

Electrochemical treatment of aqueous wastes using Boron Doped Diamond electrodes. A new mathematical approach

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In recent years some papers have been published concerning the modeling of the processes involved in the electrochemical treatment of aqueous organic wastes. The goal of some of these works is to develop models which predict the time-evolution of the most important intermediates and final products involved in the electrochemical processes¹⁻². These models use to be complex and often include several adjustable parameters. On the other hand, other authors³⁻⁵ propose simplified models, which only reproduce the behavior of a global parameter (COD). These models have a great advantage over the former ones, since they do not include adjustable parameters.

In this work a new model, with the advantages of the two previously proposed approaches, is proposed. This model has no adjustable parameters and allows the prediction of the time-evolution of the concentration of several organic products, during the electrochemical oxidation of organic pollutants on BDD electrodes.

The model has been developed for an electrochemical reactor which uses a non active electrode (BDD), operating in a batch mode under galvanostatic conditions. The model is based on several assumptions:

- The electrochemical reactor can be divided in two zones (Figure 1): a small volume close to the anode surface (or reaction zone) where electrochemical processes develop, and the remaining reactor volume (bulk zone). In both zones the concentration of every chemical compound can be considered to be constant with position, but time-depending.

- The local rate of exchange between both zones is assumed to be proportional to the concentration difference in each zone (equation 1):

$$J_i = kA \left([S_i^R] - [S_i^B] \right) \quad (1)$$

- Direct oxidation reactions rate can be evaluated using equation 2:

$$r_i = \frac{I}{F} \alpha_i \quad (2)$$

where α_i is the electrical energy fraction used for oxidizing the compound i . This parameter can be related to the oxidation potential of each compound (V_i) and to the operation cell potential (V_{cell}).

$$\alpha_i = \alpha_i(V_i, V_{cell}) \quad (3)$$

- Reactions involved in the electrochemical oxidation of an aqueous organic wastes can be summarized according to Figure 2.

- Mediated reactions carried out by very strong oxidants electrogenerated on the anode surface are considered as direct electrochemical reactions.

Figure 3 shows the experimental vs simulated data for the electrochemical oxidation of a phenol aqueous waste ($\rho = 30 \text{ mA cm}^{-2}$; $\text{pH} = 12$, $T = 25^\circ\text{C}$, $C^0 = 1000 \text{ ppm}$ phenol), using a BDD electrode. As it can be seen good agreements are achieved.

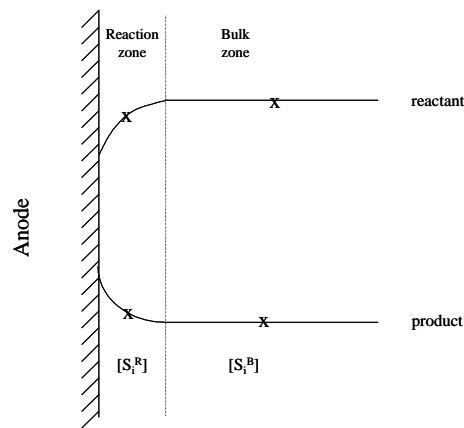


Figure 1. Electrochemical reactor scheme.

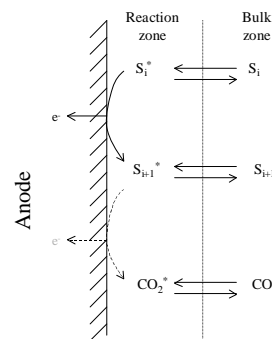


Figure 2. Reaction mechanism in a electrochemical process.

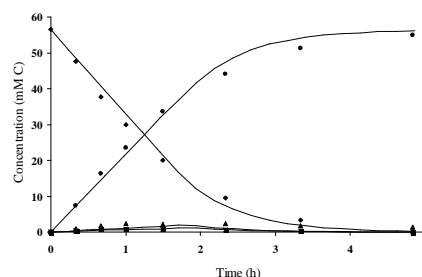


Figure 3. Experimental vs. simulated data: \blacklozenge phenol, \blacksquare maleic acid, \blacktriangle oxalic acid, \bullet carbon dioxide.

A extended study including the modelization of several experimental conditions shows that the coefficient of variation between simulated and experimental data is in most of cases below 5%.

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