Chemosphere 146 (2016) 233–237

Contents lists available at ScienceDirect

Chemosphere

journal homepage: www.elsevier.com/locate/chemosphere

Technical note

The numerical model of biosorption of Zn^{2+} and its application to the bio-electro tower reactor (BETR)

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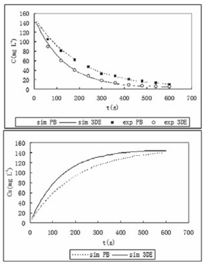
HIGHLIGHTS

- Developing a novel kinetic model to simulate the bio-electro tower reactor.
- Bio-adsorption and mass transfer process of Zn^{2+} in BETR was simulated.
- Coefficient η was created to discribe the effect in bio-electro tower reactor.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 7 July 2015
Received in revised form
27 November 2015
Accepted 28 November 2015
Available online 28 December 2015

Handling Editor: Dr. E. Brillas

Keywords:
Numerical model
Biosorption
3-Dimensional electrode
Mass transfer
BETR

ABSTRACT

A 2-D numerical kinetic model considering flow velocity and adsorption is developed to simulate the bio-electro tower reactor (BETR). This new model considers the adsorbed amount when equilibrium q_e as transient variable, which is superior to the old pseudo-first-order and the pseudo-second-order model which regards q_e as a constant. We did research on the intensifying effect of electric field upon heavy metal ions adsorption process. The calculation result matches well with the experimental data. BETR is a coupling technique whose mechanism is that outer electric field can enhance the mass transfer rate when the solute is metal ions. Two kinds of carriers, pottery ball and 3-dimensional electrode (3DE), were used to support the biofilm layer; and organic wastewater that contains Zn^{2+} is selected as a sample to validate the model. The 3DE carriers can be polarized by outer electric field, but pottery ball cannot. It is found that Zn^{2+} transfers faster in 3DE carriers than in pottery ball (insulation materials); and an intensifying coefficientη is introduced to describe this effect in BETR.

1. Introduction

Nowadays, industrial utilization of heavy metals, such as metal plating, tanning, preparation of catalysts and nuclear technology, generates large quantity of aqueous effluent that contains high levels of heavy metal (Volesky, 1990; Hatfield et al., 1996; Hatfield and Pierce, 1998; Bhatti and Hamid, 2014; Hanif et al., 2015). Therefore, it is necessary to develop harmless novel process for

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http://dx.doi.org/10.1016/j.chemosphere.2015.11.118
0045-6535/

efficiently treating this sort of wastewater (Li et al., 2001; Ahluwalia and Goyal, 2007; Zaki et al., 2007). Generally, biosorption is better than the conventional methods. Furthermore, it has been proven that the bio-electro reactor that combines electrochemistry technique with microbial way is a more effective novel process (Li et al., 2006a). The BETR (bio-electro tower reactor) that we invented (Li et al., 2006b) has an anode in the center and cathode on the tower wall. 3-dimensional electrode materials (granule or crumb-shaped) were filled between the anode and cathode and the BETR is electrified by outer electric field. These 3DE materials form the third electrodes. On the surface of the 3DE some electrochemistry reactions take place, and biofilm can be obtained through culturing and acclimating microorganism under low direct current.

Adsorption and biosorption equilibria information is extremely important for analysis and design of the reactor. There has been large research effort on the adsorption equilibria in heavy metals biosorption (Dursun, 2006; Deng et al., 2007; Hanif et al., 2007; Preetha and Viruthagiri, 2007). The equilibrium concentration is a function of temperature. Therefore, the adsorption equilibrium relationship at a given temperature is referred as adsorption isotherm. Some adsorption isotherms were adopted to correlate the biosorbent-assisted heavy metals removal; Freundlich and Langmuir equations are most widely used. However, Kinetic studies of biosorption of heavy metals need to be improved. Several adsorption kinetic models have been established to understand the adsorption kinetics. The pseudo-first-order and the pseudo-second-order kinetic model are the most frequently used to quantify the extent of uptake in biosorption (Kargi and Cika, 2007; Pamukoglu and Kargi, 2007; Miretzky et al., 2008; Guo et al., 2008; Djeribi and Hamdaoui, 2008).

The rate of adsorption is expressed as

$$\frac{dq}{dt} = k_1(q_e - q) \tag{1}$$

The pseudo-first-order kinetic expression is deduced from integration of Eq. (1)

$$q = q_e(1 - \exp(-k_1 t)) \tag{2}$$

with the boundary conditions as follow: $t = 0$, $q = 0$, and at $t = t$, $q = q$.

Similarly, pseudo-second-order model is derived from the rate of adsorption

$$\frac{dq}{dt} = k_2(q_e - q)^2 \tag{3}$$

Integration of Eq. (3) with the boundary conditions $t = 0$, $q = 0$, and at $t = t$, $q = q$, gives

$$\frac{t}{q} = \frac{t}{q_e} + \frac{1}{k_2 q_e^2} \tag{4}$$

Hypothetical models, q_e, the adsorbed amount at equilibrium, is regarded as constant during the whole process. However, an obvious logical contradiction exists because q_e actually complies with the adsorption isotherm equation. Since q_e is a time-dependent variable, the pseudo-first-order and pseudo-second-order model are not appropriate.

In this study, Zn^{2+} was selected as the simple ion in the experiment and a numeric kinetic model that considers mass transfer inside biofilm is established innovatively which contains the isotherm equation at very first time. Langmuir equation is introduced for adsorption isotherm according to our previous work (Zhang, 2005) because it is consistent with our experimental data. The model is numerically solved by calculating q_e at every single step, avoiding regarding q_e as a constant. Meanwhile, it is also the first time that the model is applied to study the biosorption under electric field. The calculated results are to be compared with experimental data. The experiment in this study consists of two portions: 1. organic wastewater purifying in the fixed bed made of pottery ball and 2. of 3DE granule. Theoretically, the mass transfer is enhanced by the electric field when the fixed bed is made of 3DE granules. For this reason, different mass transfer parameters Kα are regressed from experimental data and are used as important parameter in the simulation.

2. Method

2.1. Numeric model

We set up the numeric model of electric-biofilm system inside the tower reactor under pole coordinate. It is assumed that:

1) the supporting particles on which the microbial biofilm is located at can be treated as porous media;
2) the adsorption of metal ions on the biofilm is consistent with Langmuir equation;
3) the wall effect of the tower can be neglected;
4) the effect of acceleration on the ions movement due to the DC electric field only affects the mass transfer coefficient K.

So the governing equations of the model include:continuity equation:

$$\nabla u = 0 \tag{5}$$

and momentum equation:

$$\frac{\partial u}{\partial t} + u \cdot \nabla u = -\frac{1}{\rho}\nabla p + \nu \nabla^2 u - \Delta p \tag{6}$$

Here the last variable on the right hand side of equation comes from the particle drag. In this study, d = 0.1 m, $u = 7.42 \times 10^{-5}$ m s^{-1}. The Re number is roughly estimated to be 7.42×10^{-3} by substitution the density and viscosity of the metal ions solution with the water. Thus the flow pattern is laminar inside the tower.

Therefore, the Blake-Kozeny equation (Ergun, 1952) is applied to calculate the pressure drop in laminar flow:

$$\frac{|\Delta p|}{L} = \frac{150\mu}{D_p^2} \frac{(1-\varepsilon)^2}{\varepsilon^3} u \tag{7}$$

The governing equation of the ions concentration is as follows:

$$\frac{\partial c_L}{\partial t} + u \cdot \nabla c_L = D\nabla^2 c_L - K\alpha(c_L - c^*) \tag{8}$$

K is the mass transfer coefficient, and α is the surface area of unit volume. c^* is the equilibrium ion concentration, whose concentration inside the biofilm is c_s.

The concentration inside the biofilm c_s is the total ions accumulated during the time form 0 to t.

$$c_s = \int_0^t K\alpha(c^* - c_L)\,dt \tag{9}$$

If the equilibrium equation is $c_e = f(c_L)$, then the c^* can be expressed as