Chemical Engineering Journal 178 (2011) 183–190

Contents lists available at SciVerse ScienceDirect

Chemical Engineering Journal

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

Modeling adsorption of sodium dodecyl benzene sulfonate (SDBS) onto polyaniline (PANI) by using multi linear regression and artificial neural networks

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ARTICLE INFO

Article history:
Received 24 July 2011
Received in revised form 13 October 2011
Accepted 18 October 2011

Keywords:
Adsorption
PANI
SDBS
ANN
MLR

ABSTRACT

In the study, artificial neural network (ANN) and multi linear regression (MLR) models were used to predict the efficiency of sodium dodecyl benzene sulfonate (SDBS) removal from aqueous solutions. Polyaniline (PANI) doped with 8% $CuCl_2$ and 10% $ZnCl_2$ was used as adsorbents. Effects of operating variables (pH, adsorbent dosage, temperature, agitation period and agitation speed) were examined with laboratory batch studies. Removal efficiencies were evaluated considering calculated equilibrium adsorption capacities. Thermodynamic parameters were also calculated in the study in order to define the adsorption mechanism of SDBS molecules onto polymeric adsorbents. Data obtained from batch experiments (69 experimental sets individually for each adsorbent type) were used in MLR and ANN models. In MLR analyses, regression equations were developed to explain the effects of the tested parameters. In ANN applications, network with two hidden layers provided the highest prediction efficiencies for both of the PANI species. Considering higher determination coefficients and lower error values, it is concluded that ANN models provided more successful results compared to MLR.

1. Introduction

Surfactants are the major components of domestic wastewaters. As well as they are the main ingredient of laundry detergents they are also extensively used in cosmetics, dyeing of fabrics in textile industry and flotation applications [1]. Among the many surfactant species, sodium dodecyl benzene sulfonate (SDBS) is a well-known anionic type exhibiting recalcitrant molecular structure [2]. Due to hardly biodegradable characteristic it may remain for long periods of time in the environment [3]. Similar to other surfactants SDBS may cause foams in rivers and surface waters and by this way environmental risks can occur in aquatic ecosystems as a result of oxygen reduction. Environmental and public health authorities have focused on control and removal of surfactants due to the mentioned harmful effects noted in aqueous media [4].

There are several methods used for removal of surfactants from wastewater effluents. These methods can be listed as membrane technology [5], adsorption [6,7], chemical and electrochemical oxidation [8], chemical precipitation [9] and photocatalytic degradation [10]. Among various water treatment techniques, adsorption has been widely used as it is an effective and eco-friendly process [11]. Zeolites [12], bentonite [13], sand [14], silica gel [15], resins [16,17], and activated carbons [7,18,19] have been tested in removal of anionic surfactants. Some of the promising adsorbents which were used for removal of SDBS from aqueous solutions have been summarized in Table 1.

Due to the demand of supplying more efficient and easily available adsorbents researches have been extended to obtain novel adsorbents types.

After decision of the appropriate adsorbent type, it is essential to determine the optimum experimental conditions (pH, adsorbent dosage, agitation period, temperature, etc.) in adsorption studies. Determination of optimum conditions involves numerous time-consuming experimental tests. For practical applications of adsorption such as process design and control, it is important to model the effects of these experimental conditions. Besides the conventional adsorption isotherms (Langmuir, Freundlich, Temkin, Thomas, etc.) and kinetic models (pseudo first and second order reaction kinetics) statistical methods are also promising for providing information about adsorption behaviors. Among the various multivariate statistical methods, multiple linear regression (MLR), explaining the linear relations successfully [22] and artificial neural networks (ANNs), known with the superiority of modeling complex and non-linear problems [23,24] can be easily used for adsorption modeling purposes [25,26]. In the literature, there are novel studies about usage of ANN models for explaining adsorption processes. Turan et al. have tested efficiency of ANNs for modeling adsorption

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doi:10.1016/j.cej.2011.10.046

Table 1
Adsorption capacities of different adsorbents used for removal of SDBS.

Adsorbents	q_{max} (mg/g)	References
Acrylic ester resin (Diaion HP2MG)	405	[17]
Acrylic ester resin (YWB-13)	461	[17]
Activated carbons	260–470	[20]
Alumina	19.8	[21]
Modified natural zeolite	30.7	[4]
PANI doped with $CuCl_2$	32.3	This study
PANI doped with $ZnCl_2$	29.5	This study

of Zn(II) from leachate using hazelnut shell and obtained successful results in a recent study [27].

The major aim of this work was to evaluate efficiencies MLR and ANN for modeling adsorption behavior of SDBS onto Polyaniline (PANI) – a novel adsorbent doped with 8% $CuCl_2$ and 10% $ZnCl_2$, individually. Batch experiments were conducted in order to examine effects of pH, adsorbent dosage, temperature, agitation speed and agitation period. Thermodynamic studies were also performed in order to explain the adsorption mechanism of SDBS molecules onto doped PANI species. 69 data sets were used in the modeling applications for each PANI type, individually. Finally, performances of ANN models have been compared with MLR models considering the correlations between the predicted and experimental data.

2. Materials and methods

2.1. Experimental studies

2.1.1. Preparation of the used adsorbents

In the study, PANI doped with $CuCl_2$ and $ZnCl_2$ was used as adsorbents. PANI species doped with different metal ratios were tested to determine the most efficient adsorbent type for SDBS removal (Fig. 1).

As seen from Fig. 1, highest adsorption efficiencies were obtained as 98.09% and 99.63% for PANI species doped with 8% $CuCl_2$ and 10% $ZnCl_2$, respectively. Raw PANI could provide the efficiency of 86.45%. So, PANI species doped with 8% $CuCl_2$ and 10% $ZnCl_2$ were prepared regarding better adsorption efficiencies. With this aim 5 mL of aniline was dissolved in 70 mL of 1.5 M HCl. In order to obtain the doped PANI species, 5 mL of the required metal solutions (8% $CuCl_2$ or 10% $ZnCl_2$) were added individually into the aniline solution. On the other hand 10 g of $(NH_4)_2S_2O_8$, a strong oxidant, was dissolved in 20 mL deionized water. Then $(NH_4)_2S_2O_8$ solution was added into the previously prepared solution, gradually. The total solution was stirred at constant speed for 5 h at 25 °C. After the polymerization, solution was filtered, washed, and dried. By this way green granular PANI powders were obtained. Analytical grade reagents (Merck) were used in all experimental studies [28].

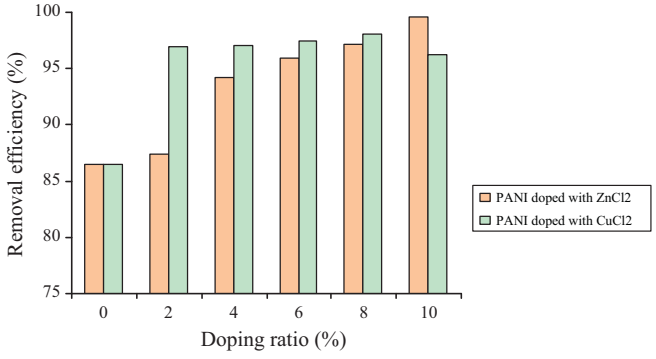

Fig. 1. Effects of doping ratio of PANI species on removal of SDBS.

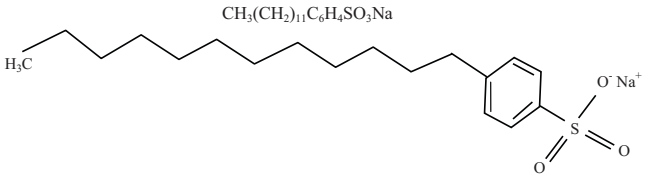

Fig. 2. Chemical structure of SDBS.

2.1.2. Batch adsorption tests

Adsorption of SDBS onto PANI was performed in NUVE ST-402 model batch reactor. Standard SDBS solutions of 100 mg/L were prepared by diluting the stock solution of 1000 mg/L. Chemical structure of the used surfactant ($C_{18}H_{29}NaO_3S$) was given the scheme in Fig. 2. The used sample volume was determined to be 100 mL in the experiments. pH adjustments were carried out using 0.1 N HCl and 0.1 N NaOH. HANNA Instrument 211 model pH-meter was used in the adjustments. Samples with adsorbent dosage in the range of 0.3–1.2 g were shaken at predetermined conditions (temperature, speed, etc.) After the required agitation period samples were taken from the reactor and then they were extracted according to MBAS (methylene blue active substances) method prior to spectrophotometric analyses (Standard Methods, 5540C). Remaining SDBS concentration in the samples was analyzed by using HACH-DR 2000 spectrophotometer at 652 nm wavelength. Effects of several factors (pH, adsorbent dosage, temperature, agitation speed and contact time) on SDBS removal were examined by applying the explained procedure.

Adsorption capacity of PANI was calculated according to the following formula [11]:

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

where q_e (mg/g) is the equilibrium adsorption capacity, C_0 and C_e (mg/L) are the initial and equilibrium concentrations of SDBS in solution, V (L) is the sample volume, and m (g) is the amount of the adsorbent.

2.1.3. Scanning electron microscopy (SEM) analysis

The SEM images are used as an innovative technique for the study of adsorption of surfactants at the solid/liquid interface. In the study, SEM images of the doped PANI species were taken before and after the adsorption processes performed in optimum conditions. The solids were drained, dried under vacuum at room temperature. JEOL 6060 type SEM was used in order to take the images of the adsorbents.

Fig. 3(a) and (b) shows the SEM images of PANI species doped with 10% $ZnCl_2$ and 8% $CuCl_2$ before SDBS adsorption. These figures illustrate irregularity in the surfaces and the existence of pores on the adsorbent.

SEM images of polymeric adsorbents after SDBS adsorption are presented in Fig. 4(a) and (b). As seen from the figures, the surfaces of polymeric adsorbents were fully covered with SDBS molecules, and zinc and copper structures completely disappeared on doped PANI species. These results confirm that SDBS molecules have been successfully adsorbed onto the surface of doped PANI species.

2.2. Statistical methods

2.2.1. Multiple linear regression (MLR)

Multiple linear regression (MLR) analysis is commonly used in environmental studies in order to model the impacts of numerous independent factors on the examined dependent variable [29–32].

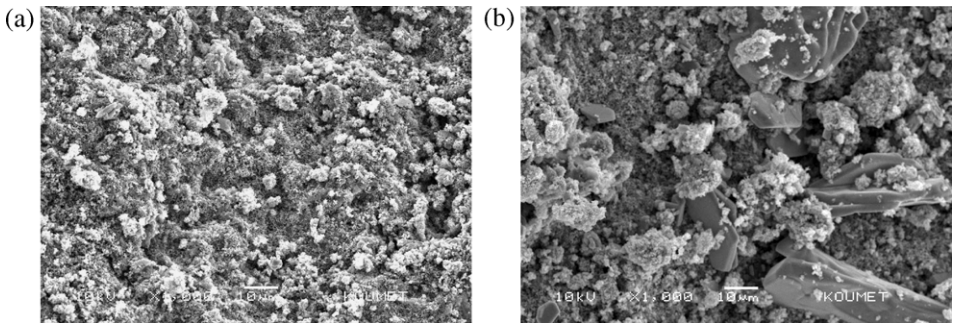

Fig. 3. SEM images of the doped PANI with (a) 10% $ZnCl_2$ and (b) 8% $CuCl_2$ before SDBS adsorption.

MLR analyses can be expressed with the following mathematical expression:

$$Y = a_0 + a_iX_i + a_2X_2 + \cdots + a_nX_n + \varepsilon \quad (2)$$

In Eq. (2) Y denotes the dependent (predicted) variable, a_i ($i = 0,\ldots,n$) are the regression coefficients, X_i ($i = 1,\ldots,n$) are the independent variables (predictors) and ε shows stochastic error of the regression.

Besides the various purposes of MLR analysis, it can be easily applied in adsorption studies to determine cumulative effect of several independent variables, such as retention time, adsorbent dosage, agitation rate and temperature of the system, on a dependent variable – the equilibrium adsorption capacity.

In the study, SPSS 17 statistical program has been used for MLR analyses.

2.2.2. Artificial neural networks (ANN)

In recent years, artificial neural network (ANN) models have been commonly used to examine relationships in complex nonlinear data sets [33]. ANN models have gained acceptance in numerous engineering fields as they provide spontaneously learning from examples and produce adequate and rapid responses to new information [34]. ANNs have been mainly consisted of three layers; input layer, hidden layer and output layers, respectively (Fig. 5). The models run with interaction of elementary processing units (neurons) by sending signals to one another along weighted connections [35]. In the system each neuron is connected to all neurons in the preceding and following layer by links.

Each input value is represented by a neuron in the input layer. Input values are weighted individually before entering the hidden layer and weighted values are transferred to the hidden layer. In the hidden layer each neuron produces outputs based on the sum of the weighted values from the input layer [33]. Outputs of a neuron can be calculated according to the following formula elementarily:

$$o = f\left(\sum_{J=0}^{n} \omega_{ji} \times x_j\right) \quad (3)$$

where n represents the number of inputs, x_j is the jth input to the neuron, ω_j is the jth synaptic weight and f is a non-linear function [36].

In the study hyperbolic tangent function that produces outputs between −1 and +1 was preferred [37]:

$$\tan\ h(x) = \frac{2}{1 + e^{-2x}} - 1 \quad (4)$$

In training process run with a data set of input and output data, weights of the network are adjusted to obtain the similar outputs as seen in the training data set. With this aim, data were divided into the two subsets for training and model validation purposes.

All data were normalized before ANN application regarding the general procedure of the method. The following equation was used for normalization:

$$NI_{ij} = \frac{I_{(i,j)} - \min(j)}{\max(j) - \min(j)} \quad (5)$$

In the equation I represents the input value, NI is the standardized value, i is the number of samples, and j shows the measured value of variables [38]:

Performances of the developed models were evaluated by considering mean standard error value (MSE) and Pearson's determination coefficient (R^2). Eqs. (6) and (7) were used with this aim, respectively:

$$\mathrm{MSE} = \frac{1}{N}\sum_{i=1}^{n}(q_{e,\mathrm{predict}} - q_{e,\mathrm{exp}})^2 \quad (6)$$

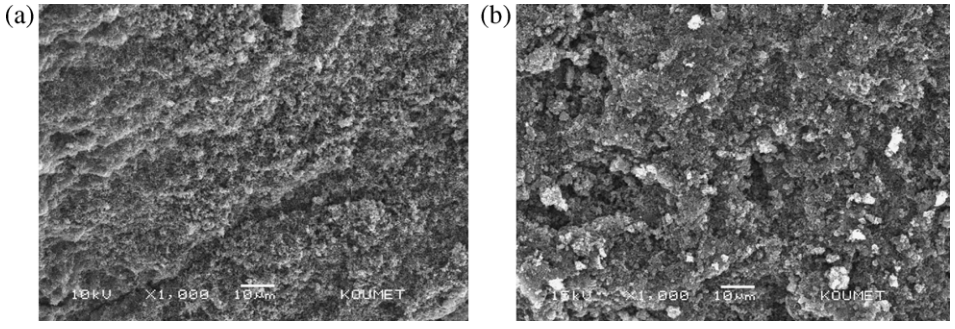

Fig. 4. SEM images of the doped PANI with (a) 10% $ZnCl_2$ and (b) 8% $CuCl_2$ after SDBS adsorption.

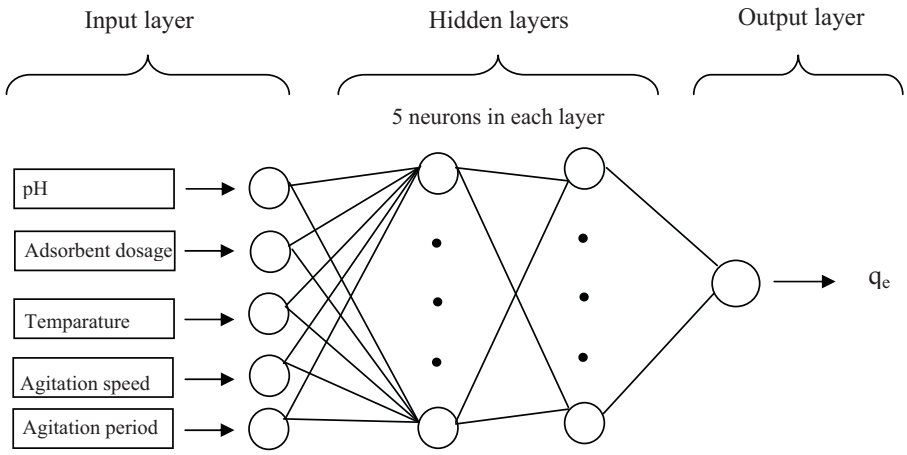

Fig. 5. Scheme of the used ANN model.

$$R^2 = \frac{\left[\sum_{i=1}^{n}(q_{e,predict} - \bar{q}_{e,predict})(q_{e,exp} - \bar{q}_{e,exp})\right]^2}{\sum_{i=1}^{n}(q_{e,predict} - \bar{q}_{e,predict})^2 \sum_{i=1}^{n}(q_{e,exp} - \bar{q}_{e,exp})^2} \quad (7)$$

In the equations $q_{e,predict}$ and $q_{e,exp}$ denote the predicted and experimental q_e values, respectively. $\bar{q}_e$ term represents the average values of the related q_e, and i: $1 \rightarrow n$, n is the total number of observations [39].

In this work, Matlab program has been used to predict q_e values.

3. Results and discussion

3.1. Experimental results

Effects of several important factors (pH, adsorbent dosage, temperature, agitation speed and period) on SDBS adsorption were examined with the conducted experiments. Although obtained results were presented in terms of q_e in the graphs, optimal conditions were determined considering the highest adsorption efficiencies in each experimental test. In this section results of these tests were explained briefly for each PANI type individually.

3.1.1. Effects of pH

The pH of the aqueous solution is one of the most important parameters affecting adsorption efficiency. This impact changes due to the adsorbent type, its behavior in the solution and type of the ions adsorbed [40].

In this study, pH has no significant effect on SDBS removal considering calculated q_e values. This indicates that electrostatic adsorbent–adsorbate interactions do not play an important role in SDBS adsorption on doped PANI species. Despite this fact, relatively higher adsorption efficiencies were obtained at lower pH values. Highest adsorption efficiencies were obtained at pH values of 2 and 3, respectively for adsorption processes using PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$ (Fig. 6).

Optimum pH values were used in further experiments examining the effects of adsorbent dosage, temperature, agitation speed and period.

3.1.2. Effects of adsorbent dosage

In adsorption processes amount of the adsorbent is another important factor affecting removal efficiencies. In general, increase in adsorbent dosage provides better removal efficiencies [41]. In the study, effect of adsorbent dosage (m) was tested by using different amounts of PANI in the range 0.3–1.2 g. Predetermined optimum pH values were used in these experiments.

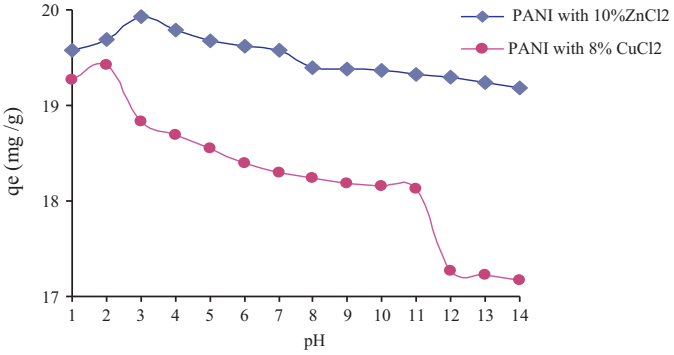

Fig. 6. Effect of pH on adsorption of SDBS by doped PANI species (initial SDBS concentration 100 mg/L, adsorbent dosage 0.5 g, agitation speed 200 rpm, contact time 120 min, temperature 23 °C).

Fig. 7 shows the effect of m on q_e values. As seen from the figure, better adsorption efficiencies were obtained in parallel with the increasing m. Optimum adsorbent dosages were determined as 0.9 g and 0.5 g, respectively for PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$.

3.1.3. Effects of temperature

Determining effects of temperature (t) is essential for explaining adsorption thermodynamics [42]. With this aim we have

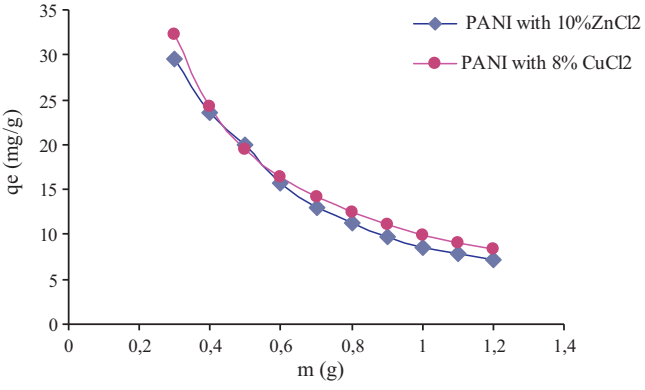

Fig. 7. Effect of adsorbent dosage on adsorption of SDBS by doped PANI species (initial SDBS concentration 100 mg/L, pH 2 and 3 agitation speed 200 rpm, contact time 120 min, temperature 23 °C).

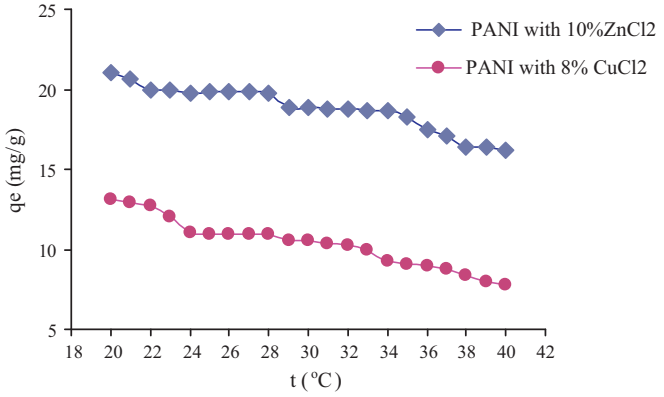

Fig. 8. Effect of temperature on adsorption of SDBS by doped PANI species (initial SDBS concentration 100 mg/L, pH 2 and 3, adsorbent dosage 0.9 and 0.5, agitation speed 200 rpm, contact time 120 min).

performed experiments in different temperature conditions in the range 20–40 °C. q_e versus t are presented in Fig. 8.

Increase in temperature caused remarkable decrease in adsorption capacity. This demonstrates the exothermic characteristic of the SDBS adsorption on PANI. Highest adsorbent capacities were obtained at 20 °C for both of the PANI species.

3.1.4. Effects of agitation speed

Adsorption processes are also influenced by mass transfer parameters. The equilibrium adsorption capacities are presented in Fig. 9 for varying agitation speeds (AS).

As seen from Fig. 9, higher removal efficiencies were obtained with the increase in agitation speed. 200 rpm was determined as optimum agitation speed for the adsorption process.

3.1.5. Effects of agitation period

Effects of agitation period (AP) were also examined by using the predetermined optimum values of pH, m, t, AS. Fig. 10 presents effects of AP on q_e values. The adsorption efficiencies increased to a certain level with increasing AP and remains almost stable after then. It can be concluded that 40 and 70 min are optimum periods for adsorption of SDBS onto PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$, respectively.

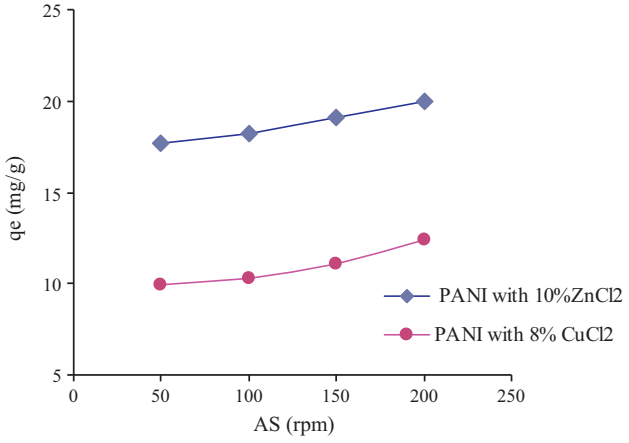

Fig. 9. Effect of agitation speed on adsorption of SDBS by doped PANI species (initial SDBS concentration 100 mg/L, pH 2 and 3, adsorbent dosage 0.9 g and 0.5 g, contact time 120 min, temperature 20 °C).

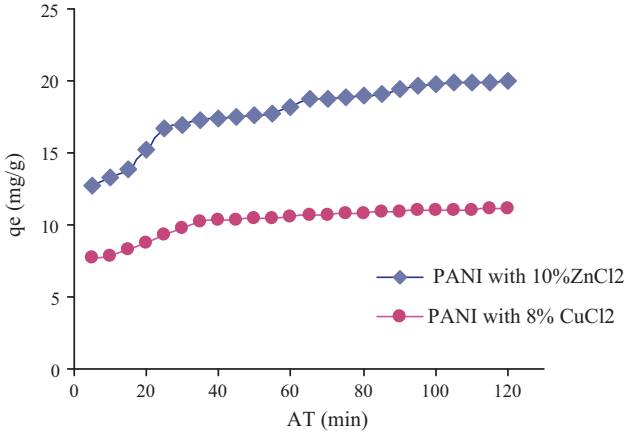

Fig. 10. Effect of agitation time on adsorption of SDBS by doped PANI species (the initial SDBS concentration 100 mg/L, pH 2 and 3, adsorbent dosage 0.9 g and 0.5 g, agitation speed 200 rpm, temperature 20 °C).

3.2. Thermodynamic studies

Thermodynamic studies were also performed in order to explain the adsorption mechanism of SDBS molecules onto polymeric adsorbents in detail. Thermodynamic parameters were calculated according to following equations [43,44]:

$$K_c = \frac{C_{ads}}{C_e} \tag{8}$$

$$lg\left(\frac{1}{C_e}\right) = lgK_c + \left(\frac{-\Delta H}{2.303RT}\right) \tag{9}$$

$$\Delta G = -RT \ \ln K_c \tag{10}$$

$$\Delta S = \frac{\Delta H - \Delta G}{T} \tag{11}$$

where, K_c is the equilibrium constant, C_{ads} is the amount of SDBS adsorbed on PANI at equilibrium (mg/g), C_e is equilibrium concentration of SDBS in solution (mg/L), T is absolute temperature (K), ΔH is the isosteric enthalpy change of adsorption (kJ/mol). R represents the gas constant (J/mol K), ΔG is the free energy change of adsorption (kJ/mol) and finally ΔS is the entropy change of adsorption (J/mol K).

All calculated thermodynamic parameters are given in Table 2. As seen from Table 2, negative values of ΔH show the exothermic characteristic of SDBS adsorption for both of the PANI species. Furthermore, physical adsorption is suggested as the absolute values of ΔH change in the range of 10–30 kJ/mol [44]. Negative ΔG values show spontaneous adsorption reactions [43] and negative ΔS values indicate regularity of the solute molecules during the process. Increase of temperature decreases the absolute ΔS values and improves randomness at the solid–liquid interface in adsorption processes [44].

3.3. Results of modeling studies

In the study MLR and ANN models were applied in order to predict the effects of the experimental conditions on adsorption of SDBS onto doped PANI adsorbents. In the models 69 data sets were used for each PANI type. Used data were presented in the graphs given in Section 3.1.

3.3.1. Results of MLR analyses

Firstly, MLR analyses were applied to model the effects of experimental conditions considering q_e values. In MLR applications, predictive equations were obtained by using experimental data.

Table 2
Calculated thermodynamic parameters for the study.

Temperature (K)	K_c		ΔG (kJ/mol)		ΔH (kJ/mol)		ΔS (J/mol K)	
	PANI with $ZnCl_2$	PANI with $CuCl_2$	PANI with $ZnCl_2$	PANI with $CuCl_2$	PANI with $ZnCl_2$	PANI with $CuCl_2$	PANI with $ZnCl_2$	PANI with $CuCl_2$
293	18.00	1.31	−7.03	−0.65	−13.28	−21.66	−21.33	−71.71
298	27.94	1.79	−8.23	−1.44	−13.07	−19.72	−16.21	−61.34
303	67.61	2.85	−10.59	−2.63	−12.85	−17.02	−7.43	−47.49
308	106.00	8.83	−11.92	−5.56	−12.62	−12.21	−2.26	−21.59
313	107.79	9.36	−12.15	−5.81	−12.43	−12.04	−0.86	−19.90

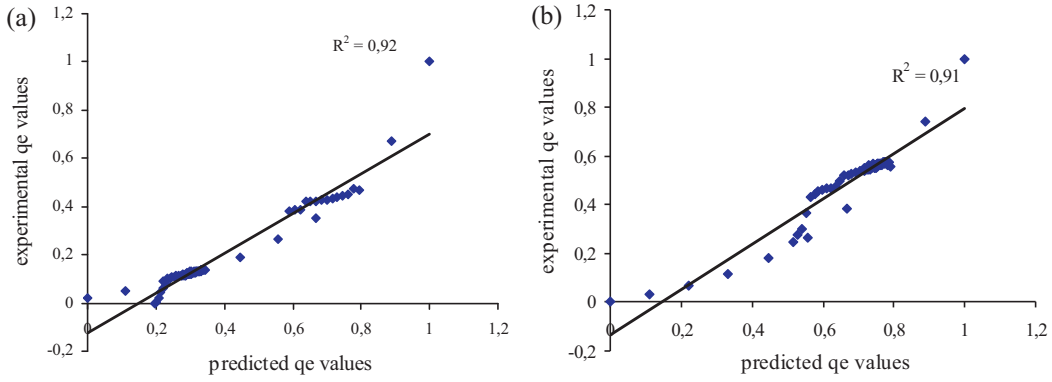

Fig. 11. Predicted and experimental q_e values for (a) PANI doped with 8% $CuCl_2$ and (b) PANI doped with 10% $ZnCl_2$ obtained with MLR models.

SPSS 17.0 statistical program has been used for this purpose. Developed regression equations are given below respectively for PANI doped with 8% $CuCl_2$ (Eq. (12)) and PANI doped with 10% $ZnCl_2$ (Eq. (13)):

$$q_{e,predict} = 29.53 - 0.32pH - 22.43m - 0.07t + 0.006AS + 0.03AP \quad (12)$$

$$q_{e,predict} = 26.57 - 0.12pH - 23.20m - 0.07t + 0.006AS + 0.05AP \quad (13)$$

$q_{e,predict}$ values were calculated by using the equations given above. Determination coefficients for the relations between $q_{e,predict}$ and $q_{e,exp}$ were calculated as 0.92 and 0.91 for adsorption processes using PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$, respectively. As seen from the equations, highest regression coefficients have been determined for adsorbent dosage. This shows the significant effect of m in the adsorption processes whereas agitation speed does not seem so effective considering lower coefficients.

Predicted q_e values versus actual q_e values were presented in Fig. 11(a) and (b) individually for each adsorbent specie. Furthermore MSE values of the models were found as 0.040 and 0.035, respectively.

3.3.2. Results of ANN models

Efficiency of ANN models was also tested for modeling adsorption behaviors of SDBS onto PANI. With this aim various network architectures were developed including different functions (training and learning functions, number of hidden layers, epochs, etc.). Among the tested architectures, backpropagation feed-forward network type with two hidden layers provided the highest modeling efficiencies for both of the PANI species. *Trainr* training function, *Learngdm* adaptation function and *Tansig* transfer function were preferred in the models.

Similar to the MLR models, R^2 and MSE values were calculated for the predictive models. Relations between $q_{e,predict}$ and $q_{e,exp}$ were explained with the R^2 values of 0.98 and 0.94 for adsorption processes using PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$, respectively (Fig. 12(a) and (b)).

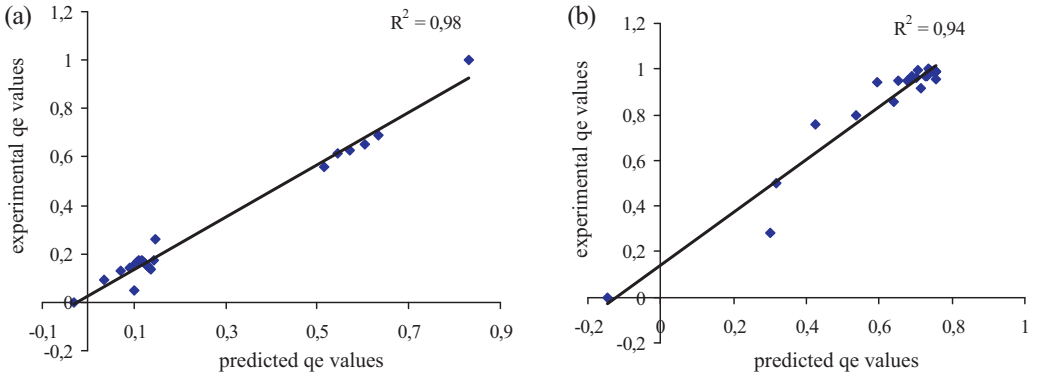

Fig. 12. Predicted and experimental q_e values for (a) PANI doped with 8% $CuCl_2$ and (b) PANI doped with 10% $ZnCl_2$ obtained with ANN models.

MSE values of the predictions were found as 0.004 and 0.006, respectively for processes using PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$.

Lower error values and higher determination coefficients stated that ANN models are more efficient for explaining adsorption behaviors of SDBS onto doped PANI species.

4. Conclusions

In this study, it was aimed to investigate adsorption behaviors of SDBS from aqueous solutions. With this aim doped PANI species were used as adsorbent. PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$, provided sufficient adsorption capacities for SDBS removal. Effects of pH, adsorbent dosage, temperature, agitation speed and agitation period were investigated by the batch experiments. Results of the thermodynamic studies indicated exothermic and spontaneous characteristics of the concerned adsorption processes. A total of 69 experimental sets were conducted for each PANI type and obtained data were used to model adsorption processes. In MLR analyses the relations between $q_{e,predict}$ and $q_{e,exp}$ could be explained with R^2 of 0.92 and 0.91 respectively, for PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$. MSE values of the predictions were calculated as 0.040 and 0.035, respectively. Furthermore efficiency of ANN models was also examined. Results of ANN applications demonstrated that a backpropagation feed-forward network type with two hidden layers provided successful modeling efficiencies for both of the PANI species. Compared to MLR models, higher R^2 values were obtained by using the selected network architecture (R^2 = 0.98 and 0.94 respectively, for PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$). MSE values of the ANN models were also lower than those of MLR models. At the end of the study, it was concluded that ANN models provide more sufficient efficiency to predict effects of experimental conditions on adsorption of SDBS onto PANI doped with 8% $CuCl_2$ and 10% $ZnCl_2$, individually.

Acknowledgements

This study was funded by the University of Kocaeli Research Fund under Project No. 2011-024.

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