Journal of Molecular Liquids 218 (2016) 354–362

Contents lists available at ScienceDirect

Journal of Molecular Liquids

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

Kinetics and thermodynamics of methyl orange adsorption from aqueous solutions—artificial neural network-particle swarm optimization modeling

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ARTICLE INFO

Article history:
Received 1 February 2016
Accepted 20 February 2016
Available online 8 March 2016

Keywords:
Anionic dye MO
Adsorption isotherm
Random forest
Artificial neural network
Partial swarm optimization

ABSTRACT

The efficiency and performance of lead oxide nanoparticles loaded activated carbon were well investigated and elucidated for the removal of methyl orange dye. The influence of variables like; pH, contact time, MO concentration and mass of adsorbent was investigated and optimized by artificial neural network-partial swarm optimization (ANN-PSO). At optimal conditions predicted by ANN-PSO, the coefficient of determination (R^2) and mean square error (MSE) correspond to test data were 0.97 and 0.00093, respectively. The maximum removal percentage (~98%) was observed at conditions set at: 0.02 g of PbO-NP-AC, 15 mg L^{-1} of MO at pH 2.0 following mixing and stirring for 20 min. The experimental data were efficiently explained by the Langmuir isotherm model at all conditions with maximum adsorption capacity of 333.33 mg g^{-1}. Kinetic studies at various adsorbent mass and initial MO concentrations revealed that maximum MO removal was achieved within 15 min. The experimental data follow the pseudo-second-order rate equation.

1. Introduction

The industrial and food stuff pollutants have more contribution on different ecosystem media such as aqueous media [1]. Dyes and their breakdown products generate high toxicity for living organisms following their entrance to rivers and other aqueous media [1]. Azo reactive dyes with high brightness in color due to the presence of azo (–N═N–) groups in cooperation with substituted aromatic structures [2, 3] have more toxicity to living organisms. Unique properties viz. high stability to light, heat and oxidizing agents are the cause of their hard and difficult degradation, while in some times more toxic compounds were appeared [4]. The previously reported disadvantages and drawbacks such as requirement of large amount of supporting material, generation of large amount of secondary waste in expensive and tedious stages and production of large amount of sludge [5–11] encourage the researchers to develop and design adsorption based efficient method. Adsorption especially based on non-toxic and very reactive material for adsorption is novel approaches for dye removal [12–17]. The nanoparticles loaded on various conventional adsorbent are used nowadays as these are advantageous because their high specific surface area (high adsorption capacity) leading to enhance their application in separation, pre-concentration and adsorption of various pollutants [18]. Their performance significantly affected by their size, surface area and interparticle interaction affinity. Methyl orange (MO; anionic category) is extensive used in textile, printing, paper manufacturing, pharmaceutical and food industries [19,20]. The effluent coming out from these industries lead to health hazards (breathing problem, vomiting, diarrhea and nausea).

Adsorption process (complex and nonlinear process) encourages the researchers to apply nonlinear models including least squares support vector machines (LS-SVM), random forest (RF), adaptive Neuro-fuzzy inference system (ANFIS) and artificial neural network (ANN) for prediction of the adsorption profile. Artificial neural network (ANN) is widely used as alternative mathematical methods to solve various problems with minor adaptations [21–28]. Back propagation neural network (BPNN) with high efficiency is able to solve non-linear and complex problems. The improvement in reliability achieved by using heuristic optimization algorithm such as genetic algorithm (GA),

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http://dx.doi.org/10.1016/j.molliq.2016.02.048
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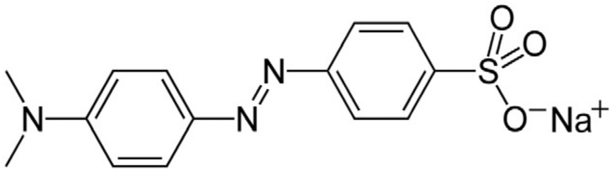

Fig. 1. Chemical structure of methyl orange.

imperialist competitive algorithm (ICA) and particle swarm optimization (PSO) combined with BPNN to avoid local minimum and achieve global convergence quickly and correctly [29–31]. A hybrid of artificial neural network and particle swarm optimization (ANN-PSO) was used for the prediction of pollutants removal from water samples [32–34].

This study is to focus on the application of ANN-PSO model to predict the MO adsorption behavior onto PbO-NP-AC. The said adsorbent was synthesized and characterized via different techniques including FT-IR, XRD and SEM analysis. Effects of various operating conditions like; pH, MO concentration, amount of adsorbent and contact time on the extent of MO removal were studied and optimized using ANN and PSO models.

2. Experimental

2.1. Instruments and reagents

The stock solution (100 mg L^{-1}) of MO (Fig. 1; formula weight: 327.34 g mol^{-1} with molecular formula of $C_{14}H_{14}N_3NaO_3S$) was prepared by adding 20 mg pure MO in 200 mL of double distilled water. Appropriate dilution was done to get desired concentration as working solution. All chemicals including NaOH, HCl, KCl and MO were purchased from Merck (Darmstadt, Germany). The details of instrument used, experimental procedure, measurements of MO uptake optimization technique, kinetic and isotherm studies were carried out according to conditions reported elsewhere [12,21–28].

2.2. Hybrid neural networks and PSO

The classical ANN training methods (back-propagation (BP)) are simply extended by particle swarm optimization (PSO) algorithm. The training starts with PSO based on global search on the net weights range in order to refine an initial random set of weights to achieve a better estimate close to the global optimum. Subsequently, the BP algorithm progresses the training and refine the solution provided by the PSO to approach the optimum solution as efficient, powerful and simple optimization algorithm [30,35]. Fig. 2 indicates the flow chart of the PSO that composed of several steps such as generation and initialization of particle array, evaluation of objective function until obtaining better position, determines new g best value, calculation of particles new velocity, update particle's position and repeating the steps [36]. PSO has several controllable parameters such as the acceleration coefficients (personal learning coefficient = c_1 and global learning coefficient = c_2), inertia weight (w), velocity clamping and swarm size (n Pop). Wrong initialization of these parameters may escort to diverge or cyclic behavior [35].

In the present study, MATLAB R2013a software (ANN-PSO) models was used to predict the removal percentage of MO as a function of three input variables including concentration (mg L^{-1}), adsorbent dosage (g), and contact time (min). Feed-forward architecture of ANN-PSO (Fig. 3) model has been used with back propagation (BP) algorithm to build the predictive models with data flow in forward direction (input layer to output layer). The connection between input, hidden and output layers consists of weights (w) and biases (b) that are considered

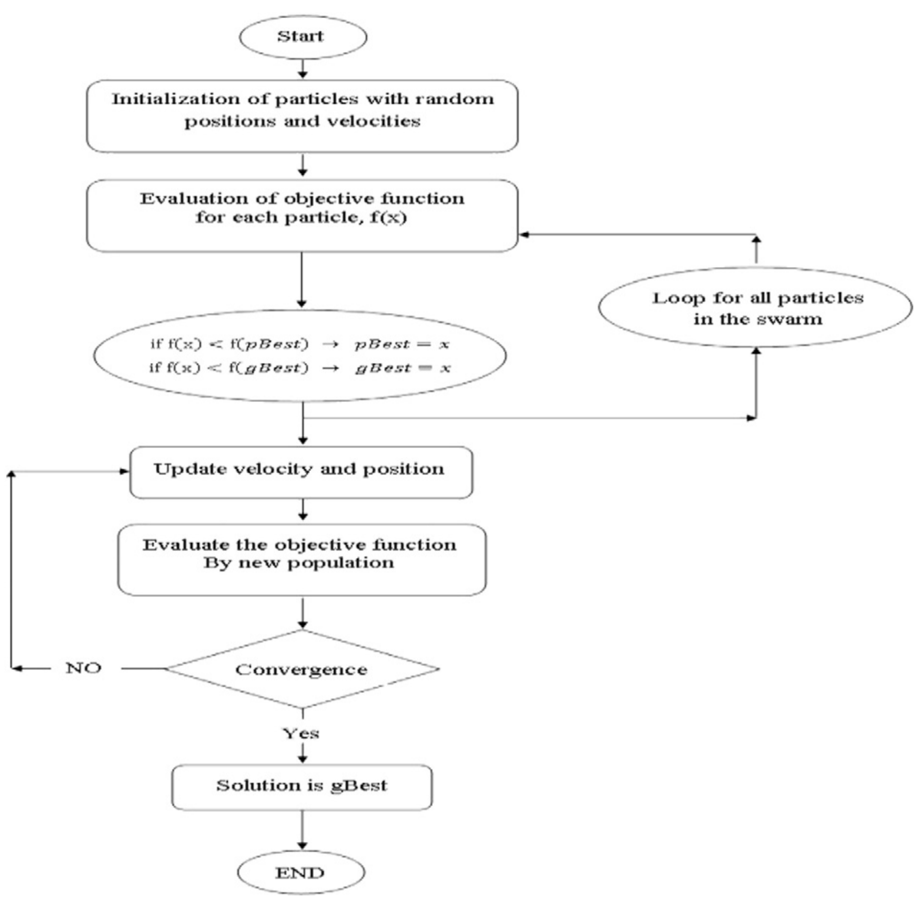

Fig. 2. Flowchart of the PSO algorithm.