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Use of artificial neural networks and genetic algorithms for prediction of sorption of an azo-metal complex dye onto lentil straw

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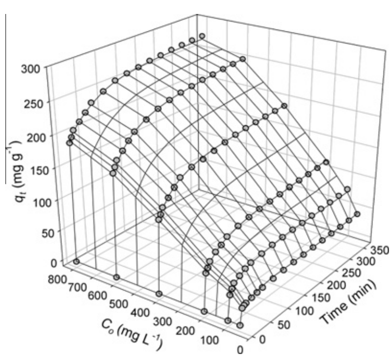
HIGHLIGHTS

- ▶ Predictive modeling of sorption of Lanaset Red (LR)G on lentil straw was studied.
- ▶ Artificial neural network (ANN) was found to be excellent model in representing the sorption kinetics data.
- ▶ The sorption at various operating factors in a single equation was described by gene expression programming (GEP).

GRAPHICAL ABSTRACT



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ABSTRACT

Artificial neural network (ANN), pseudo second-order kinetic, and gene expression programming (GEP) models were constructed to predict removal efficiency of Lanaset Red G (*LR G*) using lentil straw (*LS*) based on 1152 experimental sets. The sorption process was dependent on adsorbent particle size, pH, initial dye concentration, and contact time. These variables were used as input to construct a neural network for prediction of dye uptake as output. ANN was an excellent model because of the lowest error and the highest coefficient values. ANN indicated that initial dye concentration had the strongest effect on dye uptake, followed by pH. The GEP model successfully described the sorption kinetic process as function of adsorbent particle size, pH, initial dye concentration, and contact time in a single equation. Low cost adsorbent, *LS*, had a great potential to remove *LR G* as an eco-friendly process, which was well described by GEP and ANN.

1. Introduction

Various water treatment processes are used to remove undesired materials from industrial and domestic effluents. Sorption is an effective and eco-friendly process to remove color compounds from wastewaters due to its simplicity in operation and availability of a wide range of adsorbents (Srinivasan and Viraraghavan, 2010; Çelekli and Geyik, 2011). Sorption is highly dependent on various operating variables like adsorbent particle size, adsorbent dose, pH regime, dye concentration, temperature, ionic strength, and contact time. Operating factors consisted of multi-input variables (e.g., adsorbent dose, pH value, temperature, ionic strength, dye concentration, and contact time) and output(s) (e.g., percentage value of removal, dye adsorbed per unit of adsorbent at time *t* and at equilibrium), are closely related in sorption systems. To solve these types of complex issues, modeling of the sorption process can be achieved via artificial neural network (ANN) techniques (Khataee and Kasiri, 2010). This approach has been used to describe

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adsorption systems like sorption of reactive dyes (Dutta et al., 2010), Methylene Blue (Cavas et al., 2011), Lanaset Red G (Çelekli and Geyik, 2011), textile dyes (Balcı et al., 2011), Pb(II) (Yetilmezsoy and Demirel, 2008), Auramine O (Kumar and Porkodi, 2009), and biodegradation of dyes (Khataee et al., 2010; Yang et al., 2011).

Results of ANN give information about the relative importance of parameters driving sorption kinetics or biodegradation of dyes (Khataee et al., 2010; Çelekli and Geyik, 2011; Yang et al., 2011). Prediction of water quality as output(s) from a water treatment plant is very difficult as input water quality changes continuously. The main advantage of ANN-based models over traditional models is that they do not require mathematical description of the complex nature of the underlying process.

Genetic algorithms are used for finding precise or approximate solutions to optimize or search potential solution of problems. It is an evolutionary algorithm-based methodology. The program searches for a solution in a problem-independent manner (Goldberg, 1989; Koza, 1992). Empirical models of genetic programming have been developed by Ferreira, 2001, 2002 as gene expression programming (GEP). Parameters derived from mathematical models can be converted into information for the removal of pollutants (Çelekli et al., 2010). These parameters provide knowledge about the adsorption behavior and they are used in the design of waste-water treatment systems.

In the present study, lentil straw (*LS*) (*Lens culinaris* Medic.) was selected because it is relatively abundant and low-cost. The objectives were (i) to investigate sorption of an azo metal complex dye on *LS*, (ii) to develop an ANN model, (iii) to use pseudo second order kinetic model, and (iv) to develop a unique model to describe all studied factors by the GEP model. Since GEP gives a unique model for sorption of *LR G* on *LS* at all studied conditions to describe both kinetic and equilibrium data, removal dye concentration can be calculated from the GEP equation at the studied conditions. In order to evaluate the goodness of fitting for comparison of these models, errors and coefficients were calculated using experimental data and data predicted by the models.

2. Methods

2.1. Adsorbent

Lentil straw (*LS*) was obtained from a field in the region of South–East of Anatolia (Turkey). Dried adsorbent was ground in a mortar, sieved by use of different mesh size of sieve (125, 250, and 500 μm), and stored in air tight polyethylene bottle.

2.2. Adsorbate

The azo metal complex dye, Lanaset Red G (*LR G*) ($C_{32}H_{21}CrN_{10}O_{11}S{\cdot}2Na$, CAS No.: 70209-87-9, Huntsman, purity: 30–40%, and λ_{max} = 475 nm) was obtained from a local textile company and used without further purification and a stock dye solution (1 g L^{-1}) was prepared in distilled water. Dye solutions for sorption process were prepared by diluting the stock dye solution with distilled water.

2.3. Sorption studies

The pH of solution was adjusted to desired values (pH 1–4) with 0.1 M HCl and/or 1.0 M NaOH. Experiments were performed with 100 mL of sorption solutions with desired dye concentrations and pH and the desired amount of adsorbent in 250 mL conical flasks. The flasks were agitated on an orbital shaker at 150 rpm for 360 min to achieve equilibrium.

Samples were withdrawn and centrifuged at 1790g for 5 min and the residual *LR G* concentration in the supernatant was measured with a spectrophotometer (Jenway 6305) at 475 nm. Each data point is mean of two independent sorption studies.

The value of q_t shows the amount of *LR G* adsorbed on *LS* at time t (mg g^{-1}) calculated by use of Eq. (1).

$$q_t = \frac{(C_0 - C_t) \times V}{m} \quad (1)$$

where C_0 and C_t represent the dye concentrations (mg L^{-1}) at initial and at t time, respectively. V is the volume of solution (L), and m is the mass of adsorbent (g L^{-1}).

2.4. Kinetic modeling

2.4.1. Artificial neural network (ANN)

The ANN was trained to perform a particular (activation) function by adjusting the values of the connections (weights) between elements (neurons) as seen in Fig. 1. The activation function produced an output which it used to sum the weights of each neuron (W_i) and the bias (b_i) (a constant weight of a neuron representing the generalization error). To calculate the weight of a neuron [Eq. (2)] was multiplied by the corresponding weight of the neuron connection and each input coming to that neuron:

$$W_i = \sum_{j=1}^{n} w_{ij} x_j \quad (2)$$

where, x_j is value of input j at input layer and w_{ij} is the corresponding weight of connection between each neuron (j) in input layer and each neuron (i) in hidden layer, and also between hidden and output layers. The activation function held the final weights between neurons of all network and produced a predicted output (y_k) by Eq. (3).

$$y_k = f(W_i + b_i) \quad (3)$$

The Neural Network Toolbox V4.0 of the MATLAB 7 mathematical software was used for the prediction of sorption efficiency. In this tool, logistic transfer function with back-propagation algorithm at hidden layer and logistic transfer function at output layer activation function were used. Logistic transfer function is expressed as (Eq. (4)):

$$f(x) = \frac{1}{1 + e^{-x}} \quad (4)$$

where $f(x)$ is hidden neuron output.

A three-layer back propagation (BP) ANN structure was used. Input layer had four neurons as adsorbent particle size, initial pH value, initial dye concentration, and contact time. The output layer

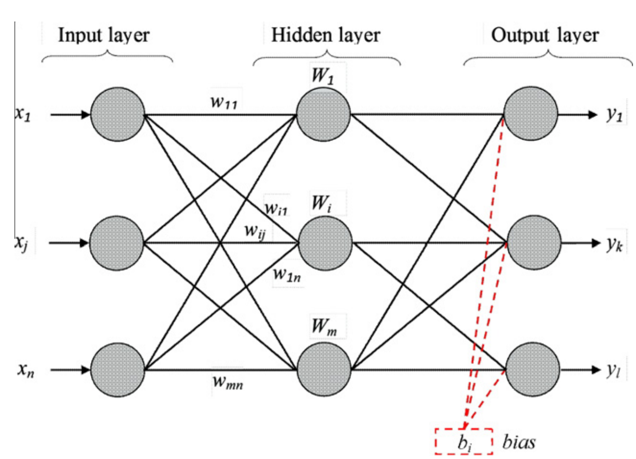

Fig. 1. Architecture of multilayer back propagation ANN.