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Discussion

Comments on "Treatment of malachite green dye containing solution using bio-degradable sodium alginate/NaOH treated activated sugarcane baggsse charcoal beads: Batch, optimization using response surface methodology and continuous fixed bed column study" and "Adsorption and oxidation of ciprofloxacin in a fixed bed column using activated sludge derived activated carbon"

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ABSTRACT

This comment analyses the results of the fixed-bed column modeling from the studies published by Gupta and Garg (2019), and Das et al. (2020), which are the last two papers on this topic published in this journal.

1. Introduction

The last two papers published in the *Journal of Environmental Management* with regard to the application of kinetic models (such as the Thomas model, the Yoon- Nelson model, and the Bohart-Adams model) in adsorption processes in fixed bed columns are the work of Gupta and Garg (2019) titled as "*Adsorption and oxidation of ciprofloxacin in a fixed bed column using activated sludge derived activated carbon*", and the work of Das et al. (2020) titled as "*Treatment of malachite green dye containing solution using bio-degradable Sodium alginate/NaOH treated activated sugarcane baggsse charcoal beads: Batch, optimization using response surface methodology and continuous fixed bed column study*". These two works provide novel and valuable information on the removal of dyes and antibiotics from wastewaters using adsorption technology. However, there are two misunderstandings regarding the application of the Bohart-Adams, Yoon-Nelson, and Thomas models that need to be discussed to avoid future confusion.

2. Discussion

2.1. The Bohart-Adams model

The two papers under discussion have used the Thomas, Yoon-Nelson, and "Adams-Bohart" models to fit the experimental data and estimate the characteristic parameters of each model. The authors of both articles have found that the Bohart-Adams model has the worst fit to the experimental data based on the correlation coefficient (R^2). The Bohart-Adams model equation used by Gupta and Garg (2019), and Das et al. (2020) in their paper is written in Equation (1).

$$\ln\left(\frac{C}{C_0}\right) = k_{AB}C_0t - k_{AB}N_0\frac{Z}{v} \quad (1)$$

where, C_0 and C (mg/L) indicated the inlet concentration and effluent concentration, k_{AB} (L/(min·mg)) is the Bohart-Adams rate coefficient, N_0 (mg/L) is the maximum volumetric adsorption capacity, Z (cm) is the bed height, and v (cm/min) is the superficial velocity. Equation (1) may be rewritten in its breakthrough form as shown in Equation (2).

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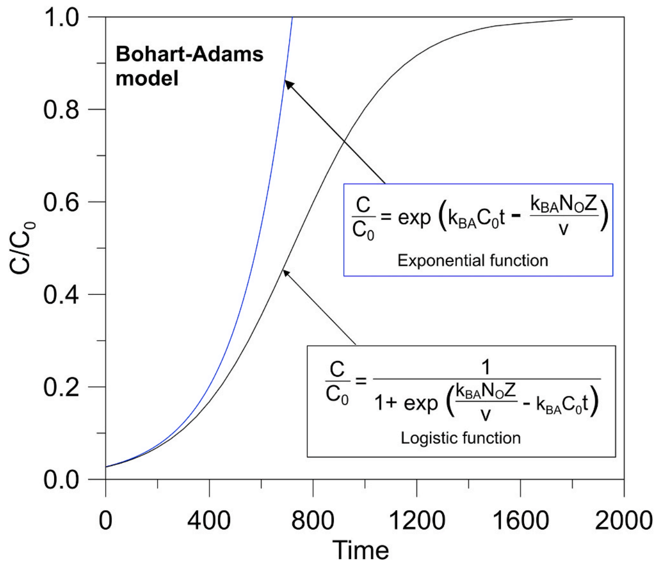

Fig. 1. Comparison of the exponential and logistic equation of the Bohart-Adams model.

$$\frac{C}{C_0} = \exp\left(k_{AB}C_0t - k_{AB}N_0\frac{Z}{v}\right) \tag{2}$$

However, it is necessary to bear in mind that Equations (1) and (2) are oversimplified versions of the Bohart-Adams model. In fact, Equation (2) is an exponential function, thus C/C_0 increases exponentially with time, obtaining C/C_0 vales higher than unity. Using Equation (2), a J-shaped curve is obtained (Fig. 1), and not an S-shaped sigmoid curve, which is characteristic of the breakthrough curve in adsorption processes. To obtain S-shaped breakthrough curves, a more general version of the Bohart-Adams model should be used given by Equations (3) and (4) (Amundson, 1948; Bohart and Adams, 1920).

$$\ln\left(\frac{C_0}{C} - 1\right) = \frac{k_{BA}N_0Z}{v} - k_{BA}C_0t \tag{3}$$

$$\frac{C}{C_0} = \frac{1}{1 + \exp\left(\frac{k_{BA}N_0Z}{v} - k_{BA}C_0t\right)} \tag{4}$$

As can be seen in Fig. 1, Equation (4) is a logistic function that produces an S-shaped breakthrough curve, which is more realistic and similar to the experimental data obtained in adsorption tests. Although the authors explain that Equation (2) was used only to study the initial region of the breakthrough curve, the paper published by Chu (2020) has shown that Equation (4) can be more accurate even in the initial region. Therefore, there are no advantages in using Equation (2) to fit experimental data.

2.2. The Bohart-Adams, Thomas, and Yoon-Nelson models

Gupta and Garg (2019), and Das et al. (2020) in their paper have used the Thomas model, the Yoon- Nelson model, and "Adams-Bohart model" as independent models. Although the equations of the three models have an independent origin and were derived by their authors independently, it is easy to show that the equations of these three models are mathematically equivalent.

Table 1 shows the equations of the Yoon-Nelson and Thomas model used by Gupta and Garg (2019), and Das et al. (2020) in their paper. These equations can be rearranged and rewritten as shown in Equations (5) and (6) for both models.

$$\text{Thomas model}: \quad \ln\left(\frac{C_0}{C} - 1\right) = \frac{k_{Th}q_0m}{Q} - k_{Th}C_0t \tag{5}$$

$$\text{Yoon} - \text{Nelson model}: \quad \ln\left(\frac{C_0}{C} - 1\right) = k_{YN}\tau - k_{YN}t \tag{6}$$

It can be seen that Equation (3) for the Bohart-Adams model, Equation (5) for the Thomas model, and Equation (6) for the Yoon-

Table 1
The Yoon-Nelson and Thomas models used by the two papers under discussion.

Model	Gupta and Garg (2019)	Das et al. (2020)
Yoon-Nelson model	$\frac{C_t}{C_0 - C_t} = \exp(k_{YN}t - k_{YN}\tau)$	$\ln\left(\frac{C}{C_0 - C}\right) = K_{YN}t - \tau K_{YN}$
Thomas model	$\ln\left(\frac{C_0}{C_t} - 1\right) = \frac{mk_{Th}q_0}{Q} - k_{Th}C_0t$	$\ln\left(\frac{C_0}{C} - 1\right) = \frac{K_{Th}q_Sm}{Q} - K_{Th}C_0t$

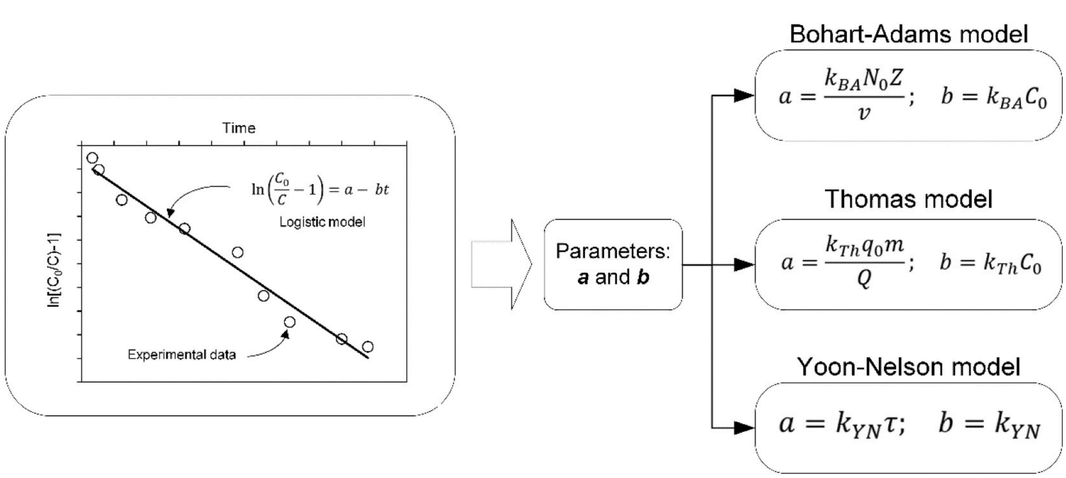

Fig. 2. Scheme to obtain the Bohart-Adams, Thomas, and Yoon-Nelson parameters using Logistic model.

Nelson model are identical to each other and reveal the same functional form. Therefore, these three equations can be expressed as a unified equation, which can be called "Logistic model" given by Equation (7).

$$\ln\left(\frac{C_0}{C}-1\right)=a-bt \tag{7}$$

where, the parameters a and b can have different definitions depending on the model (Fig. 2). Equation (7) can be rewritten in its breakthrough form as

$$\frac{C_t}{C_0}=\frac{1}{1+\exp(a-bt)} \tag{8}$$

Thus, the experimental data of the breakthrough curve should be fitted with the linear equation of the Logistic model (Equation (7)), then the slope and intercept of the plot $ln[(C_0/C)-1]$ vs t allow to obtain b and a, respectively. Finally, the parameters of the Thomas, Yoon-Nelson, and Bohart-Adams models can be computed using simple relations given in Fig. 2. Indeed, the Logistic model have been used in other papers.

By fitting the experimental data to the Logistic model, a single correlation coefficient value (R^2) is obtained. Therefore, it is not logical to treat the three models independently and compare one with the other based in their R^2 value. The Logistic model has been used in other papers and has shown a perfect fit for the breakthrough curve and can be used to predict the performance of continuous adsorption columns (Bakka et al., 2020; Celik et al., 2020; Chatterjee and Schiewer, 2011; Chu, 2020; Dima et al., 2020; Tan and Hameed, 2017; Yan et al., 2018). Taking into account that the equations of the Thomas, Yoon-Nelson, and Bohart-Adams model are mathematically equivalent, the model comparison analysis presented by Gupta and Garg (2019), and Das et al. (2020) in their paper has flaws, and their conclusions are not meaningful. It is hoped that this comment may reduce future confusion regarding fixed bed modeling.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

References

Amundson, N.R., 1948. A note on the mathematics of adsorption in beds. J. Phys. Colloid Chem. 52, 1153–1157. https://doi.org/10.1021/j150463a007.

Bakka, A., Mamouni, R., Saffaj, N., Laknifli, A., Aziz, K., Roudani, A., 2020. Removal of bifenthrin pesticide from aqueous solutions by treated patellidae shells using a new fixed bed column filtration technique. Process Saf. Environ. Protect. 143, 55–65. https://doi.org/10.1016/j.psep.2020.06.030.

Bohart, G.S., Adams, E.Q., 1920. Some aspects of the behavior of charcoal with respect to chlorine. J. Am. Chem. Soc. 42, 523–544. https://doi.org/10.1021/ja01448a018.

Celik, S., Duman, N., Sayin, F., Tunali Akar, S., Akar, T., 2020. Microbial cells immobilized on natural biomatrix as a new potential ecofriendly biosorbent for the biotreatment of reactive dye contamination. J. Water Process Eng. 101731. https://doi.org/10.1016/j.jwpe.2020.101731.

Chatterjee, A., Schiewer, S., 2011. Biosorption of cadmium(II) ions by citrus peels in a packed bed column: effect of process parameters and comparison of different breakthrough curve models. CLEAN - Soil, Air, Water 39, 874–881. https://doi.org/10.1002/clen.201000482.

Chu, K.H., 2020. Breakthrough curve analysis by simplistic models of fixed bed adsorption: in defense of the century-old Bohart-Adams model. Chem. Eng. J. 380, 122513. https://doi.org/10.1016/j.cej.2019.122513.

Das, L., Das, P., Bhowal, A., Bhattachariee, C., 2020. Treatment of malachite green dye containing solution using bio-degradable Sodium alginate/NaOH treated activated sugarcane baggsse charcoal beads: batch, optimization using response surface methodology and continuous fixed bed column study. J. Environ. Manag. 276, 111272. https://doi.org/10.1016/j.jenvman.2020.111272.

Dima, J.B., Ferrari, M., Zaritzky, N., 2020. Mathematical modeling of fixed-bed columns adsorption: hexavalent chromium onto chitosan flakes. Ind. Eng. Chem. Res. 59, 15378–15386. https://doi.org/10.1021/acs.iecr.0c02004.

Gupta, A., Garg, A., 2019. Adsorption and oxidation of ciprofloxacin in a fixed bed column using activated sludge derived activated carbon. J. Environ. Manag. 250, 109474. https://doi.org/10.1016/j.jenvman.2019.109474.

Tan, K.L., Hameed, B.H., 2017. Insight into the adsorption kinetics models for the removal of contaminants from aqueous solutions. J. Taiwan Inst. Chem. Eng. 74, 25–48. https://doi.org/10.1016/j.jtice.2017.01.024.

Yan, J., Xue, Y., Long, L., Zeng, Y., Hu, X., 2018. Adsorptive removal of As(V) by crawfish shell biochar: batch and column tests. Environ. Sci. Pollut. Res. 25, 34674–34683. https://doi.org/10.1007/s11356-018-3384-1.