



Modelling the Effect of Sorbate-Sorbent Interphase on the Adsorption of Pesticides and Herbicides by Historical Data Design

J. O. Ighalo^{1,2*}, A. A. Adelodun^{3,4}, A. G. Adeniyi¹, C. A. Igwegbe²

¹ Department of Chemical Engineering, Faculty of Engineering and Technology, University of Ilorin, Ilorin, Nigeria

² Department of Chemical Engineering, Nnamdi Azikiwe University, Awka, Nigeria

³ Environmental Engineering and Management Research Group, Ton Duc Thang University, Ho Chi Minh City, Vietnam

⁴ Faculty of Environment and Labour Safety, Ton Duc Thang University, Ho Chi Minh City, Vietnam

PAPER INFO

Paper history:

Received 05 September 2020

Accepted in revised form 16 November 2020

Keywords:

Adsorption process
 Environmental modeling
 Pesticides and herbicides
 Response surface methodology
 Surface area
 Water pollution control

ABSTRACT

Statistical modelling was employed to analyze the effect of sorbate-sorbent interphase on the adsorption of pesticides and herbicides from aqueous media. The dataset used for this study was sourced from relevant and reputable published papers in the past five years. Sixty-six lines of data were analyzed using response surface methodology (RSM) and historical data design (HDD) on Design expert. Five parameters were considered in the study: adsorbate's relative molecular mass (RMM), adsorbent specific surface area (SBET), adsorbent effective surface area eSBET (i.e., the portion of the SBET occupied by the sorbate molecules), the water solubility of adsorbate, and adsorbate preferential adsorption (i.e., the ratio of the amount of sorbate on the sorbent to the amount in solution). From the analysis of variance, it was observed that the SBET of the adsorbent was the most significant determining factor for the adsorption capacity, q (at a significance level of $p < 0.05$). Other significant factors were the RMM, eSBET, and the preferential adsorption. Generally, solubility did not show any significant influence on the q . The response surface model had an R^2 value of 0.9945 and an adjusted R^2 value of 0.9927. Conclusively, the q of an adsorbent towards an herbicide or a pesticide increases with increasing eSBET and SBET, irrespective of the sorbate's solubility and molecular mass.

doi: 10.5829/ijee.2020.11.04.02

INTRODUCTION

Pesticides and herbicides (P & H) are substances (or mixtures of various substances) used for the control of pests and herbs, respectively [1]. Their use gained attraction in the 1950s when the so-called 'green revolution' commenced [2]. However, the incessant population explosion, dynamics of lifestyle patterns, and technological advancement require the use of P & H in large quantities to cope with the huge demand for agricultural produce in modern times. Therefore, high levels of residual P & H are often found in the environment, which has rendered the chemical being regarded as emerging pollutants because their use has led to soil pollution [3, 4]. Further, P & H often leach from their point of primary application into nearby water bodies, thereby resulting in secondary water pollution and, sometimes, eutrophication [5]. Due to the high toxicity of P & H, these forms of pollution endanger human health via the food chain [6]. Especially, considering the importance of water to the livelihood and

survival of man, the presence, quantitation, and eventual mitigation of P & H in our waters cannot be trivialized or ignored [7, 8].

Adsorption by activated carbon [9, 10], biosorbents [11], clay [12], biochar [13, 14], carbon nanotubes [15], and polymers [16, 17] is a proven excellent method in remediating water pollution in general and those of P & H in particular. Therefore, the sorbate-sorbent interphase must be adequately understood because it influences the q of sorbents in aqueous media. Where q is introduced as adsorption capacity.

Within the scope of the authors' exhaustive search, so far, no study has investigated a historical dataset towards evaluating the effect of sorbate-sorbent interphase on the adsorption of P & H. Thereby, leaving open an interesting knowledge gap, which underlines the novelty of this study. Thence, response surface methodology and historical data design was utilized to investigate the effect of sorbate-sorbent interphase on the adsorption of P & H from aqueous media. The key adsorption properties considered were the adsorbent specific surface area

*Corresponding Author E-mail: oshea.ighalo@yahoo.com (J. O. Ighalo)

(S_{BET}), a derived effective surface area (eS_{BET}) (i.e., the portion of the S_{BET} occupied by the sorbate molecules), the water solubility of adsorbate, and adsorbate preferential adsorption (i.e., the ratio of the amount of sorbate on the sorbent to the amount in solution), and estimated preferential adsorption. The estimation of the eS_{BET} is relevant because the preferential attachment of a sorptive onto a surface depends on the number of active sites with sufficient affinity for the sorptive, irrespective of the S_{BET} . Since most studies reviewed here only reported the S_{BET} without providing (any, adequate, or quantitated) information on the chemical functionalities on the sorbents, the derivation of eS_{BET} came to the fore to inform on the relevance of the active sites on the surface to the q value. Thus, the eS_{BET} value would increase linearly with the relevant chemical surface functionality tethered on the S_{BET} , either naturally or engineered by chemical impregnation [18, 19]. The key index for evaluating the extent of sorbate-sorbent interphase is the mass adsorption capacity (q , mg/g) of the adsorbent for the specific pesticides or herbicides.

MATERIAL AND METHOD

Response surface methodology (RSM) and historical data design on Design Expert v10.0.1 (Stat Ease Inc., Minneapolis, USA) were used in this study. RSM has been discussed in detail elsewhere [20, 21]. Because the adsorption dataset used in this study was already available (i.e., does not require the pre-designing of experiments), historical data design was selected because of its flexibility. In other words, the adsorption dataset to be analysed was not pre-planned by a Design of experiments (DOE); therefore, it is suitable for the statistical modeling and analysis. This analytical approach affords the researcher the freedom of specifying the number of factors, the number of responses, and the number of lines of results. Historical data design has been previously used for the optimization of biodiesel production [22], machining condition [23], solvent extraction [24], photocatalytic degradation [25], and a host of other applications.

Description of dataset

The dataset used for this analysis was sourced from reliable and relevant open literature. Research papers specifically on herbicide or pesticide adsorption that were published within the past five years were considered. Due to the nature of the analysis, the minimum data specification required from each reviewed paper were those of q and S_{BET} of the adsorbent. Although the amount of adsorbent and the volume of sample solution data were required, they are usually reported in adsorption papers. From the original dataset, 33 papers reported on all the four required information, leading to 66 lines of data for analysis. The base data used

for current work is presented in the Supplementary material. Some of the adsorbate (P & H) represented in the dataset includes 2,4-D [26, 27], oxamyl [28], diuron [29], metribuzin [14], dicamba [16], tebuthiuron [17], lindane [30] and a host of others.

Data analysis

The adsorption dataset was entered into Design Expert v10.0.1 (Stat Ease Inc., Minneapolis, USA) under response surface methodology and historical data design for statistical modeling and analysis. Adequate care was taken to ensure that each string of factors corresponded with the assigned response. The designation of factors and response are summarized in Table 1. The molecular mass is the mass of a molecule of the adsorbate (in this case, the pesticide or herbicide), whereas the specific surface area refers to the total surface area of a unit mass of the adsorbent. Moreover, the effective surface area is the surface area of the adsorbent concerning the specific adsorbate. It is unique to each sorbate-sorbent system. The solubility is the chemical property of the adsorbate, which refers to its ability to dissolve in water (specifically for this case). The solubility values reported in the Supplementary material is for 25°C. The preferential adsorption is the adsorbate preference/affinity in getting adsorbed on the surface of the adsorbent, especially in light of other competing adsorbate. The data band shows the range of numeric values for each response and, by consequence, the range for which any model developed from the data is valid.

The design of a wastewater treatment system and equipment dimension that is appropriate to improve the performance of the existing of waste water treatment plant (WWTP) is based on maximum flow 150 m³/day. Secondary data from some literatures to calculate the size of the equipment dimension was also used.

RESULTS AND DISCUSSION

Determination of best fit model

First, the model of best fit for the input data was determined. The Design Expert software uses the sequential model sum of squares where the highest order polynomial whose additional terms are significant (and the model not aliased) is selected as the best fit. A model is said to be aliased when the estimate of an effect includes the influence of one or more other effects (and these are usually high order interactions). Furthermore, a lack-of-fit test is also performed to determine the non-aliased model with the most insignificant lack-of-fit. The lack-of-fit is an error that is observed when the analysis omits one or more critical factors or terms from the process model. The results of the sequential model sum of squares and the lack of fit test are shown in Tables 2 and 3, respectively. The models considered were the linear, two-factor interaction (2FI), quadratic, and cubic

TABLE 1. Designation of factors and response

Designation	Data	Unit	Data band
Factor 1	Relative molecular mass (RMM)	g/mol	100 < x < 500
Factor 2	Specific surface area (S _{BET})	m ² /g	0 < x < 3000
Factor 3	Effective surface area (eS _{BET})	mol/m ²	0 < x < 1
Factor 4	Solubility	mol/l	0 < x < 20
Factor 5	Preferential adsorption	Dimensionless (sorbate mols on sorbent/sorbate mols in solution)	0 < x < 50
Response	Mass adsorption capacity	mg/g	

models. Based on the verdicts presented in Tables 2 and 3, the quadratic model was selected as the model of choice for further analysis.

Analysis of variance (ANOVA) and model reduction

The ANOVA was conducted to determine the statistical significance of the quadratic model and all its associated model terms (at p<0.05). From the ANOVA results (Table 4), it was observed that the model is statistically significant, and the lack-of-fit is insignificant. In addition, we observed that the S_{BET} of the adsorbent is the most significant, limiting factor for the *q* value. Other significant factors were the RMM, eS_{BET}, and preferential adsorption values. Generally, the solubility of the adsorbate has no statistical significance on the *q*. In this case, statistical significance refers to an observable relationship between the response (*q*) and the factors over the range of data. The effect of each factor may be positive or negative. Such affirmation cannot be determined by ANOVA but by parametric investigations.

Based on the limiting factors, the derived model (whose ANOVA is presented in Table 4) is given in Equation (1). The range of validity for each factor is 100<A<500, 0<B<3000, 0<C<1, 0<D<20 and 0<E<50.

$$q \text{ (mg/g)} = -516.99 + 3.967A - 0.5529B - 1.26 \times 10^6C + 12650D + 17.62E + 2.554AB + 5368AC - 64.64AD - 0.1146AE + 2.125 \times 10^5BC + 2.743BD + 1.37 \times 10^{-3}BE + 2.105 \times 10^7CD - 4156CE + 2519DE - 7.23 \times 10^{-3}A^2 - 1.399 \times 10^{-5}B^2 + 1.343 \times 10^7C^2 - 296.6D^2 + 0.2674E^2 \quad (1)$$

Next in the modelling of the data was model reduction. Here, the insignificant terms in the model are sequentially removed whilst monitoring the ANOVA result and the model summary statistics (R², adjusted R²). This is done to improve the overall accuracy of the model. The first term removed from the model was the single solubility term 'D'. Upon recalculation, all the remaining terms remained significant except BE, C², and D². Therefore, by expunging those 3 terms, the final model (Equation (2)) had all terms significant.

$$q \text{ (mg/g)} = -348.93 + 2.914A - 0.4809B - 5.396 \times 10^5C + 11.13E + 2.159 \times 10^{-3}AB + 2515AC - 1.338AD - 0.0571AE + 2.145 \times 10^5BC + 1.779BD - 1.55 \times 10^6CD - 1427CE + 416.4DE - 5.92 \times 10^{-3}A^2 - 5.31 \times 10^{-6}B^2 + 0.0978E^2 \quad (2)$$

Note, the current model is a non-hierarchical polynomial regression model (and it excludes hierarchically inferior terms). Thus, it may be used only within the range of validity for each factor. This is because all analysis within the software is based on the coded equation. This means that these expressions cannot serve as a truly accurate predictor but can be used only by investigating the relationship between the factors and their respective responses.

Model diagnostics

The R-squared value is the variance of the experimental variables that is predictable by the correlation/model, and the closer the R² is to unity (1), the better the model [22].

TABLE 2. Results of the sequential model sum of squares

Source	Sum of Squares	df	Mean Square	F Value	p-value	Verdict
Mean vs Total	4.967e+6	1	4.967e+6			
Linear vs Mean	2.171e+6	5	4.342e+5	5.65	0.0002	
2FI vs Linear	4.513e+6	10	4.513e+5	233.00	< 0.0001	
Quadratic vs 2FI	64592	5	12918	18.02	< 0.0001	Suggested
Cubic vs Quadratic	32260	33	977.59			Aliased
Residual	0.000	12	0.000			
Total	1.175e+7	66	1.780e+5			

TABLE 3. Results of the lack-of-fit test

Source	Sum of Squares	df	Mean Square	F Value	p-value	Verdict
Linear	4.607e+6	58	79434	52.39	0.0189	
2FI	93820	48	1954.6	1.29	0.5340	
Quadratic	29227	43	679.72	0.45	0.8803	Suggested
Cubic	-3032.7	10	-303.26	-0.20	1.0000	Aliased
Pure Error	3032.7	2	1516.3			

TABLE 4. Analysis of variance (ANOVA) for quadratic model (Partial sum of squares - Type III)

Source	Sum of Squares	df	Mean Square	F Value	p-value	Verdict
Model	6.749e+6	20	3.374e+5	470.70	< 0.0001	significant
A-Relative molecular mass	5000.8	1	5000.1	6.98	0.0113	
B-Specific surface area	2.937e+6	1	2.937e+6	4096.7	< 0.0001	
C-Effective surface area	7644.0	1	7644.01	10.66	0.0021	
D-Solubility	1323.6	1	1323.6	1.85	0.1810	
E-Preferential adsorption	4372.5	1	4372.5	6.10	0.0174	
AB	47104	1	47104	65.71	< 0.0001	
AC	8585.5	1	8585.5	11.98	0.0012	
AD	31232	1	31232	43.57	< 0.0001	
AE	16787	1	16787	23.42	< 0.0001	
BC	2.933e+6	1	2.933e+6	4091.1	< 0.0001	
BD	9453.8	1	9453.8	13.19	0.0007	
BE	717.11	1	717.11	1.00	0.3226	
CD	1307.8	1	1307.8	1.82	0.1836	
CE	11511	1	11511	16.06	0.0002	
DE	4773.7	1	4773.7	6.66	0.0132	
A ²	25401	1	25401	35.43	< 0.0001	
B ²	2525.7	1	2525.7	3.52	0.0670	
C ²	796.97	1	796.97	1.11	0.2973	
D ²	783.25	1	783.25	1.09	0.3015	
E ²	12210	1	12210	17.03	0.0002	
Residual	32260	45	716.90			
Lack of Fit	29228	43	679.72	0.45	0.8803	not significant
Pure Error	3032.7	2	1516.3			
Cor. Total	6.781e+6	65				

The adjusted R² value is one that has been adjusted for the number of predictors in the correlation/model. The new model had an R² and adjusted R² values of 0.9945 and 0.9927, respectively. Such high reliability is impressive, considering that 66 lines of data (from nine different adsorbents against 32 different adsorbate) were used for the analysis. To achieve such high values for the coefficient of determination when a large pool of

data is analysed is rare. This is an indicator of the accuracy of the model in predicting the statistical relevance of the factors. The parity between the model prediction and the actual values are shown in Figure 1. Obviously, most of the 66 data points fell on the parity diagonal with negligible few outliers, further suggestive of the accuracy of the model for the intended purpose.

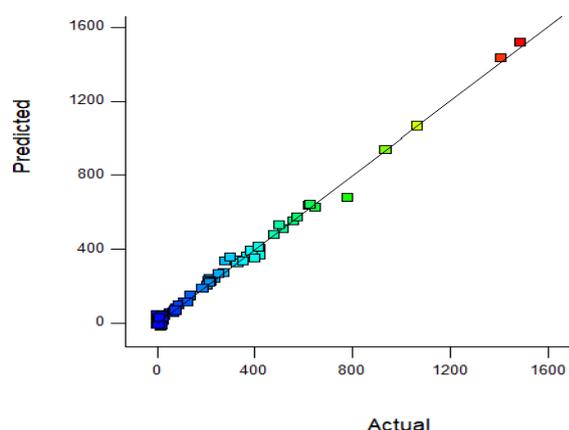


Figure 1. Parity plot of model predictions against actual results

Parametric studies

Besides, the evaluation of the statistical significance of the factors on the mass adsorption capacity, the other purpose of this paper is to conduct a parametric study. In parametric investigations, the relationship between the process parameters is evaluated in relation to the process response. Five parameters are considered in this study as factors affecting the sorbate-sorbent interactions for pesticides and herbicides. They are the adsorbate molecular mass, adsorbent specific surface area, adsorbent effective surface area, adsorbate solubility, and adsorbate preferential adsorption. The adsorbate solubility has already been shown to be a statistically insignificant factor but will be discussed also. The values on the y-axis of Figures 2-4 must be ignored as they are not the exact values because the model is a non-hierarchical polynomial regression model (and it excludes hierarchically inferior terms). The plots are chosen in such a way that all factors are discussed, and all key factor interactions are highlighted.

From Figure 2, it was observed that adsorbent having higher S_{BET} would exhibit a superior q value irrespective of the sorptive's RMM. Although the chemistry of the

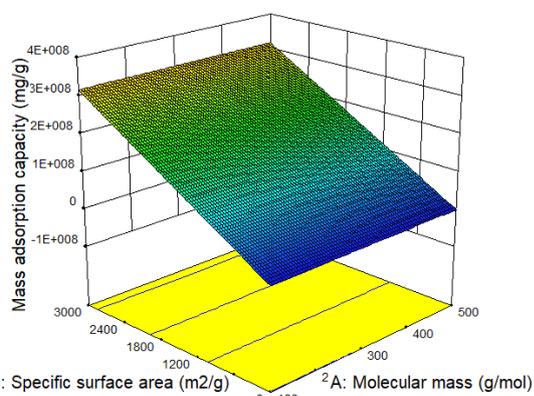


Figure 2. Effect of specific surface area and molecular mass on the mass adsorption capacity

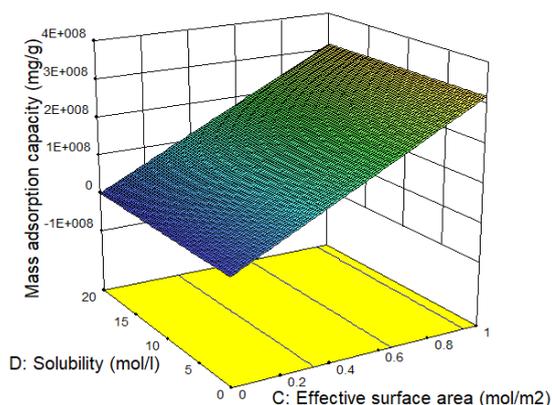


Figure 3. Effect of solubility and effective surface area on the mass adsorption capacity

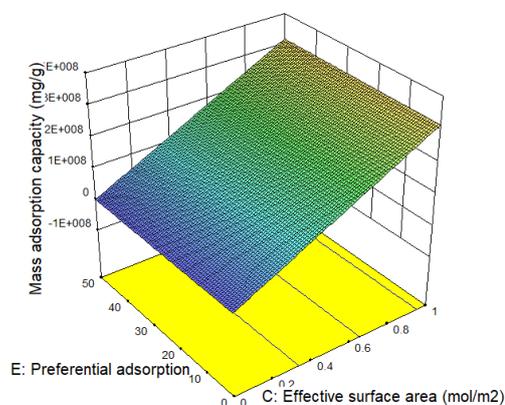


Figure 4. Effect of preferential adsorption and effective surface area on the mass adsorption capacity

sorbate-sorbent interface plays an important role in adsorption, the S_{BET} remains the primary determining factor for P & H adsorption. The initial concentration of the adsorbate is another important determining factor identified in this study with respect to P & H control. Further, it was noticed that the q increases with eS_{BET} regardless of the sorptive's solubility (Figure 3). This was expected because the eS_{BET} is a function of the active sites on the S_{BET} with an adequate affinity towards a specific adsorbate. Such specificity means that if the adsorbent has a quite S_{BET} , then more available active sites for adsorption of that specific adsorbate are expected. Therefore, other physical properties (such as pore volume and pore size distribution), and chemical properties (amount and affinity of surface chemical groups) of the adsorbent, as well as the kinetic diameter and orientation of the adsorbate often influence the q values.

The effect of dimensionless preferential adsorption (Table 1) on the adsorption capacity was barely noticed, as depicted in Figure 4, as the case was for solubility (Figure 3). This was unsurprising as solubility was not statistically significant to the response surface model

from the ANOVA. It must be emphasized that the observations from these discussions are specifically for P & H with RMM between 100 and 500 g/mol (Table 1). Thence, further inferences and wide generalizations outside this domain are not guaranteed.

CONCLUSIONS

Response surface methodology and historical data design were successfully used to investigate the effect of sorbate-sorbent interphase on the adsorption of pesticides and herbicides from aqueous media. Five parameters were considered in the study: adsorbate molecular mass, adsorbent specific surface area, adsorbent effective surface area, adsorbate solubility, and adsorbate preferential adsorption. Several important conclusions can be drawn from the study:

- i. The results of the sequential model sum of squares and the lack of fit test revealed that the quadratic model is the best fit.
- ii. From the analysis of variance (ANOVA), it was observed that the specific surface area of the adsorbent is the most significant factor affecting the adsorption capacity (at a significance level of $p < 0.05$). Other significant factors were the molecular mass, effective surface area, and the preferential adsorption.
- iii. The adsorbate's water solubility does not have a significant effect on the adsorption capacity. The model was carefully reduced to eliminate all non-significant terms before diagnostics, and parametric investigations were conducted.
- iv. The model had an R^2 value of 0.9945 and an adjusted R^2 value of 0.9927, which was quite impressive for 66 lines of data.

An adsorbent with a high specific surface area would exhibit high adsorption capacity irrespective of the relative molecular mass. The adsorption capacity of the adsorbent to the herbicide or pesticide increases at the higher effective surface area, and this holds for all domains of solubility. The effect of solubility and preferential adsorption on the adsorption capacity was barely noticed.

REFERENCES

1. Khoshnood, M., & Azizian, S., 2012, Adsorption of 2,4-dichlorophenoxyacetic acid pesticide by graphitic carbon nanostructures prepared from biomasses, *Journal of Industrial and Engineering Chemistry*, 18(5): 1796–1800. <https://doi.org/10.1016/j.jiec.2012.04.007>
2. Bezerra, C. de O., Cusioli, L. F., Quesada, H. B., Nishi, L., Mantovani, D., Vieira, M. F., & Bergamasco, R., 2020, Assessment of the use of *Moringa oleifera* seed husks for removal of pesticide diuron from contaminated water, *Environmental Technology*, 41(2): 191–201. <https://doi.org/10.1080/09593330.2018.1493148>
3. Cusioli, L. F., Bezerra, C. de O., Quesada, H. B., Alves Baptista, A. T., Nishi, L., Vieira, M. F., & Bergamasco, R., 2019, Modified *Moringa oleifera* Lam. Seed husks as low-cost biosorbent for atrazine removal, *Environmental Technology*, 1–12. <https://doi.org/10.1080/09593330.2019.1653381>
4. Yavari, S., Malakahmad, A., Sapari, N. B., & Yavari, S., 2016, Sorption-desorption mechanisms of imazapic and imazapyr herbicides on biochars produced from agricultural wastes, *Journal of Environmental Chemical Engineering*, 4(4): 3981–3989. <https://doi.org/10.1016/j.jece.2016.09.003>
5. Ioannidou, O. A., Zabaniotou, A. A., Stavropoulos, G. G., Islam, M. A., & Albanis, T. A., 2010, Preparation of activated carbons from agricultural residues for pesticide adsorption, *Chemosphere*, 80(11): 1328–1336. <https://doi.org/10.1016/j.chemosphere.2010.06.044>
6. Ayranci, E., & Hoda, N., 2005, Adsorption kinetics and isotherms of pesticides onto activated carbon-cloth, *Chemosphere*, 60(11): 1600–1607. <https://doi.org/10.1016/j.chemosphere.2005.02.040>
7. Coldebella, P. F., Fagundes-Klen, M. R., Nishi, L., Valverde, K. C., Cavalcanti, E. B., Andreo dos Santos, O. A., & Bergamasco, R., 2017, Potential effect of chemical and thermal treatment on the Kinetics, equilibrium, and thermodynamic studies for atrazine biosorption by the *Moringa oleifera* pods, *The Canadian Journal of Chemical Engineering*, 95(5): 961–973. <https://doi.org/10.1002/cjce.22756>
8. Derylo-Marczewska, A., Blachnio, M., Marczewski, A. W., Seczkowska, M., & Tarasiuk, B., 2019, Phenoxyacid pesticide adsorption on activated carbon – Equilibrium and kinetics, *Chemosphere*, 214: 349–360. <https://doi.org/10.1016/j.chemosphere.2018.09.088>
9. Hameed, B. H., Salman, J. M., & Ahmad, A. L., 2009, Adsorption isotherm and kinetic modeling of 2,4-D pesticide on activated carbon derived from date stones, *Journal of Hazardous Materials*, 163(1): 121–126. <https://doi.org/10.1016/j.jhazmat.2008.06.069>
10. Kurtoglu, A. E., & Atun, G., 2016, Competitive adsorption of 2,4-dichlorophenoxyacetic acid herbicide and humic acid onto activated carbon for agricultural water management, *Desalination and Water Treatment*, 57(53): 25653–25666. <https://doi.org/10.1080/19443994.2016.1156027>
11. Adeniyi, A. G., Ighalo, J. O., & Odetoye, T. E., 2020, Response surface modelling and optimisation of biodiesel production from Avocado plant (*Persea americana*) oil, *Indian Chemical Engineer*, 62(3): 243–250. <https://doi.org/10.1080/00194506.2019.1658546>
12. de Souza, F. M., dos Santos, O. A. A., & Vieira, M. G. A., 2019, Adsorption of herbicide 2,4-D from aqueous solution using organo-modified bentonite clay, *Environmental Science and Pollution Research*, 26(18): 18329–18342. <https://doi.org/10.1007/s11356-019-05196-w>
13. Essandoh, M., Wolgemuth, D., Pittman, C. U., Mohan, D., & Mlsna, T., 2017, Adsorption of metribuzin from aqueous solution using magnetic and nonmagnetic sustainable low-cost biochar adsorbents, *Environmental Science and Pollution Research*, 24(5): 4577–4590. <https://doi.org/10.1007/s11356-016-8188-6>
14. Essandoh, M., Wolgemuth, D., Pittman, C. U., Mohan, D., & Mlsna, T., 2017, Phenoxy herbicide removal from aqueous solutions using fast pyrolysis switchgrass biochar, *Chemosphere*, 174: 49–57. <https://doi.org/10.1016/j.chemosphere.2017.01.105>
15. Duman, O., Özcan, C., Gürkan Polat, T., & Tunç, S., 2019, Carbon nanotube-based magnetic and non-magnetic adsorbents for the high-efficiency removal of diquat dibromide herbicide from water: OMWCNT, OMWCNT-Fe₃O₄ and OMWCNT-κ-carrageenan-Fe₃O₄ nanocomposites, *Environmental Pollution*, 244: 723–732. <https://doi.org/10.1016/j.envpol.2018.10.071>
16. Pinto, M. C. E., Santos, R. M. M., Gonçalves, R. G. L., Duarte, V. G. O., Borges, P. D., Leroux, F. Tronto, J., 2018, Adsorption of Dicamba herbicide onto a carbon replica obtained from a layered double hydroxide, *Dalton Transactions*, 47(9): 3119–3127.

- <https://doi.org/10.1039/C7DT03720A>
17. da Fonseca, R. J., Segatelli, M. G., Borges, K. B., & Tarley, C. R. T., 2015, Synthesis and evaluation of different adsorbents based on poly(methacrylic acid-trimethylolpropane trimethacrylate) and poly(vinylimidazole-trimethylolpropane trimethacrylate) for the adsorption of tebuthiuron from aqueous medium, *Reactive and Functional Polymers*, 93: 1-9. <https://doi.org/10.1016/j.reactfunctpolym.2015.05.004>
 18. Shafeeyan, M. S., Daud, W. M. A. W., Houshmand, A., & Shamiri, A., 2010, A review on surface modification of activated carbon for carbon dioxide adsorption, *Journal of Analytical and Applied Pyrolysis*, 89(2): 143-151. <https://doi.org/10.1016/j.jaap.2010.07.006>
 19. Adelodun, A. A., Kim, K.-H., Ngila, J. C., & Szulejko, J., 2015, A review on the effect of amination pretreatment for the selective separation of CO₂, *Applied Energy*, 158: 631-642. <https://doi.org/10.1016/j.apenergy.2015.08.107>
 20. Khuri, A. I., & Mukhopadhyay, S., 2010, Response surface methodology, *Wiley Interdisciplinary Reviews: Computational Statistics*, 2(2): 128-149. <https://doi.org/10.1002/wics.73>
 21. Hill, W. J., & Hunter, W. G., 1966, A review of response surface methodology: a literature survey, *Technometrics*, 8(4): 571-590. <https://doi.org/10.1080/00401706.1966.10490404>
 22. Adeniyi, A. G., & Ighalo, J. O., 2019, Biosorption of pollutants by plant leaves: An empirical review, *Journal of Environmental Chemical Engineering*, 7(3): 103100. <https://doi.org/10.1016/j.jece.2019.103100>
 23. Said, M. S. M., Ghani, J. A., Kassim, M. S., Tomadi, S. H., & Haron, C. H. C., 2013, Comparison between Taguchi method and response surface methodology (RSM) in optimizing machining condition, In *Proceeding of 1st International Conference on Robust Quality Engineering*, pp. 60-68. Retrieved from http://eprints.utm.edu.my/7716/1/ICRQE_2013.pdf
 24. Widyaningsih, T. D., Widjanarko, S. B., Waziiroh, E., Wijayanti, N., & Maslukhah, Y. L., 2018, Pilot plant scale extraction of black cincau (*Mesona palustris* BL) using historical-data response surface methodology, *International Food Research Journal*, 25(2): 712-719. Retrieved from [http://www.ifrj.upm.edu.my/25 \(2\) 2018/\(38\).pdf](http://www.ifrj.upm.edu.my/25%20(2)2018/(38).pdf)
 25. Mahmoodi, N. M., Keshavarzi, S., & Rezaei, P., 2017, Synthesis of copper oxide nanoparticle and photocatalytic dye degradation study using response surface methodology (RSM) and genetic algorithm (GA), *Desalination and Water Treatment*, 72: 394-405. <https://doi.org/10.5004/dwt.2017.20639>
 26. Abdel daiem, M. M., Rivera-Utrilla, J., Sánchez-Polo, M., & Ocampo-Pérez, R., 2015, Single, competitive, and dynamic adsorption on activated carbon of compounds used as plasticizers and herbicides, *Science of The Total Environment*, 537: 335-342. <https://doi.org/10.1016/j.scitotenv.2015.07.131>
 27. Kazak, O., Eker, Y. R., Akin, I., Bingol, H., & Tor, A., 2017, Green preparation of a novel red mud@carbon composite and its application for adsorption of 2,4-dichlorophenoxyacetic acid from aqueous solution, *Environmental Science and Pollution Research*, 24(29): 23057-23068. <https://doi.org/10.1007/s11356-017-9937-x>
 28. Agarwal, S., Sadeghi, N., Tyagi, I., Gupta, V. K., & Fakhri, A., 2016, Adsorption of toxic carbamate pesticide oxamyl from liquid phase by newly synthesized and characterized graphene quantum dots nanomaterials, *Journal of Colloid and Interface Science*, 478: 430-438. <https://doi.org/10.1016/j.jcis.2016.06.029>
 29. Al Bahri, M., Calvo, L., Gilarranz, M. A., & Rodriguez, J. J., 2016, Diuron Multilayer Adsorption on Activated Carbon from CO₂ Activation of Grape Seeds, *Chemical Engineering Communications*, 203(1): 103-113. <https://doi.org/10.1080/00986445.2014.934447>
 30. Ignatowicz, K., 2011, A mass transfer model for the adsorption of pesticide on coconut shell based activated carbon, *International Journal of Heat and Mass Transfer*, 54(23-24): 4931-4938. <https://doi.org/10.1016/j.ijheatmasstransfer.2011.07.005>

Persian Abstract

DOI: 10.5829/ijee.2020.11.04.02

چکیده

از مدل آماری برای تجزیه و تحلیل تأثیر اینترفاز جاذب مواد در جذب سموم و علفکش‌ها از محیط‌های آبی استفاده شد. مجموعه داده‌های مورد استفاده برای این مطالعه از مقالات معتبر منتشر شده در پنج سال گذشته تهیه شده است. شصت و شش خط داده با استفاده از روش سطح پاسخ (RSM) و طراحی داده‌های تاریخی (HDD) در Expert Design مورد تجزیه و تحلیل قرار گرفت. پنج پارامتر در این مطالعه در نظر گرفته شد: توده مولکولی نسبی جاذب (RMM)، سطح خاص جاذب (SBET)، جاذب سطح موثر (Esber) به عنوان مثال، بخشی از SBET اشغال شده توسط مولکول‌های جاذب، حلالیت آب جاذب. جذب ترجیحی و جاذب (یعنی نسبت مقدار جاذب روی جاذب به مقدار محلول). از تجزیه واریانس مشاهده شد که SBET جاذب برای تعیین ظرفیت جذب، q در سطح معنی داری $p < 0.05$ مهمترین بود. عوامل مهم دیگر RMM ، $esBe$ و جذب ترجیحی بودند. به طور کلی، حلالیت تأثیر قابل توجهی در q نشان نمی‌دهد. مدل سطح پاسخ دارای ارزش $R^2 = 0.9945$ و مقدار R^2 تنظیم شده 0.9927 بود. به طور حتم، q ماده جاذب نسبت به علف کش یا سموم دفع آفات با افزایش $SBET$ و $Esber$ ، صرف نظر از محلول بودن مواد جاذب و جرم مولکولی، افزایش می‌یابد.
