mathematical model is applied to fit the experimental data, for instance MPSD, HYBRID, SSE, ARED and RMSD. Different statistical tools such as Pearson correlation coefficient, coefficient of determination, the chi-square test, F-test, Student's T-test can be used to analyze the experimental data and investigate the applicability of mathematical model[7)]

Several researchers performed error analysis in the field of adsorption to estimate the best isotherm model and corresponding isotherm parameters. For instances, Chan et al.[8)] performed the error analysis of isotherm models for bamboo–derived activated carbon (AC)/acid dyes. The experimental data were analyzed using various models with five different error evaluation functions. Kumar et al.[9)] compared various error evaluation functions in estimating the optimum isotherm by linear and non-linear regression analysis. Six different error evaluation functions and three isotherms were studied and showed that non-linear regression found to be better way to obtain the isotherm parameters and also the model. Sreńscek-Nazzal et al.[10)] compared the optimized isotherm models and error functions for AC/CO_2 pair. Sips isotherm model was found the best fitted model for all the experimental data. Error analysis showed that hybrid fractional error evaluation function and SSE provide the minimum error. Different kinds of isotherm models and error evaluation functions can be found elsewhere [1,3,5,11,12)].

The literature review indicates that the error analysis can help to select the appropriate model for their corresponding experimental data. However, there is dearth of evidence to use statistical analysis for finding the best fitting isotherm model and corresponding isotherm parameters. Consequently, this study focuses on statistical evidence to find the best isotherm model and optimum isotherm parameters set for the experimental data of a particular pair.

Miller[13)], Pitt & Myung[14)], and Zucchini[15)], suggested several model selection criteria in different situations. This model selection technique mainly discussed log likelihood functions with simple penalty terms namely, Akaike’s Information Criterion[16)], Bozdogan’s consistent AIC[17)], the Bayesian Information Criterion[18)], and the adjusted BIC[19)]. For multiple comparison problem, grouping of the categories of a contingency table and analysis of variance using logit model in contingency table AIC is used[20)]. Corrected AIC also proposed here. Extension of AIC called CAIC and makes AIC asymptotically stable and penalize over parameterization more rigorously to choice the true models[17)]. Auther showed that, for separating latent classes, if sample size adjustment included in the penalty terms then provide a plausible solution[21)]. AIC can be verified as Bayesian and BIC can be obtained as a non- Bayesian result. Comparison between AIC and BIC for model selection cannot be from a Bayes versus frequentist perspective[22)].

In this study, the equilibrium adsorption data of ethanol onto Maxsorb III and water onto RD silica gel are investigated to find the optimum isotherm model and corresponding parameter set. The experimental data are analyzed with frequently used models, namely, Freundlich, Langmuir, Dubinin-Astakhov (D-A), Tòth, Redlich-Peterson, and Hill isotherm models. Five different error evaluation functions are used to calculate the isotherm parameters, including; sum of the squares of errors (SSE); root mean square deviation (RMSD); Marquardt’s percent standard deviation (MPSD); hybrid fractional error function (HYBRID); and average relative error deviation (ARED). The sum of normalized method (SNE) is considered on the error analysis to decide the appropriate error evaluation function for candid explanation for the experimental data, and consequently, the most accurate prediction of the isotherm parameters. This study also considers the applicability of six statistical tools and seven model selection criteria for finding optimum isotherm model.

2. Adsorption isotherm models

2.1 Freundlich isotherm model

For describing adsorption mechanism, this model is the most primitive model and can be written as[1)]:

$$\frac{W}{W_0} = \left(\frac{P}{P_s} \right)^{1/n} \tag{1}$$

Here, n denotes the heterogeneity factor. If n = 1 the Freundlich equation reduces to Henry’s law[8)].

2.2 Langmuir isotherm model

Langmuir model describes the monolayer adsorption process of adsorbent/adsorbate pair. This model is based on the assumption that the adsorbent is homogeneous i.e. all sites of adsorbent are energetically equivalent and identical. It is expressed as[1,8)]:

$$\frac{W}{W_0} = \frac{b_0 e^{\frac{Q}{RT}} P}{1 + b_0 e^{\frac{Q}{RT}} P} \tag{2}$$

2.3 Dubinin-Astakhov (D-A) model

The D-A can be described by the Eq.3. This model usually suitable for carbon based adsorbent to explain the heterogeneity of adsorbent[11,23)].

$$\frac{W}{W_0} = \exp\left[-\left(\frac{RT}{E} \ln\left(\frac{P_s}{P} \right) \right)^n \right] \tag{3}$$

Where, the parameter n describes the surface heterogeneity. When n = 2, the D-A equation reduces to the D-R model.

2.4. Tòth model

The Freundlich equation cannot properly explains the adsorption process at low and high pressure region. However, Tòth equation satisfies both the two end pressure limits and can be written as the following form [11,24)]:

$$\frac{W}{W_0}=\frac{b_0 e^{\frac{Q}{RT}}.P}{\left(1+\left(b_0 e^{\frac{Q}{RT}}.P\right)^t\right)^{1/t}} \tag{4}$$

When $t = 1$, the above equation reduces to the Langmuir equation. Hence, the parameter t is supposed to characterize the system heterogeneity.

2.5 Redlich-Peterson model

This model does not follow the ideal monolayer adsorption characteristics. It is the combined form of both Langmuir and Freundlich model and is given by[9,25]:

$$\frac{W}{W_0}=\frac{A_{RP}\left(\frac{P}{P_s}\right)}{1+K_{RP}\left(\frac{P}{P_s}\right)^{\beta}} \tag{5}$$

β is Redlich-Peterson constant. When $\beta = 1$, it becomes a Langmuir model and $\beta = 0$, it reads like the Henry's Law equation.

2.6 Hill model

This equation is used to describe the binding ability of different gas molecules onto homogeneous adsorbent and can be written as[24]:

$$\frac{W}{W_0}=\frac{\left(\frac{P}{P_s}\right)^{n_H}}{K_D+\left(\frac{P}{P_s}\right)^{n_H}} \tag{6}$$

Where, K_D and n_H represents the Hill constant and Hill cooperativity coefficient of the binding interaction, respectively. Hence, three possibilities can occur

$n_H > 1$, positive cooperativity in binding

$n_H = 1$, non-cooperative or hyperbolic binding

$n_H < 1$, negative cooperativity in binding

3. Objective function of error evaluation

There are mainly two types of error are associated with an experimental result, measurement error and fitting error. Measurement error is the difference between a measured value and the true value. This error reduces if system accuracy is improved. In this study, measurement error of adsorption data for Maxsorb III/ethanol was very negligible, due to the use of highly precise magnetic suspension balance, which is ±1 μm[3]. In case of volumetric adsorption measurement of RD silica gel/water, authors[2] only presented the component error. Fitting error occurs when the experimental data correlated with the isotherm models. In this study only fitting error is considered as an error evaluation function.

In this study, five different error evaluation functions are used to estimate the parameters of each isotherm model. The description of the error evaluation functions is given in the following sub-sections.

3.1 The sum of squares of the errors (SSE)

It is the most commonly used error evaluation function and the mathematical form of the SSE can be written as:

$$SSE=\sum_{i=1}^{n_1}\left(W_{\exp}-W_{cal}\right)_i^2 \tag{7}$$

At the high pressure region, isotherm parameters estimated using this error evaluation function provides better fit. This is due to the magnitude of the errors and hence square of the errors increases as the pressure increases.

3.2 Root mean square deviation (RMSD)

RMSD is also widely used error evaluation function and the mathematical form is[1]:

$$RMSD=\sqrt{\frac{\sum_{i=1}^{n_1}\left(W_{\exp}-W_{cal}\right)_i^2}{n_1}} \tag{8}$$

In this error evaluation function, if the deviation is large between experimental and predicted value, square provides large value relative to other. RMSD mainly tells to avoid the models that give occasional large error. It fulfills the triangle inequality distance metric property. It follows the normal distribution which is the basis for fitting of ordinary least square regression models.

3.3 The Marquardt's Percent Standard Deviation (MPSD)

MPSD was previously used by notable researchers in various fields and is very popular in adsorption parameter estimation. It has some similarity to the geometric mean error distribution which was modified according to the number of degrees of freedom of the system[7,10].

$$MPSD=100*\sqrt{\frac{1}{n_1-p}\sum_{i=1}^{n_1}\left(\frac{W_{cal}-W_{\exp}}{W_{\exp}}\right)_i^2} \tag{9}$$

3.4 The hybrid fractional error function (HYBRID)

Hybrid error evaluation function was developed by Porter et al.[26] in order to improve the fit at low pressure region compared to the sum of the squares of errors (SSE). In this error function, each SSE values is divided by the measured adsorption values[8]. In addition, degrees of freedom are included as a divisor in the equation. So, various isotherms with different number of parameters can be compared in terms of HYBRID error evaluation function. The hybrid error evaluation function is expressed as:

$$HYBRID = \frac{100}{n_1 - p} * \sum_{i=1}^{n_1} \left[\frac{\left(W_{cal} - W_{\exp}\right)^2}{W_{\exp}} \right]_i \tag{10}$$

3.5 The average relative error deviation (ARED)

The ARED is defined by the following equation[24]:

$$ARED = \frac{100}{n_1} * \sum_{i=1}^{n_1} \left| \frac{W_{cal} - W_{\exp}}{W_{\exp}} \right|_i \tag{11}$$

ARED minimizes the fractional error distribution across the all-inclusive range of pressure in the adsorption system[7]. It is actually an error measurement relative to the experimental measurement. In case of Laplacian or proportional error distribution, ARED error function is the best to use.

4. Error optimization

Estimation of isotherm parameters can be affected by the choice of error evaluation function. It is difficult to identify the optimum isotherm parameters because different error evaluation functions provide different set of isotherm parameters[8,10]. The parameter sets can be compared meaningfully by calculating the sum of the normalized errors (SNE) [26]. The calculation procedure of SNE is given below [24]:

i) At first, one isotherm model and one error evaluation function are selected. By minimizing the selected error evaluation function, the parameter set of that isotherm model is determined.

ii) Using this optimized parameter set, the values of all other error evaluation functions are calculated.

iii) Process (i) and (ii) are applied for all other parameter sets and error functions.

iv) From the selection of each error measured, the maximum error value is determined. After that, selected error is divided by the maximum error which is called normalized error.

v) For each isotherm parameter set, all the normalized errors are summed which is called sum of normalized error(SNE).

In the same way, all the SNEs for different parameter sets are determined where the smallest SNE can be selected as the optimum for that isotherm model. It is assumed that there is no bias in the data sampling and selected error methods.

5. Statistical tools

5.1 Pearson correlation coefficient (r)

The Pearson product-moment correlation coefficient is a measure of the strength of the linear relationship between two variables. It is a sampling index, varying from -1 to +1, reflecting the degree of linearity between two variables. The value of r close to +1 and -1 means strong positive and strong negative relationship between two variables, respectively. The Pearson correlation coefficient is expressed as[7]:

$$r = \frac{n_1 \sum_{i=1}^{n_1} x_i y_i - \left(\sum_{i=1}^{n_1} x_i \right) \left(\sum_{i=1}^{n_1} y_i \right)}{\sqrt{\left[n_1 \sum_{i=1}^{n_1} x_i^2 - \left(\sum_{i=1}^{n_1} x \right)^2 \right] \left[n_1 \sum_{i=1}^{n_1} y_i^2 - \left(\sum_{i=1}^{n_1} y \right)^2 \right]}} \tag{12}$$

Here, x and y denote experimental uptake and predicted uptake, respectively.

5.2 Coefficient of determination (R^2)

The coefficient of determination, R^2, is used to examine how changes in the dependent variable can be explained by changing in independent variable. The range of R-squared value is 0 to 1 i.e. 0% to 100% of the variation of dependent variable can be explained by the independent variable. The coefficient of determination can be calculated as:

$$R^2 = \frac{S_{xy}^2}{S_{xx} S_{yy}} \tag{13}$$

Where, S_{xy} represents the sum of squares of the product of x and y, S_{xx} is the sum of squares of x and S_{yy} denotes the sum of square of y.

5.3 Student's T-test

Assumptions:

i) Paired samples

ii)The differences of the pairs follow a normal distribution or the number of pairs is large.

Hypothesis:

$H_0 : \mu_1 = \mu_2$ ("the paired population means are equal")

$H_0 : \mu_1 \neq \mu_2$ ("the paired population means are not equal"), Alternatively,

$H_0 : \mu_d = 0 \; vs$ $H_1 : \mu_d \neq 0$ or $H_0 : \mu_d = 0 \; vs$ $H_1 : \mu_d > 0$ or, $H_0 : \mu_d = 0 \; vs$ $H_1 : \mu_d < 0$

Let d = differences between the pairs of data,

Then $\bar{d}$ = mean of these differences.

The test statistic:

$$t = \frac{\bar{d}}{s_d / \sqrt{n_1}} \tag{14}$$

which is distributed as Student's t distribution with (n_1-1) degrees of freedom.

5.4 Equality of variance test

F-test of equality of variances is a test for the null hypothesis that two normal populations have the same variance. F-test can be regarded as a comparison of two variances.

Hypothesis:

$H_0 : \sigma_1^2 = \sigma_2^2$ *vs*

$H_1 : \sigma_1^2 > \sigma_2^2$ (Upper tailed test)

$OR, H_1 : \sigma_1^2 < \sigma_2^2$ (Lower tailed test)

$OR, H_1 : \sigma_1^2 \neq \sigma_2^2$ (Two tailed test)

Test statistic:

$$F = \frac{s_1^2}{s_2^2}$$

Where, s_1 and s_2 are the sample standard deviation. The more this ratio deviates from 1, the stronger the evidence for unequal population variances.

5.5 Mann-Whitney U-test

Mann–Whitney U-test is a non-parametric test that can be used to determine whether two independent samples are selected from population having the same distribution or not.

H_0: The difference of location between the samples is equal to 0. *vs*

H_1: The difference of location between the samples is different from 0.

5.6 Kolmogorov-Smirnov (KS) test

It is a nonparametric test and does not assume that data are come from Gaussian distributions (or any other defined distributions).

H_0: The two samples follow the same distribution. *vs*

H_1: The two samples follow the different distribution.

If H_0 is false, it means two populations have different medians, variances, or different distributions. If the outcome variables are categorical, KS test should not be used.

5.7 Probability value (P-value)

Only the error analysis does not provide the enough evidence to select the best isotherm model for a particular pair. To determine whether the predicted uptake based on the isotherm model is statistically significant or not, calculating the P-value between experimental data and predicted data is a good approach. The P-value, or calculated probability value, is the probability of finding the observed, or more extreme results when the null hypothesis (H_0) of this study question is true. More appropriately, P-value is the smallest level of significance for which the null hypothesis is rejected. There are different tests in statistics depends on null hypothesis.

6. Information-based criterion for model selection

The general form of the classical penalized-likelihood information criteria (*IC*), i.e., *-2l + f(n,p)* contains a goodness of fit term *(-2l)* and a penalty function, *f(n, p)* [19,27,28]. The goal of these criteria is to select the “best model” which defines the relationship in the data. These criteria are based on the theory that the best model is one which sacrifices the minimum information when it is used to estimate the truth. The aim of the information-based model selection criteria is to find a model for which the loss of information is as minimum as possible compared to all studied models.

6.1 The AIC

Akaike (1969) developed a model selection criterion based on the relationship between the relative K-L distance and the maximized log-likelihood. This criterion plays the significant role in practical and theoretical development in various models selection and complex data analysis[17]. Author first showed that, the maximized log-likelihood method is biased upward. Second, he showed that under certain conditions, this bias is approximately equal to *p* which is the number of estimable parameters in the studied model. Consequently, an approximately unbiased estimator of the relative expected *K-L* information is $\log\left(L\left(\hat{\theta}|(y)\right)\right) - p$ or *l-p*. For historical reasons, instead of finding the highest value of *l* minus a penalty (*l-p)*, the generalized information criteria (GIC, Atkinson (1980)) considers the lowest value of *-2l* plus a penalty *f(n,p)*[29]. Occasionally, the *GIC* is stated in the form *GIC = -2l +* $A_n p$.

where A_n is some constant or some function of *n* and *p*. AIC was proposed by Akaike (1969), and select a model that minimizes *AIC = -2l + 2p*, where *l* is the likelihood of the model and *p* is the number of parameter in the model[27].

6.2 Criteria Related to AIC

In the perspective of regression and time series models, numerous researchers[20,22,30] have been recommended using a corrected version, AIC_c which applies slightly heavier penalty depending on *p* and *n*.

A second order variant of *AIC* called AIC_c[30] derived by Sugiura (1978). Further, Hurvich and Tsai (1989) added small-sample bias adjustment in the second order which led to a criterion that is called AIC_c and denoted by $AIC_c = -2l + 2p\left(n/(n-p-1)\right)$ [30]. For small *n*, Hirvich and Tsai (1989) found that AIC_c sometimes perform better than that of *AIC*. If there are so many parameters in relation to the size of the sample[28], *AIC* may perform poorly. But, the correction term, *n/(n-p-1)* is negligible if *n* is large with respect to *p*. The *AIC* should then perform equally well as AIC_c. Unless *n* is large with respect to the number of parameters AIC_c is recommended[31].

Phoa et al.[27] suggested a modified *AIC* named *mAIC* which employs quadratic penalty for the model complexity, instead of the linear penalty in *AIC*. Hence, the *mAIC* increases in a higher rate than *AIC* for each additional effect in the competing model. For *mAIC* the model stinginess is the inspiring goal, which in turn confirms lower Type I error than that of AIC.

The modification *AIC3* uses $A_n = 3$ instead of 2 in AIC was suggested by some researchers[21,28,32] in the perspective of mixture models such as *LCA*. However, it has little theoretical basis, regardless of comparable simulation performance.

6.3 The BIC

BIC was proposed by Schwarz (1978). It has a similar form to AIC except that the log-likelihood is penalized by *plog(n)* instead of *2p*, selecting the model that minimizes BIC = *-2l* + *plog(n)*, where *n* is the number of observations[18)]. The highest posterior probability in the model is expected the one with lowest BIC.

6.4 Criteria Related to BIC

Based on the work of Rissanen (1978), Boekee and Buss (1981), and Sclove (1987) suggested ABIC (adjusted BIC). It used *f(n,p)* = *pln((n+2)/24)* as a substitute for *ln(n)*[28,33)]. A similar version of BIC (despite the name), is the CAIC proposed by Bozdogan (1987)[17)]. The goal was of using *f(n,p)* = *p(ln(n)* + *1)* rather than *pln(n)* is to select more parsimonious model and more under fitting than BIC. Different model selection criteria are used this study presented in Table 1.

Table 1: Formula for different model selection criteria.

Criterion	Form
AIC	$-2l+2p$
BIC	$-2l+p\ln(n)$
AICc	$-2l+2p\left(\dfrac{n}{n-p-1}\right)$
mAIC	$-2l+2p^2$
AIC3	$-2l+3p$
CAIC	$-2l+p\left(\ln(n)+1\right)$
ABIC	$-2l+p\ln\left((n+2)/24\right)$

where, $2l=-n(\log 2\pi+\log(error)-\log n+1)$

7. Results and discussion

In this analysis, six isotherm models and five objective function of error evaluation are employed to fit the experimental isotherm data of Maxsorb III/ethanol[3)] and RD silica gel/water [2)] pairs. Equilibrium adsorption uptake of ethanol onto Maxsorb III and water onto RD silica gel are presented in Fig. 1 and Fig. 2, respectively at different temperatures and pressures. The different lines represent the different isotherm models whereas the circle denotes the experimental adsorption uptake. From the Fig. 1, it is observed that Freundlich, Langmuir, Redlich-Peterson and Hill model do not fit well with the experimental data for Maxsorb III/ethanol pair. However, D-A and Tòth model fits well with the experimental data compared to other isotherm models. It should be highlighted that Tòth is found the best fitted isotherm model for both the Maxsorb III/ethanol and RD silica gel/water pairs compared to other studied isotherm models. This conclusion is made based on the error analysis using five error evaluation functions. The details of the error analysis with numerical values are presented in Fig. 3 and Fig. 4.

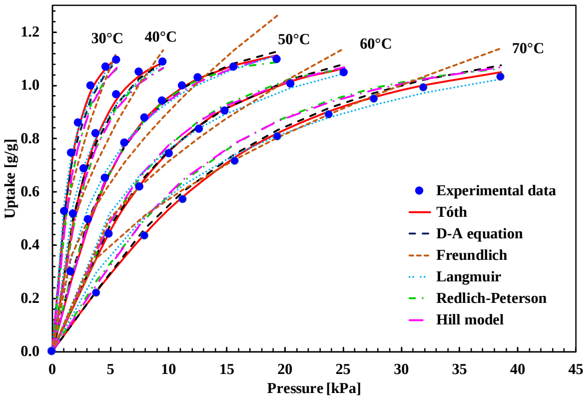

Fig. 1: Adsorption isotherm of Maxsorb III/ethanol pair (data are fitted with Tòth model, D-A equation, Redlich-Peterson model and Hill model using HYBRID error evaluation function).

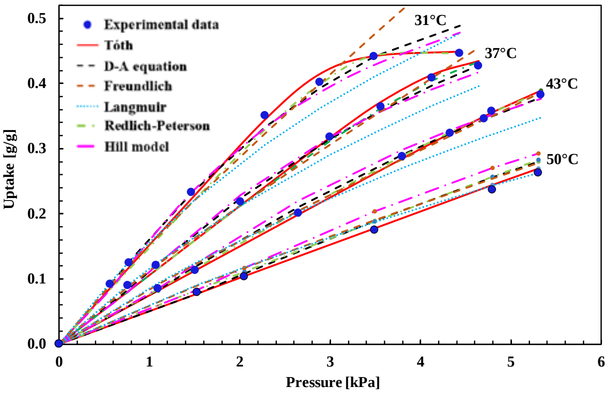

Fig. 2: Adsorption isotherm of silica gel/water pair (data are fitted with Tòth model, D-A equation, Redlich-Peterson and Hill model using ARED error evaluation function).

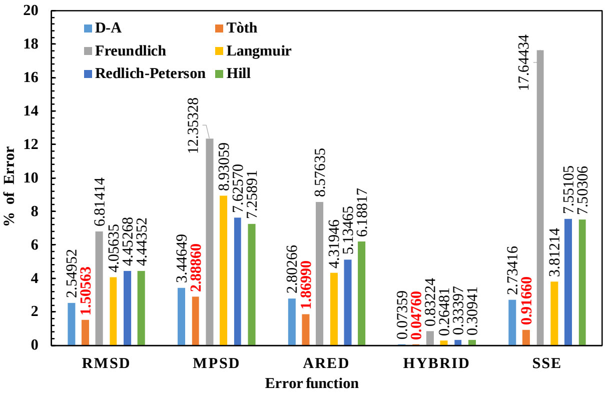

Fig. 3: Isotherm error deviation data for Maxsorb III/ethanol pair using five commonly used error evaluation functions. (Bold and red colored values indicate minimum error values).

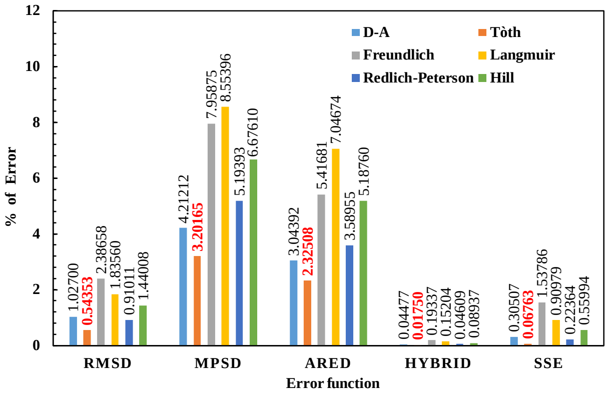

Fig. 4: Isotherm error deviation data for silica gel/water pair using five commonly used error evaluation functions. (Bold and red colored values indicate minimum error values).

The isotherm error deviation data related to Maxsorb III/ethanol and RD silica gel/water pairs considering six isotherm models and five well known error evaluation function are shown in Fig. 3 and Fig. 4, respectively. Non-linear optimization technique using Excel Solver is employed to calculate optimized error deviation between experimental uptake and predicted uptake by six isotherm models. Less error means better fitting of the isotherm model. Optimized error value of Tòth model for five error functions shows minimum compared to other models (see in Fig. 3), so the Tòth model can be considered as the best model for Maxsorb III/ethanol pair. Tòth model is also found the most acceptable model for describing the RD silica gel/water pair (see in Fig. 4). Actually, for both pairs, the non-linear optimized value of RMSD, MPSD, ARED, HYBRID and SSE are smaller.

Tòth and Redlich-Peterson are four parameters model while D-A, Langmuir and Hill are three parameters and Freundlich is two parameters models. Therefore, in that context, it has to be emphasized that the error obtained from MPSD and HYBRID evaluation functions which considers the effect of the number of parameters in the model seem essentially meaningful and justified.

The estimated optimum isotherm parameters of different models and the corresponding SNE calculation are shown in Table 2. Here, Pair-I represents the adsorption of ethanol onto Maxsorb III whereas Pair-II denotes adsorption of water onto RD silica gel. Non-linear optimization technique is used to estimate the parameters of an isotherm model using different error evaluation functions. The five different errors calculated from the same isotherm model are different but the value of the parameters are quite similar.

For the Maxsorb III/ethanol pair, on the basis of SNE, HYBRID objective function of error evaluation is appropriate for the fitting of D-A, Freundlich, and Hill models whilst ARED evaluation function is suitable for the fitting of Tòth and Langmuir. In the case of Redlich-Peterson model, RMSD error evaluation function is appropriate for this pair.

In the case of silica gel/water pair, on the basis of SNE, HYBRID error function is suitable for the fitting of all isotherm models except Tòth. For Tòth model fitting, the SSE error evaluation function is appropriate.

The lowest value of SNE with the corresponding evaluation function of error implies optimum isotherm parameter set for particular isotherm model.

Here, for comparing two populations (experimental and predicted data), mean tests (T-tests), variance tests (F-tests), location tests (Mann-Whitney-U tests), and distribution tests (KS-tests) are performed. P-value of all studied tests, also correlation coefficient and regression coefficient are presented in the Table 3 and Table 4 for the Maxsorb III/ethanol and silica gel/water pairs, respectively. From the Table 3, except the F-test, all the other statistical test is suitable to determine the most appropriate fitting model which is Tòth model for Maxsorb III/ethanol pair. The correlation coefficient of Tòth model is 0.997924 which is higher than other model. So, it can be concluded that for Tòth model the strength of linear relationship between the experimental uptake and predicted uptake is higher than that of other models. The coefficient of determination of Tòth is also higher than the other models which is 0.9958537, i.e. 99.58 percent variation of the model can be explained by the experimental uptake. Since, all P-values are greater than 0.05 or 0.1, so all models are statistically significant. However, the model which P-value is greater, implies that model is the best fit. Therefore, according to T-test, P-value is 0.9860 for Tòth model which is higher, which indicates the population mean of experimental data and predicted data are equal. Mann-Whitney U and Kolmogorov Smirnov test are for location test and distribution test, respectively. Since the P-value for both the test is higher in case of Tòth model, so this model can be considered the best fitting model.

On the basis of correlation coefficient (r), coefficient of determination (r^2), T-test and Kolmogorov-Smirnov test, Tòth model is better fitting than that of other models for RD silica gel/water pair in Table 4.

The values of different classical model selection criteria for different isotherm models for Maxsorb III/ethanol and RD silica gel/water are presented in Table 5(a) and 5(b) respectively. Putting the value of "error" in the equation (15), the value of $2l$ can be obtained. The value of different model selection criteria are then calculated using equation mentioned in Table 1.

$$2l = -n(\log 2\pi + \log(error) - \log n + 1) \qquad (15)$$

Second column of Table 5(a) and 5(b) shows optimized error (%) of different isotherm model. Here five different sets of calculation have been calculated for five error evaluation functions. For RMSD evaluation function, all the calculated value of model selection criteria of Tòth isotherm model is small compare to other isotherm model. Since small value of IC's means less information loss, accordingly, Tòth isotherm is found less information loss compare to other isotherm model. Similar result was observed in the case of ARED, HYBRID and SSE error evaluation function. For MPSD error function, except mAIC all IC's are smaller for Tòth isotherm than other isotherm model. Overall, on the basis of model selection criteria the adsorption of ethanol onto Maxsorb III, Tòth isotherm model is better fit than other isotherm model.

Table 5(b) shows the model selection criteria RD silica gel/water pair. For RMSD, HYBRID and SSE evaluation function of error, all the calculated value of model selection criteria of Tòth isotherm model are found small compare to other isotherm model and for MPSD & ARED all IC's are smaller except the mAIC. So Tòth isotherm model has less information loss (fit better) compare to other isotherm models.

Table 2: Isotherm parameters with error analysis using SNE for Maxsorb III/ethanol (Pair-I) and RD silica gel/water (Pair-II).

Model Parameters		**RMSD [%]**		**MPSD [%]**		**ARED [%]**		**HYBRID [%]**		**SSE [%]**	
		Pair-I	Pair-II	Pair-I	Pair-II	Pair-I	Pair-II	Pair-I	Pair-II	Pair-I	Pair-II
D-A	W_0	1.17	0.4715	1.1507	0.4908	1.160	0.490	1.165	0.4798	1.18	0.4715
	E	143	200.18	142.93	193.59	143	195.87	142.5	198.10	144	200.18
	n	1.9	1.442	1.98	1.2836	1.98	1.3225	1.96	1.3584	1.87	1.40
	RMSD	2.5495	1.0270	2.4913	1.2221	2.4493	1.1520	2.4803	1.0811	2.6823	1.0630
	MPSD	3.6964	5.6828	3.4464	4.2121	3.4670	4.4067	3.4660	4.4739	4.0179	4.8864
	ARED	2.9150	3.9256	2.7772	3.1867	2.8026	3.0439	2.8039	3.3679	3.1742	3.6972
	HYBRID	0.0792	0.0517	0.0737	0.0494	0.0726	0.0480	0.0735	0.0447	0.0943	0.0468
	SSE	2.4700	0.2847	2.3586	0.4032	2.3796	0.3582	2.2378	0.3155	2.7341	0.3050
	SNE	4.3390	4.5464	4.3060	4.5074	4.2990	4.3089	**4.2689**	**4.1770**	5	4.3327
Tòth	W_0	1.2	0.4486	1.2	0.4483	1.21	0.4497	1.20	0.4514	1.23	0.4485
	b_0	3.1E-9	2.7E-9	3.1E-9	2.7E-9	3.E-9	2.7E-9	3.E-9	2.7E-9	3.1E-9	2.7E-9
	Q	47635	47172	47435	47219	47640	47185	47470	47173	4744	47182
	t	1.69	10	1.80	9.5	1.70	10	1.87	9.5	1.69	9
	RMSD	1.5056	0.5435	1.5294	0.6109	1.4044	0.5630	1.5965	0.5448	1.5545	0.4936
	MPSD	3.0699	3.6354	2.8885	3.2016	2.7689	3.4664	3.1067	3.6192	2.8832	3.5360
	ARED	1.9592	2.3900	2.0286	2.1998	1.8699	2.3250	1.9874	2.4107	2.0696	2.2891
	HYBRID	0.0433	0.0181	0.0419	0.0167	0.0364	0.0178	0.0475	0.0175	0.0423	0.0167
	SSE	0.8614	0.0783	0.8889	0.0882	0.7494	0.0851	0.9686	0.0801	0.9165	0.0676
	SNE	4.6773	4.7687	4.6676	4.7158	**4.2135**	4.7836	4.9602	4.7601	4.7375	**4.4183**
Freundlich	W_0	1.48208	0.5377	1.6848	0.5716	1.5907	0.5986	1.5678	0.5564	1.4820	0.5377
	n	2.2141	1.2563	1.7489	1.1147	1.9402	1.1020	1.9716	1.1644	2.2141	1.2563
	RMSD	6.81413	**2.3865**	8.5975	2.7085	7.3790	3.0630	7.2561	2.5178	6.8141	2.3865
	MPSD	16.4475	12.029	12.353	7.9587	13.333	8.8174	13.516	8.5297	16.447	9.5445
	ARED	8.95444	9.0278	9.1370	5.9967	8.5763	5.4168	8.5790	6.2798	8.9544	9.0287
	HYBRID	0.9553	0.2366	0.9694	0.2063	0.8362	0.2542	0.8322	0.1933	0.9553	0.2366
	SSE	17.6443	1.5378	28.088	1.9807	20.6913	2.5331	20.007	1.7116	17.644	1.5378
	SNE	4.38616	4.3169	4.7510	3.8035	4.2067	4.3329	**4.1754**	**3.6631**	4.3861	4.1105
Langmuir	W_0	1.38	1.2089	1.4	1.1592	1.41	1.1606	1.39	1.1896	1.39	1.2084
	b_0	3.1E-09	3E-09	3.1E-9	3E-09	3.1E-9	3E-09	3.1E-9	3E-09	3.0E-9	3E-09
	Q	48600	44998	48400	44960	48300	44947	48400	44987	48400	44998
	RMSD	7.22307	1.8356	7.4903	2.3480	6.6758	2.3900	6.6156	1.9156	6.7561	1.8356
	MPSD	17.0654	10.064	14.292	8.5539	10.727	8.5501	14.290	9.1088	14.346	10.041
	ARED	10.5751	7.5920	9.9889	7.0854	8.230	7.0467	9.3283	7.3431	9.4738	7.5874
	HYBRID	1.1330	0.1600	0.9386	0.1883	0.6319	0.1931	0.8436	0.1521	0.8629	0.1596
	SSE	19.8256	0.9097	21.320	1.4884	16.935	1.5423	16.631	0.9908	17.345	0.9097
	SNE	4.8942	4.1865	4.6105	4.7058	**3.6502**	4.7777	4.1273	**4.1036**	4.2137	4.1818
Redlich-Peterson	W_0	1.2913	0.4734	1.2671	0.4747	1.3668	0.4737	1.2571	0.4735	1.30	0.4734
	A_{rp}	4.427	1.4084	4.1043	1.4124	4.2402	1.4093	4.3515	1.4089	4.4089	1.4084
	K_{rp}	4.1992	0.5057	3.9664	0.5034	4.2709	0.504	4.0634	0.5047	4.1992	0.5057
	β	1.2973	4.3072	1.4308	3.9997	1.335	4.297	1.3499	4.2537	1.2973	4.3072
	RMSD	4.45267	0.9101	4.5626	0.9171	4.5050	0.9107	4.5053	0.9105	4.4526	0.9101
	MPSD	7.99707	5.2119	7.6256	5.1939	8.2917	5.2085	8.2913	5.2077	7.9974	5.2118
	ARED	5.23801	3.5927	5.4536	3.5999	5.1330	3.5896	6.1624	3.5858	5.2379	3.5927
	HYBRID	0.33930	0.0461	0.3403	0.0464	0.3550	0.0461	0.3550	0.0461	0.3393	0.0461
	SSE	7.5340	0.2236	7.9107	0.2271	7.7122	0.2240	7.7134	0.2240	7.5340	0.2236
	SNE	**4.69824**	4.9686	4.7631	4.9965	4.7951	4.9704	4.9624	**4.9667**	4.6983	4.9686

Hill	W_0	1.26689	0.6839	1.2711	0.7136	1.3239	0.68	1.2713	0.7898	1.2667	0.6839
	n_h	1.32196	1.4167	1.3316	1.3155	1.1957	1.3661	1.3223	1.284	1.3220	1.4166
	K_d	0.08029	0.4124	0.0818	0.4964	0.1110	0.4156	0.0820	0.5983	0.0802	0.4124
	RMSD	0.04443	1.4400	0.0449	1.5514	0.0450	1.5192	0.0445	1.4940	0.0444	1.4400
	MPSD	7.5054	7.5535	7.3618	6.6761	8.1193	7.3876	7.4042	6.4954	7.4958	7.5508
	ARED	6.10137	5.5214	6.1624	5.3640	6.1881	5.1876	6.1334	4.9758	6.1038	5.5199
	HYBRID	0.31918	0.0987	0.3203	0.0964	0.3415	0.1074	0.3182	0.0894	0.3204	0.0986
	SSE	0.07503	0.5599	0.0766	0.6498	0.0772	0.6232	0.0753	0.6027	0.0750	0.5599
	SNE	4.80250	4.7083	4.8303	4.7523	5	4.8559	**4.7989**	**4.4832**	4.8055	4.7074

Bold numerical values indicate minimum sum of normalized error (SNE)

Table 3: Isotherm error deviation estimation for Maxsorb III/ethanol pair using statistical tools (using SSE error evaluation function).

Model	**Correlation of coefficient (*r*)**	**Coefficient of determination (r^2)**	**F-test**	**T-test**	**Mann-Whitney U-test**	**Kolmogorov-Smirnov Test**
D-A	0.993970	0.9879781	0.9398	0.8969	0.88912	0.9997822
Tòth	**0.997924**	**0.9958537**	0.9450	**0.9860**	**0.995880**	**0.9999999**
Freundlich	0.957893	0.917559	0.6329	0.9678	0.88912	0.7307010
Langmuir	0.996970	0.9939503	0.4746	0.9474	0.78431	0.9844246
Redlich-Peterson	0.981985	0.9642959	0.9012	0.9655	0.93005	0.9999999
Hill	0.99250	0.9851	**0.9624**	0.9796	0.9055	0.9999000

Bold numerical values indicate maximum correlation coefficient (*r*), regression coefficient and p-value of different tests.

Table 4: Isotherm error deviation estimation for silica gel/water pair using statistical tools (using SSE error evaluation function).

Model	**Correlation of coefficient (*r*)**	**Coefficient of determination (r^2)**	**F-test**	**T-test**	**Mann-Whitney U-test**	**Kolmogorov-Smirnov Test**
D-A	0.99781	0.99563	**0.99054**	0.81755	0.85030	0.99870
Tòth	**0.99950**	**0.99900**	0.93753	**0.98863**	0.93160	**0.99999**
Freundlich	0.98829	0.97673	0.86851	0.96466	**0.98630**	0.95860
Langmuir	0.99349	0.98702	0.84976	0.94678	0.94530	0.95860
Redlich-Peterson	0.99828	0.99656	0.99343	0.84727	0.91800	0.99870
Hill	0.99569	0.99140	0.99530	0.98330	0.85030	0.95860

Bold numerical values indicate maximum correlation coefficient (*r*), regression coefficient and p-value of different tests.

Table 5(a): Model selection criteria for Maxsorb III/ethanol pair using different error evaluation functions.

RMSD								
Model	**Error [%]**	**AIC**	**BIC**	**AICc**	**mAIC**	**AIC3**	**CAIC**	**ABIC**
D-A	2.550	11.1906	16.10343	11.8965	23.19067	14.1906	19.1034	6.72314
Tòth	1.506	**-6.82375**	**-0.27340**	**-5.61162**	**17.17625**	**-2.8237**	**3.72660**	**-12.7804**
Freundlich	6.814	46.5483	49.82350	46.8911	50.54833	48.5483	51.8235	43.5699
Langmuir	4.056	28.8371	33.74989	29.5430	40.83713	31.8371	36.7498	24.3696
Redlich-Peterson	4.453	34.3795	40.92990	35.5916	58.37956	38.3795	44.9299	28.4228
Hill	4.444	32.3013	37.21410	33.0072	44.30135	35.3013	40.2141	27.8338
MPSD								
D-A	3.44649	22.6458	27.5586	23.3517	**34.6458**	25.6458	30.5586	18.1783
Tòth	2.88860	**17.9356**	**24.4860**	**19.1477**	41.9356	**21.9356**	**28.4860**	**11.9789**
Freundlich	12.3532	69.1554	72.4306	69.4982	73.1554	71.1554	74.4306	66.1770
Langmuir	8.93059	58.8267	63.7394	59.5326	70.8267	61.8267	66.7394	54.3591
Redlich-	7.62570	54.8243	61.3746	56.0364	78.8243	58.8243	65.3746	48.8676

Peterson								
Hill	7.25891	50.9511	55.8638	51.6570	62.9511	53.9511	58.8638	46.4836
ARED								
D-A	2.80266	14.7879	19.7007	15.4938	26.7879	17.7879	22.7007	10.3204
Tòth	1.86990	**1.4100**	**7.9603**	**2.6221**	**25.4100**	**5.4100**	**11.9603**	**-4.5467**
Freundlich	8.57635	55.2887	58.5638	55.6315	59.2887	57.2887	60.5638	52.3103
Langmuir	4.31946	31.2253	36.1381	31.9312	43.2253	34.2253	39.1381	26.7578
Redlich-Peterson	5.13465	39.7948	46.3451	41.0069	63.7948	43.7948	50.3451	33.8381
Hill	6.18817	44.8866	49.7994	45.5925	56.8866	47.8866	52.7994	40.4191
HYBRID								
D-A	0.07359	-123.523	-118.6109	-122.8178	-111.5237	-120.523	-115.610	-127.991
Tòth	0.04760	**-138.082**	**-131.5326**	**-136.8708**	**-114.0829**	**-134.082**	**-127.532**	**-144.039**
Freundlich	0.83224	-33.3519	-30.0767	-33.0090	-29.3519	-31.3519	-28.0767	-36.3302
Langmuir	0.26481	-74.8662	-69.9535	-74.1603	-62.8662	-71.8662	-66.9535	-79.3338
Redlich-Peterson	0.33397	-64.0479	-57.4976	-62.8358	-40.0479	-60.0479	-53.4976	-70.0046
Hill	0.30941	-68.9505	-64.0377	-68.2446	-56.9505	-65.9505	-61.0377	-73.4180
SSE								
D-A	2.734	13.8476	18.76036	14.5534	25.84760	16.8476	21.7603	9.38008
Tòth	0.917	**-25.6830**	**-19.13273**	**-24.4709**	**-1.68308**	**-21.683**	**-15.1327**	**-31.6397**
Freundlich	17.644	82.7021	85.97729	83.0449	86.70212	84.7021	87.9772	79.7237
Langmuir	3.812	26.4775	31.39030	27.1834	38.47755	29.4775	34.3903	22.0100
Redlich-Peterson	7.551	54.4504	61.00076	55.6625	78.45042	58.4504	65.0007	48.4937
Hill	7.503	52.2081	57.12092	52.9140	64.20816	55.2081	60.1209	47.7406

Bold numerical values indicate minimum value of different model selection criterion.

Table 5(b): Model selection criteria for silica gel/water pair using different error evaluation function.

RMSD								
Model	**Error [%]**	**AIC**	**BIC**	**AICc**	**mAIC**	**AIC3**	**CAIC**	**ABIC**
D-A	1.0270	-5.6348	-1.7473	-4.5913	6.3652	-2.6348	1.2527	-11.0670
Tòth	0.5435	**-20.8150**	**-15.6317**	**-18.9968**	**3.1850**	**-16.8150**	**-11.6317**	**-28.0580**
Freundlich	2.3866	15.1322	17.7239	15.6322	19.1322	17.1322	19.7239	11.5107
Langmuir	1.8356	10.0450	13.9325	11.0885	22.0450	13.0450	16.9325	4.6128
Redlich-Peterson	0.9101	-6.8972	-1.7138	-5.0790	17.1028	-2.8972	2.2862	-14.1402
Hill	1.4401	3.4928	7.3804	4.5363	15.4928	6.4928	10.3804	-1.9394
MPSD								
D-A	4.2121	32.4710	36.3585	33.5145	**44.4710**	35.4710	39.3585	27.0387
Tòth	3.2016	**27.0649**	**32.2483**	**28.8831**	51.0649	**31.0649**	**36.2483**	**19.8219**
Freundlich	7.9587	47.6513	50.2430	48.1513	51.6513	49.6513	52.2430	44.0298
Langmuir	8.5540	51.5986	55.4861	52.6421	63.5986	54.5986	58.4861	46.1663
Redlich-Peterson	5.1939	40.1282	45.3115	41.9464	64.1282	44.1282	49.3115	32.8852
Hill	6.6761	44.9065	48.7940	45.9500	56.9065	47.9065	51.7940	39.4743
ARED								
D-A	3.0439	23.7009	27.5884	24.7444	**35.7009**	26.7009	30.5884	18.2686
Tòth	2.3251	**18.4274**	**23.6107**	**20.2456**	42.4274	**22.4274**	**27.6107**	**11.1843**
Freundlich	5.4168	37.2627	39.8543	37.7627	41.2627	39.2627	41.8543	33.6411
Langmuir	7.0467	46.3652	50.2527	47.4087	58.3652	49.3652	53.2527	40.9329
Redlich-Peterson	3.5896	30.1527	35.3360	31.9709	54.1527	34.1527	39.3360	22.9097
Hill	5.1877	38.0957	41.9832	39.1391	50.0957	41.0957	44.9832	32.6634
HYBRID								
D-A	0.0448	-90.2197	-86.3322	-89.1762	-78.2197	-87.2197	-83.3322	-95.6520
Tòth	0.0175	**-113.5812**	**-108.3979**	**-111.763**	**-89.5812**	**-109.581**	**-104.397**	**-120.824**
Freundlich	0.1934	-52.7187	-50.1271	-52.2187	-48.7187	-50.7187	-48.1271	-56.3402
Langmuir	0.1520	-57.2111	-53.3236	-56.1677	-45.2111	-54.2111	-50.3236	-62.6434

Redlich-Peterson	0.0461	-87.4383	-82.2550	-85.6202	-63.4383	-83.4383	-78.2550	-94.6814
Hill	0.0894	-71.5588	-67.6713	-70.5154	-59.5588	-68.5588	-64.6713	-76.9911
SSE								
D-A	0.3051	-38.4084	-34.5209	-37.3650	-26.4084	-35.4084	-31.5209	-43.8407
Tòth	0.0676	**-77.0834**	**-71.9001**	**-75.2653**	**-53.0834**	**-73.0834**	**-67.9001**	**-84.3265**
Freundlich	1.5379	3.2665	5.8581	3.7665	7.2665	5.2665	7.8581	-0.3551
Langmuir	0.9098	-8.9068	-5.0193	-7.8633	3.0932	-5.9068	-2.0193	-14.3391
Redlich-Peterson	0.2236	-44.7923	-46.4732	-42.9741	-20.7923	-40.7923	-35.6089	-52.0353
Hill	0.5599	-22.0123	-23.2729	-20.9688	-10.0123	-19.0123	-15.1248	-27.4445

Bold numerical values indicate minimum value of different model selection criterion.

8. Conclusions

Equilibrium adsorption uptake of Maxsorb III/ethanol and RD silica gel/water pairs are modeled using Freundlich, Langmuir, Dubinin-Astakhov, Tòth, Redlich-Peterson, and Hill models through non-linear regression analysis with five different error evaluation function. The error values of Tòth model using all error evaluation functions shows smaller values compared to other models for both pairs. It has to be emphasized that the error obtained from MPSD and HYBRID evaluation functions which considers the effect of the number of parameters in the model seem essentially meaningful and justified because all studied models does not consider equal number of parameters.

Secondly, error analysis using sum of normalized (SNE) error suggests that HYBRID error evaluation function is suitable for D-A, Freundlich, and Hill models for both adsorption pairs whereas ARED evaluation function is appropriate for Tòth and Langmuir models for the adsorption of ethanol onto Maxsorb III. RMSD for Redlich-Peterson and SSE for Tòth are found to be suitable for the adsorption of ethanol onto Maxsorb III and water onto RD silica gel, respectively. Overall, HYBRD error evaluation function is the best for optimizing the isotherm parameters.

Thirdly, six statistical tools reasonably determine the best fitting isotherm model. The analysis result indicates that Tòth is the most suitable model for the adsorption of ethanol onto Maxsorb III except the F-test.

Lastly, on the basis of model selection criterion the present study recommends that Tòth isotherm gives less information loss compared to other isotherm models for both type of adsorption pairs.

Nomenclature

A_{RP}	Redlich-Peterson isotherm constant [1/kPa]
b_0	equilibrium constant of Tòth and Langmuir model [1/kPa]
E	adsorption characteristic energy of D-A model [kJ/mol]
K_D	Hill constant [-]
K_{RP}	Redlich-Peterson isotherm constant [-]
n_H	Hill cooperativity coefficient of the binding interaction [-]
n	surface heterogeneity constant of D-A and Freundlich isotherm model [-]
n_1	number of data points [-]
p	number of parameters in the model [-]
P	equilibrium pressure [kPa]
P_s	saturated pressure [kPa]
Q	isostatic heat of adsorption of Tòth and Langmuir model [J/mol]
R	universal gas constant [J/(mol.K)]
T	temperature [K]
W	instantaneous uptake [g/g]
W_{cal}	calculated uptake [g/g]
W_{exp}	experimental uptake [g/g]
W_0	maximum uptake [g/g]

Abbreviations

ABIC	adjusted BIC
AIC	Akaike Information Criterion
AICc	corrected Akaike Information Criterion
ARED	average relative error deviation
BIC	Bayesian Information Criterion
CAIC	modified of Bayesian Information Criterion
HYBRID	hybrid fractional error function
IC	information criterion
mAIC	modified Akaike Information Criterion
MPSD	Marquardt's percent standard deviation
RMSD	root mean square deviation
SNE	sum of normalized error
SSE	sum of squares of error

Greek Letters

β	Redlich-Peterson constant [-]
σ_1	first population variance [-]
σ_2	second population variance [-]

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References

1) A. Pal, H.-S. Kil, S. Mitra, K. Thu, B. B. Saha, S.-H. Yoon, J. Miyawaki, T. Miyazaki, and S. Koyama, *Appl. Therm. Eng.* **122,** 389–397 (2017).
2) H. T. Chua, K. C. Ng, A. Chakraborty, N. M. Oo, and M. A. Othman, *J. Chem. Eng. Data* **47,** 1177–1181 (2002).
3) I. I. El-Sharkawy, K. Uddin, T. Miyazaki, B. B. Saha, S. Koyama, J. Miyawaki, and S.-H. H. Yoon, *Int. J. Heat Mass Transf.* **73,** 445–455 (2014).
4) A. Pal, K. Uddin, K. Thu, and B. B. Saha, *Evergreen, Jt. J. Nov. Carbon Resour. Sci. Green Asia Strateg.* **5,** 58–66 (2018).
5) K. Uddin, I. I. . El-Sharkawy, T. Miyazaki, B. B. Saha, and S. Koyama, *Evergreen, Jt. J. Nov. Carbon Resour. Sci. Green Asia Strateg.* **1,** 25–31 (2014).
6) K. Uddin, M. A. Islam, S. Mitra, J.-B. Lee, K. Thu, B. B. Saha, and S. Koyama, *Appl. Therm. Eng.* **129,** 117–126 (2018).
7) M. C. Ncibi, *J. Hazard. Mater.* **153,** 207–212 (2008).
8) L. S. Chan, W. H. Cheung, S. J. Allen, and G. McKay, *Chinese J. Chem. Eng.* **20,** 535–542 (2012).
9) K. V. Kumar, K. Porkodi, and F. Rocha, *J. Hazard. Mater.* **150,** 158–165 (2008).
10) J. Sreńscek-Nazzal, U. Narkiewicz, A. W. Morawski, R. J. Wróbel, and B. Michalkiewicz, *J. Chem. Eng. Data* **60,** 3148–3158 (2015).
11) A. Pal, K. Thu, S. Mitra, I. I. El-Sharkawy, B. B. Saha, H.-S. Kil, S.-H. Yoon, and J. Miyawaki, *Int. J. Heat Mass Transf.* **110,** 7–19 (2017).
12) D. Ringot, B. Lerzy, K. Chaplain, J. P. Bonhoure, E. Auclair, and Y. Larondelle, *Bioresour. Technol.* **98,** 1812–1821 (2007).
13) A. Miller, *Chapman & Hall/CRC* (A CRC Press Company, 2002).
14) M. A. Pitt, and I. J. Myung, *Trends Cogn. Sci.* **6,** 421–425 (2002).
15) W. Zucchini, *J. Math. Psychol.* **44,** 41–61 (2000).
16) H. Akaike, *Econ. Lett.* 267–281 (1973).
17) H. Bozdogan, *Psychometrika* **52,** 345–370 (1987).
18) G. Schwarz, *Ann. Stat.* **6,** 461–464 (1978).
19) L. S. Sclove, *Psychometrika* **52,** 333–343 (1987).
20) N. Sugiura, *Commun. Stat. - Theory Methods* **7,** 13–26 (1978).
21) C. C. Yang, and C. C. Yang, *J. Classif.* **24,** 183–203 (2007).
22) K. P. Burnham, and D. R. Anderson, *Sociol. Methods Res.* **33,** 261–304 (2004).
23) A. Li, A. B. Ismail, K. Thu, M. W. Shahzad, K. C. Ng, and B. B. Saha, *Evergreen, Jt. J. Nov. Carbon Resour. Sci. Green Asia Strateg.* **1,** 37–45 (2014).
24) K. Y. Foo, and B. H. Hameed, *Chem. Eng. J.* **156,** 2–10 (2010).
25) R. R. Karri, J. N. Sahu, and N. S. Jayakumar, *J. Taiwan Inst. Chem. Eng.* **80,** 472–487 (2017).
26) J. F. Porter, G. McKay, and K. H. Choy, *Chem. Eng. Sci.* **54,** 5863–5885 (1999).
27) C. Koukouvinos, K. Mylona, and A. Skountzou, *Commun. Stat. Simul. Comput.* **40,** 484–496 (2011).
28) J. J. Dziak, D. L. Coffman, S. T. Lanza, and R. Li, *Peer J Prepr. Corte Madera* 1–20 (2015).
29) A. C. Atkinson, *Biometrika* **67,** 413–418 (1980).
30) C. M. Hurvich, and C.-L. Tsai, *Biometrika* (1989).
31) D. B. K. Anderson, 515 (2002).
32) R. L. Andrews, and I. S. Currim, *J. Mark. Res.* (2003).
33) J. Rissanen, *Automatica* **14,** 465–471 (1978).