Data Article

Experimental data on antibiotic cephalexin removal using hydrogen peroxide and simulated sunlight radiation at lab scale: Effects of pH and H$_2$O$_2$

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**ABSTRACT**

Cephalexin (CPX) is a β-lactam antibiotic widely used to treat bacterial infections in the respiratory tract, skin, bones, and ear; a situation that has contributed to its discharge into wastewater (mainly through excretion after ingestion) and its accumulation in water bodies. CPX presence on environmental compartments could interfere in the physiological functions of animals and humans due to the induction of mutagenic and carcinogenic effects.

Different technologies have been evaluated to remove CPX from aqueous matrices. In this way, this work presents the main data regarding the use of the combination of hydrogen peroxide and simulated sunlight radiation in CPX removal. Effects of H$_2$O$_2$ initial concentration and solution pH were evaluated using a face-centered, central composite design and the response surface methodology. Optimized conditions, under the evaluated experimental range, were established. In addition, data about the total organic carbon and anions content in treated samples were collected.

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https://doi.org/10.1016/j.dib.2020.105437

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These data can be useful for the evaluation of the use of H₂O₂ and light radiation on organic pollutants removal, the comparison of the effectiveness of different technologies on CPX elimination, and as a starting point to carry out this type of process at pilot or real scale.

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## Specifications table

| Subject          | Chemical Engineering |
|------------------|----------------------|
| Specific subject area | Advanced oxidation technologies |
| Type of data | Table |
| Figure |
| How data were acquired | Data were obtained by High Performance Liquid Chromatography (HPLC). Solutions Total Organic Carbon (TOC) and anions content (nitrates and sulfates) were determined using the Standard Methods for the Examination of Water and Wastewater (2017) methods 526D (High temperature combustion method) and 4110B (Determination of anions by ion chromatography). Statgraphics Centurion XVI software was employed for the statistical analysis of data. |
| Data format | Raw |
| Analyzed |
| Parameters for data collection | Data were collected at fixed experimental conditions. Effects of hydrogen peroxide initial concentration and pH on cephalixin removal were evaluated. |
| Description of data collection | All experimental data were obtained at lab-scale. Optimized conditions, under evaluated experimental range, were established using the Statgraphics Centurion XVI software. |
| Data source location | Grupo Diagnóstico y Control de la Contaminación (GDCON), Engineering College, Universidad de Antioquia (UdeA), Medellín-Colombia. |
| Data accessibility | Data are available only in this article |

## Value of the data

- Data show that UV/hydrogen peroxide is an appropriate technique to remove antibiotic cephalixin from water.
- Data could benefit researches and institutions working on wastewater treatment, organic pollutants elimination, and advanced oxidation technologies application.
- Data can be employed for the evaluation of the potential use of H₂O₂ and light radiation on organic pollutants removal, and as a starting point to carry out this type of process at pilot or real scale.
- Data present optimized conditions that allow to increase CPX removal using H₂O₂ and sunlight.
- Data include information regarding the variation of the total organic carbon, nitrates and sulphates of treated samples.
- Data may be useful in future research on antibiotics removal from aquatic environments.

## 1. Data description

Data presented in this work describes the cephalixin removal by the combination of H₂O₂ and simulated sunlight. UV/H₂O₂ technology consists in the H₂O₂ decomposition under UV light presence to generate hydroxyl radicals (OH•) according to Eq. (1) [1,2]. OH• is able to oxidize
organic pollutants [3].

$$\text{H}_2\text{O}_2 + \text{hv} \rightarrow 2 \text{OH}$$

(1)

The reaction kinetics of the UV/H$_2$O$_2$ process is a function of the solution pH, the peroxide initial concentration and the physicochemical properties of the target pollutant [4]. In addition, as part of the solar radiation has a wavelength corresponding to the UV range, there is a possibility of implementing photo-treatment systems using solar light and H$_2$O$_2$ for water treatment [5].

The potential application of H$_2$O$_2$ and simulated sunlight was evaluated considering a face-centered central composite experimental design and the response surface methodology (response: pollutant removal after 30 min of reaction). Table 1 shows the factors and levels evaluated on antibiotic removal using simulated sunlight and H$_2$O$_2$; and Table 2 corresponds to the experimental results obtained after carried out the proposed experimental design. Total number of experiments: 11.

Table 1
Factors and levels evaluated on CPX removal using simulated sunlight and H$_2$O$_2$.

| Factor         | Low level | Medium level | High level |
|----------------|-----------|--------------|------------|
| pH             | 3.0       | 6.0          | 9.0        |
| H$_2$O$_2$ initial concentration (mg L$^{-1}$) | 2.3       | 4.6          | 6.9        |

Table 2
Experimental design for CPX removal using simulated sunlight and H$_2$O$_2$ (pollutant initial concentration 2.0 mg L$^{-1}$, reaction time 30 min, irradiance 500 W m$^{-2}$).

| Test | pH  | H$_2$O$_2$ initial concentration (mg L$^{-1}$) | Pollutant removal (%) | Predicted pollutant removal (%) |
|------|-----|---------------------------------------------|-----------------------|---------------------------------|
| 1    | 3.0 | 6.9                                         | 91.4                  | 88.7                            |
| 2    | 9.0 | 2.3                                         | 10.3                  | 14.7                            |
| 3    | 6.0 | 4.6                                         | 14.7                  | 17.6                            |
| 4    | 3.0 | 2.3                                         | 83.2                  | 82.5                            |
| 5    | 9.0 | 4.6                                         | 32.9                  | 24.7                            |
| 6    | 3.0 | 4.6                                         | 83.3                  | 86.3                            |
| 7    | 6.0 | 4.6                                         | 18.1                  | 17.6                            |
| 8    | 6.0 | 2.3                                         | 15.0                  | 10.7                            |
| 9    | 6.0 | 4.6                                         | 16.4                  | 17.6                            |
| 10   | 9.0 | 6.9                                         | 31.0                  | 33.3                            |
| 11   | 6.0 | 6.9                                         | 23.9                  | 23.1                            |

Fig. 1 shows the obtained response surface for CPX removal under simulated sunlight radiation and H$_2$O$_2$, which allows to predict the pollutant removal under different combinations of pH and H$_2$O$_2$ initial conditions.

Fig. 2 corresponds to the associated main effects plot for CPX removal. This figure is useful to determine the effect of each factor on CPX removal without considering the effect of the other variables that intervene in the process.

Fig. 3 is the associated Pareto chart and indicates the magnitude and significance of the effect of each factor and interaction on pollutant elimination.

Statgraphics Centurion XVI software allowed to determine the model (Eq. (2)) that relates the response factor with the evaluated experimental parameters. According to model, conditions that conduct to a higher CPX removal were pH 3.0 and 6.9 mg L$^{-1}$ H$_2$O$_2$ initial concentration. Coefficient of determination, $R^2$, between experimental data and model was 0.986. In addition, Table 2 presents the calculated values regarding CPX removal using the proposed model, which shows that equation predicts CPX elimination, under the studied conditions,
Fig. 1. Response surface for CPX removal using simulated sunlight radiation and H$_2$O$_2$ (pollutant initial concentration 2.0 mg L$^{-1}$, irradiance 500.0 W m$^{-2}$, reaction time 30 min).

Fig. 2. Main effects plot for CPX removal using simulated sunlight radiation and H$_2$O$_2$ (pollutant initial concentration 2.0 mg L$^{-1}$, irradiance 500.0 W m$^{-2}$, reaction time 30 min).

adequately.

CPX removal (%) = 227.83 – 62.85 pH + 1.28 H$_2$O$_2$ + 4.21 pH$^2$ + 0.45 pH*H$_2$O$_2$ – 0.14 H$_2$O$_2^2$  

(2)

Table 3 and Fig. 4 show CPX removal under different experimental conditions including H$_2$O$_2$/sunlight radiation at optimized conditions, photolysis, hydrolysis (at pH 3.0), oxidation with H$_2$O$_2$ and the effect of the presence of a scavenger agent (isopropyl alcohol).

Finally, Fig. 5 presents information regarding the total organic matter (TOC), nitrates and sulfates content in treated samples.
Fig. 3. Pareto chart for CPX removal using simulated sunlight radiation and H₂O₂ (pollutant initial concentration 2.0 mg L⁻¹, irradiance 500.0 W m⁻², reaction time 30 min).

Table 3
Data regarding CPX removal under optimized conditions using simulated sunlight radiation and H₂O₂ (pollutant initial concentration 2.0 mg L⁻¹, irradiance 500.0 W m⁻², pH 3.0, H₂O₂ initial concentration 6.9 mg L⁻¹).

| Sample | Time(min) | C/C₀ | Optimized conditions | Photolysis | Hydrolysis | Oxidation with H₂O₂ | Isopropyl alcohol presence (100 mg L⁻¹) |
|--------|-----------|------|----------------------|------------|------------|---------------------|----------------------------------------|
| 1      | 0         | 1.00 | 1.00                 | 1.00       | 1.00       | 1.00                | 1.00                                   |
| 2      | 5         | 0.86 | 0.99                 | 0.96       | 1.00       | 0.94                | 0.95                                   |
| 3      | 10        | 0.73 | 0.96                 | 1.00       | 0.92       | 0.95                | 0.95                                   |
| 4      | 15        | 0.58 | 0.94                 | 1.00       | 0.90       | 0.93                | 0.93                                   |
| 5      | 20        | 0.41 | 0.94                 | 1.00       | 0.88       | 0.92                | 0.92                                   |
| 6      | 25        | 0.24 | 0.91                 | 1.00       | 0.87       | 0.91                | 0.91                                   |
| 7      | 30        | 0.18 | 0.89                 | 0.99       | 0.85       | 0.91                | 0.91                                   |
| 8      | 40        | 0.05 | 0.85                 | 0.99       | 0.83       | 0.89                | 0.89                                   |
| 9      | 50        | 0.00 | 0.82                 | 0.99       | 0.81       | 0.85                | 0.85                                   |
| 10     | 60        | 0.00 | 0.76                 | 0.99       | 0.79       | 0.83                | 0.83                                   |

2. Experimental design, materials, and methods

2.1. Materials

All the aqueous solutions were prepared using ultra-pure water (Milli-Q water, 18.2 MΩ cm). Cephalexin (98.0%, AK Scientific), H₂O₂ (35.0% w/w, Merck) and isopropyl alcohol (99.9%, Merck) were used to carry out the experiments. Control of pH was done using concentrated solutions of NaOH (0.1 N) and HCl (1.0 N) obtained from Alfa-Aesar. Sodium thiosulfate pentahydrate (Na₂S₂O₅•5H₂O, Sigma Aldrich) was employed for quenching remaining H₂O₂ after sampling process; and acetonitrile for chromatographic analysis was of LC/MS grade.

2.2. Photocatalytic system

Pyrex flasks containing 50.0 mL of solution (CPX initial concentration 2.0 mg L⁻¹) were used for photo-treatment. Solutions pH was adjusted after the additon of CPX and H₂O₂. Experiments were carried out using a Suntest CPS+ (Atlas) photosimulator equipped with a xenon lamp that
Fig. 4. CPX removal under optimized conditions using simulated sunlight radiation and \( \text{H}_2\text{O}_2 \) (pollutant initial concentration 2.0 mg L\(^{-1}\), irradiance 500.0 W m\(^{-2}\), pH 3.0, \( \text{H}_2\text{O}_2 \) initial concentration 6.9 mg L\(^{-1}\)).

delivered light with a spectrum similar to that of the sun. Irradiance during experiments was 500 W m\(^{-2}\). Distance from the lamp to the liquid surface was \( \sim 20.0 \) cm, and the liquid depth inside the flasks was \( \sim 5.0 \) cm.

2.3. Experimental design

The effects of solution pH and \( \text{H}_2\text{O}_2 \) initial concentration were evaluated using a face-centered central composite design, and considering the levels presented by Table 1. The total number of experiments was 11 (three central points). Data were analyzed using the Statgraphics Centurion XVI software with a confidence level of 95.0%.

Optimized conditions were selected having into account the polynomial model stablished, after a non-linear regression of data, by the statistical software (Eq. (2))

Tests regarding pollutants removal under optimized conditions, hydrolysis, photolysis, oxidation with \( \text{H}_2\text{O}_2 \) and effect of an scavenger agent presence were done in triplicate.

2.4. Analytical methods

Samples of 0.75 mL were withdrawn at different time intervals during the experiments, then 0.25 mL of \( \text{Na}_2\text{S}_2\text{O}_3\cdot5\text{H}_2\text{O} \) (100 mg L\(^{-1}\)) were added to inhibit the potential oxidative effect of remaining \( \text{H}_2\text{O}_2 \).

CPX concentration was determined using an Agilent 1200 Series HPLC system, a Kinetex C18 column (silica with 100 Å pore diameter, 2.5 \( \mu \text{m} \), 4.6 \( \times \) 150 mm), and a diode array detector set to 261.4 nm. A mixture of acetonitrile/water (90:10, v/v) was used as mobile phase (flow rate 0.55 mL min\(^{-1}\)). injection volume was 80 \( \mu \text{L} \), and column temperature was 35.0 °C.

Total Organic Carbon (TOC), nitrates and sulfates were determined using an APOLLO 9000 Combustion TOC Analyzer (Teledyne Tekmar) and a Dionex Integrion HPIC system (Thermo
Fig. 5. a. Total organic carbon, b. Nitrates and c. sulfate variation during CPX removal under optimized conditions using simulated sunlight radiation.
Scientific) respectively. Standard Methods for the Examination of Water and Wastewater (2017) [6] methods 526D (High temperature combustion method) and 4110B (Determination of anions by ion chromatography) were also employed.

Acknowledgments

Authors thank Vicerrectoría de Investigación-Universidad de Antioquia for the financial support provided to this project.

Conflict of Interest

The authors declare that they have no known competing financial interests or personal relationships which have, or could be perceived to have, influenced the work reported in this article.

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