Data Article

Data on modeling of UV/Na₂S₂O₈/FeS₂ process in amoxicillin removal using Box-Behnken methodology

Roshanak Rezaei Kalantarya, Massuomeh Rahmatinia, Masoud Moradi

Article history:
Received 3 June 2018
Received in revised form 14 June 2018
Accepted 27 June 2018
Available online 2 July 2018

Keywords:
Amoxicillin
Box-Behnken
UV/Na₂S₂O₈/FeS₂

Abstract

Among the pharmaceutical compounds, antibiotics have been paid specific consideration, due to their acute and chronic toxic effects on organisms. Amoxicillin (AMX) is used widely for treatment of bacterial infections. About 80% of amoxicillin excreted unchanged and enters the aquatic environment through different routes including disposal of municipal wastewaters, hospital wastewaters and farm wastewaters. In this study degradation of amoxicillin by UV/Na₂S₂O₈/FeS₂ process was evaluated. According to the results, the R-squared and adjusted R-squared were 0.9877 and 0.9828, respectively. The AMX removal efficiency was 93% at optimum conditions. Thus, UV/Na₂S₂O₈/FeS₂ process is a useful process for amoxicillin removal.

© 2018 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).
**Specifications Table**

| Subject area               | Environmental engineering          |
|----------------------------|----------------------------------|
| More specific subject area | Advanced oxidation process       |
| Type of data               | Figures and tables                |
| How data was acquired      | All degradation tests were done in a reactor batch (Volume of 1 L), equipped with a UV-C lamp (16 W). Three level of each parameter was evaluated using BOX-Behnken design. A High Liquid Performance Chromatography (HPLC) was used for the determination of AMX concentration. |
| Data format                | Analyzed                         |
| Experimental factors       | Measuring of AMX concentrations under various levels of initial AMX concentration, solution pH, Persulfate concentration, dose of FeS$_2$ and contact time to obtain optimum AMX removal from aqueous solutions. |
| Experimental features      | Optimization of AMX degradation using BOX-Behnken design. |
| Data source location       | Iran University of Medical sciences, Tehran, Iran |
| Data accessibility         | Data are available within paper. |

**Value of data**

- The synthesized catalyst has properties include earth abundant, low cost, high absorption coefficient and good photocatalytic activity. Also, pyrite catalyst is reusable.
- This research shows a statistical method (Box-Behnken design) to optimize AMX removal from aqueous solution.
- The obtained data will be appropriate for AMX removal from water and wastewater.

1. **Data**

The level of variables and their codes are shown in Table 1. For optimization of UV/Na$_2$S$_2$O$_8$/FeS$_2$ process, Box–Behnken design (BBD) was applied as a response surface method [1–3]. The adequacy of the model was checked using analysis of variance (ANOVA) (Table 2). P-values $< 0.05$ showed that the model is statistically significant [4]. Five variables (initial AMX concentration, pyrite dose, per sulfite concentration, time and pH) had linearly significant effect with p-value $< 0.05$. The R-Squared value (0.9828) is close to adjusted R-squared (0.9877) implying high importance of the model [5]. The diagrams of normal probability of the studentized residuals and the predicted against experimental values are shown in Figs. 1 and 2, respectively. Fig. 3 shows the interaction effects of variables on AMX removal efficiency. According to the results, a quadratic equation between dependent variable (AMX removal %) and independent variables was obtained as follows:

**Table 1**
Levels of independent variables and experimental range in Box–Behnken design.

| Factors                        | Range and level |
|--------------------------------|-----------------|
| A: Initial AMX (mg/l)          | 10  40  70      |
| B: catalyst load (g/l)         | 1   2   3       |
| C: per sulfite concentration (mM)| 0.5  2  3.5     |
| D: Time(min)                   | 30  45  60      |
| E: pH                          | 3   6   9       |

R.R. Kalantary et al. / Data in Brief 19 (2018) 1810–1815
Table 2
ANOVA test for quadratic model.

| Source | Sum of squares | Degree of freedom | Mean square | F value | P-value | Prob > F |
|--------|----------------|-------------------|-------------|---------|---------|----------|
| Model  | 14,539.55      | 13                | 111.43      | 198.39  | < 0.0001| Significant |
| A      | 1440.1         | 1                 | 1440.1      | 255.44  | < 0.0001| Significant |
| B      | 41.93          | 1                 | 41.93       | 7.44    | 0.0103  | Significant |
| C      | 603.56         | 1                 | 603.56      | 107.6   | < 0.0001| Significant |
| D      | 7428.72        | 1                 | 7428.72     | 1317.74 | < 0.0001| Significant |
| E      | 3693           | 1                 | 3693        | 639.12  | < 0.0001| Significant |
| AD     | 21.58          | 1                 | 21.58       | 3.83    | 0.0479  | Significant |
| BD     | 22.52          | 1                 | 22.52       | 3.99    | 0.0490  | Significant |
| CD     | 0.22           | 1                 | 0.22        | 0.038   | 0.0592  | Not Significant |
| A²     | 49.09          | 1                 | 49.09       | 8.71    | < 0.0059| Significant |
| B²     | 890.71         | 1                 | 890.71      | 158     | < 0.0001| Significant |
| C²     | 168.96         | 1                 | 168.96      | 29.97   | < 0.0268| Significant |
| D²     | 30.48          | 1                 | 30.48       | 5.93    | < 0.0241| Significant |
| E²     | 31.59          | 1                 | 31.59       | 5.60    | < 0.0278| Significant |
| Residual | 180.40        | 32                | 5.64        |         |         |          |
| Lack of Fit | 142.54    | 27                | 5.28        | 0.70    | 0.7559  | Not significant |
| Pure Error | 37.86         | 5                 | 7.57        |         |         |          |
| Cor Total | 14,719.95     | 45                |             |         |         |          |
| R-square | 0.9877        |                   |             |         |         |          |
| Adj R-square | 0.9828 |                   |             |         |         |          |
| Pred R-squared | 0.9700 |                   |             |         |         |          |
| Adequate precision | 55.813 |                   |             |         |         |          |

Fig. 1. Normal probability plot of studentized residuals.
2. Experimental design, materials and methods

2.1. Materials

AMX (CAS 26787-78-0) and Sodium persulfate (Na$_2$S$_2$O$_8$ 98%) were obtained from Sigma- Aldrich. FeS$_2$ rock sample (Pyrite) was purchased from Department of Mine Engineering, university of Tehran.

2.2. Catalyst preparation

Firstly, pyrite rock sample by a ceramic mortar was milled and for 5 min in ethanol (95%) was ultra-sonicated. For removal of impurities was washed with 1 M nitric acid, rinsed with deionized water and ethanol, respectively. Subsequently, pyrite was dried at 30 °C. Finally, pyrite was sieved (80 μm) [6].

2.3. Determination of AMX concentration

The AMX concentration of all samples was measured by A High Liquid Performance Chromatography (HPLC, CE4200-c Cecil, England). The equation below was applied for obtaining the removal efficiency (η %) as follows [7–9]:

\[
\text{AMX removal(\%)} = 55.35 - 9.49A - 1.62B + 6.14C + 21.55D + 15.01E + 2.32AD - 2.37BD - 0.23CD + 2.37A^2 - 10.10B^2 - 4.40C^2 + 1.87D^2 - 1.90E^2
\]

Where, $C_0$ is the initial concentration and $C_f$ is residual concentration of AMX.
Fig. 3. Response surface plots for AMX removal by UV/Na$_2$S$_2$O$_8$/FeS$_2$ (a) AMX removal versus initial AMX and time (b) AMX removal versus AMX catalyst load and time (c) AMX removal versus persulfate dose and time (d) AMX removal versus pH and time.
2.4. Experimental design

2.4.1. Box–Behnken design experiments

The experiments designed by Design-Expert software (version 7), based on Box–Behnken design (BBD) and total experiments were 46 runs. BOX-Behnken design was used to analyze five parameters i.e. pH, concentration of per sulfate, Fe S₂ concentration, contact time and initial AMX concentration on AMX removal efficiency and removal optimum conditions.

2.4.2. AMX removal experiments

Firstly, the stock solution of 1000 mg/L AMX was prepared to obtain different concentration. Then, the effects of variables such as initial AMX (10–80 mg/L), solution pH (3–9), contact time (30–60 min), pyrite dose (1–3 g/L) and persulfate concentration (0.5–3.5 mM) were evaluated.

Funding sources

This research was supported by Iran University of Medical Sciences under Grant no. 30049.

Transparency document. Supporting information

Transparency data associated with this article can be found in the online version at https://doi.org/10.1016/j.dib.2018.06.109.

References

[1] M. Shams, M.H. Dehghani, R. Nabizadeh, A. Mesdaghinia, M. Alimohammadi, AA. Najafpoor. Adsorption of phosphorus from aqueous solution by cubic zeolitic imidazolate framework-8: modeling, mechanical agitation versus sonication, J. Mol. Liq. 224 (2016) 151–157.
[2] M.H. Dehghani, M. Ghadermazi, A. Bhatnagar, P. Sadighara, G. Jahed-Khaniki, B. Heibati, et al., Adsorptive removal of endocrine disrupting bisphenol A from aqueous solution using chitosan, J. Environ. Chem. Eng. 4 (2016) 2647–2655.
[3] M. Dehghani, F. Changani, The effect of acoustic cavitation on chlorophyceae from effluent of wastewater treatment plant, Environ. Technol. 27 (2006) 963–968.
[4] B. Kakavandi, A. Takdastan, N. Jaafarzadeh, M. Azizi, A. Mirzaei, A. Azari, Application of Fe3O4@ C catalyzing heterogeneous UV-Fenton system for tetracycline removal with a focus on optimization by a response surface method, J. Photochem. Photobiol. A: Chem. 314 (2016) 178–188.
[5] A.T. Nair, A.R. Makwana, M.M. Ahamed, The use of response surface methodology for modelling and analysis of water and wastewater treatment processes: a review, Water Sci. Technol. (2014) 464–478.
[6] M. Moradi, R.R. Kalantary, A. Esrafil, A.J. Jafari, M. Gholami, Visible light photocatalytic inactivation of Escherichia coli by natural pyrite assisted by oxalate at neutral pH, J. Mol. Liq. 248 (2017) 880–889.
[7] A. Assadi, M.H. Dehghani, N. Rastkari, S. Nasserri, A.H. Mahvi, Photocatalytic reduction of hexavalent chromium in aqueous solutions with zinc oxide nanoparticles and hydrogen peroxide, Environ. Prot. Eng. 38 (2012) 5–16.
[8] M. Yousefi, S.M. Arami, H. Takallo, M. Hossein, M. Radfard, H. Soleimani, et al., Modification of pumice with HCl and NaOH enhancing its fluoride adsorption capacity: kinetic and isotherm studies, Human. Ecol. Risk Assess.: Int. J. (2018) 1–13.
[9] H.N. Saleh, M.H. Dehghani, R. Nabizadeh, A.H. Malvi, F. Hossein, M. Ghaderpoori, et al., Data on the acid black 1 dye adsorption from aqueous solutions by low-cost adsorbent-Cerastoderma Lamarcki shell collected from the northern coast of Caspian Sea, Data Brief. 17 (2018) 774–780.