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# Optimization of removal of toluene from industrial wastewater using RSM Box– Behnken experimental design

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# Optimization of removal of toluene from industrial wastewater using RSM Box–Behnken experimental design

Dariush Jafari[1,2*], Morteza Esfandyari[3] and Mehdi Mojahed[4]

**Abstract**

The study is concerned with the adsorption of toluene from real wastewater using granular beads of activated carbon. The adsorbent was analyzed before and after the process using Scanning Electron Microscope analysis to characterize its surface characteristics. The adsorption parameters including solution pH, contact time, dosage of adsorbent, temperature and toluene initial concentration were optimized using response surface methodology (RSM) Box-Behnken experimental design to maximize the toluene adsorption. The adsorption capacity of the adsorbent was 298 mg $g^{-1}$ and the maximum toluene removal was 99.5% which was achieved in the following optimal conditions: pH: 2, 100 min, adsorbent dosage: 0.7 g $L^{-1}$, 40 °C and initial concentration: 30 mg $L^{-1}$. The adjusted coefficient of determination of the model was over 0.99 which denotes that the model was quite appropriate and accurate and also it was effective in the optimization of toluene adsorption. Finally, the activated carbon adsorbent was applied to remove toluene from a real sample of wastewater under the optimal operating conditions and the uptake percentage of 96.9% was achieved which was in accordance with the output of the removal of toluene from synthetic wastewater.

**Keywords** Optimization, Activated carbon, Toluene, Adsorption, Box-Behnken, Real Wastewater

## 1 Introduction

As a result of development of technology and increasing growth of industrial activities, environmental pollutants have become the today's worldwide critical challenge [1]. Although crude oil has always been playing a key role in global economy, its increasing usage pollutes and threatens the environment due to its irreparable damages in ecosystems [2]. The most important hydrocarbon pollutants are gasoline, diesel fuel, oil and other petroleum derived compounds which enter the environment from the leakage of reservoir tanks, gas stations, or improper discharge of industrial wastewaters of refineries, petrochemical plants, and explosion or leakage in crude oil transmission pipelines and tankers used for the transmission of petroleum or chemical products. Most hydrocarbon pollutants contain organic compounds including phenolic combinations. Several techniques such as membrane separation, electrochemical techniques and reverse osmosis have been used for the removal of these compounds, most of which are neither low-cost nor completely effective. However, adsorption by activated carbon adsorbent has proved its efficiency as a low-cost, efficient technique [3].

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Several researchers investigated the removal of chemical compounds from wastewaters. Visa et al. used coal derived activated carbon for the adsorption of phenol. They modified the achieved carbon from coal burning by sodium hydroxide and hexadecyltrimethylammonium bromide and optimized the operating conditions to achieve the maximum efficiency [4]. Pourzamani et al. used an experimental design to optimize toluene removal using single-walled carbon nanotube-magnetized nanoparticles. Their results showed that the proposed adsorbent had an excellent potential for the adsorption of toluene from aqueous solutions since they acquired the removal percentage of over 99% [5]. Khare and Kumar studied the uptake of phenol from sludge using activated carbon derived from *Terminalia chebula* as an agricultural based adsorbent. The maximum adsorption capacity of the synthesized activated carbon was 295 mg $g^{-1}$ and denotes the adsorbent's high efficiency for the removal of phenolic compounds from aquatic systems [6]. In another research carried out by Ameri et al., toluene was successfully adsorbed using clay activated by acid. Analysis of variance (ANOVA) data showed that time and temperature were significant parameters for the removal of toluene and both of the optimization and experimental results were successfully fitted by response surface methodology (RSM) model [7]. Mojoudi et al. used activated carbon achieved from oily sludge for the adsorption of phenol. It was observed that the maximum adsorption capacity ($q_m$) of the derived activated carbon was 434 mg $g^{-1}$ and the process was fast under the optimal operating conditions [8]. In research carried out to find the optimal operating conditions for the toluene removal using RSM, Khoshakhlagh et al. applied oxidized activated carbon (OAC), microporous composites of Cu (Cu- 1,4-benzenedicarboxylate (BDC)) and Cu-BDC@OAC in various operating conditions. Based on their results, Cu-BDC@OAC outperformed in comparison with the other two adsorbents [9]. In recent research, Kyzas et al. studied the removal of toluene and benzene from aqueous medium using $Fe_3O_4$/zeolite imidazolate framework nanoparticles. The synthesized adsorbent presented excellent uptake percentages towards these two pollutants [10].

Several parameters affect the performance of an adsorbent used in adsorption process including contact time, solution pH, pollutant initial concentration, adsorbent dosage, temperature and stirring rate. Regarding the number of these parameters and their testing levels, high cost and time are required to assess the total effect of these parameters. In order to avoid them and study the effects of the operating parameters properly, a regular design is applied for the optimization of experiments and the desired information can be achieved from a smaller number of experiments without affecting the output of the tests. This can be done by experimental design concept. Several designs have been recently used in various fields including response surface methodology (RSM) [11], Central Composite Design (CCD) and Box-Behnken design [12, 13]. Multivariable optimization techniques are low-cost, effective statistical methods which yield the best experimental conditions for a specific output. In comparison with the common single-variable methods, they have advantages such as possibility of the assessment of effective factors during the optimization and investigation of interactions between parameters and other variables with the lowest number of required tests [14].

This study aims to optimize the removal of toluene, a hazardous and toxic component found in wastewaters, using activated carbon as an efficient and cost-effective adsorbent. The Box-Behnken method was used to design experiments and determine the optimal values for adsorption operating parameters, such as pH, adsorbent dosage, toluene initial concentration, time, and temperature. This method enabled the researchers to achieve maximum toluene removal with the least amount of cost and time. The findings of this study suggest that the optimization of pollutant removal from wastewater can be improved using activated carbon and the Box-Behnken method.

## 2 Materials and methods

### 2.1 Chemicals

Toluene (99.9%) was purchased from Merck (Germany) and was applied without further purification. The stock solution of toluene was prepared by adding a specified amount toluene (11.5 mL) in 1 L of deionized water to produce a solution containing 10,000 ppm toluene. Since toluene is volatile, the concentration of remaining toluene was measured at most for 4 h after each test. The activated carbon which was applied as the adsorbent in this study was purchased from Vazin Carbon (Iran). The specifications of the applied activated carbon are presented in Table 1.

### 2.2 Sampling procedure

The real wastewater samples were initially analyzed to determine the composition of the pollutants. Several samples were collected from the wastewater stream of a Natural Gas liquid (NGL) plant and were preserved in dark tightened capped glass bottles. The samples were prepared for the experiments based on Standard Methods for the Examination of Water & Wastewater (21st Edition) and Manual of Oceanographic Observations and Pollutant Analyses Methods 1999.

### 2.3 Experiments

In this work, batch experiments were performed to assess the effect of operating parameters on the removal of toluene

**Table 1** Specifications of activated carbon

| Specification | Magnitude | Unit |
|---|---|---|
| Size | 0.4–1.2 | mm |
| Total surface area (BET) | 900 | $m^2\ g^{-1}$ |
| Apparent density | 480–500 | $kg\ m^{-3}$ |
| Ash content | 12 | mass % |
| pH | 7–9 | - |
| Moisture (as packed) | 3 | mass % |

from aquatic medium using granular beads of activated carbon. Batch experiments were carried out in 250-mL Erlenmeyer flasks, and the average values of three repetitions were reported as the final output of each parameter. During these experiments the effects of variation of operating parameters on the removal percentage were studied in the following ranges: pH (2–10), adsorbent dosage (0.1–0.8 g $L^{-1}$), contact time (5–150 min), temperature (30–50 °C) and toluene initial concentration (30–200 mg $L^{-1}$). The experiments were initiated with the preparation of 100 mL of the toluene solution (e.g. 50 mg $L^{-1}$) by dilution of the stock solution. Then the appropriate content of the adsorbent (e.g. 0.3 g $L^{-1}$) was added to the solution and the process was carried out based on the level of parameters determined from Box-Behnken design method (e.g. temperature: 30 °C, time: 80 min and pH: 7). After each test, the solution and adsorbent were filtered using Whatman No. 42 filter paper and the content of the remained toluene was determined using spectrophotometer (HACH DR-5000) to achieve the toluene adsorption efficiency at the wavelength of 260 nm. The adsorption percentage (R) and adsorption capacity ($q_e$) were calculated by Eqs. 1 and 2, respectively:

$$R(\%) = \frac{C_i - C_e}{C_i} \times 100 \tag{1}$$

$$q_e = \frac{C_i - C_e}{m} \tag{2}$$

In these equations, $C_i$ (mg $L^{-1}$), $C_e$ (mg $L^{-1}$), $q_e$ (mg $g^{-1}$), m (g) and V (L) are toluene initial concentration of, the toluene equilibrium concentration, adsorption capacity, mass of the adsorbent, and volume of the tested solution, respectively [15, 16].

The effect of main factors of the process and their interactions were investigated using a 2-level factorials design of experiments screening method. Five main factors are solution pH (A), contact time (B), adsorbent dosage (C), temperature (D) and toluene initial concentration (E). The modeling and optimization of the effects of these main parameters were performed by Box-Behnken technique which is a RSM model. The modeling was done using Design Expert software. In this method, it is hypothesized that a polynomial (Eq. 3) is used to express the relationship between the independent variables and response where, y is the response variable or the removal percentage, $\beta_0$ is the constant value of polynomial, $\beta$, $\beta_{ii}$ and $\beta_{ij}$ are the regression coefficients for mutual interactions, $X_j$ and $X_i$ are the independent variables and $\varepsilon$ is the random error.

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum_{1 \le i \le j}^{k} \beta_{ii} X_i X_j \tag{3}$$

Based on the selected operating conditions, the number of experiments was 46. The main goal of the current design is the optimization of operating parameters to achieve the maximum adsorption efficiency. Table 2 represents the information of the design parameters.

## 3 Results and discussion

### 3.1 Design of experiments and statistical analysis

As mentioned before, 46 rotatable runs were performed to investigate the effect of 5 variables on the response variable (%R) based on Box-Behnken design. Rotatability refers to the variance of the response function. A rotatable design exists when there is an equal prediction variance for all points a fixed distance from the center, 0. The accuracy of the proposed model can be assessed by the data reported in Table 3. It is clear that the quadratic

**Table 2** The information of the selected factors

| Factor | Name | Units | Lower code (-1) | Upper code (1) | Mean | Std. Dev. |
|---|---|---|---|---|---|---|
| A | pH | - | 2 | 10 | 6 | 2.4 |
| B | Contact time | min | 5 | 150.00 | 77.5 | 35.8 |
| C | Adsorbent dosage | $g\ L^{-1}$ | 0.1 | 0.8 | 0.45 | 0.18 |
| D | Temperature | °C | 30 | 50 | 40 | 9 |
| E | Initial concentration | $mg\ L^{-1}$ | 30 | 200 | 115 | 51 |

**Table 3** ANOVA results for the BB quadratic model

| Source | Sum of Squares | df | Mean Square | *F*-value | *p*-value |
|---|---|---|---|---|---|
| Model | 2662 | 20 | 133 | 529 | < 0.0001 |
| A-pH | 5 | 1 | 5 | 19 | 0.0002 |
| B-Contact time | 527 | 1 | 527 | 2098.12 | < 0.0001 |
| C-Absorbent dosage | 525 | 1 | 525 | 2089 | < 0.0001 |
| D-Temperature | 140 | 1 | 140 | 557.69 | < 0.0001 |
| E-Initial concentration | 1318 | 1 | 1318 | 5241.33 | < 0.0001 |
| AB | 1.77 | 1 | 1.77 | 7.03 | 0.0137 |
| AC | 2.61 | 1 | 2.61 | 10.37 | 0.0035 |
| AD | 1.90 | 1 | 1.90 | 7.57 | 0.0109 |
| AE | 7.24 | 1 | 7.24 | 28.77 | < 0.0001 |
| BC | 3.08 | 1 | 3.08 | 12.25 | 0.0018 |
| BD | 4.45 | 1 | 4.45 | 17.70 | 0.0003 |
| BE | 0.13 | 1 | 0.13 | 0.53 | 0.4735 |
| CD | 6.20 | 1 | 6.20 | 24.66 | < 0.0001 |
| CE | 4.88 | 1 | 4.88 | 19.42 | 0.0002 |
| DE | 42.84 | 1 | 42.84 | 170.34 | < 0.0001 |
| $A^2$ | 6.27 | 1 | 6.27 | 24.95 | < 0.0001 |
| $B^2$ | 40.42 | 1 | 40.42 | 160.73 | < 0.0001 |
| $C^2$ | 38.87 | 1 | 38.87 | 154.57 | < 0.0001 |
| $D^2$ | 26.11 | 1 | 26.11 | 103.82 | < 0.0001 |
| $E^2$ | 17.57 | 1 | 17.57 | 69.86 | < 0.0001 |
| Residual | 6.29 | 25 | 0.25 | | |
| Lack of Fit | 6.29 | 20 | 0.31 | 7.86 | 0.2425 |
| Pure Error | 0 | 5 | 0 | | |
| Cor Total | 2668.34 | 45 | | | |

model was in accordance with the produced data. Moreover, *p*-value was lower than 0.001 which denotes that the model was significant. In addition, Lack of Fit (0.24) was not significant in comparison with the pure error. Furthermore, the accurate predictions of the model approve such a negligible Lack of Fit.

It should be noted that *p*-values less than 0.05 indicate that the terms of the model are significant. For the current model A, B, C, D, E, AB, AC, AD, AE, BC, BD, CD, CE, DE, $A^2$, $B^2$, $C^2$, $D^2$, $E^2$ are significant. The terms are not significant when *p*-values are higher than 0.1. If there are many insignificant model terms, the model can be improved through model reduction. Considering the achieved *p*-values, the model performance can be promoted by omitting BE factor. The correlation coefficients of the model after the modification are presented in Table 4.

The Predicted $R^2$ of 0.9909 is in reasonable agreement with the Adjusted $R^2$ of 0.9958; Adeq Precision determines the signal to noise ratio and for values than 4 it is desirable. Regarding these data, the ratio value of 93.9 denotes an adequate signal, which delineates that this model can be used to navigate the design space. Equation 4 shows the relationship between the input variables and the target value in terms of coded factors:

$$\begin{aligned} Removal(\%) = {} & 81.91 - 0.5456A + 5.74B + 25.73C + 2.96D \\ & - 9.08E - 0.6650AB - 0.8075AC - 0.69AD \\ & + 1.35AE - .8775BC + 1.05BD + 0.1825BE \\ & + 1.24CD - 1.11CE - 3.27DE - 0.8479A^2 \\ & - 2.15B^2 - 2.11C^2 - 1.73D^2 - 1.42E^2 \end{aligned} \quad (4)$$

**Table 4** Statistical parameters of the model

| Std. Dev. | Mean | C.V. % | $R^2$ | Adjusted $R^2$ | Predicted $R^2$ | Adeq Precision |
|---|---|---|---|---|---|---|
| 0.5 | 79 | 63 | 0.9976 | 0.9958 | 0.9909 | 94 |

Figure 1 depicts the validation of the proposed model. The simultaneous effects of 5 main effective factors on the removal percentage are presented in Fig. 1a. It is clear that the parameter E and then C and B have more deviations from the reference point defined by the software in comparison with D and A. In addition, the least deviation belongs to parameter A which denotes that this parameter is non-significant compared to the other parameters. The measured values versus the predicted response are illustrated in Fig. 1b. Since the majority of the parameters are approximately located on 45° line, the prediction error values were minor which delineates on the agreement between the experimental values and predicted data. Figure 1c illustrates the values predicted by statistical model versus the real data achieved from experiments. The uniform distribution and low distance of the points from 45° line denotes the high cohesion of the results and high accordance between the values predicted by the software and the experimental data. Such an accordance confirms the capability of the proposed model in prediction of the

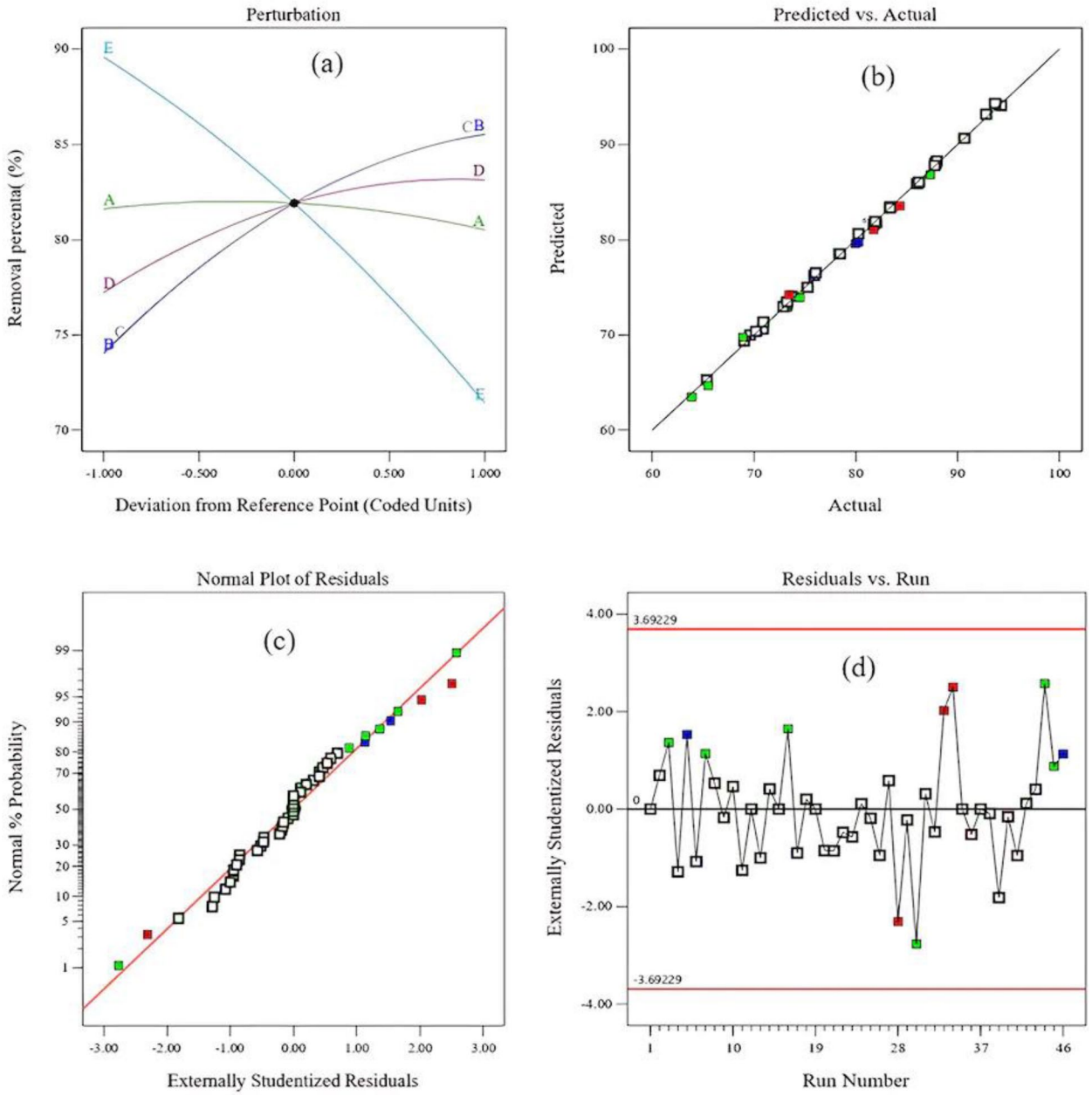


**Fig. 1** **a** Perturbation plot of variables; **b** Experimental (actual) values plotted versus the predicted data; **c** normal probability plot; **d** Residual values plotted versus the run number

response. Additionally, the agreement between the predicted values and the real data and the uniform distribution of the achieved outputs on the normal line delineates the uniform distribution of errors. Figure 2d shows the effect of experiments on the responses presented by the software. When a single experiment is located out of the range, it will have a negative effect on the overall output of the software. It should be noted that such a situation is controlled well for the current experiments.

Figure 2 reveals the graphical forms of regression equations as 3D surface diagrams which are used for the better description of the interactions between variables in the desired ranges and determination of the optimal values of these variables. The variation of toluene removal with the operating parameters is illustrated in this figure. As can be seen, factors E and A are the most and least significant factors, respectively. Based on these diagrams, toluene initial concentration (E), adsorbent dosage (C) and contact time (B) are the most effective parameters on the removal of toluene.

### 3.2 Optimization

In this study, the optimization was performed without adjustment of factor values which is called infinite optimization. For this type of optimization, all factors are in their corresponding ranges while the response is set in its maximum value. Figure 3 represents the results of this optimization. It can be seen

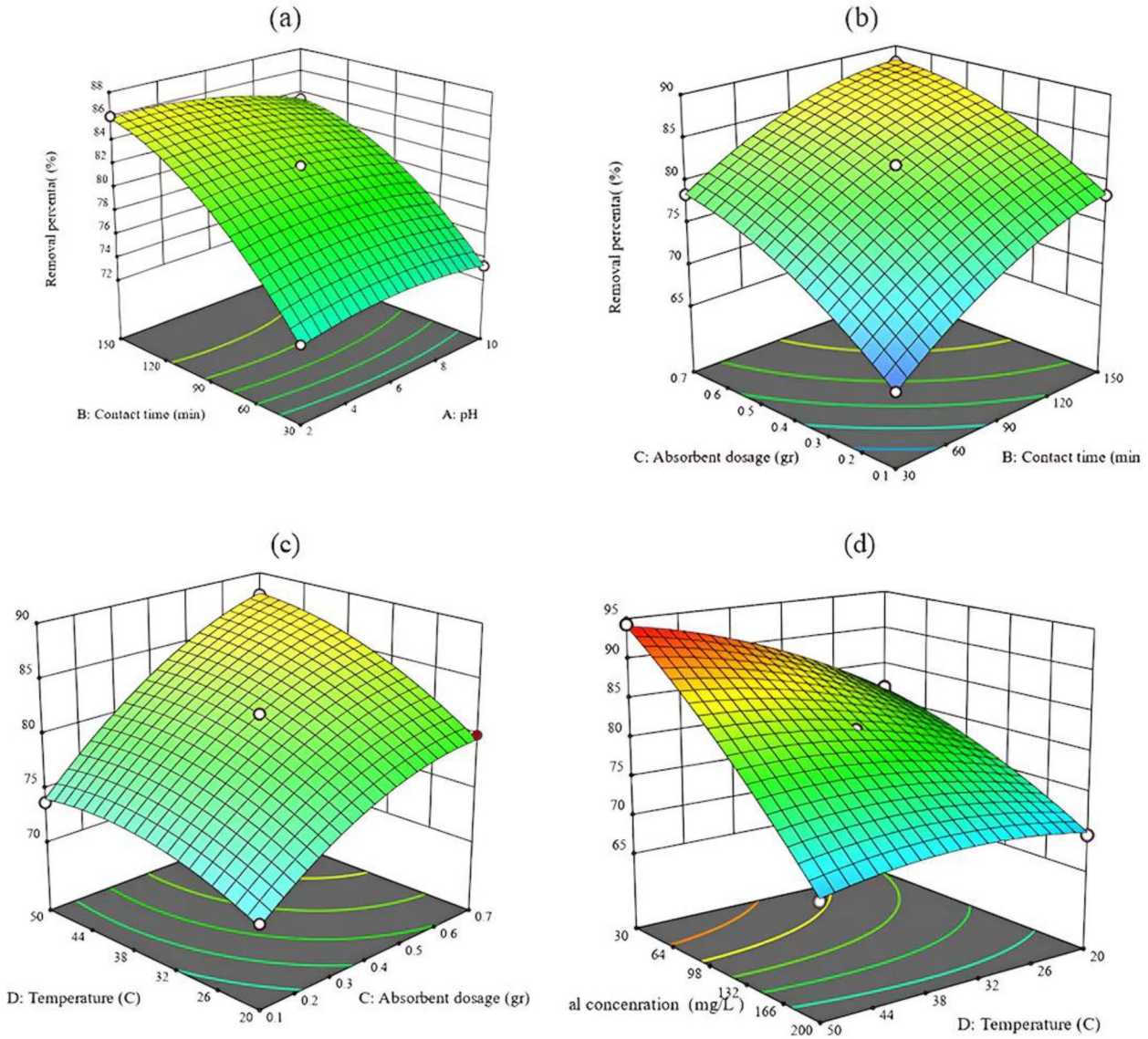


**Fig. 2** Response surface graphs showing the interaction between (**a**) pH and contact time (**b**) adsorbent dosage and contact time (**c**) temperature and absorbent dosage (**d**) effect of interactions between initial concentration and temperature on removal percentage

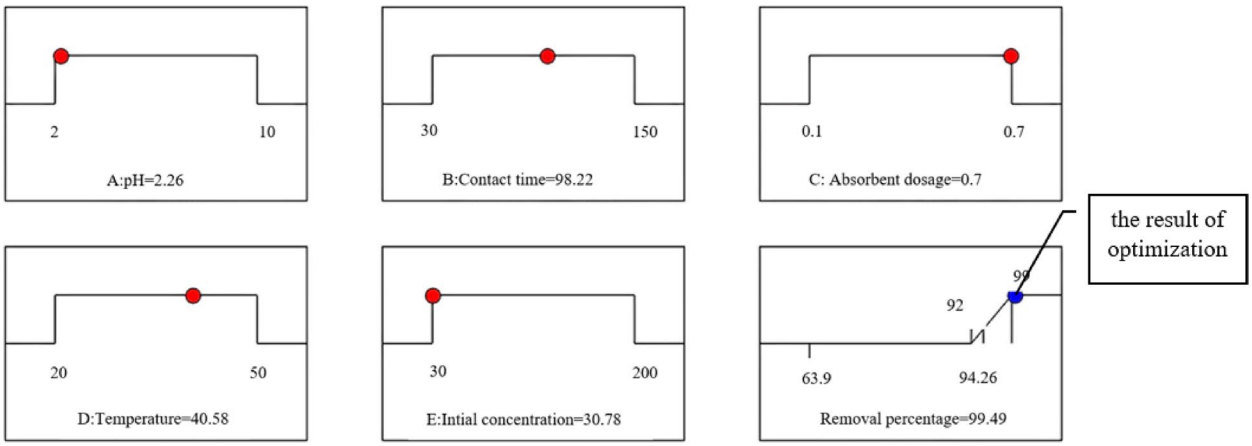


**Fig. 3** Optimal operating conditions achieved from the Design Expert software for the maximum removal percentage

that the result of optimization for the model data was 99.5%. Since the achieved optimal values are decimal figures, the rounded values were applied during the experiments performed for the validation of the model (Table 5).

### 3.3 Adsorption results

#### *3.3.1 Solution pH*

As a crucial parameter, solution pH affects the process by changing the charge of the adsorbent, ionization degree and the nature of the adsorbate during the process [17]. Considering Fig. 4a, increase of pH from 2 to 10 results in the drop of removal efficiency. Such an observation can be interpreted through the fact that by the variation of solution pH the surface charge of the adsorbent will be changed which is followed by the separation of the adsorbed toluene from the active sites of the adsorbent, therefore, they return into the solution. On the other hand, the removal of the pollutants is defined based on the competition between the pollutant ions and $H^+$ and $OH^-$ at low and high solution pH values, respectively. Since toluene is a weak acid [18] and cannot compete with $OH^-$ ions for binding to the active sites of the adsorbent surface, the adsorption falls off in high pH values. In addition, the electrostatic repulsion between the positive charge of the adsorbed surface and toluene ions barricades the attachment of toluene to the adsorbent surface. Based on this plot, the maximum efficiency (83%) was achieved in pH = 2.

Additionally, the results of $pH_{ZPC}$ studies are presented in Fig. 4b. As it can be seen, the $pH_{ZPC}$ value for the current adsorbent is 2.6. For pH values equal to $pH_{ZPC}$, the surface of the adsorbent is neutral. Additionally, for values higher than $pH_{ZPC}$, the surface charge of the adsorbent was negative, while it was positively charged for $pH < pH_{ZPC}$ [16]. Toluene is a weak acid. If pH of the solution is greater than pHpzc, the surface becomes negative and repulses toluene from its surface. These observations accord with the results of inspections of solution pH effect on the adsorption.

**Table 5** The toluene removal percentage at the point optimized by the model

| Factor | Name | value | Rounded values |
|---|---|---|---|
| A | pH | 2.26 | 2 |
| B | Contact time (min) | 98 | 100 |
| C | Adsorbent dosage (g $L^{-1}$) | 0.7 | 0.70 |
| D | Temperature (°C) | 40.6 | 40 |
| E | Initial concentration (mg $L^{-1}$) | 30.8 | 30 |

#### *3.3.2 Adsorbent dosage*

The adsorbent dosage affects the adsorption efficiency through its surface area and binding sites. Therefore, finding the proper adsorbent dosage is crucial [19]. The effect of adsorbent dosage on the removal of toluene was investigated in the range of 0.1–0.8 g $L^{-1}$. Figure 4c shows that increase of the dosage of adsorbent between 0.1 and 0.6 g $L^{-1}$ is accompanied by rise in the uptake percentage, since more free active sites are available for the pollutant to occupy. Although there are more active sites on the adsorbent surface, more pollutants are not available in the solution to bind the free active sites of the adsorbent and beyond 0.6 g $L^{-1}$, the adsorbent amount is in excess. In this research, the maximum efficiency was 95% which was achieved in 0.7 g $L^{-1}$. This value is in agreement with the model results.

#### *3.3.3 Contact time*

One of the significant parameters of the adsorption process is contact time since it delineates the

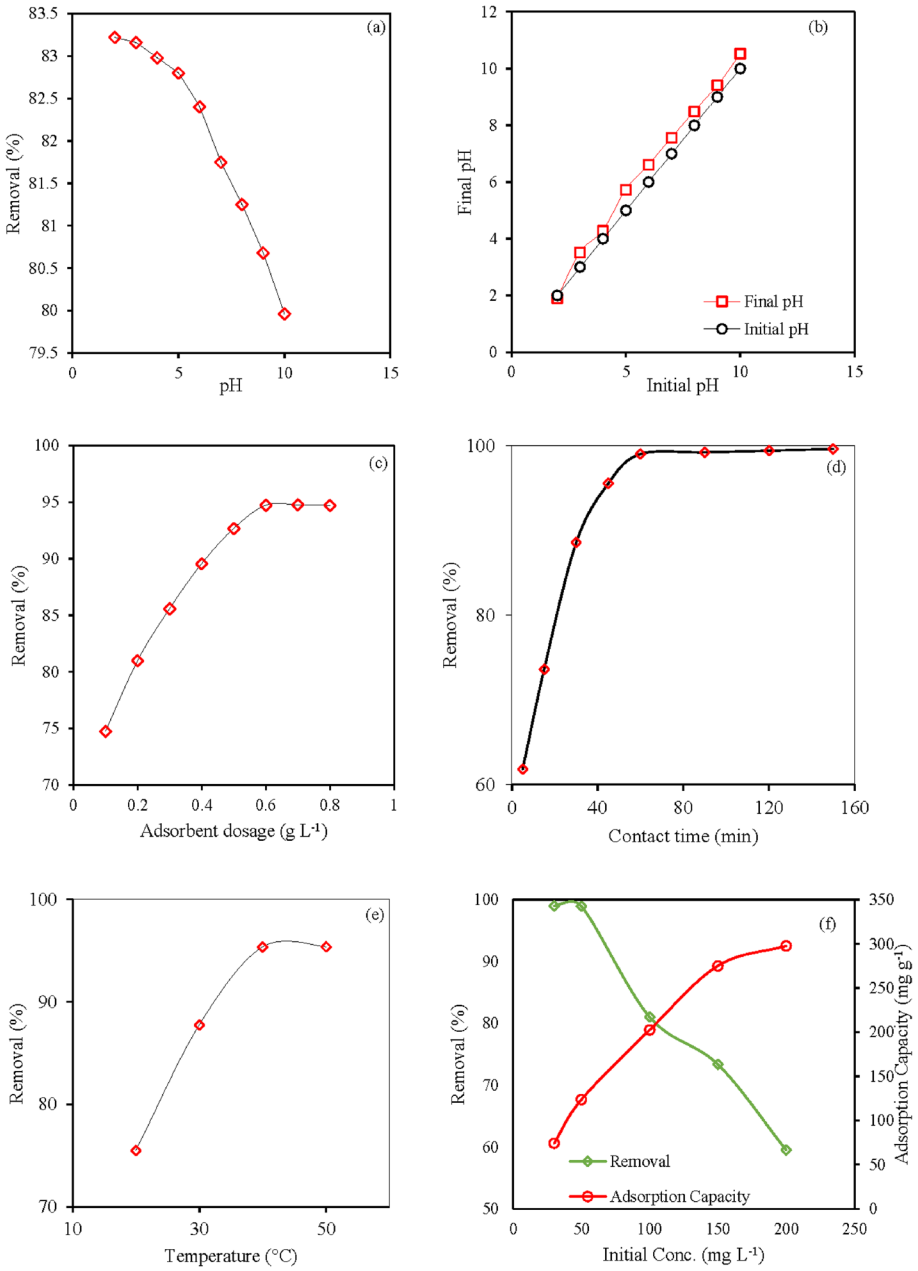


**Fig. 4** Parameters affecting toluene adsorption. **a** pH, **b** Point of zero charge ($pH_{ZPC}$) of the biosorbent, **c** adsorbent dosage, **d** Contact time, **e** Temperature, **f** Initial toluene concentration

equilibrium time between the adsorbent and adsorbate [20]. The effect of contact time was investigated from 5 to 150 min and is presented in Fig. 4d. As can be seen, the adsorption rose sharply with time initially and then became approximately unchanged after 80 min. The initial increase of the adsorption can be related to the fact the pollutant has more time to occupy the free active sites of the adsorbent with the increasing the contact time. However, after the equilibrium time the rate of removal of pollutant is equal to the rate of their desorption. As a result, 80 min was considered as the equilibrium contact time in this study in which the removal of 99% was achieved. It should be noted that although the optimal contact time specified by the model was 100 min which is far from 80 min, the uptake efficiency in both of these levels were approximately equal.

#### *3.3.4 Temperature*

The effect of temperature on the removal percentage of toluene from aqueous medium was investigated in the range of 30–50 °C and the result are shown in Fig. 4e. From this figure, it can be observed that the adsorption efficiency increased with temperature. This can be related to the increase in attraction between the adsorbent active sites and adsorbate toluene. Since the adsorption was approximately unchanged between 40 and 50 °C, therefore, the former was selected as the optimal operating temperature which is consistent with the output of the model.

#### *3.3.5 Toluene initial concentration*

The initial concentration of the pollutant is a crucial parameter in determination of the capacity of an adsorbent and the driving force of adsorption [21]. The effect of toluene initial concentration on removal and equilibrium adsorption capacity is presented in Fig. 4f. It can be clearly seen that these two parameters showed opposite responses to the increase of initial concentration of toluene. While the adsorption decreased with initial concentration, the equilibrium capacity rose in the tested range. By increase of the pollutant concentration, the number of toluene molecules in the solution which can occupy the active sites of the adsorbent increased, while the number of free actives sites was constant; as a result, the efficiency decreased [22]. On the other hand, the adsorption capacity rose from 74 to 298 mg $g^{-1}$ with the concentration increase from 30 to 200 m $gL^{-1}$. This can be attributed to the easier migration of the pollutant molecules from the solution to the surface of the adsorbent as the result of high driving force which defeats the mass transfer resistance of toluene between the aqueous phase and the adsorbent phase and therefore all the active sites are occupied by the pollutant molecules. As the result, higher capacities are obtained [23, 24].

### 3.4 Adsorbent characterization

SEM (TESCAN MIRA3-FEG model (Czech Republic)) analysis was used to study the variations of the surface characteristics and morphology of the activated carbon adsorbent before and after the adsorption of toluene and the results are presented in Fig. 5. Comparison between Fig. 5a and b shows that the surface of the adsorbent was probably covered with pollutant particles after the process. Considering the SEM images, it can be seen that the surface of the activated carbon is altered after the adsorption of toluene, and some impurities can be seen on this surface which was not present on the surface of the activated carbon prior to adsorption. These impurities can be pollutant particles which are attached to the surface of the adsorbent during adsorption process.

### 3.5 Adsorption from real wastewater sample

In this study, Gas Chromatography (GC) (Varian-cp-3800) (fused-silica capillary column DB-1 (30 m × 0.32 mm i.d) was used for the analysis of a real wastewater sample to confirm the presence of toluene in the sample as a major constituent. The system was equipped by a flame ionization detection and a 30 mm capillary column and the carrier gas was helium. Initially, after 60 s the temperature was increased from 150 to 220 °C with the pace of 10 °C $min^{-1}$ and it was

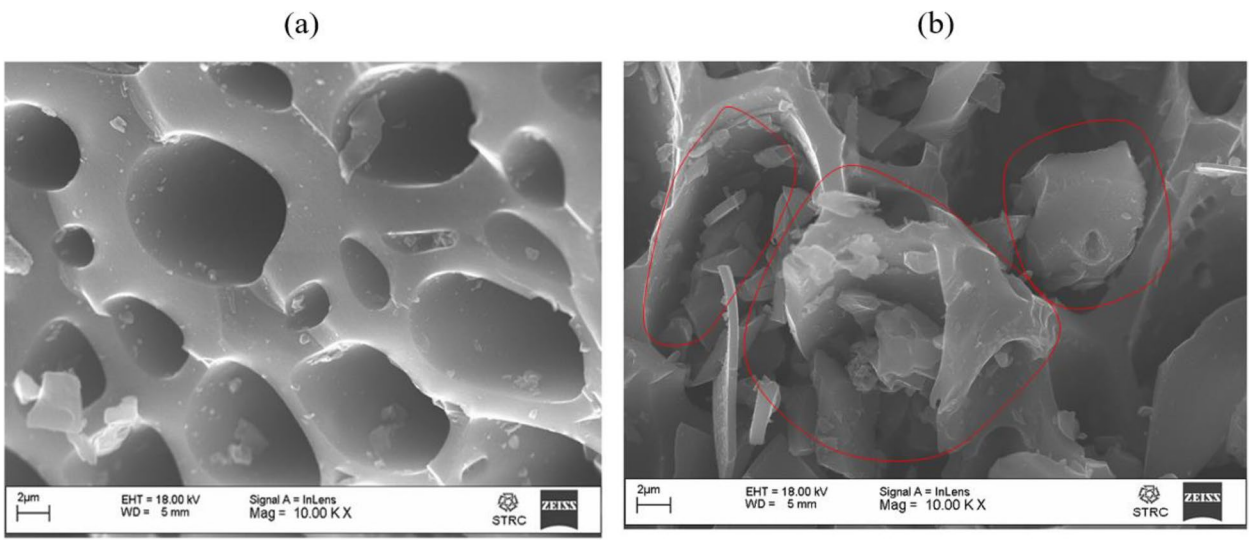


**Fig. 5** SEM analysis of the activated carbon: **a** before and **b** after the adsorption of toluene

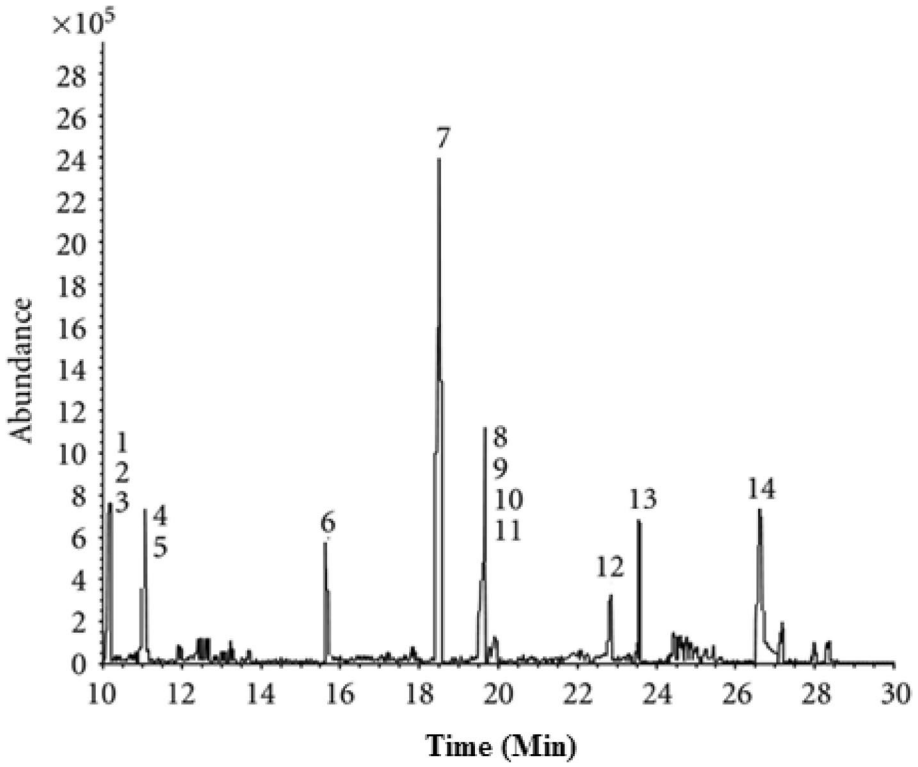


**Fig. 6** GC of the real wastewater sample

kept constant for 2 min. Then it was raised to 235 °C at the rate of 7 °C $min^{-1}$ and was kept at this temperature for 2 min. Afterwards, it was heated to 255 °C with the same rate and kept for 1 min. Finally, the temperature was increased to 268 °C with the rate of 10 °C $min^{-1}$ and was kept constant for 30 min. The result of GC analysis of the real wastewater sample which was collected from the waste stream of a NGL plant is presented in Fig. 6. The peaks appeared in this diagram is as follows:

1: 2-methoxy-2-methylpropane; 2: cyclopropane; 3: benzaldehyde; 4: methyl-tetrabutyl ether; 5: phenol; 6: 2,3,5,6-tetramethylphenol; 7: toluene; 8: xylene; 9: 2,4-dimethylphenol (xylenol); 10: 2,5-dimethyl-3-ethylphenol; 11: octamethylcyclotetrasiloxane; 12: tetradecane; 13: 4-chloro-3-methylphenol; and 14: 3-tert-butylphenol.

As it can be seen, peak number 7 belongs to toluene which denotes that it has the highest content (43%) in the wastewater sample; therefore, the applied adsorbent was used to treat the collected real sample and assess its efficiency in removal of toluene. The adsorption experiment was carried out in the achieved optimal conditions (pH: 2, 100 min, adsorbent dosage: 0.7 g $L^{-1}$, 40 °C) and the efficiency of 97% was achieved which is in agreement with the result of the model and the synthetic wastewater experiments.

## 4 Conclusions

To summarize, the adsorption of toluene from aqueous medium by activated carbon was investigated and the optimal operating conditions were achieved using RSM Box–Behnken experimental design method. Based on the achieved results the maximum removal of toluene was 99.5% which was achieved in the following optimized operating conditions: pH: 2, adsorbent dosage: 0.7 g $L^{-1}$, initial concentration: 30 mg $L^{-1}$, contact time: 100 min, and 40 °C. Such a removal percentage denotes that the current process was successful and reliable for the removal of toluene from aqueous systems. The model showed a good performance in fitting the experimental data and its p-value was lower than 0.001 which shows that the model was significant. In addition, toluene initial concentration and solution pH were the most and least significant factors, respectively. Moreover, the effect of factors including solution pH, adsorbent dosage, contact time, initial concentration and temperature on the adsorption efficiency was investigated. Additionally, the maximum adsorbent capacity was equal to 298 mg $g^{-1}$. The removal percentage of toluene from real wastewater was 97%.

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**Authors' contributions**
Dariush Jafari: Equilibrium, Kinetic, and Thermodynamic Studies, Methodology, Optimization. Writing – review & editing. Morteza Esfandyari: Design Expert, Methodology, Project administration, Software, Validation, Writing – original draft. Mehdi Mojahed: draft manuscript preparation, experimental, analysis and interpretation of results.

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**Availability of data and materials**
The datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

## Declarations

**Ethics approval and consent to participate**
All authors have read, understood, and have complied as applicable with the statement on "Ethical responsibilities of Authors" as found in the Instructions for Authors and are aware that with minor exceptions, no changes can be made to authorship once the paper is submitted.

**Consent for publication**
All authors agreed on the publication of this research work.

**Competing interests**
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.

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