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Adaptive Neuro-Fuzzy Inference system analysis on adsorption studies of Reactive Red 198 from aqueous solution by SBA-15/CTAB composite

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ABSTRACT

In this study, the Mesoporous material SBA-15 were synthesized and then, the surface was modified by the surfactant Cetyltrimethylammoniumbromide (CTAB). Finally, the obtained adsorbent was used in order to remove Reactive Red 198 (RR 198) from aqueous solution. Transmission electron microscope (TEM), Fourier transform infra-red spectroscopy (FTIR), Thermogravimetric analysis (TGA), X-ray diffraction (XRD), and BET were utilized for the purpose of examining the structural characteristics of obtained adsorbent. Parameters affecting the removal of RR 198 such as pH, the amount of adsorbent, and contact time were investigated at various temperatures and were also optimized. The obtained optimized condition is as follows: pH = 2, time = 60 min and adsorbent dose = 1 g/l. Moreover, a predictive model based on ANFIS for predicting the adsorption amount according to the input variables is presented. The presented model can be used for predicting the adsorption rate based on the input variables include temperature, pH, time, dosage, concentration. The error between actual and approximated output confirm the high accuracy of the proposed model in the prediction process. This fact results in cost reduction because prediction can be done without resorting to costly experimental efforts. SBA-15, CTAB, Reactive Red 198, adsorption study, Adaptive Neuro-Fuzzy Inference systems (ANFIS).

1. Introduction

In recent years, the treatment of industrial waste water has gained increasing importance as industrial effluents contain dyes which can result in more pollution of ecosystems [1]. Dyes are used in different industries, especially in textile, leather, pulp, paper, food, plastics, pharmaceutical, cosmetics, and dyestuffs, to name but a few; in particular, textile industries are in the forefront of the use of dyes and the discharge of the largest amount of colored effluent into the environment [2]. Over 70,000 tons of approximately 10,000 different dyes and pigments are used in industries annually worldwide; 20–30% of the dyes are lost in industrial effluents during dyeing and finishing processes due to inefficiencies of the industrial dyeing process [3]. Azo dyes are the largest class of dyes, constituting 60–70% of all dyes produced [4]. Reactive Red 198 (RR 198) is one of the Azo dyes that used for cotton dyeing in textile industry. Removal process of this dye is very difficult due to its high solubility. RR 198 may be toxic to some aquatic organisms, animals and humans because of its carcinogenicity which leads to mutagenic [5].

A wide range of methods have been developed for the removal of dyes and other colored contaminants from industrial waste water including chemical precipitation, electrolysis, aerobic/anaerobic biological degradation, chemical coagulation, membrane filtration, flocculation, photochemical degradation and chemical oxidation. However, these methods suffer from one or more limitations and are unable to adequately reduce dyes concentrations to desired levels [6,7]. Adsorption is one method which is widely used because of its high efficiency, easy operations and low running cost [8]. Various adsorbents such as Fe_3O_4/polyaniline nano composite [9], activated carbon/polyaniline composite [10], eggshell biocomposite dead [11] have been used for the removal of RR 198 from waste water.

In recent years, new hybrid organic- inorganic mesoporous ordered structures are widely investigated as adsorbents for the removal of heavy metal ions, organic dyes, and other organic compounds [12]. SBA-15 is a new kind of ordered mesoporous molecular sieve exhibiting large and uniform pore size distribution, thick amorphous silica walls, large surface area and remarkable thermal and hydrothermal stability [13,14,15]. In addition, the surface of SBA-15 can be readily modified by organic groups that can significantly enhance its adsorption capacity and selectivity [16,17].

Using simulations helps researchers study the effect of various input parameters on the output more easily. This idea results in cost reduction since doing several experiments on all possible combinations of input data is no longer needed [18]. The model which was used in this study is ANFIS. In [19], ANFIS is introduced as a very suitable model in different

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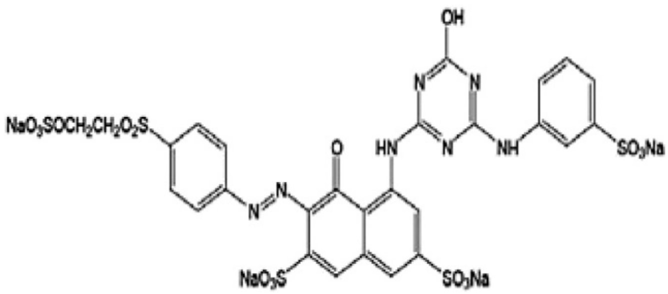

Fig. 1. Chemical structure of RR 198.

environmental engineering aspects. In [20], ANFIS is used for quantitative evaluation of woven fabrics pilling resistance. In [21], it is applied to the prediction of water absorption of geo polymers made from wasted ashes. In [22], ANFIS modelling is used to predict the iodine numbers of activated carbons made from Tabas anthracite. Ghaedi et al. used ANFIS model for modelling the adsorption of 1,3,4-thiadizanole-2, 5-dithiol onto gold nanoparticles-activated carbon [23]. In [24], the authors focused on using ANFIS based-method for the removal of arsenic and chromium from water using a ZEDA hybrid material. In [25], the application of ANFIS modelling in the biodegradation of penicillin-G wastewater using AHR (Anaerobic Hybrid Factor) is discussed. In [26], the effect of annatto dye on Salmonella enteritidis in mayonnaise is predicted using ANFIS model. They also used ANFIS model to predict inactivation of Salmonella enteritidis by ultrasound [27]. In [28], ANFIS model is used to find the best techno economical reactive Blue 19 elimination conditions according to RSM design.

In the present work, SBA-15 was functionalized with Cetyltrimethylammoniumbromide (CTAB) and used as an adsorbent for the removal of reactive Red 198 from aqueous solutions. Also ANFIS model is drived to predict the adsorption rate based on the input variables include temperature, pH, time, dosage, concentration.

2. Experimental

2.1. Materials

Materials such as Pluronic P123 surfactant ($EO_{20}PO_{70}EO_{20}$, $Mw=$ 5800), Tetraethylorthosilicate (TEOS, 98%), Hydrochloric acid 37% and sodium hydroxide 99%, Cetyl trimethyl ammonium bromide (CTAB) were supplied from Sigma-Aldrich and Merck. Reactive Red 198 (Reactive Red RB), an anionic dye, was prepared from Dystar (Fig. 1 & Table 1) and was used as received without further purification. A stock solution of RR 198 (1000 mgl^{-1}) was prepared and diluted with the required initial concentration. This dye shows an intense adsorption peak in the visible region at 515 nm. This wave length corresponds to the maximum adsorption peak of RR 198 ($\lambda max = 515$).

2.2. SBA-15 synthesis

According to Zhao et al. [29], Mesoporous SBA-15 was synthesized as follows: 12.5 ml of P123 as surfactant and 375 ml of distilled water as well as 75 ml (0.1 N) of HCl were stirred at 42 °C. After that, 31.5 ml of TEOS, representing the silica source, was added to the homogeneous mixture. The obtained gel was kept in static conditions at 42 °C for 24 h. Next, the temperature was raised to 138 °C and maintained for 24 h. After filtration, the obtained powder was transferred to a furnace for calcinations at 550 °C for 5 h for the purpose of removing existing organics from its pores.

2.3. SBA-15/CTAB synthesis

10 *ml* of Distilled water is poured into a beaker and 0.02 g of CTAB as well as 0.1 g of SBA-15 is added to it; then, all these materials are stirred by a mechanical stirrer for 20 min. Finally, the obtained mixture is filtered by filter papers, washed by distilled water and dried in oven at 70 °C for 5 h.

2.4. Instrumentation

Transmission electron microscope (TEM) image was taken by Hitachi, HF2000. Field emission scanning electron microscope (FESEM) images were obtained using a TESCAN MIRA3 microscope. Low angle X-ray spectra patterns in the range of 0.6â€“9 were determinedby XPERT-PRO40 *kV* spectrometer using Cu Kα radiation ($\lambda = 1.5406\ A$). FT-IR results were recorded via Shimadzu 4100 Fourier transform infrared spectroscopy. The surface area of SBA-15 and the size of holes before and after the Sited CTAB on SBA-15 were measured by Quanta chrome, Chemo BET 3000 TPR/TPD. Thermo gravimetric analysis (TGA) was done with a Shimadzu TGA50H instrument.

2.5. Adsorption studies

Batch experiments were carried out through contacting different amounts of adsorbent (SBA-15/CTAB) with 100 ml dye (RR 198) solution with different initial concentrations (20–400 ppm) at various pH values ($2-12$) and temperatures of 25, 35 and 45 °C. In order to control pH in the adsorption process, a buffer solution was added. The products were placed in a shaker with 150 rpm velocity for different times (5–120 min). At the end of the process, the adsorbent was separated by centrifuging at 4000 rpm in 30 min. The amount of dye in the solution before and after adsorption process was measured by Jenway 6505 UV–visible spectrophotometer. The quantity of dye adsorbed on SBA-15/CTAB and dye removal precentage (removal efficiency %) were estimated using the following Eq. 1 and 2 [30]:

$$q_e = \frac{(C_0 - C_e)V}{W} \quad (1)$$

where, q_e is the quantity of dye adsorbed on SBA-15/CTAB (mg/g), C_0 and C_e are the initial and final dye concentrations (mg/l), respectively. V is the volume of dye bath (l) and W is the weight of adsorbent (SBA-15/CTAB) (g).

$$R\% = \frac{A_1 - A_2}{A_1} \times 100 \quad (2)$$

where $R\%$ is the removal percentage, A_1 and A_2 are the initial adsorption of dye before and after adsorption process, respectively.

2.6. Modelling using adaptive Neuro-Fuzzy Inference systems (ANFIS)

2.6.1. Fuzzy inference system

Fuzzy modelling is a common approach to modelling the input-output relationship in complex nonlinear systems. Using the fuzzy methodology enables us to define this relationship based on relatively simple calculations on linguistic terms rather than complicated calculations. A general fuzzy system basically includes four parts, namely,

Table 1
Characteristics of RR 198.

Name	CAS number	C.I. number	Formula	Molecular weight	λmax
Reactive Red 198	145017-98-7	18221	$C_{27}H_{18}ClN7O_{15}S_{5.4}Na$	968.21 g/mol	515 nm