Data Article

Data for efficiency comparison of raw pumice and manganese-modified pumice for removal phenol from aqueous environments—Application of response surface methodology

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A B S T R A C T

Present deadest collection was aimed to evaluate the efficiency of raw pumice (RWP) and Mn-modified pumice (MMP). Response surface methodology (RSM) based on the central composite designs (CCD) was applied to evaluate the effects of independent variables including pH, adsorbents dosage, contact time and adsorbate concentration on the response function and the best response values were predicted. The Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) and scanning electron microscopy (SEM) were used to characterize the adsorbents. Based on acquired data, the maximum efficiency removal of phenol was obtained 89.14% and 100% for raw and Mn-modified pumice respectively. The obtained data showed pH was effective parameter on phenol removal among the different variables. Evaluation of data using isotherms and kinetics
models showed the fitted with Langmuir isotherm and pseudo second order kinetic for both adsorbents. According to obtained data was observed that modification of pumice can improve the efficiency removal of phenol to meet the effluent standards.

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### Specifications table

| Subject area                      | Environmental Health Engineering |
|-----------------------------------|----------------------------------|
| More specific subject area        | Environmental Chemistry          |
| Type of data                      | Tables, figures, text file       |
| How data was acquired             | The performance of RWP and MMP were evaluated to removing of phenol from aqueous solution. The characteristics of adsorbents were conducted by SEM, XRD and FTIR analysis. The response surface methodology (RSM) was used for analyzing the effects of several independent variables (pH, adsorbate concentration, contact time and adsorbents dosage) on the response. Moreover, obtained data were evaluated 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             | 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 [2]. |

### Value of the data

- The obtained data of this dataset showed that Mn-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 dataset 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 dataset.
- The raw data of this dataset was analyzed using the RSM method [3–6]. Therefore, the data related to the optimization conditions and the determination of the effect of each parameter will be very understandable for other researchers.
1. Data

Table 1 shows the experimental conditions and results of central composite design. The obtained data indicated the maximum efficiency removal of phenol was obtained 89.14% and 100% for RWP and MMP respectively. Tables 2 and 3 revealed the estimated regression coefficients and ANOVA dataset from the central composite design experiments for RWP and MMP respectively. Table 4 indicated Analysis of variance (ANOVA) for fit of Phenol removal efficiency by RWP and MMP. Table 5 shows the parameters of Langmuir and Freundlich isotherms for phenol adsorption on RWP and MMP. The acquired data indicated the data were obeyed the Langmuir isotherm for RWP (R² = 0.9798) and MMP (R² = 0.9944). Also, Table 6 indicates kinetic model parameters. The revealed data were obey the pseudo second order for RWP (R² = 0.9748) and MMP (R² = 0.9971). Fig. 1 illustrates the Fourier transform infrared spectroscopy (FTIR) and XRD patterns of RWP and MMP. Fig. 2 demonstrates the SEM images of RWP and MMP. Fig. 3 shows trend of phenol removal efficiency by RWP. Fig. 4 shows the response surface plots for phenol removal efficiency by RWP. Fig. 5 indicated the normal probability plot of residual related to phenol removal efficiency by RWP. Fig. 6 shows the response surface plots for phenol removal efficiency by MMP. Fig. 7 indicated the normal probability plot of residual related to phenol removal efficiency by MMP.

Table 1
Experimental conditions and results of central composite design.

| Run | Variable | Response (Phenol removal by RWP) | Response (Phenol removal by MMP) |
|-----|----------|----------------------------------|----------------------------------|
|     | Factor 1 | Factor 2 | Factor 3 | Factor 4 | Actual | Predicted | Actual | Predicted |
|     | A: pumice dosage (g/l) | B: Contact time (min) | C: pH | D: Phenol concentration (mg/l) | % | % | % | % |
| 1   | 1        | 20      | 11      | 50      | 19.31  | 18.97     | 29.6  | 27.87     |
| 2   | 0.2      | 20      | 11      | 50      | 6.21   | 6.9       | 11.7  | 12.31     |
| 3   | 1        | 20      | 3       | 50      | 79.68  | 81.46     | 89.64 | 91.7      |
| 4   | 0.6      | 80      | 7       | 150     | 70.52  | 67.65     | 78.92 | 73.91     |
| 5   | 1        | 100     | 11      | 50      | 29.32  | 27.89     | 34.55 | 32.23     |
| 6   | 0.6      | 60      | 7       | 150     | 65.76  | 65.42     | 71.98 | 73.28     |
| 7   | 1        | 100     | 3       | 250     | 68.61  | 65.04     | 76.46 | 75.28     |
| 8   | 0.6      | 60      | 7       | 150     | 65.76  | 65.42     | 72.28 | 73.28     |
| 9   | 0.6      | 60      | 7       | 100     | 66.27  | 69.58     | 76.87 | 76.72     |
| 10  | 0.2      | 100     | 3       | 250     | 49.84  | 52.97     | 61.25 | 63.6      |
| 11  | 0.6      | 40      | 7       | 150     | 58.57  | 63.19     | 65.86 | 70.1      |
| 12  | 0.6      | 60      | 7       | 150     | 65.76  | 65.42     | 72.67 | 73.28     |
| 13  | 0.6      | 60      | 7       | 200     | 60.73  | 61.26     | 69.41 | 68.79     |
| 14  | 0.6      | 60      | 7       | 150     | 65.76  | 65.42     | 72.67 | 73.28     |
| 15  | 0.6      | 60      | 7       | 150     | 65.76  | 65.42     | 72.67 | 73.28     |
| 16  | 0.2      | 100     | 11      | 50      | 14.17  | 15.82     | 11.7  | 15.73     |
| 17  | 0.6      | 60      | 9       | 150     | 53.06  | 48.87     | 58.97 | 56.18     |
| 18  | 1        | 100     | 3       | 50      | 89.14  | 90.38     | 100   | 102.85    |
| 19  | 0.2      | 20      | 11      | 250     | 3.94   | -1.03     | 10.36 | 8.12      |
| 20  | 0.4      | 60      | 7       | 150     | 57.44  | 59.23     | 64.82 | 67.94     |
| 21  | 0.8      | 60      | 7       | 150     | 69.07  | 65.26     | 78.64 | 74.75     |
| 22  | 0.6      | 60      | 5       | 150     | 73.6   | 75.76     | 82.96 | 84.98     |
| 23  | 0.2      | 100     | 11      | 250     | 8.53   | 7.89      | 14.88 | 12.25     |
| 24  | 1        | 100     | 11      | 250     | 15.19  | 19.96     | 20.64 | 23.36     |
| 25  | 1        | 20      | 3       | 250     | 59.04  | 56.12     | 66.85 | 63.44     |
| 26  | 1        | 20      | 11      | 250     | 8.93   | 11.04     | 15.44 | 18.3      |
| 27  | 0.2      | 20      | 3       | 250     | 41.01  | 44.05     | 50.95 | 52.7      |
| 28  | 0.2      | 20      | 3       | 50      | 70.38  | 69.38     | 77.68 | 75.58     |
| 29  | 0.2      | 100     | 3       | 50      | 81.34  | 78.31     | 89.21 | 85.78     |
| 30  | 0.6      | 60      | 7       | 150     | 65.76  | 65.42     | 74.5  | 73.28     |
2. Experimental design, materials and methods

2.1. Pumice preparation and its modification using manganese

Early preparations of raw scoria powder (RSP) were performed according to Moradi et al. study [2]. The coating of particles with manganese (Mn) was carried out as follows: 150 mL of 0.01 M Mn (NO₃)₂ solution and certain amount of raw pumice powder were transferred to a beaker. Then, pH was adjusted via HCl and NaOH 0.5 M. The beaker was putted on shaker at ambient temperature (25 °C ± 1 °C) for 72 h and dried at 105 °C for 24 h. The uncoated Mn was removed several times by distilled water and dried in 105 °C for 24 h [7].

| Table 2 | Estimated regression coefficients and corresponding to ANOVA results from the data of central composite design experiments before elimination of insignificant model terms: (RWP). |
|---------|----------------------------------------------------------------------------------------------------------|
| MT      | CE         | SE      | SS       | DF  | MS        | FV  | PV        | S/NS |
| Quadratic model | –          | –       | 18,744.97 | 14  | 1338.93   | 128.20 | < 0.0001  | Significant |
| A       | 6.04       | 0.80    | 601.40   | 1   | 601.40    | 57.58  | < 0.0001  | Significant |
| B       | 4.46       | 0.80    | 328.43   | 1   | 328.43    | 31.45  | < 0.0001  | Significant |
| C       | –26.89     | 0.80    | 11,932.03| 1   | 11,932.03 | 1142.47| < 0.0001  | Significant |
| D       | –8.32      | 0.80    | 1141.34  | 1   | 1141.34   | 109.28 | < 0.0001  | Significant |
| AB      | 0.18       | 0.81    | 0.55     | 1   | 0.55      | 0.052  | 0.8220 Not significant |
| AC      | –0.88      | 0.81    | 12.25    | 1   | 12.25     | 1.17   | 0.2959 Not significant |
| AD      | 0.19       | 0.81    | 0.60     | 1   | 0.60      | 0.058  | 0.8137 Not significant |
| BC      | –0.62      | 0.81    | 6.25     | 1   | 6.25      | 0.60   | 0.4512 Not significant |
| BD      | –0.57      | 0.81    | 5.22     | 1   | 5.22      | 0.50   | 0.4904 Not significant |
| CD      | 4.35       | 0.81    | 302.93   | 1   | 302.93    | 29.01  | < 0.0001  | Significant |
| A²      | –7.91      | 7.92    | 10.40    | 1   | 10.40     | 1.00   | 0.3341 Not significant |
| B²      | –2.75      | 7.92    | 1.25     | 1   | 1.25      | 0.12   | 0.7337 Not significant |
| C²      | –7.61      | 7.92    | 9.63     | 1   | 9.63      | 0.92   | 0.3522 Not significant |
| D²      | –6.93      | 7.92    | 7.98     | 1   | 7.98      | 0.76   | 0.3958 Not significant |

| Table 3 | Estimated regression coefficients and corresponding to ANOVA results from the data of central composite design experiments before elimination of insignificant model terms: (MMP). |
|---------|----------------------------------------------------------------------------------------------------------|
| MT      | CE         | SE      | SS       | DF  | MS        | FV  | PV        | S/NS |
| Quadratic model | –          | –       | 20,758.16 | 14  | 1482.73   | 118.25 | < 0.0001  | Significant |
| A       | 6.81       | 0.87    | 765.14   | 1   | 765.14    | 61.02  | < 0.0001  | Significant |
| B       | 3.82       | 0.87    | 240.55   | 1   | 240.55    | 19.18  | 0.0005    | Significant |
| C       | –28.80     | 0.87    | 13,683.74| 1   | 13,683.74 | 1091.28| < 0.0001  | Significant |
| D       | –7.94      | 0.87    | 1039.74  | 1   | 1039.74   | 82.92  | < 0.0001  | Significant |
| AB      | 0.24       | 0.89    | 0.89     | 1   | 0.89      | 0.071  | 0.7937 Not significant |
| AC      | –0.14      | 0.89    | 0.32     | 1   | 0.32      | 0.026  | 0.8748 Not significant |
| AD      | –1.35      | 0.89    | 29.03    | 1   | 29.03     | 2.31   | 0.1490 Not significant |
| BC      | –1.70      | 0.89    | 46.00    | 1   | 46.00     | 3.67   | 0.0747 Not significant |
| BD      | 0.17       | 0.89    | 0.49     | 1   | 0.49      | 0.039  | 0.8465 Not significant |
| CD      | 4.67       | 0.89    | 349.60   | 1   | 349.60    | 27.88  | < 0.0001  | Significant |
| A²      | –7.73      | 8.68    | 9.95     | 1   | 9.95      | 0.79   | 0.3871 Not significant |
| B²      | –5.09      | 8.68    | 4.32     | 1   | 4.32      | 0.34   | 0.5662 Not significant |
| C²      | –10.79     | 8.68    | 19.38    | 1   | 19.38     | 1.55   | 0.2328 Not significant |
| D²      | –2.09      | 8.68    | 0.73     | 1   | 0.73      | 0.058  | 0.8128 Not significant |

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

2. Experimental design, materials and methods

2.1. Pumice preparation and its modification using manganese

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Table 4
Analysis of variance (ANOVA) for fit of phenol removal efficiency by RWP and MMP from central composite design after elimination of insignificant model terms.

| Adsorbent | Model       | SMT  | SD    | R²     | Adj. R²  | CV    | AP    | PRESS | PV     | FV     | PLF    |
|-----------|-------------|------|-------|--------|----------|-------|-------|-------|--------|--------|--------|
| RWP       | Quadratic   | A,B,C,D, CD | 3.23  | 0.991  | 0.984    | 6.26  | 40.03 | 1090.93 | <0.0001 | 128.2  | 0.081  |
| MMP       | Quadratic   | A,B,C,D, CD | 3.54  | 0.991  | 0.982    | 5.99  | 37.83 | 1280.44 | <0.0001 | 118.2  | 0.004  |

Removal phenol by RWP(%) = 6.04A + 4.46B - 26.89C - 8.32D + 4.35CD + 65.47
Removal phenol by MMP(%) = 6.81A + 3.82B - 28.80C - 7.94D + 4.67CD + 73.28

R²: Determination Coefficient, Adj. R²: Adjusted R², 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 5
Isotherm equation parameters for phenol adsorption on RWP and MMP.

| Adsorbent | Langmuir isotherm | Freundlich isotherm |
|-----------|-------------------|---------------------|
| RWP       | qₘ (mg/g)        | 27.61               |
|           | b                 | 0.4                 |
|           | r²                | 0.9798              |
| MMP       | qₘ (mg/g)        | 41.68               |
|           | b                 | 0.095               |
|           | r²                | 0.9944              |

Freundlich isotherm

| RWP       | nₜ                   | 7.25                |
|           | Kₚ (mg/g)(L/mg)ⁿ       | 14.31               |
|           | r²                   | 0.5332              |
| MMP       | nₜ                   | 5.36                |
|           | Kₚ (mg/g)(L/mg)ⁿ       | 15.86               |
|           | r²                   | 0.9078              |

Table 6
Kinetic model parameters for the adsorption phenol at different concentration on FSP.

| Kinetic model parameters | Kinetic parameters | Adsorbent type |
|-------------------------|--------------------|----------------|
|                        |                    | RWP  | MMP |
| Pseudo-first-order      | K₁                 | 0.227| 0.206|
|                         | R²                 | 0.9654| 0.9852|
| Pseudo-second-order     | K₁                 | 0.002| 0.004|
|                         | R²                 | 0.9948| 0.9971|
| Pore diffusion          | Kᵢ                 | 1.03 | 0.9535|
|                         | R²                 | 0.945 | 0.8968|
| Elovich                 | A                  | 0.0973| 0.22|
|                         | B                  | 3.28 | 2.85|
|                         | R²                 | 0.982 | 0.9705|
2.2. Characteristics of RWP and MMP

The Fourier transform infrared spectroscopy (FTIR) analysis was conducted by WQF-510 Model. The chemical characteristics and surface morphology were determined by an XRD (Shimadzu XRD-6000) and scanning electron microscope (SEM; Philips XL30) respectively were used to Characteristics of RWP and MMP [8–11].

Fig. 1. A) Fourier transform infrared spectroscopy (FTIR) and B) XRD patterns of RWP and MMP.

Fig. 2. SEM images of A) RWP and B) MMP.
2.3. Experimental design using RSM

Because the existence of many parameters which affected the results of experiments, achieve to the optimal conditions of experiments is an important strategy for determining the effective parameters and reducing the costs. Hence, attention to mathematical methods was developed to evaluate the obtained data. RSM based on central composite design (CCD) is a proper method to determine the best conditions of experiments for minimization of number of experiments and to survey of the relationship between the measured responses (phenol removal) and number of independent variables with the goal of optimizing the response [12–16]. (Design Expert 8.0, Stat-Ease Inc., Minneapolis, MN, USA) Table 7 illustrated- the experimental range and level of the independent variables.

2.4. Batch sorption studies

The sorption experiments were carried out in batch reactor. Initial concentration of phenol (50, 100, 150, 200 and 250 mg/l), adsorbent dose (0.1–1 g/L), pH (3, 5, 7, 9 and 11), contacted time
(20, 40, 60, 80 and 100 min) and ambient temperature (25 °C) were selected as variables. The residual phenol was determined by UV/VIS spectrophotometer (Hitachi Model 100-40) at $\lambda_{\text{max}}$ 500 nm [17–19].

2.5. Adsorption isotherms and kinetics

The adsorbent capacity could be described using sorption isotherm. In the present study the adsorption data of phenol were evaluated by Langmuir and Freundlich isotherms. The linear Langmuir isotherm presented as follow:

$$\frac{C_e}{q_e} = \frac{1}{bq_m} + \frac{C_e}{q_m}$$  \hspace{1cm} (1)

Where the $C_e$ is equilibrium concentration (mg/l), $q_e$ is phenol adsorbed at equilibrium (mg/g), $q_o$ and $b$ are the Langmuir constants related to the capacity and energy of adsorption, respectively [20,21].

Freundlich adsorption isotherm is an empirical expression that describes adsorption on a heterogeneous surface. The linear Freundlich isotherm could be illustrated as fallow:

$$\ln q_e = \ln k_f + n^{-1} \ln C_e$$  \hspace{1cm} (2)
Where $K_f$ and $n$ are Freundlich constants corresponded to adsorption capacity and adsorption intensity, respectively [22–24]. The kinetics were investigated via adsorption of certain concentration of phenol at different contact time. Kinetic study is essential for provide information on the factors affecting it reaction speed.

Several kinetics include pseudo-first-order, pseudo-second-order, intraparticle diffusion and elovich were used to controlling mechanisms of the adsorption process. The equations of kinetic models are expressed as follows [25–30]:

**Pseudo-first-order:**

$$\ln(q_e - q_t) = ln q_e - k_1 t$$

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**Fig. 5.** Normal probability plot of residual (A), predicted vs. actual values plot (B), and plot of residual vs. predicted response (C) related to phenol removal efficiency by RWP.
Pseudo-second-order:

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

(4)

Intraparticle diffusion:

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

(5)

Elovich:

\[ q_t = \beta \ln(\alpha \beta) + \beta \ln t \]  

(5)

Fig. 6. Response surface plots for phenol removal efficiency by MMP with respect to contact time and pumice dosage (A), pH and phenol concentration (B), pH and contact time (C).
Fig. 7. Normal probability plot of residual (A), predicted vs. actual values plot (B), and plot of residual vs. predicted response (C) related to phenol removal efficiency by MMP.

| Table 7  |
|----------|
| **Variables** | **Range and level** |
| | $-\alpha(-1.5)$ | $-1$ | $0$ | $1$ | $+\alpha(1.5)$ |
| Contact Time, min | 20 | 40 | 60 | 80 | 100 |
| Adsorbent Dosage, g/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 |
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Transparency document. Supporting information

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