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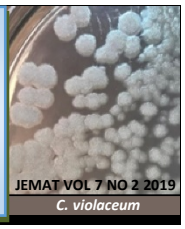

Kinetics of the Removal of Polybrominated Diphenyl Ethers from Aqueous Solutions by Using pressure steam–washed Black Tea

Jaafar, I.N.M.[1], Sabullah, K.[2], Othman, A.R.[3], Yasid, N.A.[1], Halmi, M.I.E.[4], Shukor, M.Y.[1]*

[1]Department of Biochemistry, Faculty of Biotechnology and Biomolecular Sciences, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, D.E, Malaysia.
[2]Biotechnology Programme, Faculty of Science and Natural Resources, Universiti Malaysia Sabah, 88400 Kota Kinabalu, Sabah
[3]Department of Chemical Engineering, Faculty of Engineering and Built Environment, Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Selangor, D.E, Malaysia.
[4]Department of Soil Management, Faculty of Agriculture, Universiti Putra Malaysia, 43400 UPM Serdang, Selangor, D.E, Malaysia.

*Corresponding author:
Prof. Dr. Mohd Yunus Shukor,
Department of Biochemistry,
Faculty of Biotechnology and Biomolecular Sciences,
Universiti Putra Malaysia,
43400 UPM Serdang, Selangor,
Malaysia.
Email: mohdyunus@upm.edu.my

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ABSTRACT

Established approaches for the management of contaminants include things like membrane separation, ion exchange, precipitation, transformation and biosorption. Of all of these technologies, biosorption has lots of features that include low running expenditures, very effective detoxification of toxicants at low levels, low quantity of removal components as well as does not require nutrient needs as with bacterial-based remediation, theaforementioned being restricted to the existence of heavy metals and other toxicants. The biosorption of BDE-3 on spent black tea was successfully fitted to three models—pseudo-1st, pseudo-2nd and Elovich. Statistical analysis based on root-mean-square error (RMSE), adjusted coefficient of determination (adjR^2), accuracy factor (AF), bias factor (BF), corrected AICc Bayesian Information Criterion (BIC), (Akaike Information Criterion) and Hannan–Quinn information criterion (HQC) showed that the pseudo-second order model is the best model giving valuable parameters such as the equilibrium sorption capacity q_e and the pseudo-second-order rate constant, k_2, which can be further utilized in isothermal modelling analysis. Further analysis is needed to provide proof for the chemisorption mechanism usually tied to this kinetic.

INTRODUCTION

Polybrominated diphenyl ethers (PBDEs) flame retardants are extensively incorporated into many consumer products such as plastics, electronic appliances, textiles, building materials, wire insulation and upholstery foam [1,2] to meet fire safety regulations since the 1970s by prolonging flame dispersion and interfering with the combustion of polymeric materials [3]. There are 209 possible congeners in PBDE family, and two of them, namely 4-bromodiphenyl ether (BDE-3) and 4,4-dibromodiphenyl ether (BDE-15) are two of the most ubiquitously used as flame-retardant additives. Unlike reactive brominated flame retardants (BFRs) that are chemically bonded onto the polymer, additive BFRs like PBDEs which are blended physically, do not form chemical bonds with the polymeric matrix and tend to leach out into the surroundings [4,5]. As BDE-3 and BDE-15 are the most abundant photodegradation products of higher brominated PBDEs, considerable levels of both congeners have been found in the environment [6–8].

The United Nations Environment Programs (UNEP) officially identified PBDE as a new class of persistent organic pollutants (POPs) in 2009 [9]. Several traits contributed to their persistence in the environment including chemical stability, long half-life, low vapor pressure, high lipid solubility, and resistance to degradation [10]. These lipophilic PBDEs have chemical structures that are very similar to that of thyroid hormones, hence they are regarded as endocrine disruptors that can trigger cancer and cause neurodevelopmental deficits [11,12]. Toxicity effects of PBDEs have become a global concern, thus the quest for the best remediation methods of PBDE-contaminated environment is of the utmost importance. At present, three remediation

mechanisms often applied for PBDEs are anaerobic biodegradation, photochemical degradation and adsorption. PBDE-47 for instance have been reported to be photodegraded in the presence of non-ionic surfactant solutions Brij 35, Brij 58, Tween 80, with the best performance showed by Brij 35, and the most predominant photoproducts were BDE-28, BDE-15 and BDE-3 [13].

Despite its extensive use as effective adsorbent to remove numerous organic pollutants, the high amount of money required to operate activated carbon-based adsorption is a limitation to many. Hence, low-cost and safe, non-hazardous adsorbents are urgently needed. These alternative adsorbents could be biosorbents and wastes generated from the agricultural or industrial sectors. Among the adsorbents reported to effectively treat pollutants like heavy metals and dyes are agricultural wastes such as spent tea leaves [14] and pineapple leaf [15] and inexpensive materials like chitosan and zeolites [16]. Notably, agricultural wastes application as alternative adsorbents came into the limelight, due to these four attractive factors; a) highly abundant; b) no/simple pre-treatment or activation process prior to use; c) regeneration-free, contrary to activated carbon which requires regeneration; adsorption process require less supervision and maintenance. Unfortunately, post-application disposal and lack of documentation in real wastewater systems negatively affect the use of these potential adsorbents in wastewater treatment [3].

In a previous study, the evaluation of spent black tea as a potential low-cost adsorbent for removing BDE-3 and BDE-15 from aqueous solutions was attempted [17]. The correct assignment of the kinetics and isotherms of biosorption is urgently needed in order to understand the mechanism of biosorption of glyphosate. The linearization from of an obviously nonlinear curve can provide issues on the error structure of the data making it extra difficult to estimate uncertainty of the parameters of the kinetics which are commonly shown in the form of a 95% confidence interval range [18]. In addition, the transformation of data for linearization can result in the introduction of error into the independent variable. In addition, alteration of the weight placed on each data point can occur that normally leads to differences in the fitted parameter values between linear and nonlinear versions of the Langmuir model [19]. In this study the published data from the biosorption of BDE-3 and BDE-15 from black tea [17] was remodeled with several more kinetic models (**Table 1**) and then regressed using nonlinear regression method and assessment of the best mode was carried out using various error function analysis.

Table 1. Kinetic models utilized in this study.

Model	Equation	Reference
Pseudo-1st order	$q_t = q_e(1 - e^{-K_1 t})$	[20]
Pseudo-2nd order	$q_t = \frac{K_2 {q_e}^2 t}{(1 + K_2 q_e t)}$	[21]
Elovich	$q_t = \frac{1}{\beta ln\alpha\beta} + \frac{1}{\beta lnt}$	[22]

METHODS

Data acquisition, handling and fitting

Data from **Fig. 1** from a published work [17] were digitized using the software Webplotdigitizer 2.5 [23]. Digitization using this software has been acknowledged for its reliability [24,25]. In the original published work, the data was not converted into the sorption capacity at time t or q_t of which this study did to be able to calculate the sorption capacity at equilibrium or q_e. will convert which is the amount of PBDE absorbed per g of adsorbent. The data were then nonlinearly regressed using the curve-fitting software CurveExpert Professional software (Version 1.6).

Statistical analysis

Commonly used statistical discriminatory methods such as corrected AICc (Akaike Information Criterion), Bayesian Information Criterion (BIC), Hannan and Quinn's Criterion (HQ), Root-Mean-Square Error (RMSE), bias factor (BF), accuracy factor (AF) and adjusted coefficient of determination (R^2).

The RMSE was calculated according to **Eq. (1)**, [18], n is the number of experimental data, Ob_i and Pd_i are the experimental and predicted data while p is the number of parameters. Smaller number of parameters is expected to give a smaller RMSE values. This error function puts up a penalty for models having more parameters.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(Pd_i - Ob_i)^2}{n-p}} \quad \textbf{(Eqn. 1)}$$

As R^2 or the coefficient of determination ignores the number of parameters in a model, the adjusted R^2 is utilized to overcome this issue. In the equation (**Eqns. 2** and **3**), the total variance of the y-variable is denoted by S_y^2 while RMS is the Residual Mean Square. This error function puts up a penalty for models having more parameters.

$$Adjusted\left(R^2\right) = 1 - \frac{RMS}{S_Y^2} \quad \textbf{(Eqn. 2)}$$

$$Adjusted\left(R^2\right) = 1 - \frac{\left(1-R^2\right)(n-1)}{(n-p-1)} \quad \textbf{(Eqn. 3)}$$

The Akaike Information Criterion (AIC) is based on the information theory. It balances between the goodness of fit of a particular model and the complexity of a model [26]. To handle data having a high number of parameters or a smaller number of values corrected Akaike information criterion (AICc) is utilized [27]. The AICc is calculated as follows (**Eqn. 4**), where p signifies the quantity of parameters and n signify the quantity of data points. A model with a smaller value of AICc is deemed likely more correct [27].

$$AICc = 2p + n\ln\left(\frac{RSS}{n}\right) + 2(p+1) + \frac{2(p+1)(p+2)}{n-p-2} \quad \textbf{(Eqn. 4)}$$

Aside from AICc, Bayesian Information Criterion (BIC) (**Eqn. 5**) is another statistical method that is based on information theory. This error function penalizes the number of parameters more strongly than AIC [28].

$$BIC = n.\ln\frac{RSS}{n} + k.\ln(n) \quad \textbf{(Eqn. 5)}$$

A further error function method based on the information theory is the Hannan–Quinn information criterion (HQC) (**Eqn. 6**). The HQC is strongly consistent unlike AIC due to the ln ln *n* term in the equation [27];

$$HQC = n \times ln\frac{RSS}{n} + 2 \times k \times ln(\ln n) \qquad \textbf{(Eqn. 6)}$$

Further error function analysis that originates from the work of Ross [29] are the Accuracy Factor (AF) and Bias Factor (BF). These error functions test the statistical evaluation of models for the goodness-of-fit but do not penalize for number of parameter (**Eqns. 7 and 8**). These error function, however do not put up a penalty for models having more parameters.

$$\text{Bias factor} = 10^{\left(\sum_{i=1}^{n}\log\frac{(Pd_i/Ob_i)}{n}\right)} \qquad \textbf{(Eqn. 7)}$$

$$\text{Accuracy factor} = 10^{\left(\sum_{i=1}^{n}\log\frac{|(Pd_i/Ob_i)|}{n}\right)} \qquad \textbf{(Eqn. 8)}$$

RESULTS AND DISCUSSION

The absorption kinetics data from a published work [17] on the biosorption of BDE-3 from black tea were analyzed using three models—pseudo-1st, pseudo-2nd and Elovich, and fitted using non-linear regression. The Elovich model was the poorest in fitting the curve based on visual observation followed by Pseudo-1st order (**Figs. 1-3**). Statistical analysis based on root-mean-square error (RMSE), adjusted coefficient of determination (adjR^2), bias factor (BF), accuracy factor (AF), corrected AICc (Akaike Information Criterion), Bayesian Information Criterion (BIC) and Hannan–Quinn information criterion (HQC) that showed that the pseudo-second order model is the best model.

Kinetic analysis using the pseudo-second order model gave a value of equilibrium sorption capacity q_e for 0.01 g per L adsorbent of 459.94 mg g^{-1} (95% confidence interval from 452.36 to 467.51) and a value of the pseudo-second-order rate constant, k_2 of 0.0005 (95% confidence interval from 0.00035 to 0.00064) while the equilibrium sorption capacity q_e for 0.01 g per L adsorbent of 472.75 mg g^{-1} (95% confidence interval from 464.61 to 480.88) and a value of the pseudo-second-order rate constant, k_2 of 0.00019 (95% confidence interval from 0.00016 to 0.00021). The vast discrepancy from the originally published works is as a result of the values of the data was not converted into the sorption capacity at time t or q_t of which will ot give the calculated the sorption capacity at equilibrium or q_e.

Table 2. Error function analysis of regressed models of the biosorption of 3-BDE on 0.01 g per L of spent black tea.

Model	*p*	RMSE	*adR*^{2}	AICc	BIC	HQC	AF	BF
Pseudo-1st order	2	9.895	0.996	47.73	33.63	32.40	1.014	1.000
Pseudo-2nd order	2	4.499	0.999	36.70	22.59	21.36	1.006	1.000
Elovich	2	9.200	0.996	46.71	32.61	31.38	1.016	0.998

Note:
RMSE Root mean Square Error
p no of parameters
adR^2 Adjusted Coefficient of determination
BF Bias factor
AF Accuracy factor
AICc Adjusted Akaike Information Criterion

Table 2. Error function analysis of regressed models of the biosorption of 3-BDE on 0.02 g per L of spent black tea.

Model	p	RMSE	*adR*^{2}	AICc	BIC	HQC	AF	BF
Pseudo-1st order	2	16.547	0.987	54.93	40.82	39.59	1.028	0.999
Pseudo-2nd order	2	4.329	0.999	36.16	22.05	20.82	1.007	1.000
Elovich	2	8.822	0.996	46.13	32.02	30.79	1.014	1.000

Note:
RMSE Root mean Square Error
p no of parameters
adR^2 Adjusted Coefficient of determination
BF Bias factor
AF Accuracy factor
AICc Adjusted Akaike Information Criterion

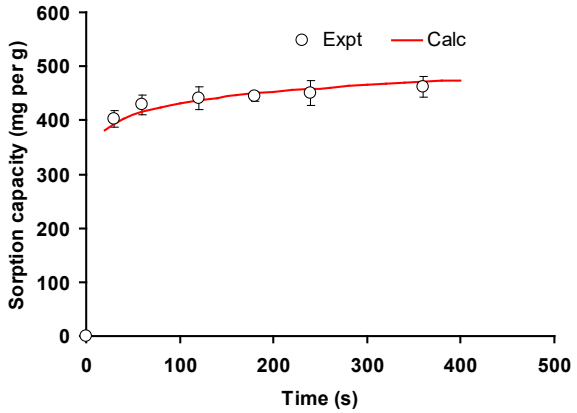

Fig. 1. Kinetics of on the biosorption of BDE-3 on 0.01 g per L spent black tea modelled using the Elovich model.

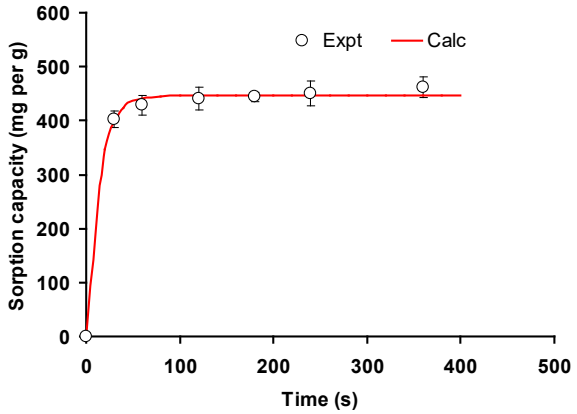

Fig. 2. Kinetics of on the biosorption of BDE-3 on 0.01 g per L spent black tea modelled using the pseudo-1st order model.

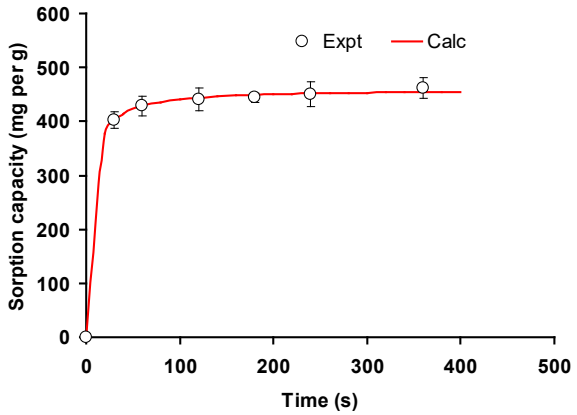

Fig. 3. Kinetics of on the biosorption of BDE-3 on 0.01 g per L spent black tea modelled using the pseudo-2nd order model.

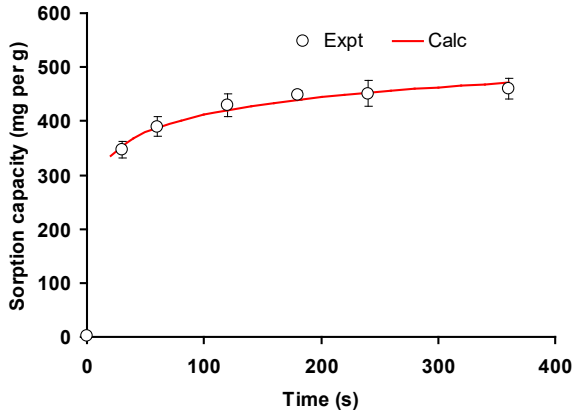

Fig. 4. Kinetics of on the biosorption of BDE-3 on 0.02 g per L spent black tea modelled using the Elovich model.

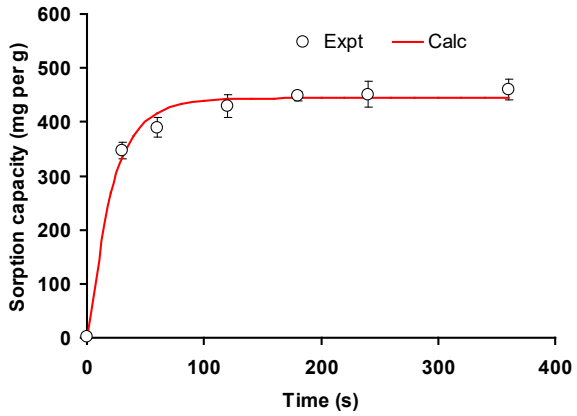

Fig. 5. Kinetics of on the biosorption of BDE-3 on 0.02 g per L spent black tea modelled using the pseudo-1st order model.

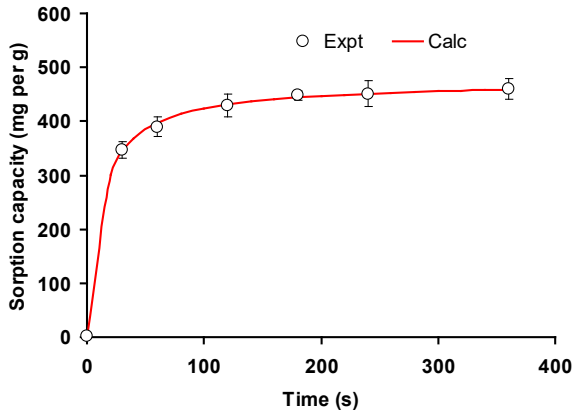

Fig. 6. Kinetics of on the biosorption of BDE-3 on 0.02 g per L spent black tea modelled using the pseudo-2nd order model.

Table 2. Constants obtained from the modelling exercise for BDE-3 using 0.01 g per L adsorbent (black tea).

Kinetic model	Parameter	Values (95% confidence interval)	Values from [17]
Pseudo-first order	q_e (mg per g)	446.72 (434.87 to 458.58)	-n.a.
	k_1 (s^{-1})	0.075 (0.055 to 0.095)	-n.a.
Pseudo-second order	q_e (mg per g)	459.94 (452.36 to 467.51)	-n.a.
	K_2 (s^{-1})	0.0005 (0.00035 to 0.00064)	-n.a.
Elovich	α (mg per g per s)	0.032 (0.030 to 0.034)	-n.a.
	β (g per mg)	338832 (97654 to 580010)	-n.a.

Note: -n.a. not available

Table 3. Constants obtained from the modelling exercise for BDE-3 using 0.02 g per L adsorbent (black tea).

Kinetic model	Parameter	Values (95% confidence interval)	Values from [17]
Pseudo-first order	q_e (mg per g)	444.039 (423.06 to 465.03)	-n.a.
	k_1 (s^{-1})	0.046 (0.033 to 0.059)	-n.a.
Pseudo-second order	q_e (mg per g)	472.75 (464.61 to 480.88)	4.79
	K_2 (s^{-1})	0.00019 (0.00016 to 0.00021)	0.0257
Elovich	α (mg per g per s)	0.02 (0.015 to 0.027)	-n.a.
	β (g per mg)	3075 (-3938 to 10088)	-n.a.

Note: -n.a. not available

The possible rate controlling steps and mechanism of sorption such as mass transport processes and physical or chemical reactions can be investigated via kinetic models such as the pseudo-1st order equation, the pseudo-2nd order equation as well as the Elovich equation.

The pseudo-1st order and pseudo-2nd order rate laws are two types of adsorption kinetics that are generally used. The pseudo-1st order kinetics (hereafter denoted by K11) was first introduce by Lagergren at the end of the 19th century [8]. The pseudo-2nd order kinetics was introduced in the middle of the 80's [9,10] and gain prominence in 1999 when Ho and McKay suggest the pseudo-2nd order kinetics to be the dominant mechanism and the thousands of literature citations have proven this point [30].

In the pseudo first order reaction there is a constant concentration of the adsorbate as it is set at saturation level resulting in the adsorbate to be adsorbed at a constant rate. In the event film diffusion controls the rate, the inverse relationship between rate and particle size, the distribution coefficient and the film thickness can be overcome by stirring the system and using smaller particle size adsorbent. In this situation, the label physisorption is given as the rate-limiting step is diffusion and is independent on the level of both reactant (physical exchange).

In a reaction governs by a pseudo-2nd order reaction, it is anticipated that chemical reaction controls the rate-controlling step, a process known as chemisorption. Under these conditions, the sorption kinetics follow a reversible second order reaction at low adsorbate/adsorbent ratios while at higher sorbate/sorbent ratios, two competitive reversible second order reactions will arise [31].

Nevertheless, critics have advised against jumping to the conclusion that the mechanism is a chemisorption based only on kinetics data. It is suggested that further proofs need to be supplemented which include the evaluation results of the activation energies by repeating the experiment at numerous temperatures and also by checking out the process rates dependences to the sizes of the adsorbent particle [32]. In addition, increasing the data points to more than twenty especially at earlier times can statistically discriminate better whether a reaction is 1st or 2nd order. In addition, various error functions needed to be utilized instead of the popular correlation coefficient value as the sole discriminant error function [33–35].

The pseudo-2nd order kinetics model was utilized in the original work without resorting to existing mathematical model comparison but the fact that the PSO model is the best model indicates its wide application and suitability in biosorption works. The PSO model has been reported to be the best model in several studies [36–39] including flame retardants such as tetrabromobisphenol A [40,41], BDE-47 [42], 4-BDE [35], hexabromocyclododecane [43], and the sorption of the OPFRs; tri(n-butyl) phosphate (TnBP), tris(2-butoxyethyl) phosphate (TBEP), and tris(2-chloroethyl) phosphate (TCEP) on Pahokee peat soil [44], the adsorption of tetrakis (hydroxymethyl) phosphonium chloride (THPC) on biochar [45] and the adsorption of tricresyl phosphate onto graphene nanomaterials [46] while the adsorption of tris-(2,3-dibromopropyl) isocyanurate are best modelled using a pseudo-first order [47].

CONCLUSION

The biosorption of BDE-3 on spent black tea was successfully fitted to three models—pseudo-1st, pseudo-2nd and Elovich. Statistical analysis based on root-mean-square error (RMSE), adjusted coefficient of determination (adjR^2), accuracy factor (AF), bias factor (BF), corrected AICc Bayesian Information Criterion (BIC), (Akaike Information Criterion) and Hannan–Quinn information criterion (HQC) showed that the pseudo-second order model is the best model giving valuable parameters such as the equilibrium sorption capacity q_e and the pseudo-second-order rate constant, k_2, which can be further utilized in isothermal modelling analysis.

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