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Artificial neural network-genetic algorithm based optimization for the adsorption of methylene blue and brilliant green from aqueous solution by graphite oxide nanoparticle

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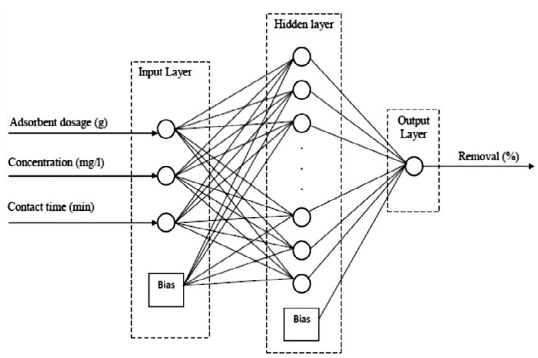
HIGHLIGHTS

- A novel nanomaterial has been used as reusable support for removal of dyes.
- A high efficiency removal technology is proposed for fast removal of dyes.
- Removal of dyes can be significantly enhanced under application of nanoparticles.
- The novel sorbent was characterized by FT-IR, SEM and BET analysis.
- This model is applicable for rapid removal of large quantity of these dyes.

GRAPHICAL ABSTRACT



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ABSTRACT

In this study, graphite oxide (GO) nano according to Hummers method was synthesized and subsequently was used for the removal of methylene blue (MB) and brilliant green (BG). The detail information about the structure and physicochemical properties of GO are investigated by different techniques such as XRD and FTIR analysis. The influence of solution pH, initial dye concentration, contact time and adsorbent dosage was examined in batch mode and optimum conditions was set as pH = 7.0, 2 mg of GO and 10 min contact time. Employment of equilibrium isotherm models for description of adsorption capacities of GO explore the good efficiency of Langmuir model for the best presentation of experimental data with maximum adsorption capacity of 476.19 and 416.67 for MB and BG dyes in single solution. The analysis of adsorption rate at various stirring times shows that both dyes adsorption followed a pseudo second-order kinetic model with cooperation with interparticle diffusion model. Subsequently, the adsorption data as new combination of artificial neural network was modeled to evaluate and obtain the real conditions for fast and efficient removal of dyes. A three-layer artificial neural network (ANN) model is applicable for accurate prediction of dyes removal percentage from aqueous solution by GO following conduction of 336 experimental data. The network was trained using the obtained experimental data at optimum pH with different GO amount (0.002–0.008 g) and 5–40 mg/L of both dyes over contact time of 0.5–30 min. The ANN model was able to predict the removal efficiency with Levenberg–Marquardt algorithm (LMA), a linear transfer function (purelin) at output layer and a tangent sigmoid transfer

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function (tansig) at hidden layer with 10 and 11 neurons for MB and BG dyes, respectively. The minimum mean squared error (MSE) of 0.0012 and coefficient of determination (R^2) of 0.982 were found for prediction and modeling of MB removal, while the respective value for BG was the MSE and R^2 of 0.001 and 0.981, respectively. The ANN model results show good agreement with experimental data.

Nomenclature

Symbols

y	normalized value of x_i
ANN	artificial neural network
x_i	input or output of the network
x_{min}	lower extreme value of x_i
x_{max}	upper extreme value of x_i
MSE	mean squared error
N	the number of data points
$y_{prd,i}$	the network prediction
$y_{exp,i}$	the experimental response
i	index of the data
y_m	average of the experimental value
C_t	dye concentration (mg/L) at time t
Q_e	equilibrium adsorption capacity (mg/g)
C_e	dye concentration (mg/L) at equilibrium
V	volume of solution (L)
W	weight of adsorbent (g)
K_1	rate constant of pseudofirst order adsorption (L/min)
K_2	second-order rate constant of adsorption (g mg^{-1} min^{-1})
h	initial adsorption rate (mg g^{-1} min^{-1})
α	initial adsorption rate (mg g^{-1} min^{-1})
β	desorption constant (g mg^{-1})
C	intercept of intraparticle diffusion (related to the thickness of the boundary layer)
K_{dif}	rate constant of intraparticle diffusion (mg g^{-1} min$^{-1/2}$)
F	fraction of solute adsorbed at any time t (mg/g)
D_i	effective diffusion coefficient of adsorbate in adsorbent
r^2	radius of adsorbent particles (m)
Q_m	maximum adsorption capacity reflected a complete monolayer (mg/g) in Langmuir isotherm model
K_a	Langmuir constant or adsorption equilibrium constant (L/mg) that is related to the apparent energy of sorption
R_L	dimensionless equilibrium parameter (separation factor)
K_F	isotherm constant indicate the capacity parameter (L/mg) related to the intensity of the adsorption
N	isotherm constant indicate the empirical parameter (g L^{-1}) related to the intensity of the adsorption
T	absolute temperature in Kelvin
R	universal gas constant (8.314 J K^{-1} mol^{-1})
β_1	related to the heat of adsorption ($\beta_1 = RT/b$)
ε	Polanyi potential at the D–R isotherm
b_T	constant related to the heat of adsorption
K_T	equilibrium binding constant
B	constant related to the adsorption energy at the D–R isotherm (mol^2/(kJ^2))
q_s	theoretical saturation capacity at the D–R isotherm

Introduction

The dyes and pigments usage in recent years (more than107 kg per year) in human life and industries like textile, paints, pulp and paper, carpet and printing wastewater extensively was increased [1]. Therefore, their effluents are highly color and cause water pollution [2]. The dyes are highly toxic and generate permanent hazard to humans and animals [3]. Among various branch of dyes including anionic, cationic, non-ionic and zwitterionic, the highest toxicity is attributed to cationic dyes [4,5]. In despite of low toxicity of MB, it can because harmful effects such as vomiting enhance in heart rate, diarrhea, shock, cyanosis, jaundice, quadriplegia and human tissue necrosis [6]. Brilliant green (BG) is applied as dermatological agent, veterinary medicine and as inhibitor of mold propagation and following contact with skin and eye, inhalation and ingestion generates toxic to the lungs and other tissues and lead to target-organ damage [7]. There are many dyes removal procedures such as flocculation, chemical coagulation, oxidation, adsorption, precipitation, filtration, and degradation of dyes using photocatalytic activity [8–10], while among them, adsorption is good and superior candidate technique for the pollutants removal from aqueous solutions [11–15]. The priority of adsorption is in term of cheap approach and instrument, adsorbent versatility, high efficiently and less sludge generation. The application of high adsorption capacity and readily available non-toxic adsorbent is highly recommended requirement [16–22]. GO is good candidate for MB and BG removal due to its large specific surface area, low density, chemical stability and high adsorption capacity [23]. This adsorbent as precursor in the formation of graphene layers is highly-oxidized planar material with 25–30% (w/w) oxygen due to formation of oxygen-containing functional groups such as carboxyl, hydroxyl, epoxy easily can be prepared by chemical modification in the presence of strong oxidizing agent such as potassium chlorate, permanganate, dichromate and chlorine dioxides. GO was previously applied to remove cationic dyes [24,25]. Modeling and studying the optimization of variables which influences the adsorption process must be associated with at least experiments, while be able to consider the interaction of variables. One of the most powerful tools for this purpose is artificial neural network (ANN) that introduces mathematical functions for both linear and non-linear systems. It has been widely used in various research areas to obtain experimental information to design water treatment model [26]. Daneshvar et al. studied ANN model to predict the performance of decolorization efficiency of C.I. Basic Yellow 28 removal from solutions via the electrocoagulation method [27]. Salari et al., also applied the artificial neural network modeling to investigate the effect of variables and their relationship in the peroxi-coagulation process (R^2 = 0.97) for decolorization of C.I. Basic Yellow 2 (BY2) in aqueous solutions [28]. Balci et al. applied ANN model to estimate the adsorption capability of bed systems toward textile dyes (Basic Blue 41-BB41 and Reactive Black 5-RB5) and found good agreement of the ANN-predicted results with the experimental values. They also found that mean square errors in BB41 and RB5 test data were 0.00620594 and 0.00119229, respectively [29]. In this study, the GO-NP as an effective and excellent adsorbent for the removal of BG and MB dyes is used.