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Artificial neural network and particle swarm optimization for removal of methyl orange by gold nanoparticles loaded on activated carbon and Tamarisk

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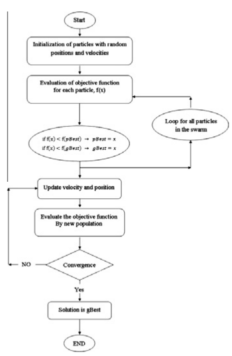
HIGHLIGHTS

- A novel nanoparticle has been used as reusable support for removal of dye EY.
- A high efficiency removal technology is proposed for fast removal of dye.
- Removal of dye can be significantly enhanced under application of nanoparticle.
- The adsorption process was modeled by artificial neural network.
- This model is applicable for rapid removal of large quantity of the dye.

GRAPHICAL ABSTRACT



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ABSTRACT

The influence of variables, namely initial dye concentration, adsorbent dosage (g), stirrer speed (rpm) and contact time (min) on the removal of methyl orange (MO) by gold nanoparticles loaded on activated carbon (Au-NP-AC) and Tamarisk were investigated using multiple linear regression (MLR) and artificial neural network (ANN) and the variables were optimized by partial swarm optimization (PSO). Comparison of the results achieved using proposed models, showed the ANN model was better than the MLR model for prediction of methyl orange removal using Au-NP-AC and Tamarisk. Using the optimal ANN model the coefficient of determination (R^2) for the test data set were 0.958 and 0.989; mean squared error (MSE) values were 0.00082 and 0.0006 for Au-NP-AC and Tamarisk adsorbent, respectively. In this study a novel and green approach were reported for the synthesis of gold nanoparticle and activated carbon by Tamarisk. This material was characterized using different techniques such as SEM, TEM, XRD and BET. The usability of Au-NP-AC and activated carbon (AC) Tamarisk for the methyl orange from aqueous solutions was investigated. The effect of variables such as pH, initial dye concentration, adsorbent dosage (g) and contact time (min) on methyl orange removal were studied. Fitting the experimental equilibrium data to various isotherm models such as Langmuir, Freundlich, Tempkin and Dubinin–Radushkevich models show the suitability and applicability of the Langmuir model. Kinetic models such as pseudo-first order, pseudo-second order, Elovich and intraparticle diffusion models indicate that the second-order equation and intraparticle diffusion models control the kinetic of the adsorption process. The small amount of proposed Au-NP-AC and activated carbon (0.015 g and 0.75 g)

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is applicable for successful removal of methyl orange (>98%) in short time (20 min for Au-NP-AC and 45 min for Tamarisk-AC) with high adsorption capacity 161 mg g^{-1} for Au-NP-AC and 3.84 mg g^{-1} for Tamarisk-AC.

Introduction

As we know, perform experiments for problem solving in engineering are normally costly and time-consuming. Therefore, we can analyze experimental data to discover many scientific relationships and apply computational modeling to solve complex engineering problems. Modeling is a simplification of reality and well-accepted engineering technique. Computational modeling assists us to analyze and figure out what is going on in a process and confirm results achieved from experiments. The selection of appropriate procedures for constructing the models is a main factor to build an accurate prediction. Often used statistical methods such as simple, but interpretable multiple linear regression (MLR) [1] and nonlinear, highly predictive methods include fuzzy inference system (FIS) [2], adaptive Neuro-fuzzy inference system (ANFIS) [3,4], support vector machine (SVM) [5,6], artificial neural networks (ANN) [7–12], and random forest [13]. Unlike classical optimization algorithm, the meta-heuristic optimization algorithms are efficient and flexible models. Different heuristic optimization algorithms have been used to solve the reliability redundancy allocation problem. Sometimes, some impressive ideas are motivated from biological, physical, and social processing [14,15]. Particle swarm optimization (PSO) is a stochastic optimization approach inspired from the simulation of simplified social behavior of bird flocking, firstly introduced by Kennedy and Eberhart [16]. Khajeh et al., used response surface methodology (RSM) and combine of artificial neural network-particle swarm optimization (ANN-PSO) for prediction and optimization of removal of methylene blue using silver nanoparticles from water samples. Their results indicated that the modeling capability of the ANN was better than RSM with comparative less value of RMSE and more the value of correlation coefficient [17]. Khajeh et al. proposed response surface methodology (RSM) and combine of artificial neural network-particle swarm optimization (ANN-PSO) to develop predictive models for simulation and optimization of tea waste extraction process. They have shown that the result of the ANN was better than the RSM model [18]. Dyes are one of the most hazardous materials in industrial effluents, which can cause severe health problems in human beings, since they exhibit high biotoxicity and potentially mutagenic and carcinogenic effects [19,20]. Therefore, the removal of dye from colored effluents has attracted increasing attention. Several technologies including biological treatment, adsorption, coagulation, flocculation, chemical oxidation, membrane separation and ion exchange have been developed [21–23]. Among these methods, adsorption has been considered to be simple, highly efficient, and ease of operation. A wide range of materials has been reported for dye removal, including activated carbon, zeolite, clay, polymer, etc. [24–26]. In view of pollutant control at present, it is still indispensable for the development of new adsorbent materials with high adsorption capacities and removal efficiencies. Methyl Orange is widely used for coloration of cellulosic textiles. Some of the applied techniques for the treatment of dye contaminated wastewaters are flocculation, coagulation, precipitation, adsorption, membrane filtration, electrochemical techniques, ozonation and fungal decolorization [27,28]. Among them, the adsorption based procedure widely utilized due to its high efficiency, capacity and ability for large scale dye removal application (with potential for adsorbent regeneration) [29–33]. The nontoxic, low cost and easy availability adsorbents are the best choice for wastewater treatment. Due to the unique properties of nanoparticles such as a high number of reactive atoms, high mechanical and thermal strength, large number of vacant reactive surface sites metallic or semi-metallic behavior and high surface area widely applied for removal of various toxic materials [34]. Activated carbon as one of the most common building blocks of nanotechnology is the low cost and general material as support for loading nanomaterial. In such activated carbon based adsorbents the various reactive sites such as AC functional group and nanoparticle material synergies ally adsorb trace amount of different pollutant. Due to its unique molecular structure, AC has an extremely high affinity for many classes of dyes and controlled by the AC characteristics. In this technique application of nanoscale materials with high surface area enhance the removal percentage and adsorption capacity of AC based adsorbent. Metallic nanoparticles such as gold as well as gold are of great importance in the analytical chemistry, catalytic applications, and electromagnetic devices. In this investigation, MLR and ANN models have been used to study linear and nonlinear relationships exist among variables while PSO used to optimize the influence of variables concern to the adsorption of methyl orange by Au-NP-AC and AC. The results achieved from the introduced models were compared with the experimental values. The Au-NP-AC was synthesized and subsequently characterized via various techniques such as scanning electron microscopy (SEM) and X-ray diffraction (XRD) analysis. Then the adsorption kinetics and isotherms of methyl orange removal on this adsorbent was studied and its applicability for treatment of wastewater and this dye removal was investigated. The adsorption rates were evaluated by fitting the experimental data to traditional kinetic models such as pseudo-first and second-order and intraparticle diffusion models. The proposed sorbent is useful for quantitative adsorption of the methyl orange with high sorption capacities in short time.

Experimental

Instruments and reagents

The stock solution (1000 mg L^{-1}) of Methyl Orange (formula weight: 327.34 g mol^{-1} and molecular formula: $C_{14}H_{14}N_3NaO_3S$) was prepared by dissolving appropriate amount of the solid dye in double distilled water and the working concentrations daily were prepared by its diluting (Fig. 1). The pH measurements were carried out using Metrohm 692 pH/Ion meter (Metrohm, Switzerland, Swiss) and the methyl orange concentration was determined using Jasco UV–Vis spectrophotometer model V-530 (Jasco, Japan) at a wavelength of 465 nm. The morphology of the Au-NP-AC and AC was observed by scanning electron microscopy (SEM; Hitachi S-4160, Japan) under an acceleration voltage of 15 kV. X-ray diffraction (XRD) pattern was recorded by an automated Philips X'Pert X-ray diffractometer (Philips, Netherland) (40 kV and 30 mA) for 2θ values over 10–80°. A BET surface analyzer (Quantachrome NOVA 2000, USA) was used to measure nitrogen adsorption–desorption isotherm at 77 K while before the measurement, the samples were degassed using helium at 553 K for 3 h. The BET surface area, total pore volume, and micropore area were obtained from the adsorption isotherms. All chemicals, including