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# Electrochemical oxidation of sulfamethoxazole using Ti/SnO<sub>2</sub>–Sb/Co–PbO<sub>2</sub> electrode through ANN-PSO

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Abstract: Even in a trace amounts, the presence of antibiotics in aqueous solution is getting more and more attention. Accordingly, appropriate technologies are needed to efficiently remove these compounds from aqueous environments. In this study, we have examined the electrochemical oxidation (EO) of sulfamethoxazole (SMX) on a Co modified PbO<sub>2</sub> electrode. The process of EO of SMX in aqueous solution followed the pseudo-first-order kinetics, and the removal efficiency of SMX reached the maximum value of 95.1 % within 60 min. The effects of major factors on SMX oxidation kinetics were studied in detail by single-factor experiments, namely current density (1-20 mA cm<sup>-2</sup>), solution pH value (2-10), initial concentration of SMX (10-500 mg L<sup>-1</sup>) and concentration of electrolytes (0.05-0.4 mol L<sup>-1</sup>). An artificial neural network (ANN) model was used to simulate this EO process. Based on the obtained model, particle swarm optimization (PSO) was used to optimize the operating parameters. The maximum removal efficiency of SMX was obtained at the optimized conditions (e.g., current density of 12.37 mA cm<sup>-2</sup>, initial pH value of 4.78, initial SMX concentration of 74.45 mg L<sup>-1</sup>, electrolyte concentration of  $0.24 \text{ mol } L^{-1}$  and electrolysis time of 51.49 min). The validation results indicated that this method can ideally be used to optimize the related parameters and predict the anticipated results with acceptable accuracy.

*Keywords*: sulfamethoxazole; electrochemical oxidation; artificial neural networks; particle swarm optimization.

# INTRODUCTION

Synthetic antimicrobial agents in aqueous environments are attracting more and more attention from the scientific community due to their potentially hazardous impacts on the aquatic environment and human health. Widespread detection of these compounds in water bodies, even at minute concentrations, has already raised public health concerns. The adverse health effects, such as enhancement of

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antibiotic resistance, have been increasingly reported, but the consequences caused by long-lasting exposure to trace amounts of such synthetic antimicrobial agents remain uncertain.<sup>1–5</sup> In this study, sulfamethoxazole (SMX), a typical broad-spectrum sulfonamide antibiotic used to combat Gram-positive and Gram-negative aerobic bacteria, was selected as a model pollutant.<sup>6,7</sup> In recent years, SMX has been detected in surface water, hospital effluents, and drinking water, thus posing a potential environmental risk.<sup>8–10</sup> Besides, its antibacterial property impedes effective abatement using conventional biological treatment processes.<sup>5,11</sup> Therefore, effective methods are sorely needed to prevent dangerous accumulation of SMX in aqueous environments.

The electrochemical oxidation (EO) process has been proved to be an effective method for the removal of a broad spectrum of organic matters due to its ease of operation, low cost and environmental friendliness.<sup>12-14</sup> In EO, organic pollutants are either removed by direct oxidization (e.g., electrons are transferred to the anode directly) or by indirect oxidization (i.e., some hydroxyl radicals are generated and act as mediators in the degradation process).<sup>15–19</sup> EO is a thoroughly studied advanced oxidation process (AOP) for all kinds of wastewater applications, with most studies focused on the anode material, operating factors and design of the EO reactor.<sup>18-21</sup> The performance of EO is highly dependent on the activity and stability of the anode. Various anodes such as, PbO<sub>2</sub>, dimensionally stable anodes, and boron-doped diamond (BDD) have shown outstanding rem-oval efficiency for SMX.<sup>7,19,22</sup> However, the possibility of releasing lead ions during the EO process is a major drawback of the PbO<sub>2</sub> anode. The BDD anode seems to be the best choice, as it exhibits the highest oxygen evolution reaction overpotential and better oxidation performance than alternative approaches. In addition, it has been reported that BDD anodes almost completely mineralize SMX and its intermediates, achieving high SMX removal efficiency ( $\approx 100$  %). chemical oxygen demand (COD > 90 %) and total organic carbon (TOC > 90%).<sup>23</sup> However, the price of BDD anodes is relatively high (\$15,000–22,000/m<sup>2</sup>), which limits its industrial applications.<sup>24</sup>

As an engineering method, modeling can help to comprehensively understand the EO process.<sup>25</sup> Nevertheless, few studies have focused specifically on optimizing relevant parameters and predicting results to reach optimal conditions. The characteristics of current density, pH value, the initial concentration of SMX, electrolyte concentration and degradation time also play key roles in the EO of the antibiotic in aqueous solution. The mechanism of EO is very complicated and the relationships among these parameters are nonlinear. It is difficult to explain such problems by using conventional mathematical models. An artificial neural network (ANN) is a universal and highly flexible mathematical tool for the modeling and analysis of some complicated problems in which the data relationships are unknown. Compared to the conventional modeling methods, ANNs

perform better in extracting a pattern in nonlinear, complex and noisy data sets to detect the trends with higher accuracy. ANNs have proved useful in a variety of biological, medical and economic aspects.<sup>26–28</sup> Particle swarm optimization (PSO), which was originally inspired by the regularity of the behavior of bird flocks, obtains the optimal solution by sharing information among the groups.<sup>29,30</sup> With advantages such as less parameters, ease of adjustment, local and global integration and fast convergence, PSO has been successsfully applied to many cases including ANN training, function optimization and pattern classification.<sup>31</sup>

The present study describes an efficient method for the degradation of SMX in aqueous solution. The effects of the major factors on the kinetics were investigated in detail, particularly current density, electrolyte concentration, solution pH value, and initial concentration of SMX. An ANN was developed to model the SMX removal through the EO process. Moreover, the ANN model coupled with PSO was applied to predict the optimized parameters required for maximizing the SMX removal efficiency. The outcomes of this study may contribute to the further application of EO for the removal of synthetic antimicrobial agents in aqueous medium.

## EXPERIMENTAL

## Material and reagents

All reagents and materials were analytical grade and all solutions were prepared with deionized water (resistivity = 18 M $\Omega$  cm at 25 °C) using a Milli-Q<sup>TM</sup> system (Millipore Corp., Bedford, MA, USA). Titanium foil with a reaction area of 37.5 cm<sup>2</sup> (50 mm×75 mm) was selected as the metal matrix. SMX was purchased from Sigma-Aldrich (Saint Louis, MO, USA).

# Preparation of electrodes

In this study, the anode contained three coatings. First, before use, the titanium plates were chemically degreased in a NaOH solution (5%) at 90 °C for 1 h and then etched in a boiling oxalic acid solution (10%) for 2 h. Second, the SnO<sub>2</sub>–Sb<sub>2</sub>O<sub>3</sub> bottom coating was prepared by the sol–gel method. The titanium plate was symmetrically brushed with the sol–gel, consisting of SbCl<sub>3</sub>, SnCl<sub>4</sub>·4H<sub>2</sub>O and isopropyl alcohol, dried under vacuum for 10 min at 130 °C and annealed for 15 min at 515 °C. This process was repeated 15 times, followed by annealing for 60 min. Ultimately, the Co-doped modified  $\beta$ -PbO<sub>2</sub> active coating was electrodeposited in an acidic electrolyte containing 0.5 M Pb(NO<sub>3</sub>)<sub>2</sub>, 0.1 M HNO<sub>3</sub>, 0.01 M NaF and 0.006 M Co(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O.

#### Electrochemical oxidation experiments

The EO processes of SMX were performed in an electrochemical system with an effective volume of 100 ml. A 1.5-mm-thick Co-doped modified  $PbO_2$  electrode with dimensions of 7.5 cm (length)×5 cm (width) was selected as the anode, and same-sized stainless steel plates (SS304) were used as cathode. The electrode spacing was maintained at 1.5 cm. A 1000-ml reservoir contained the test solution, which was kept in a constant state of flow by pumping it through the electrochemical system before being returned to the reservoir (Scheme 1). In each experiment, an SMX aqueous solution (10–500 mg L<sup>-1</sup>) containing 0.05–0.4 M NaCl electrolyte solution was used and the current density was adjusted in the range from 1 to 20 mA cm<sup>-2</sup> with alternating current power. In each experiment, samples were taken from the reservoir at predetermined time intervals.



1: Power, 2:Anode, 3:Cathode, 4: Reservoir, 5: Peristaltic pump Scheme 1. Configuration of the electrochemical oxidation experiments.

### Analytical methods

The concentration of SMX was determined by high-performance liquid chromatography (HPLC) on an Agilent HPLC system (Agilent Technologies, Santa Clara, CA, USA) equipped with an Agilent Eclipse XRD-C18 column (4.5 mm×250 mm with 5  $\mu$ m pore size) using 36 mM KOH as eluent at a flow rate of 1.0 ml L<sup>-1</sup>. The pH value was determined with a 766 laboratory pH meter (Knick International, Berlin, Germany).

## ANN-PSO modelling and optimization

A standard ANN consists mainly of network topology, activation functions between neurons, and learning algorithms. In this study, a three-layer network with a back propagation algorithm was designed to build the predictive mathematical model. The input layer consists of five neurons, including current density, pH value of the solution, the initial SMX concentration, electrolyte concentration and electrolysis time, with the tangent sigmoid (Eq. (1)) as the activation function. The output layer comprises one neuron, described as the SMX removal efficiency, with a linear function (Eq. (2)) as the transfer function:

$$f(x) = \frac{1}{1 + e^{-x}} \tag{1}$$

$$f(x) = x \tag{2}$$

Although there are formulas for reference, the stability of the network structure is particularly sensitive to the number of neurons. Therefore, this study compares the mean square error (MSE) when training the networks under different hidden layer neurons to determine the optimal number of neurons. (Eq. (3)):

$$MSE = \frac{\sum_{i=1}^{n} \left( X_{i,\text{cal}} - X_{i,\text{exp}} \right)^2}{n}$$
(3)

Since the unit data and the order of magnitude of the sample data are different, the input data for developing the ANN model were normalized in the range of -1 to 1, using Eq. (4).

$$x_{\rm i} = \frac{2X_{\rm i}}{X_{\rm max} - M_{\rm min}} - 1 \tag{4}$$

Based on the obtained model, PSO was used to optimize the operating parameters. The hybrid program comprising the ANN and PSO is shown in Scheme 2. In this study, MATLAB version R2012a (MathWorks, Inc., Natick, MA, USA) was used to perform all calculations and analyze the experimental data.



Scheme 2. Flow chart of the ANN in combination with PSO.

# RESULTS AND DISCUSSION

# Kinetics of the electrochemical oxidation of SMX

The effects of the applied current density  $(1-20 \text{ mA cm}^{-2})$ , pH of the solution (2–10), the initial concentration of SMX (10–500 mg L<sup>-1</sup>) and electrolyte concentration (0.05–0.4 mol L<sup>-1</sup>) on the removal of SMX were systematically evaluated. Based on the results, the kinetics of the EO of SMX were calculated according to the pseudo-first-order kinetics model, as described in Eq. (5):

$$\ln \frac{c_0}{c_t} = kt \tag{5}$$

where  $c_0 / \text{mg} \cdot \text{L}^{-1}$  is the initial sulfamethoxazole concentration;  $c_t / \text{mg} \cdot \text{L}^{-1}$  is the sulfamethoxazole concentration at time t / min. The kinetic parameters, rate constant, k, and half-life,  $t_{1/2}$ , and coefficient  $R^2$  are summarized in Table I.

# Operating parameters influencing the electrochemical oxidation of SMX

*Effects of current density*. In the process of EO, the current density plays a very important role as it determines the removal rate of pollutants by controlling electron transport and the generation of reactive oxidants.<sup>7,15,19,20</sup> The current density was variously set to 1, 5, 10, 15 and 20 mA cm<sup>-2</sup>, and the removal efficiency of SMX during the degradation at each current density is shown in Fig. 1. These

results reveal that the increase of the current density has a positive effect on the SMX removal efficiency. When the current density was 10 mA cm<sup>-2</sup>, the SMX removal efficiency was 92.3 % after 60 min, and reached 95.1 % when the current density was increased to 15 mA cm<sup>-2</sup>. In addition, when the current density was increased to a certain level, its influence on the SMX removal efficiency would gradually become insignificant. For instance, as the current density was increased by 0.9 %. These findings were consistent with the previous reports that increasing current density enhances the pollutant removal efficiency.<sup>23,32</sup>

TABLE I. Efficiency and kinetics of SMX electrochemical degradation

$j / \text{mA cm}^{-2}$	Degradation efficiency, %	$k / 10^{-2} \min^{-1}$	$t_{1/2} / \min$	$R^2$	
1	72.1	1.97	35.2	0.936	
5	77.9	2.41	28.8	0.961	
10	92.3	4.14	16.7	0.994	
15	95.1	5.08	13.6	0.995	
20	96.0	5.34	13.0	0.995	
Initial pH					
2	90.8	3.73	18.6	0.989	
4	89.3	3.38	20.5	0.981	
6	87.2	3.16	21.9	0.981	
8	78.8	2.38	29.1	0.964	
10	72.2	1.99	34.8	0.96	
$c_{\rm SMX}$ (initial) / mg L <sup>-1</sup>					
10	94.1	4.66	14.9	0.995	
50	89.4	3.59	19.3	0.961	
100	82.7	2.98	23.3	0.970	
200	78.8	2.49	27.8	0.943	
500	79.9	2.1	33.0	0.950	
$c_{\text{electrolyte}} / \text{mol } \text{L}^{-1}$					
0.05	88.1	3.59	19.3	0.992	
0.1	91.2	4.10	16.9	0.995	
0.2	93.9	4.67	14.8	0.995	
0.3	94.5	3.43	13.9	0.995	
0.4	87.2	3.38	20.5	0.970	

As shown in Table I, the coefficient of determination ( $R^2$ ) was always >0.94, suggesting that the removal of SMX by EO followed the pseudo-first-order kinetics pattern. At the same time, at the current densities of 1, 5, 10, 15 and 20 mA cm<sup>-2</sup>, the degradation kinetic constants were  $1.97 \times 10^{-2}$ ,  $2.41 \times 10^{-2}$ ,  $4.14 \times 10^{-2}$ ,  $5.08 \times 10^{-2}$  and  $5.34 \times 10^{-2}$  min<sup>-1</sup>, respectively. However, when the current density exceeded 15 mA cm<sup>-2</sup>, the removal efficiency of SMX and the kinetic constant were not significantly increased. The results can be interpreted from two aspects: *i*) the anodic oxidation takes place on the surface of the electrode, and the mass

transfer efficiency is limited. Once the current density is reaching the limiting current density, the rate of degradation is only related to mass transfer; ii) the undesirable parasitic reactions such as OH<sup>-</sup> to O<sub>2</sub> or to  $^{\circ}$ OH<sub>2</sub> were enhanced with the increasing current density.<sup>15,16</sup>



Fig. 1. Effects of the current density on the dynamics of the electrochemical oxidation of SMX.

*Effects of the pH value of the solution*. It is well known that the pH value has a significant impact on the EO of organic pollutants.<sup>14,18,33</sup> The removal efficiency of SMX during degradation was determined at various solution pH values (2, 4, 6, 8 and 10), and the results are shown in Fig. 2. Under acidic conditions (pH of 2, 4 and 6), the SMX removal efficiency was 90.8, 89.3 and 87.2 %, res-



Fig. 2. Effects of the initial pH value on the dynamics of the electrochemical oxidation of SMX.

pectively, while, under alkaline conditions, the maximum removal efficiency of SMX was 78.8 %. As shown in Table I, the kinetic constant (*k*) values changed significantly with the various pH values evaluated. For example, at an initial pH value of 2, the *k* value  $(3.73 \times 10^{-2} \text{ min}^{-1})$  was about 1.9 times higher than that  $(1.99 \times 10^{-2} \text{ min}^{-1})$  at an initial pH value of 10.

The acid dissociation constant ( $pK_a$ ) of SMX is reported to be 1.8, suggesting that acidic conditions have a positive impact on the diffusivity of SMX.<sup>22</sup> On the other hand, the oxygen evolutions on the anode surface were decreased under acidic condition (Eq. (6) and (7)) and the polymerization reactions were also accelerated under this condition.<sup>34</sup> Furthermore, the active chlorine was present in the form of Cl<sub>2</sub> at the pH range from 0 to 3.3, as HClO at the pH range from 3.3 to 7.2, and mainly as ClO<sup>-</sup> at pH higher than 7.2. Among these chlorine forms, the oxidizing organic matter of HClO is significantly stronger than that of the other two forms:

$$2OH^{-} \rightarrow O_2 + 2H^{+} + 2e^{-}$$
 (6)

$$2H_2O \to O_2 + 4H^+ + 4e^-$$
 (7)

*Effects of initial SMX concentration.* The removal efficiency of SMX during degradation was determined at various initial SMX concentrations (10, 50, 100, 200 and 500 mg  $L^{-1}$ ) and the results are shown in Fig. 3.



Fig. 3. Effects of the initial SMX concentration on the dynamics of the electrochemical oxidation of SMX.

They reveal that as the initial concentration of SMX increased from 10 to 500 mg L<sup>-1</sup>, the removal efficiency of SMX decreased from 94.0 to 69.9 %, meanwhile, the k values were consistent with the tendency. These findings can be explained by the following aspects: *i*) direct oxidation was controlled by mass transfer. Besides, SMX and some intermediate products can be adsorbed on the

surface of the electrode, which contaminate the electrode and also hinders the diffusion of other pollutants to the electrode surface;<sup>33,35</sup> ii) the number of hydroxyl radicals and active sites on the electrode surface at a given current density have been identified. As the concentration of SMX increases, more and more intermediates are formed, and these compounds compete with SMX for hydroxyl radicals and active sites on the electrode surface.<sup>18</sup>

Effects of electrolyte concentration. In order to promote the transfer of electrons and ionic conduction, NaCl was added to SMX solution. The removal efficiency of SMX during degradation was determined at various electrolyte concentrations (0.05, 0.1, 0.2, 0.3 and 0.4 mol  $L^{-1}$ ) and the results are shown in Fig. 4. The results indicated that an increase in the electrolyte concentration from 0.05 to 0.2 mol  $L^{-1}$  improved the SMX removal efficiency and k values, and reached the maximum removal efficiency at the NaCl concentration of 0.2 mol L<sup>-1</sup> after 60 min. Thus, it is clear that increasing the concentration of electrolyte in a certain concentration range was beneficial to the degradation of SMX. This is probably due to the addition of electrolyte, which can effectively reduce the solution resistance and increase the conductivity, thereby increasing the amount of 'OH generated on the electrode surface and accelerating the degradation of SMX. Besides, in an electrochemical system, increasing chlorides under high applied potential will produce more active chlorine compounds, such as Cl<sub>2</sub> (Eq. (8)), HClO (Eq. (9)) and  $OCI^{-}$  (Eq. (10)) which are active oxide species, leading to the rapid elimination of organic matter:<sup>36</sup>

$$2\mathrm{Cl}^- \to \mathrm{Cl}_2 + 2\mathrm{e}^- \tag{8}$$

$$Cl_{2} + H_{2}O \rightarrow HOCl + H^{+} + Cl^{-}$$

$$HOCl \rightarrow H^{+} + OCl^{-}$$
(9)
(10)

$$OCl \to H^+ + OCl^- \tag{10}$$



Fig. 4. Effects of the electrolyte concentration on the dynamics of the electrochemical oxidation of SMX.

However, the SMX removal efficiency decreased from 94.5 to 87.2 % when the NaCl was further increased from 0.3 to 0.4 mol  $L^{-1}$ . These results suggest that if the optimum concentration of electrolyte is exceeded, the removal rate will not increase but rather decrease, likely due to the formation of a layer salt on the surface of the anode, which exerted a negative influence on the direct and indirect oxidation.<sup>37</sup>

# ANN modelling and optimization of parameters

Establishment of ANN model. The 125 data sets used in this experiment were divided into two groups. One group consists of 110 data sets, which are used for the training of the network and are called training sample sets. The other group is called the test network and was evaluated with the remaining 15 data sets. Different hidden layer nodes (5-20) were selected to establish a network and determine the optimal number of neurons by training the MSE for training the network using different neuron number conditions. The relationship between the MSE and the number of neurons is illustrated in Fig. 5. The results show that the network with fewer neurons or more than 11 in the hidden layer cannot effectively converge, thus the topology of 5-11-1 seem to be the optimal topology to develop the model.



Fig. 5. Relationship between the MSE and number of neurons in the hidden layer.

*Evaluation of the ANN model.* The relationship between the number of epochs and the MSE was evaluated. The results shown in Fig. 6 reveal that the training of the ANN achieved convergence after 645 epochs with the minimum *MSE*, suggesting that the proposed ANN model successfully predicted the results of SMX removal through the EO process.



Fig. 6. The relationship between the number of epochs and MSE.

To further validate the current ANN model, the regression analysis and the standardized residual analysis were also conducted. As shown in Fig. 7, the coefficient of determination for the training, test and all data sets were 0.9845, 0.9644 and 0.9826, respectively. The representation of the predicted SMX removal efficiency versus experimental data for both training and test data shows the good predictive ability of the proposed ANN model. The high value of the coefficient of determination suggests that the current ANN model is suitable for the prediction of data which has not been used during the training of the model. In addition, the histograms (Fig. 8) of the standardized residual of the model is subject to normal distribution, which confirms that the ANN model has high accuracy to predict results.<sup>38</sup>





Optimization of parameters by ANN-PSO. Based on the obtained ANN model, the optimization of experimental parameters was performed. With the objective of maximizing the removal efficiency of SMX, the PSO technique was

used to optimize the input layer of the ANN model. The values of the PSO parameters used in the optimization simulation are as follows: number of particles in swarm = 20, cognitive component = 2, social component = 2, maximum velocity = 1, minimum inertia weight = -1, and maximum inertia weight = 0.9. As shown in Fig. 9, the maximum removal efficiency was obtained after 100 generations.



Fig. 8 Standardized residual distribution of predicted and experimental values.





The operating conditions of the optimized solution were obtained at a current density of 12.37 mA cm<sup>-2</sup>, an SMX concentration of 74.45 mg L<sup>-1</sup>, a reaction time of 51.49 min, a pH of 4.78, and a NaCl dose of 0.24 mol L<sup>-1</sup>. The ANN-PSO prediction of SMX removal efficiency under the optimized process conditions was 93.70 %. In order to effectively verify the prediction results, the above-mentioned optimal conditions were used for the test, and the validation tests were performed in three parallel tests. The results of the verification tests are listed in Table II, and the actual SMX removal efficiency of 92.03 $\pm$ 2.30 % was achieved under the same optimized conditions. The absolute error between

the verification test results and the predicted value was 1.67 %. Thus, the validation results indicated that this method can be ideally used to optimize the related parameters and predict the anticipated results with acceptable accuracy

No. of verifi- cation test	$j mA cm^{-2}$	pН	$c_{\rm SMX}$ mg L <sup>-1</sup>	$c_{\rm E} \mod {\rm L}^{-1}$	t min	Removal efficiency, %	Relative standard deviation, %
1	12.37	4.78	74.45	0.24	51.49	91.9%	1.27
2	12.37	4.78	74.45	0.24	51.49	89.8%	2.75
3	12.37	4.78	74.45	0.24	51.49	94.4%	0.49

Table II. The results of the verification test

## CONCLUSION

In this study, the Co modified PbO<sub>2</sub> electrode was used to degrade the SMX in aqueous solution. The EO of SMX in aqueous solution followed the pseudofirst-order kinetics pattern, and the oxidation process was more favorable at high current density, acidic pH and low initial SMX concentration. Once the electrolyte exceeds a certain concentration, the removal rate does not increase but instead decreases. An ANN with 5–11–1 topology was used to develop a predictive model for simulating this EO process. The training of the ANN achieved convergence after 645 epochs, with the minimum *MSE*. The correlation coefficient for the training, test and all data sets are 0.9845, 0.9644 and 0.9826, respectively, indicating an excellent fit between the predicted and experimental values. The optimized operation conditions (*i.e.*, a current density of 12.37 mA cm<sup>-2</sup>, an initial pH of 4.78, an initial SMX concentration of 74.45 mg L<sup>-1</sup>, an electrolyte concentration of 0.24 mol L<sup>-1</sup>, and an electrolysis time of 51.49 min) were obtained through PSO. The results of the verification tests suggest that the proposed ANN--PSO model can successfully model and optimize the SMX removal process.

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#### ИЗВОД

# ИСПИТИВАЊЕ ЕЛЕКТРОХЕМИЈСКЕ ОКСИДАЦИЈЕ СУЛФАМЕТОКСАЗОЛА НА РЬО<sub>2</sub> ЕЛЕКТРОДИ МОДИФИКОВАНОЈ КОБАЛТОМ ПРИМЕНОМ МОДЕЛА ВЕШТАЧКИХ НЕУРОНСКИХ МРЕЖА И ОПТИМИЗАЦИЈЕ ЗАСНОВАНЕ НА МОДЕЛУ РОЈЕВА ЧЕСТИЦА

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Присуство антибиотика у водотоковима, чак и у траговима, изазива све већу пажњу. У складу с тим, неопходне су одговарајуће технологије за ефикасно уклањање ових једињења из водених раствора. У овом истраживању је испитивана електрохемијска оксидација сулфаметоксазола (SMX) на електроди од PbO<sub>2</sub> која је модификована кобалтом. Нађено је да оксидација SMX следи кинетику псеудо-првог реда и да ефикасност уклањања SMX достиже максималну вредност од 95,1 % у току 60 min. Ефекат

главних фактора на кинетику оксидације SMX је испитиван у једнофакторним експериментима у којима је густина струје износила 1–20 mA cm<sup>-2</sup>, вредност pH раствора 2–10, почетна концентрација SMX 10-500 mg L<sup>-1</sup> и концентрација електролита 0,05–0,4 mol L<sup>-1</sup>. За симулацију електрохемијске оксидације SMX коришћен је модел вештачке неуронске мреже, а затим је урађена оптимизација радних параметара заснована на моделу ројева честица. Показано је да се максимална ефикасност уклањања SMX добија под оптимизованим радним условима, тј. при густини струје од 12,37 mA cm<sup>-2</sup>, почетној вредности pH од 4,78, почетној концентрацији SMX од 74,45 mg L<sup>-1</sup>, концентрацији електролита од 0,24 mol L<sup>-1</sup> и трајању електролизе од 51,49 min. Резултати провере ваљаности добијених параметара показали су да се описана метода може успешно користити за оптимизацију сродних параметара и предвиђање очекиваних резултата са прихватљивом тачношћу.

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#### ELECTROCHEMICAL OXIDATION OF SULFAMETHOXAZOLE

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