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# Isotherms for adsorption of boron onto new fibrous adsorbent containing glycidol ligands: linear and nonlinear regression methods

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**Abstract.** The most appropriate way to design and evaluate an adsorption system performance is by having an idea of the equilibrium relationship, which is also known as adsorption isotherms. The adsorption isotherms provide information on how pollutants such as boron are interacting with adsorbent materials. A novel glycidol-containing adsorbent for selective boron removal was synthesised by radiation-induced grafting of N-vinylformamide (NVF) onto non-woven polyethylene/polypropylene (PE/PP) fiber, followed by hydrolysis and chemical treatment. The adsorbent equilibrium behaviour was investigated using the Langmuir, Freundlich, and Redlich-Peterson isotherms. Comparison of linear and non-linear regression methods was used to determine the most suitable isotherm that best describes the boron adsorption by the new adsorbent. The non-linear method is a better way of obtaining isotherm parameters. The best-fitting isotherm was found to be the Redlich-Peterson ( $R^2 > 0.99$ ) and Langmuir isotherms ( $R^2 = 0.99$ ).

## 1. Introduction

In recent times, the increasing industrial and anthropogenic activities have led to contamination of water and wastewater by various contaminants in which boron is one of them. Boron is a non-metallic contaminant capable of causing adverse health effects to humans, animals and plants when its concentration exceeds the 2.4 mg/L recommended by the WHO and other agencies [1]. As a result, different approaches have been employed for its removal from water among which adsorption has been proven as an effective process for removing boron from water and wastewaters. Adsorption of boron onto the selective adsorbents arose from the OH group in the adsorbent responsible for binding boron via the formation of neutral boron esters or complexes of borate anions [2].

Different adsorption parameters, and the underlying thermodynamic assumptions of equilibrium models, can often shed light on the adsorption mechanism, as well as the adsorbent's surface characteristics and affinity. The most appropriate way to design and evaluate an adsorption system



performance is by having an idea of the equilibrium relationship, also known as adsorption isotherms. The adsorption isotherms provide information on how pollutants such as boron are interacting with the adsorbent materials. They are thus, of the utmost importance for optimizing the adsorption mechanism pathways, the capacities of adsorbents, expression of the surface properties and effective design of the adsorption systems. The linear regression has been of frequent used for the determination of the most fitted isotherm. However, depending on how the equation of the isotherm is linearized, the error distribution may switch whether to the better or the worst [3,4]. Hence, using the linearization method alone to estimate the isotherm equilibrium parameters will be ineffective.

In this work, a comparative study between the linear isotherm (which is mostly used for determination of the best-fit isotherm) and non-linear isotherm (which is used to avoid errors affecting  $R^2$  during linearity) methods of three different isotherms which include Langmuir, Freundlich, and Redlich–Peterson for boron adsorption by glycidol-containing adsorbent was examined to establish the best and most appropriate isotherm that fit the adsorption process. A process based on trial and error for the nonlinear method was adopted with solver add-in from Microsoft's spreadsheet tool, Microsoft Excel. The complexities and problems of the transformation of non-linear to linear equations are also discussed.

## 2. Materials and methodology

### 2.1. Materials

Polyethylene/polyethylene (PE/PP) non-woven fibrous sheet was acquired from Kurashiki Co., Japan. N-vinylformamide (NVF) (purity  $\geq 98\%$ ), Glycidol ( $\geq 96\%$ ) were purchased from Sigma Aldrich (Saint Louis, MO, USA). The chemicals were all used without any treatment or purification.

### 2.2. Adsorbent preparation

PE/PP fibrous sheet was irradiated with an electron beam at 300 kGy and grafted with 20% NVF monomer in an evacuated glass ampoule. The reaction was carried out at 70 °C for 3 h. The grafted fiber was hydrolysed with a 2 M solution of sodium hydroxide for 4 h. The hydrolysed grafted fiber was subsequently treated with 10 % glycidol moiety for 2 h to obtain the glycidol-containing adsorbent [2,5].

### 2.3. Adsorption experiments

A 1000 mg/L of standard boric acid stock solution was prepared accordingly by dissolving 5716 mg of  $H_3BO_3$  in de-ionized water. Subsequent dilutions were carried out to obtain the desired concentrations for the experiment. The batch adsorption experiment was performed at 30 °C by adding the fibrous glycidol-containing adsorbent of known weight (0.5 g) to a capped 250 mL PE conical flasks having 150 mL boric acid solutions with a concentration range of 10 mg/L to 200 mg/L. The flasks containing the mixtures were agitated using an incubator shaker at a constant speed of 210 rpm for 3 h. The pH and temperature of the solution were respectively fixed at 7 and 30 °C. After shaking, the samples were filtered, and the adsorbent was separated from the solutions. The adsorption capacity  $q_e$  (mg/g) was estimated using Equation 1.

$$q_e = [(C_o - C_e)V]/W \quad (1)$$

where, the initial and equilibrium concentrations of boron in the liquid phase were respectively represented with  $C_o$  and  $C_e$ .  $W$  is the weight of the dry adsorbent (g), and  $V$  is the liquid phase volume utilised (mL).

## 3. Results and discussion

Table 1 shows both linear and non-linear expressions for the Langmuir, Freundlich and Redlich-Peterson isotherms. It can be observed from the table that, the linearized form of Langmuir isotherm has four

different types of formulas. The type 1, type 2, type 3 and type 4 Langmuir isotherm parameters can be calculated by plotting  $C_e/q_e$  vs  $C_e$ ,  $1/q_e$  vs  $1/C_e$ ,  $q_e$  vs  $q_e/C_e$  and  $q_e/C_e$  vs  $q_e$ , respectively. Consequently, the Freundlich isotherm parameters can be calculated from the plot of  $\log q_e$  vs  $\log C_e$ , while the Redlich-Peterson isotherms parameters were evaluated by plotting  $\ln(AC_e/q_e - 1)$  vs  $\ln C_e$ . The Langmuir and Freundlich isotherms each possess only two parameters, while the Redlich-Peterson isotherm has three parameters. Thus, a trial-and-error procedure is to be adopted for the estimation of parameters to maximize the  $R^2$  value using the solver add-in, Microsoft Excel.

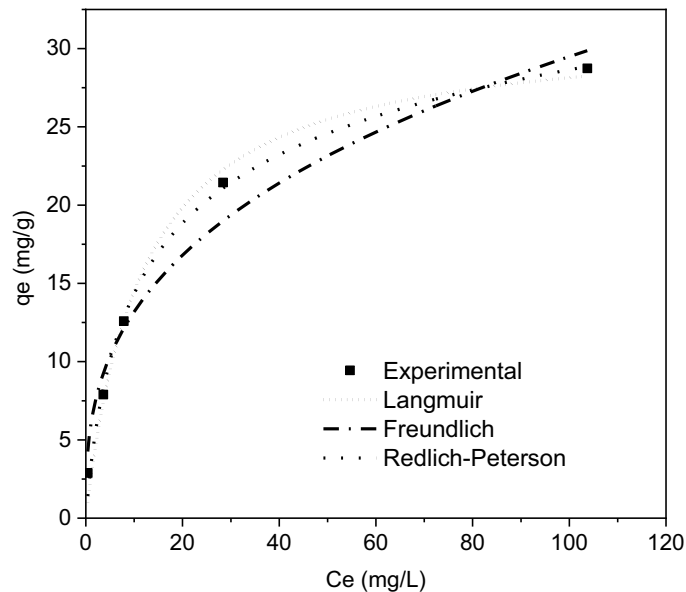
**Table 1.** The various types of isotherms in linear and non-linear form [3].

Types of isotherms	Non-linear	Linear	Plots
Langmuir 1		$\frac{C_e}{q_e} = \frac{1}{q_m} C_e + \frac{1}{K_a q_m}$	$\frac{C_e}{q_e}$ vs $C_e$
Langmuir 2		$\frac{1}{q_e} = \left( \frac{1}{K_a q_m} \right) \frac{1}{C_e} + \frac{1}{q_m}$	$\frac{1}{q_e}$ vs $\frac{1}{C_e}$
Langmuir 3	$q_e = \frac{q_m K_a C_e}{1 + K_a C_e}$	$q_e = q_m - \left( \frac{1}{K_a} \right) \frac{q_e}{C_e}$	$q_e$ vs $\frac{q_e}{C_e}$
Langmuir 4		$\frac{q_e}{C_e} = K_a q_m - K_a q_e$	$\frac{q_e}{C_e}$ vs $q_e$
Freundlich	$q_e = K_F C_e^{1/n}$	$\text{Log}(q_e) = \text{Log}(K_F) + 1/n \text{Log}(C_e)$	$\text{Log}(q_e)$ vs $\text{Log}(C_e)$
Redlich-Peterson	$q_e = \frac{AC_e}{1 + BC_e^g}$	$\ln \left( A \frac{C_e}{q_e} - 1 \right) = g \ln (C_e) + \ln (B)$	$\ln \left( A \frac{C_e}{q_e} - 1 \right)$ vs $\ln (C_e)$

The various estimated isotherm parameters from the non-linear and linear fittings are displayed (Table 2). The best fits for the linear expressions were observed to be Langmuir (type 1) and Redlich-Peterson isotherm with correlation coefficients  $>0.99$ , respectively. The low  $R^2$  value ( $<0.99$ ) from the Freundlich isotherm indicates that it is not a suitable isotherm for explaining the equilibrium adsorption phenomena of boron adsorption onto the new fibrous glycidol-containing adsorbent. Meanwhile, from the four types of linearized Langmuir isotherm expression parameters, it was found that the  $R^2$  values vary and are therefore all different from each other as seen in Table 2. The adsorption capacity of type 2, type 3 and type 4 Langmuir isotherms were found to be all low apart from type 1 which is closer to the experimental capacity. Thus, the different outcomes are indicating the problems and complexities of the linearized method for estimation of isotherm parameters. Those outcomes from the linear equations are owing to the variation in error structure upon linearization of the non-linear form of equation. So, the way the isotherm was linearized might alter the distribution of error to become either worst or better [4]. As a result, the non-linear method would be a superior means of determining the isotherm parameters to avoid such inaccuracies arising from the errors.

In the non-linear method, the parameters of the isotherm were estimated by minimization of the respective coefficients of determination between the isotherm and experimental data using the solver add-in with Microsoft's spreadsheet, Microsoft Excel, by application of computational trial-and-error procedure. The predicted and experimental equilibrium data using the non-linear method for adsorption of boron onto fibrous glycidol-containing adsorbent is as shown in Figure 1. The distribution of error was not altered in the non-linear method since all of the isotherm parameters were fixed on the same axis. The listed isotherm parameters in Table 2 show the coefficients of determination ( $R^2$ ) to be 0.99, 0.97, and

>0.99 for the non-linear Redlich-Peterson, Freundlich and Langmuir isotherm, respectively. Both Redlich-Peterson and Langmuir isotherm have higher  $R^2$  values, but the Redlich-Peterson isotherm was found to be more appropriate for the description of this adsorption system. Similarly, adsorption of boron onto NMDG functionalized Nylon fibrous adsorbent was also found to follow the Redlich-Peterson isotherm [6].

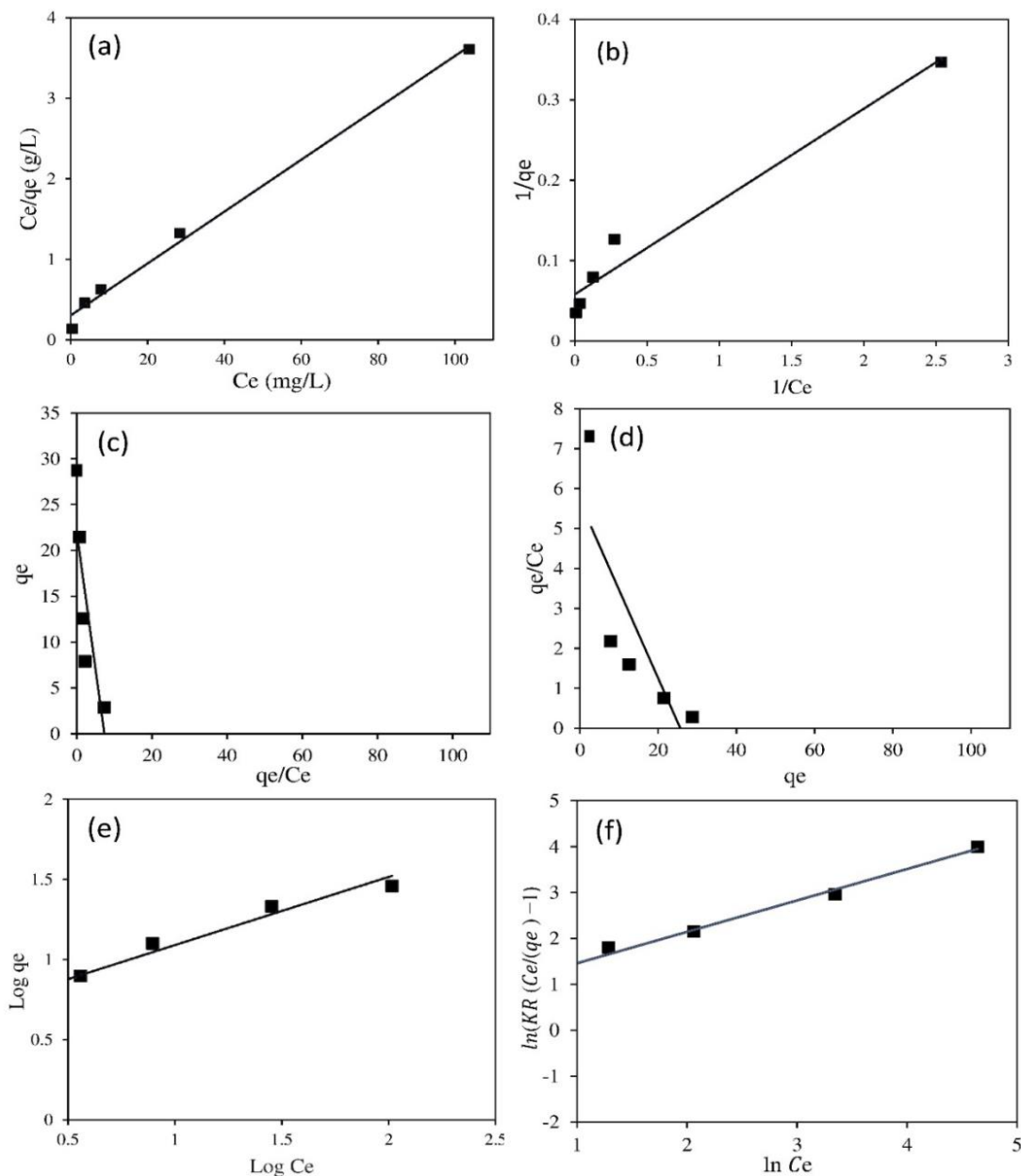


**Figure 1.** Plots of isotherms for boron adsorption using the non-linear method.

**Table 2.** Isotherm parameters obtained using the linear and non-linear method.

	Type 1	Type 2	Type 3	Type 4
Langmuir isotherm constants (linear method)				
$R^2$	0.99350	0.96580	0.66120	0.66120
$K_L$ (L/g)	0.10624	1.99482	0.13610	0.03895
$q_m$ (mg/g)	31.0559	8.65801	0.33463	4.52080
Freundlich isotherm constants (linear method)				
$R^2$	0.98320			
$n$	2.35073			
$K_F$	4.62168			
Redlich-Peterson isotherm constants (linear method)				
$R^2$	0.99570			
$A$	15.34000			
$B$	2.16994			
$g$	0.68460			
Langmuir isotherm constants (non-linear method)				
$R^2$	0.98941			
$K_L$ (L/g)	0.08560			
$q_m$ (mg/g)	31.42898			

	Type 1	Type 2	Type 3	Type 4
Freundlich isotherm constants (non-linear method)				
$R^2$	0.97411			
$n$	2.86146			
$K_F(\text{mg/g})(\text{L/g})^n$	5.89810			



**Figure 2.** Plots of: (a) Langmuir 1, (b) Langmuir 2, (c) Langmuir 3, (d) Langmuir 4, (e) Freundlich (f) Redlich-Peterson isotherms for boron adsorption using the linear method.

**Table 2.** Isotherm parameters obtained using the linear and non-linear method (continued).

	Type 1	Type 2	Type 3	Type 4
Redlich-Peterson isotherm constants (non-linear method)				
R <sup>2</sup>	0.99422			
A (L/g)	3.97194			
B (1/mg)	0.24335			
g	0.86157			

#### 4. Conclusion

The boron adsorption onto new prepared glycidol-containing adsorbent from aqueous solution was investigated on basis of equilibrium studies. For the Langmuir linear forms of isotherm, the (type 1) was the most fitted isotherm. The Redlich-Peterson is the most suitable isotherm in both linear and non-linear methods of boron adsorption onto the glycidol-containing adsorbent. Both non-linear and linear regression approaches were found to adequately describe the equilibrium data. However, the non-linear method was found to describe the boron adsorption more appropriately onto the new glycidol-containing adsorbent.

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