

Applicability of some statistical tools to predict optimum adsorption isotherm after linear and non-linear regression analysis

Mohamed Chaker Ncibi ^{a,b,*}

^a “Applied Chemistry and Environment” Research Unit, Military Academy of Sousse, 4000, Tunisia

^b Laboratory of Chemistry, High Institute of Agronomy, Chott Meriem, 4042 Sousse, Tunisia

Received 4 April 2007; received in revised form 14 August 2007; accepted 15 August 2007

Available online 19 August 2007

Abstract

In any single component isotherm study, determining the best-fitting model is a key analysis to mathematically describe the involved sorption system and, therefore, to explore the related theoretical assumptions. Hence, several error calculation functions have been widely used to estimate the error deviations between experimental and theoretically predicted equilibrium adsorption values ($Q_{e,exp}$ vs. $Q_{e,theo}$ as X - and Y -axis, respectively), including the average relative error deviation, the Marquardt's percent standard error deviation, the hybrid fractional error function, the sum of the squares of the errors, the correlation coefficient and the residuals. In this study, five other statistical functions are analysed to investigate their applicability as suitable tools to evaluate isotherm model fitness, namely the Pearson correlation coefficient, the coefficient of determination, the Chi-square test, the F -test and the Student's T -test, using the commonly-used functions as references. The adsorption of textile dye onto *Posidonia oceanica* seagrass fibres was carried out, as study case, in batch mode at 20 °C. Besides, and in order to get an overall approach of the possible utilization of these statistical functions within the studied item, the examination was realized for both linear and non-linear regression analysis. The related results showed that, among the five studied statistical tools, the χ^2 and Student's T -tests were suitable to determine the best-fitting isotherm model for the case of linear modelling approach. On the other hand, dealing with the non-linear analysis, despite the Student's T -test, all the other functions gave satisfactorily results, by agreeing the commonly-used error functions calculation.

© 2007 Elsevier B.V. All rights reserved.

Keywords: Adsorption; Isotherm; Modelling; Error calculation; *Posidonia oceanica*; Textile dye

1. Introduction

The removal of dyes from industrial effluents is a field of research receiving increasing attention in the scientific community. The presence of very low concentrations of dyes in effluent is highly visible and undesirable. Moreover, they are very stable and difficult to degrade due to their resistance to heat, light, water and oxidising agents [1]. Among several dye removal technologies including nanofiltration membranes [2], chemical catalysis [3] and microbial degradation [4], the biosorption seems to have a real promising potential to be widely used as an eco-friendly and cheap method for textile effluents decontamination [5–7].

Equilibrium data, commonly known as adsorption isotherms, are the basic requirements for the design of adsorption systems. In order to optimize the design of a specific sorbate/sorbent system to remove dyes from effluents, it is important to establish the most appropriate correlation for the experimental equilibrium data (curves). Previously, some researches were carried out within such issue [8–10]. Many isotherm equations are commonly appearing in the biosorption literature including Langmuir [11], Freundlich [12], Redlich–Peterson [13], Temkin [14] and Elovich [15]. Besides, to sufficiently use the theoretical assumptions behind these mathematical equations, several error deviation functions have been used to adequately measure the goodness of fit of the models, such as the correlation coefficient (R^2), the sum of the squares of the errors (SSE), the average relative error deviation (ARED), the Marquardt's percent standard error deviation (MPSED), the hybrid fractional error function (HYBRID) and the residual analysis (RESID).

* Correspondence address: Laboratory of Chemistry, High Institute of Agronomy, Chott Meriem, 4042 Sousse, Tunisia. Tel.: +216 73348546; fax: +216 73348691.

E-mail address: ncibi.mc@yahoo.com.

The main aim of this research was to investigate, for both linear and non-linear analysis, the applicability of other known statistical tools, namely the Pearson correlation coefficient (r), the coefficient of determination (r^2), the Chi square test (χ^2), the F -test and the Student's T -test in determining the best-fitting isotherm model(s). In the present research work, the single component sorption study case was the biosorption of direct Solophenyl Brown textile dye onto Mediterranean *Posidonia oceanica* fibrous biomass in liquid-phase batch system. The theoretically predicted isotherm data were determined using the Microsoft Excel for linear analysis and SPSS 13.0 statistic software for non-linear assessment. The random initial values used to perform the non-linear analysis were the ones deduced from the linear analysis, in order to optimize the iteration procedure. Furthermore, for the special case of three parameters Redlich–Peterson model, the runs were performed using three random initial values (i.e. \pm values deduced from the linear analysis).

2. Materials and methods

2.1. Biomass and dye solution preparation

P. oceanica biomass was harvested from Chott Mariem bay (Sousse, Tunisia). The fibres were dried, crushed, and washed thoroughly with distilled water to remove the adhering dirt. They were air dried in an oven at 40 °C for 48 h. After drying, the biosorbent was blended then sieved through a 2 mm mesh size and stored in desiccators.

An accurately weighed quantity of Azo direct dye Solophenyl Brown was dissolved in distilled water to prepare stock solution (500 mg/L). Experimental solutions of the desired concentrations were obtained by successive dilutions. Spectrophotometric scanning of dilute dye solutions was performed and absorbance maximum was identified as 420 nm. Optimum pH range was adjusted between 2 and 2.5 by addition of dilute HCl solution [16].

2.2. Batch biosorption protocol

Biosorption equilibrium assays were carried out by adding the dried sorbent (2.5 g) in 250 ml of dye solution with desired concentration and pH at 20 °C in a shaking water bath at 100 rpm. After 24 h (needed time to reach equilibrium [16]), the suspension was filtered and the final concentration of dye in solution was measured using the spectrophotometric technique. The amount of dye adsorbed onto *P. oceanica* fibres, Q_e (mg/g), was calculated by a mass balance relationship:

$$Q_e = \frac{(C_0 - C_e) \times V}{W} \text{ (mg/g)} \quad (1)$$

where C_0 and C_e are the initial and equilibrium liquid-phase concentrations of dye, respectively (mg/L), V the volume of the solution (L), and W the weight of the dry sorbent used (g).

2.3. Best-fitting isotherm model estimation

2.3.1. Commonly used error functions

2.3.1.1. Average relative error deviation (ARED). The main advantage of this error function is the minimization of the fractional error distribution across the entire studied concentration range [17]

$$\text{ARED} = \frac{1}{N} \sum \left| \frac{Q_{e,\text{cal}} - Q_{e,\text{exp}}}{Q_{e,\text{exp}}} \right| \times 100 \quad (2)$$

where N is the number of experimental data points, $Q_{e,\text{cal}}$ (mg/g) is the theoretically calculated adsorption capacity at equilibrium and $Q_{e,\text{exp}}$ (mg/g) is the experimental adsorption capacity at equilibrium.

2.3.1.2. The sum of the squares of the errors (SSE). This error estimation method is represented by Eq. (3).

$$\text{SSE} = \sum (Q_{e,\text{cal}} - Q_{e,\text{exp}})^2 \quad (3)$$

Despite its wide use, this function has a major drawback. Indeed, the calculated isotherm parameters derived from such error function will provide a better fit at the higher end of the liquid-phase concentration range. This is because the magnitude of the errors and hence the square of the errors will increase as concentration increases [18].

2.3.1.3. The Marquardt's percent standard deviation (MPSED).

This error estimation tool [19] was previously used by many researches in different research fields [20,21]. It is similar to a geometric mean error distribution which was modified to allow for the number of degrees of freedom of the system.

$$\text{MPSED} = \sqrt{\frac{\sum [(Q_{\text{exp}} - Q_{\text{cal}})/Q_{\text{exp}}]^2}{N - P}} \times 100 \quad (4)$$

where P is the number of parameters in each isotherm model.

2.3.1.4. The hybrid fractional error function (HYBRID).

This error function (Eq. (5)) was developed [22] in order to improve the fit of the SSE method at low concentration values. In this approach, each SSE value was divided by the experimental solid-phase concentration Q_e value. Furthermore, a divisor was included as a term for the number of degrees of freedom for the system (i.e. the number of data points minus the number of parameters within the isotherm equation).

$$\text{HYBRID} = \frac{1}{N - P} \sum \left| \frac{Q_{e,\text{exp}} - Q_{e,\text{cal}}}{Q_{e,\text{exp}}} \right| \times 100 \quad (5)$$

2.3.2. Alternative statistical functions

2.3.2.1. Correlation coefficient of Pearson (r). The Pearson correlation coefficient (Eq. (6)) is a sampling index, varying from -1 to 1 , reflecting the degree linearity of between two

Download English Version:

<https://daneshyari.com/en/article/583101>

Download Persian Version:

<https://daneshyari.com/article/583101>

[Daneshyari.com](https://daneshyari.com)