Data Article

Kinetic and modeling data on phenol removal by Iron-modified Scoria Powder (FSP) from aqueous solutions

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Article history:
Received 1 May 2018
Received in revised form 11 August 2018
Accepted 21 August 2018
Available online 29 August 2018

Keywords:
Phenol
Iron-Modified scoria
RSM
Aqueous environment

Abstract
Phenol present in industrial effluents is a toxicant matter which causes pollution of environments aqueous. In this work, scoria was modified by iron in order to increasing of adsorbent efficiency and effective removing of phenol. Effects of independent variables including pH, adsorbents dosage, contact time and adsorbate concentration on removing of phenol were studied by response surface methodology (RSM) based on the central composite designs (CCD). The characterization of raw scoria powder (RSP) and Iron-modified Scoria Powder (FSP) was determined via Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), scanning electron microscopy (SEM) and Energy-dispersive X-ray spectroscopy (EDS). The obtained data showed modification by iron caused the growth of new crystalline of iron oxide on the surface of FSP. Evaluated data by RSM indicated the all variables especially pH are effective in removing of phenol (P-value < 0.001) and optimum condition was obtained at pH = 5, phenol concentration = 50 mg/l, adsorbent dosage = 1 g/l and contact time = 100 min to
the value of 94.99% with desirability of 0.939. Results revealed that data were fitted by Langmuir isotherm \((R^2 = 0.9938)\) and pseudo second order kinetic \((R^2 = 0.9976)\). It was found that iron causes increasing the site active of scoria and let to significant removal of phenol.

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### Specifications Table

| Subject area | Environmental Health Engineering |
|--------------|----------------------------------|
| More specific subject area | Environmental Chemistry |
| Type of data | Tables, figures |
| How data was acquired | XRD, FTIR, SEM and EDS techniques were used to determine the characteristics of adsorbent. Response surface methodology (RSM) was used to analyzing of experiments data to determine the effects of independent variables and define the optimum condition. Moreover, the obtained data were fitted by isotherms and kinetics equations |
| Data format | Raw, analyzed |
| Experimental factors | All samples were kept in polyethylene bottles in a dark place at room temperature. |
| Experimental features | Phenol was prepared and measured according to standard methods. Scoria was modified by iron in order to removal of phenol from aqueous solution. The all above mentioned parameters were analyzed according to the standard method for water and wastewater treatment handbook [1]. |
| Data source location | Kermanshah city, Iran |
| Data accessibility | Data are included in this article |
| Related research article | M. Moradi, A.M. Mansouri, N. Azizi, J. Amini, K. Karimi, K. Sharafi, Adsorptive removal of phenol from aqueous solutions by copper (Cu)-modified scoria powder: process modeling and kinetic evaluation, Desalin Water Treat. 57 (2016) 11820–11834. (Published). |

### Value of the data

- The obtained data of this study showed that Iron modification effect on adsorbent led to increasing of equilibrium sorption capacity for removal of phenol.
- Due to cheap and high availability of this type of adsorbent in Iran, the efficiency of it can be improved by making these simple modifications and so the application of it in water and wastewater treatment will be increased.
- The obtained data of present study can be used for design and development of future similar studies. Because in this study, the optimal conditions for the removal of phenol by FSP are determined. Therefore, the range of future study variables can be determined based on the optimal conditions of this study.
- The raw data of this study was analyzed using the RSM method. Therefore, the results related to the optimization conditions and the determination of the effect of each parameter will be very understandable for other researchers.

### 1. Data

The maximum efficiency of for phenol removal was obtained at \(\text{pH} = 3\), phenol concentration \(= 50\,\text{mg/l}\), adsorbent dosage \(= 1\,\text{g/l}\) and contact time \(= 100\,\text{min}\) (Table 1). Results demonstrated
| Run | Variables | Responses |
|-----|-----------|-----------|
|     | Factor 1 | Factor 2 | Factor 3 | Factor 4 | Phenol removal by RSP | Response Phenol removal by FSP |
|     | A: pumice dosage (gr/l) | B: Contact time (min) | C: pH | D: Phenol concentration (mg/l) | Actual % | Predicted % | Actual % | Predicted % |
| 1   | 1        | 20       | 11      | 50       | 19.31           | 18.97     | 31.4    | 29.67     |
| 2   | 0.2      | 20       | 11      | 50       | 6.21            | 6.9       | 13.2    | 13.98     |
| 3   | 1        | 20       | 3       | 50       | 79.68           | 81.46     | 92.6    | 93.95     |
| 4   | 0.6      | 80       | 7       | 150      | 70.52           | 67.65     | 82.14   | 76.37     |
| 5   | 1        | 100      | 11      | 50       | 29.32           | 27.89     | 35.6    | 33.11     |
| 6   | 0.6      | 60       | 7       | 150      | 65.76           | 65.42     | 72.65   | 75.34     |
| 7   | 1        | 100      | 3       | 250      | 68.61           | 65.04     | 79.26   | 77.06     |
| 8   | 0.6      | 60       | 7       | 150      | 65.76           | 65.42     | 73.71   | 75.34     |
| 9   | 0.6      | 60       | 7       | 100      | 66.27           | 69.58     | 78.65   | 79.19     |
| 10  | 0.2      | 100      | 3       | 250      | 49.84           | 52.97     | 61.96   | 65.16     |
| 11  | 0.6      | 40       | 7       | 150      | 58.57           | 63.19     | 67.45   | 72.57     |
| 12  | 0.6      | 60       | 7       | 150      | 65.76           | 65.42     | 75.64   | 75.34     |
| 13  | 0.6      | 60       | 7       | 200      | 60.73           | 61.26     | 72.33   | 71.14     |
| 14  | 0.6      | 60       | 7       | 150      | 65.76           | 65.42     | 75.64   | 75.34     |
| 15  | 0.6      | 60       | 7       | 150      | 65.76           | 65.42     | 75.64   | 75.34     |
| 16  | 0.2      | 100      | 11      | 50       | 14.17           | 15.82     | 13.2    | 17.04     |
| 17  | 0.6      | 60       | 9       | 150      | 53.06           | 48.87     | 60.28   | 57.67     |
| 18  | 1        | 100      | 3       | 50       | 89.14           | 90.38     | 100     | 103.81    |
| 19  | 0.2      | 20       | 11      | 250      | 3.94            | 1.03      | 10.87   | 8.52      |
| 20  | 0.4      | 60       | 7       | 150      | 57.44           | 59.23     | 65.49   | 69.6      |
| 21  | 0.8      | 60       | 7       | 150      | 69.07           | 65.26     | 81.26   | 76.5      |
| 22  | 0.6      | 60       | 5       | 150      | 73.6            | 75.76     | 84.39   | 86.56     |
| 23  | 0.2      | 100      | 11      | 250      | 8.53            | 7.89      | 16.65   | 13.87     |
| 24  | 1        | 100      | 11      | 250      | 15.19           | 19.96     | 22.36   | 25.76     |
| 25  | 1        | 20       | 3       | 250      | 59.04           | 56.12     | 67.29   | 64.91     |
| 26  | 1        | 20       | 11      | 250      | 8.93            | 11.04     | 17.48   | 20.03     |
| 27  | 0.2      | 20       | 3       | 250      | 41.01           | 44.05     | 52.32   | 53.39     |
| 28  | 0.2      | 20       | 3       | 50       | 70.38           | 69.38     | 80.2    | 78.26     |
| 29  | 0.2      | 100      | 3       | 50       | 81.34           | 78.31     | 91.7    | 87.73     |
| 30  | 0.6      | 60       | 7       | 150      | 65.76           | 65.42     | 76.33   | 75.34     |
The optimum condition was obtained for pH = 5, phenol concentration = 50 mg/l, adsorbent dosage = 1 g/l and contact time = 100 min to the value of 94.99% with desirability of 0.939 (Table 4). The percent of error between mathematical design and experimental study is 3.81% that suggested the close value of both actual and predicted data (Table 5). Results revealed that data were fitted by Langmuir isotherm ($R^2 = 0.9938$) and obeyed the pseudo second order kinetic ($R^2 = 0.9976$) (Tables 6 and 7).

Fig. 1 showed the XRD patterns, Fourier transform infrared spectroscopy (FTIR), SEM images and EDS analysis of RSP and FSP. Trend of phenol removal efficiency with respect to scoria dosage, contact time, pH, and phenol concentration was showed in Fig. 2. The response surface plots for phenol removal efficiency with respect to scoria dosage, pH, phenol concentration, and contact time were showed in Fig. 3. In addition, Normal probability plot of residual, predicted vs. actual values plot, and plot of residual vs. predicted response were showed by Fig. 4.

2. Experimental design, materials and methods

2.1. Pumice preparation and its modification using iron

Early preparations of raw scoria powder (RSP) were performed according to Moradi et al. [15] study [2]. The raw scoria powder (RSP) was kept in Fe(NO₃)₃ 3.9H₂O (0.5 m) solution at pH = 12 and

| MT | CE | SE | SS | DF | MS | FV | PV | S/NS |
|----|----|----|----|----|----|----|----|------|
| Quadratic model | – | – | 21,092.82 | 14 | 1506.63 | 95.66 | < 0.0001 | Significant |
| A | 75.34 | 1.10 | 784.53 | 1 | 784.53 | 49.81 | < 0.0001 | Significant |
| B | 6.90 | 0.98 | 238.37 | 1 | 238.37 | 15.13 | 0.0014 | Significant |
| C | 3.80 | 0.98 | 13,773.74 | 1 | 13,773.74 | 874.52 | < 0.0001 | Significant |
| D | – | 28.89 | 1069.97 | 1 | 1069.97 | 67.93 | < 0.0001 | Significant |
| AB | – | 8.05 | 0.15 | 1 | 0.15 | 9.29E-03 | 0.9245 | Not significant |
| AC | – | 0.096 | 1.56E-04 | 1 | 1.56E-04 | 9.92E-06 | 0.9975 | Not significant |
| AD | – | 3.125E-003 | 3.77E + 02 | 1 | 3.77E + 02 | 2.39E + 01 | 0.0002 | Significant |
| BC | – | 1.04 | 41.12 | 1 | 41.12 | 2.61 | 0.1270 | Not significant |
| BD | – | 1.60 | 5.26 | 1 | 5.26 | 0.33 | 0.5721 | Not significant |
| CD | 0.57 | 0.99 | 3.77E + 02 | 1 | 3.77E + 02 | 2.39E + 01 | 0.0002 | Significant |
| A² | 4.85 | 0.99 | 13.92 | 1 | 13.92 | 0.88 | 0.3621 | Not significant |
| B² | – | 9.14 | 9.73 | 2 | 9.73 | 0.13 | 0.7267 | Not significant |
| C² | – | 3.46 | 27.71 | 1 | 27.71 | 1.76 | 0.2045 | Not significant |
| D² | – | 12.90 | 9.73 | 0.078 | 0.078 | 4.95E-03 | 0.9448 | Significant |

CE: Coefficient Estimate, SE: Standard Error, MT: Model Terms, SS: Sum of squares, DF: Degree of Freedom, MS: Mean square, FV: F-value, PV: P-value, S: Significant, NS: Not significant.

Table 3
Analysis of variance (ANOVA) for fit of Phenol removal efficiency from central composite design after elimination of insignificant model terms: (FSP).

| Model | SMT | SD | $R^2$ | Adj. $R^2$ | CV | AP | PRESS | PV | FV | PLF |
|-------|-----|----|-------|------------|----|----|--------|----|----|-----|
| Quadratic model | A, B, C, D, CD | 3.97 | 0.989 | 0.978 | 7.51 | 33.95 | 1500.74 | < 0.0001 | 95.66 | 0.079 |

$R^2$: Determination Coefficient, Adj. $R^2$: Adjusted $R^2$, AP: Adequate Precision, SMT: Significant Model Terms, SD: Standard Deviation, CV: Coefficient Of Variation, PRESS: Predicted Residual Error Sum Of Squares, FV: F-value, PV: P-value, PLF: Probability For Lack Of Fit.
Table 4
Numerical optimization for central composite design for phenol removal by FSP.

| Number | A: Scoria dosage (gr/l) | B: Contact time (min) | C: pH | D: Phenol concentration (mg/l) | Phenol removal by FSP (%) | Desirability |
|--------|-------------------------|-----------------------|-------|-------------------------------|---------------------------|--------------|
| 1      | 1                       | 100                   | 5     | 50                            | 94.9999                   | 0.939        |
| 2      | 1                       | 100                   | 5     | 52                            | 94.9991                   | 0.939        |
| 3      | 1                       | 100                   | 5     | 50                            | 95.0002                   | 0.938        |
| 4      | 1                       | 100                   | 5     | 55                            | 95.0002                   | 0.937        |
| 5      | 1                       | 100                   | 5     | 59                            | 95                        | 0.936        |
| 6      | 1                       | 100                   | 5     | 61                            | 95.0001                   | 0.935        |
| 7      | 1                       | 100                   | 5     | 64                            | 95.0001                   | 0.934        |
| 8      | 1                       | 97                    | 5     | 50                            | 94.9801                   | 0.931        |
| 9      | 1                       | 100                   | 5     | 50                            | 93.8081                   | 0.929        |
| 10     | 1                       | 100                   | 5     | 81                            | 95.0002                   | 0.926        |
| 11     | 1                       | 100                   | 5     | 65                            | 93.7232                   | 0.923        |
| 12     | 1                       | 100                   | 4     | 91                            | 95.0002                   | 0.922        |
| 13     | 1                       | 100                   | 4     | 98                            | 95.0002                   | 0.92          |
| 14     | 1                       | 100                   | 4     | 100                           | 95.0002                   | 0.919        |
| 15     | 1                       | 100                   | 4     | 105                           | 95.0001                   | 0.917        |
| 16     | 1                       | 100                   | 4     | 106                           | 95.0002                   | 0.917        |
| 17     | 1                       | 100                   | 3     | 114                           | 95.0002                   | 0.916        |
| 18     | 1                       | 100                   | 3     | 115                           | 95.0002                   | 0.916        |
| 19     | 1                       | 100                   | 5     | 82                            | 94.0105                   | 0.913        |
| 20     | 1                       | 100                   | 3     | 126                           | 95                        | 0.902        |

Optimized Phenol removal calculated from central composite design

Selected
25 °C (room temperature) for 72 h, and dried at 110 °C for 14 h. Not doped iron was removed via washing of modified scoria by distilled water, afterwards, FSP dried at 105 °C for 14 h [2–4].

2.2. Characteristics of SP and FSP

The functional groups of adsorbents were determined by Fourier transform infrared spectroscopy (FTIR) (WQF-510 Model), X-ray diffraction (XRD) model Shimadzu XRD-6000 were used for study of chemical characteristics and surface morphology of adsorbent. Scanning electron microscope (SEM) model Philips XL30 was used to evaluation the sample’s surface topography and composition. Energy Dispersive X-Ray Spectroscopy (EDS) model EM-30AX Plus was applied for determination of chemical characterization and elemental analysis of adsorbents [5,6].

Table 5
Confirmation between optimized phenol removals calculated from mathematical design and experimental study.

| A: Scoria dosage (gr/l) | B: Contact time(min) | C: pH | D: Phenol concentration (mg/l) | Phenol removal by FSP (%) |
|-------------------------|----------------------|------|-------------------|---------------------------|
|                         | 1                    | 100  | 3                 | 50                        | 103.81                    |
| Confirmation study of optimized Phenol removal (experimental value) | 1 | 100 | 3 | 50 | 100 |

Error (%) = \( \frac{\text{Actual value} - \text{predicted value}}{\text{Actual value}} \times 100 \)

3.81%

Table 6
Isotherm equation parameters for phenol adsorption on FSP.

| Adsorbent | Langmuir isotherm | Freundlich isotherm |
|-----------|-------------------|---------------------|
| FSP       |                   |                     |
| \( q_m \) (mg/g) | 43.06            | 5.68                |
| \( b \)       | 0.11              | 17.44               |
| \( R^2 \)     | 0.9938            | 0.9315              |

Table 7
Kinetic model parameters for the adsorption phenol at different concentration on FSP.

| Kinetic model parameters | Kinetic parameters | FSP |
|--------------------------|--------------------|-----|
| Pseudo-first-order       | \( K_1 \)          | 0.1922|
|                          | \( R^2 \)          | 0.9177|
| Pseudo-second-order      | \( K_1 \)          | 0.00487|
|                          | \( R^2 \)          | 0.9976|
| Pore diffusion           | \( K_i \)          | 0.9336|
|                          | \( R^2 \)          | 0.8766|
| Elovich                  | \( A \)            | 0.279 |
|                          | \( B \)            | 2.75  |
|                          | \( R^2 \)          | 0.9625|
2.3. Experimental design by response surface methodology (RSM)

Design of experiments (DOE) software was used to design of experiments (the required sample size). Table 8 illustrated the experimental range and level of the independent variables. The RSM based on central composite design (CCD) as statistical tool was used to minimization of experiments.

Fig. 1. XRD patterns (A), Fourier transform infrared spectroscopy (FTIR) (B), SEM images (C) and EDS analysis of SP and FSP (D).

Fig. 2. Trend of phenol removal efficiency with respect to scoria dosage (A), contact time (B), pH (C), and phenol concentration (D).

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number. On the other hand, optimum condition was determined through consideration of relationship between the measured responses (phenol removal) and number of independent variables [7–10].

2.4. Samples preparation and batch sorption studies

Phenol with molecular formula C₆H₅OH and molecular weight of 94.11 g/mol was purchased from the Merck Company-Germany (CAS. 108-92-5). Different concentrations of phenol (50, 100, 150, 200 and 250 mg/l) were prepared from phenol stoke (1000 mg/l). The phenol adsorption by FSP was conducted under following conditions: adsorbent dose (0.1–1 g/l), pH (3, 5, 7, 9 and 11), contacted time (20, 40, 60, 80 and 100 min) and room temperature (25 °C). The residual phenol was determined by UV/VIS spectrophotometer (Hitachi Model 100-40) at λₘₐₓ 500 nm [3,11,12].

2.5. The study of adsorption isotherms

Langmuir and Freundlich isotherms are the main mathematical equations for description of reaction between adsorbents adsorbate. The equilibrium adsorption capacity by adsorbent was
Fig. 4. Normal probability plot of residual (A), predicted vs. actual values plot (B), and plot of residual vs. predicted response (C).

Table 8
Experimental range and level of the independent variables.

| Variables               | Range and level |
|------------------------|-----------------|
|                        | $-\alpha(1.5)$ | $-1$  | $0$   | $1$   | $+\alpha(1.5)$ |
| Contact Time, min      | 20              | 40    | 60    | 80    | 100            |
| Adsorbent Dosage, gr/l | 0.2             | 0.4   | 0.6   | 0.8   | 1              |
| pH                     | 3               | 5     | 7     | 9     | 11             |
| Phenol concentration (mg/l) | 50          | 100   | 150   | 200   | 250            |
calculated as follows [13–16]:

\[ q_e = \frac{(C_0 - C_e)V}{m} \]  

where,

- \( q_e \) (mg/g) is the equilibrium adsorption capacity
- \( C_0 \) and \( C_e \) are the initial and equilibrium concentration of phenol (mg/l)
- \( V \) is the volume of solution (l)
- \( M \) is the weight of adsorbent (g).

2.5.1. Langmuir isotherm

The Langmuir isotherm is used to describe the monolayer adsorption of adsorbate on the adsorbent surface. This isotherm assumed the uniform number of adsorption sites. The nonlinear equation of Langmuir was depicted (Eq. (2)). Several equations related to Langmuir isotherm were derived from nonlinear equation (Eqs. (3)–(5)) [15–17].

\[ q_e = \frac{(q_m b C_e)}{1 + b C_e} \]  

\[ \frac{C_e}{q_e} = \frac{1}{b q_m} + \frac{C_e}{q_m} \]  

\[ \frac{1}{q_e} = \frac{1}{b q_m C_e} + \frac{1}{q_m} \]  

\[ q_e = b q_m - b q_e \]  

2.5.2. Freundlich isotherm

The Freundlich isotherm assumed the multi-layer adsorption on heterogeneous adsorbent sites with unequal and non-uniform energies. The nonlinear and linear equations are presented as follow respectively [18–23]:

\[ q_e = K_F (C_e)^b \]  

\[ \ln q_e = \ln K_F + n^{-1} \ln C_e \]  

2.6. The study of adsorption kinetics

The reaction kinetics was used to study of the factors affecting the reaction rate. The kinetics equations of pseudo-first-order (Eq. (8)), pseudo-second-order (Eq. (9)), intraparticle diffusion (Eq. (10)) and Elovich (Eq. (11)) were presented as follow:

\[ \ln(q_e - q_t) = lnq_e - k_1 t \]  

\[ \frac{1}{q_t} = \frac{1}{q_e} + k_2 t \]  

\[ q_t = k_0 t^{0.5} \]  

\[ q_t = \beta \ln(\alpha \beta) + \beta lnt \]
Acknowledgment

The authors gratefully acknowledge the Research Council of Kermanshah University of Medical Sciences, Kermanshah, Iran (Grant Number:93053) for the financial support.

Transparency document. Supplementary material

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.08.068.

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