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Application of non-linear regression and soft computing techniques for modeling process of pollutant adsorption from industrial wastewaters

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Abstract

The process of pollutant adsorption from industrial wastewaters is a multivariate problem. This process is affected by many factors including the contact time (T), pH, adsorbent weight (m), and solution concentration (ppm). The main target of this work is to model and evaluate the process of pollutant adsorption from industrial wastewaters using the non-linear multivariate regression and intelligent computation techniques. In order to achieve this goal, 54 industrial wastewater samples gathered by Institute of Color Science & Technology of Iran (ICSTI) were studied. Based on the laboratory conditions, the data was divided into 4 groups (A-1, A-2, A-3, and A-4). For each group, a non-linear regression model was made. The statistical results obtained showed that two developed equations from the A-3 and A-4 groups were the best models with R^2 being 0.84 and 0.74. In these models, the contact time and solution concentration were the main effective factors influencing the adsorption process. The extracted models were validated using the t-test and F-value test. The hybrid PSO-based ANN model (particle swarm optimization and artificial neural network algorithms) was constructed for modelling the pollutant adsorption process under different laboratory conditions. Based on this hybrid modeling, the performance indices were estimated. The hybrid model results showed that the best value belonged to the data group A-4 with R^2 of 0.91. Both the non-linear regression and hybrid PSO-ANN models were found to be helpful tools for modeling the process of pollutant adsorption from industrial wastewaters.

1. Introduction

With a rapid population growth and the economic development as well as for responding to the growing demand for irrigation, industry, and food, water is needed to provide higher standards in the public life [1]. An important element in the management of water resources is the effective wastewater reclamation and reuse of wastewaters [2]. In addition, wastewater treatment can prevent the infection of the low reserves of water [3]. Industrial wastewaters create a wide variety of pollution so that even they differ from one process to another in the industry [4]. Colors and dyes are among the types of pollutant materials that heavily pollute the environment. Increase in the production of paints and their various global applications lead to the production of wastewaters with a high pollution rate. These wastewaters lead to the environmental pollution concerns [5, 6]. Most of the substances contained in wastewaters are toxic and even carcinogenic [7]. Various industries such as the textile, paper, color images, pharmaceutical, food, cosmetics, and electrical industries use dyeing materials abundantly [8]. According to the researchers, about 15% of the colors used in the coloring process remain as residues in wastewaters [9]. The colors are the most dangerous group of chemical compounds found in the industrial effluents because they will

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reduce light penetration capability and disrupt the process of photosynthesis in water resources [10, 11]. The effluent treatment methods include biological treatment, coagulation, adsorption, oxidation, filtration, etc. [12-16]. On the other hand, these methods include the physical, chemical (coagulation/flocculation adsorption of surface, oxidation, separation by the membrane), and biological (biodegradable using the battery) methods [17]. The adsorption process is a highly known method among the available options. The adsorption process has a high potential in the removal of small molecules (dyes and organic matters). Thus it seems that it is one of the best methods to remove dyes from wastewaters of industries [18]. Many other techniques are effective for color removal from wastewaters but they are very expensive and require advanced technologies. In the past, the adsorption process due to the simple design and low cost with high efficiency was a suitable method for the removal of dyes, pigments, and other chemicals from wastewaters [19]. In this regard, several studies to date have been conducted for the development of effective adsorbents. There are a number of studies in this case, the most important of which are carried out with absorbents waste sugarcane, corn husks, rice bran, waste of banana, coconut, and waste of sludge, and raw materials such as carbon, coal, and petroleum coke [20-26]. A study conducted by Patil investigated the potential of fruit and vegetable wastes as new bio-adsorbents [27]. In another study conducted by Wang and Chen in 2009, evaluation of biological sorbents to remove heavy metals was considered; they investigated the capacity of different bio-adsorbents for the removal of heavy metals [28]. Another study carried out in this regard that can be noted for the potential of waste and agricultural by-products used to remove heavy metals from wastewater is the study conducted by Nguyen et al. [29]. In another study, Ashutosh Tripathi and Manju Rawat Ranjan investigated the possibility of removing heavy metals from industrial wastewaters using low-cost adsorbents [30]. Aryafar et al. used the support vector machine for assessment of heavy metal pollution in Shour River in Sharcheshmeh Copper Mine [31]. Rasalingam et al. examined a method to remove pollutants from wastewaters using a combination of TiO_2 SiO_2 and an oxidized material [32]. The ability of adsorbing metal ions from sewage and wastewaters with an adsorbent in agriculture was analyzed by Emenike et al. [33]. Methods of removing heavy metals from industrial effluents were studied in the research work of Gunatilake [34]. In this work, the statistical analysis, Particle Swarm Optimization (PSO) algorithm, Hybrid PSO-based ANN, and Hybrid Modeling were applied for modeling pollutant adsorption from industrial wastewaters.

2. Methodology

2.1. Materials and methods

In the present study, 54 industrial wastewater samples gathered by Institute of Color Science & Technology of Iran (ICSTI) were used for evaluation of metallic and dye pollutant adsorption from industry. The dye pollutant was green Malachite and the metallic pollutant was Nickel. The data was kinetically produced during the process of adsorption of pollutants from industrial wastewaters using Perlite adsorbent. The effects of some factors including pH, contact time, solution concentration, and adsorbent mass were investigated during laboratory (experimental) tests. The data was divided into four groups (A-1, A-2, A-3, and A-4) based on different laboratory conditions and types of pollutant [35]. In this work, the statistical analysis and soft computing techniques were applied to investigate the factors affecting the process of adsorption of metallic and dye pollutants from industrial wastewaters.

2.2. Statistical analysis

The adsorption process was affected by many factors such as the contact time, pH, solution concentration, and adsorbent mass. For this reason, simple regression models could not be used for such problems. In this research work, the laboratory test results were studied using the multivariate regression. Regression analysis was performed using the computing software "Statistical Package for the Social Sciences (SPSS)". Among the four factors involved, the adsorbent mass had the same role for each group of data because the adsorbent weight was constant during different conditions of laboratory tests. The other factors changed under the laboratory conditions [35]. The non-linear multivariate regression models were constructed based on 3 factors. These models are given in Eqs. 1-8. In these equations, A is the adsorption value (per %), T is the contact time (per minute), pH is the potential of log $[H^+]$, and P is the solution concentration (per ppm). As shown in the extracted models, in some models (Eqs. 3-6), three factors influenced the adsorption value, and in the others (Eqs.1, 2, 7, 8), two factors affected

the adsorption process. In all models, the contact time and solution concentration were the main effective factors that affected the adsorption process, and therefore, these two factors had to be controlled and optimized significantly. The statistical results of the models are given in Table 1.

$$A = 0.114T - 0.933P + 74.332 \quad \text{A-4} \quad (1)$$

$$A = \frac{10^{2.676} \times T^{0.239}}{P^{1.24}} \quad \text{A-4} \quad (2)$$

$$A = 0.461T + 0.745pH - 0.604P + 36.486 \quad \text{A-1} \quad (3)$$

$$A = \frac{10^{1.671} \times T^{0.134} \times pH^{0.059}}{P^{0.106}} \quad \text{A-1} \quad (4)$$

$$A = 0.2441T + 1.08pH - 0.962P + 58.78 \quad \text{A-2} \quad (5)$$

$$A = \frac{10^{1.079} \times T^{0.489} \times pH^{0.084}}{P^{0.145}} \quad \text{A-2} \quad (6)$$

$$A = 0.2291T - 0.844P + 61.604 \quad \text{A-3} \quad (7)$$

$$A = \frac{10^{1.728} \times T^{0.658}}{P^{1.066}} \quad \text{A-3} \quad (8)$$

Table 1. Statistical results of the multiple regression models.

Model	Independent variables	Coefficients	Std. Error	t	t*	F	F*	R^2
Eq. (1)	Constant	74.332	4.965	14.970	±1.96	115.12	±5.02	0.62
	Time	0.114	0.055	2.078				
	ppm	-0.933	0.063	-14.859				
Eq. (2)	Constant	2.676	0.127	21.009	±1.96	350.32	±5.02	0.84
	Time	0.239	0.06	3.959				
	ppm	-1.24	0.048	-25.952				
Eq. (3)	Constant	36.486	13.13	2.779	±2	16.37	±3.92	0.5
	Time	0.461	0.067	6.891				
	pH	0.745	1.762	0.423				
	ppm	-0.604	0.502	-1.203				
Eq. (4)	Constant	1.671	0.12	13.961	±2	6.12	±3.92	0.31
	Time	0.134	0.034	3.889				
	pH	0.059	0.107	0.549				
	ppm	-0.106	0.062	-1.72				
Eq. (5)	Constant	58.78	3.956	14.56	±1.96	53.7	±3.68	0.5
	Time	0.244	0.022	11.202				
	pH	1.08	0.55	1.964				
	ppm	-0.962	0.168	-5.744				
Eq. (6)	Constant	1.079	0.127	8.508	±1.96	76.74	±3.68	0.5
	Time	0.489	0.032	15.09				
	pH	0.084	0.125	0.67				
	ppm	-0.145	0.08	-1.805				
Eq. (7)	Constant	61.604	11.352	5.427	±2.05	13.42	±5.61	0.5
	Time	0.229	0.136	1.681				
	ppm	-0.844	0.172	-4.901				
Eq. (8)	Constant	1.728	0.289	5.982	±2.05	38.8	±5.61	0.74
	Time	0.658	0.106	6.184				
	ppm	-1.066	0.17	-6.273				

a. Dependent Variable: adsorption (%), t^*: Tabulated t value, F^*: Tabulated F value

The determination coefficient of Eqs. (2) and (8) are 0.84 and 0.74, respectively; these values are appropriate but they do not necessarily identify the valid model. The F-test, the t-test, and the plot of predicted versus observed values were used to confirm the developed models. The t-test was used to determine the significance of R^2. This test compares the obtained t-value with the tabulated t-value by use of the null hypothesis. If the obtained t-value is greater than the tabulated t-value, the null hypothesis is rejected. This means that r is significant; otherwise, r is not notable. In these models, the confidence level of 97.5% was chosen to evaluate the significance of R^2. As it can be seen in Table 1, the obtained t-value is greater than the tabulated t-value for the models (Eqs. 2 and 8). This means that the models are valid. The F-test with the degrees of freedom $df_1 = 1$ and $df_2 = 141$ for Eq. (2) and $df_1 = 1$ and $df_2 = 28$ for Eq. (8) were used to evaluate the significance of the regressions. In this test, a 97.5% level of confidence was chosen. If the obtained F-value from model is greater than the tabulated F-value, the null hypothesis is rejected. This means that there is a real relation between the dependent and independent variables. According to Table 1, the obtained F-value is greater than the tabulated F-value. This means that the null hypothesis is rejected. Therefore, it can be concluded that the models are valid. In order to evaluate the capability of prediction of the derived model, the scatter diagrams of the actual and predicted values were plotted. The predicted adsorption values were plotted against the actual adsorption values (Figures 1 and 2). Ideally, on a plot of actual versus predicted values, the points should be scattered around the 1:1 diagonal straight line. The distance that each data point plots from the 1:1 diagonal line can display the error in the predicted value. A point lying on the line indicates an exact estimation. In the plots for models 2 and 8, the points are nearly scattered around the 1:1 diagonal line. This means that the prediction capability of models 2 and 8 are appropriate.

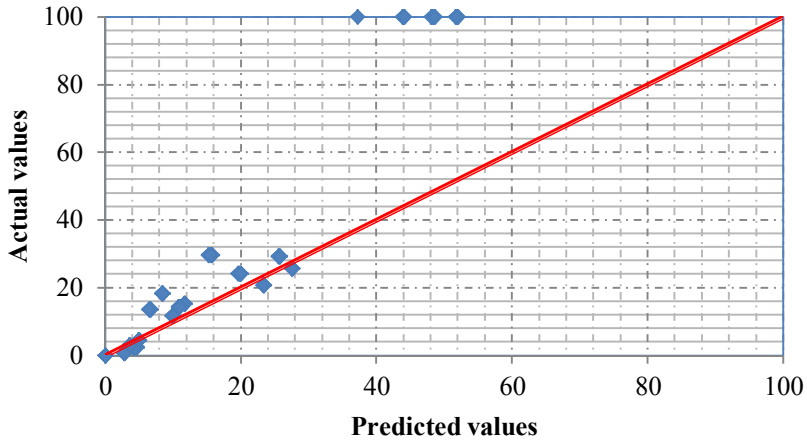

Figure 1. Predicted values versus actual values for model 2.

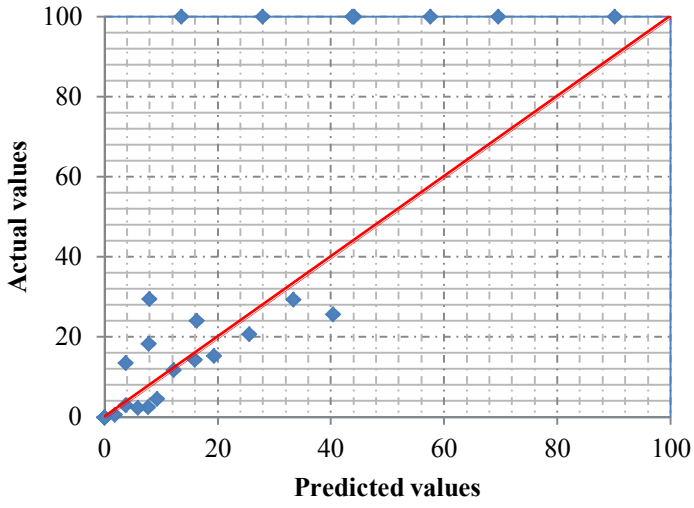

Figure 2. Predicted values versus actual values for model 8.

2.3. Particle swarm optimization (PSO) algorithm

In order to solve the optimization problems, the main objective is to determine the best possible response considering the conditions of the problems. Many optimization methods based on the artificial intelligence have been developed, and the meta-heuristic algorithms are one of the main branches of these techniques. Finding the different answers for complex and dynamic problems is the main attractive feature of these algorithms [36-39]. The PSO algorithm is one of the most influential meta-heuristic algorithms in the area of optimization, which was proposed for the first time by Kennedy and Eberhart based on the group and social behavior patterns of birds and fish flock [40, 41]. According to these researchers, each particle in the PSO algorithm is the representative of a random answer in the search and optimal solution area, and based on the experience and behavior of each particle as well as its neighboring particles, it can move in the problem space. In addition, each particle has a velocity vector, and based on any change in this vector, the particle will constantly search the problem space. The movement of each particle depends on three factors including the current position of particle (X_i^k), the best position of particle (Pbest), and the best position of total particles (Gbest). Movements of particles can be calculated by Equations (9) and (10) [42] as follow:

$$V_i^{(k+1)} = w V_i^k + c_1 r_1.(pbest_i - X_i^k) + c_2 r_2.(gbest - X_i^k) \quad (9)$$

$$X_i^{(k)} = X_i^k + V_i^k \quad (10)$$

where $V_i^{(k+1)}$ is a new velocity vector and V_i^k is the i[th] particle's velocity. N is the size of swarm i = (1, 2, 3, ..., N) and k = (1, 2, 3, …) determining the number of iterations. W is the inertia weight that controls the effect of the previous velocity on the current one. r_1 and r_2 are random numbers in the range of [0, 1]. Furthermore, C_1 and C_2 are the acceleration constants, and based on the empirical evidence, Equation (11) is satisfied [43]. A flowchart of the basic form of the PSO algorithm is illustrated in Figure 3.

$$c_1 + c_2 \leq 4 \quad (11)$$

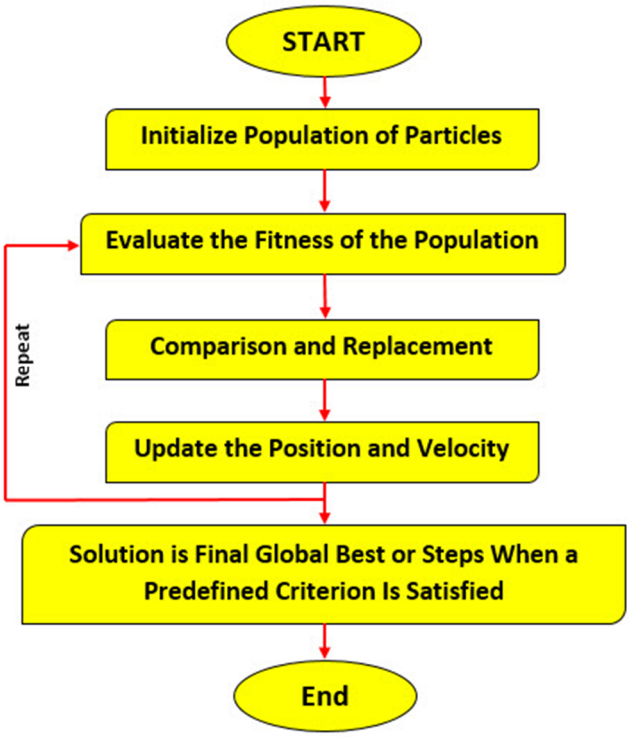

Figure 3. Basic form of PSO flowchart.

2.4. Hybrid PSO-based ANN

Nowadays, in the post-industrial world and in different fields of applied sciences, dynamic and optimization models have various significant applications including artificial intelligence and engineering optimization, which have introduced the scientific-practical concept of these models to the industry sector's administrators and academic researchers [44-48].

Among the proposed optimization models, artificial neural networks that use the brain dynamic structure and system have significantly been improved in terms of development, analysis, and implementation of the models with a complex and uncertain structure in technical and engineering problems and sciences. Overall, artificial neural networks relying on two fundamental characteristics of power-based mapping and parallel structure and generalizability had appropriate performances while dealing with complex systems. In fact, in the artificial neural network, based on the comparison between the input and output data, a linear or non-linear mapping was determined and set to match this network output with the target, and created the most optimal condition. Artificial neural networks have a diverse structure, the most practical of which is Hopfield, the multi-layer perceptron network [49].

In a research work conducted by Alizadeh and Kavianpour, the function of artificial neural networks in anticipating several water quality parameters in Hilo Bay, Pacific Ocean was studied [50]. In the recent years, with the emergence of meta-heuristic optimization algorithms and for improving the performance of artificial neural networks, the application of neural networks with optimization algorithms has become significantly important for determining the most optimal value for weights and biases [51]. It led to the creation of a very accurate and powerful network in the identification of learning pattern and power, and many research works have been conducted in different engineering fields including geotechnics, mining, and environment. In a study conducted by Alizadeh et al., a combination of four different meta-heuristic algorithms including genetic algorithm (GA), imperialist competitive algorithm (ICA), bee algorithm (BA) and cuckoo search (CS) algorithm, and neural networks was used to evaluate and anticipate the longitudinal dispersion coefficient in rivers [52]. In this work, the pollutant adsorption process of industrial wastewaters was evaluated using the PSO-ANN hybrid algorithm. Furthermore, it should be noted that ANN is a multi-layer perceptron (MLP), and PSO is utilized to optimize ANN networks in this research work.

2.5. Hybrid modeling

Two factors influencing the data modelling and analysis in hybrid algorithms are control parameters and performance indices. In this section, to build the model and conduct the required analyses, first, the control parameters of the hybrid algorithm are proposed. In fact, the control parameters in meta-heuristic algorithms have a key role in improving and enhancing the accuracy of optimization processes. For this reason, according to the previous studies and the contribution of experienced experts, as an example, the control parameters for modeling the A-1 group data were Swarm Size = 250 and Max Iteration = 25. In addition, 75% of the total dataset was used randomly for the training dataset and the remaining 25% was considered as the testing data for the PSO-ANN model [53-55]. Furthermore, the performance indices for data analysis based on Equations (12)-(14) included value account for (VAF), root mean square error (RMSE), and coefficient of determination (R^2).

$$VAF = \left[1 - \frac{\mathrm{var}(x_i - y_i)}{\mathrm{var}(x_i)}\right] \quad (12)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2} \quad (13)$$

$$R^2 = \frac{[\sum_{i=1}^{n}(x_i - x_{mean})^2] - [\sum_{i=1}^{n}(x_i - y_i)^2]}{[\sum_{i=1}^{n}(x_i - x_{mean})^2]} \quad (14)$$

Where n explains the number of datasets. y_i and x_i are the forecasted and measured adsorption values, respectively. Note that in a modeling with a high and acceptable accuracy, VAF is equal to 100 (%) and the values for RMSE and R^2 should be close to 0 and 1, respectively, demonstrating the best approximation. The results derived from the hybrid algorithm based on the stochastic optimization technique for modeling the pollutant adsorption process of industrial wastewaters including 4 groups of data are given in Table 2.

Based on the performance indices in Table 2, it can be observed that the best performance indices belong to A-4. Furthermore, according to the modeling results, the predicted adsorption values were plotted against the actual adsorption values for A-1, A-2, A-3, and A-4 in Figures 4-7, respectively.

Table 2. Results of performance indices using PSO-ANN modeling.

	A-1	A-2	A-3	A-4
VAF	65.32	69.69	76.03	90.79
RMSE	0.27	0.21	0.43	0.27
R^2	0.65	0.7	0.77	0.91

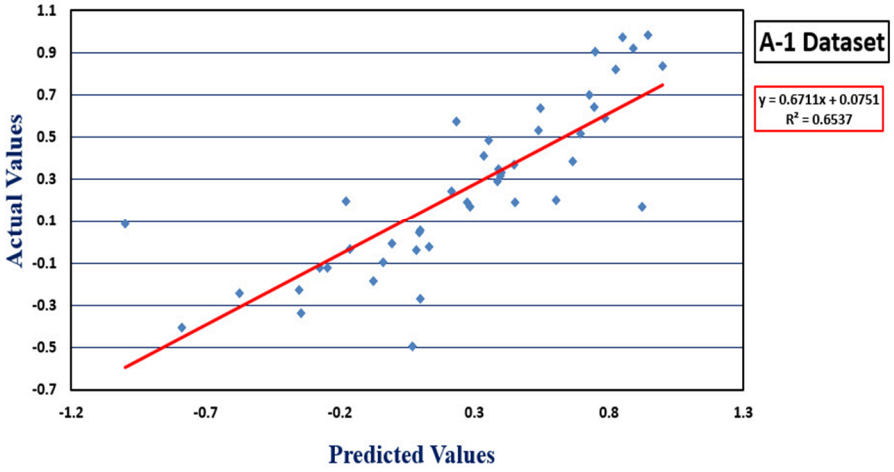

Figure 4. Predicted values versus actual values for A-1.

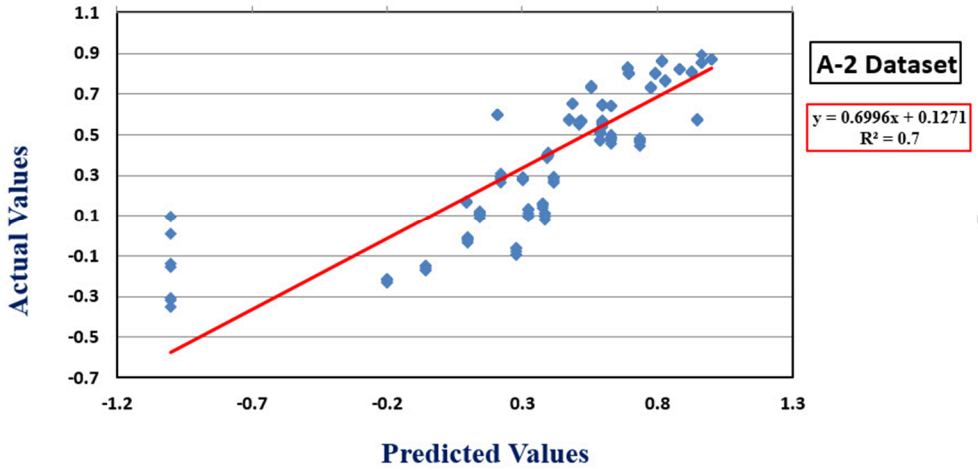

Figure 5. Predicted values versus actual values for A-2.

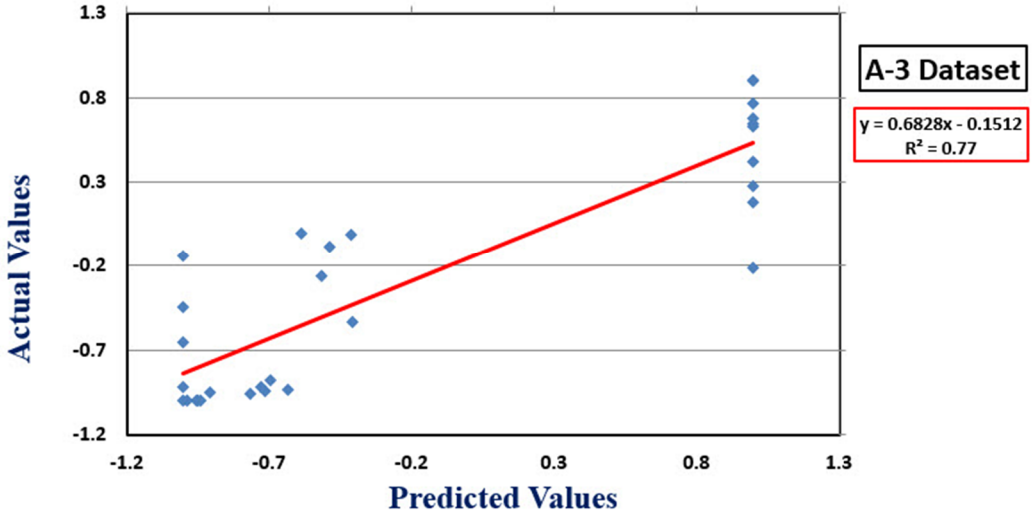

Figure 6. Predicted values versus actual values for A-3.

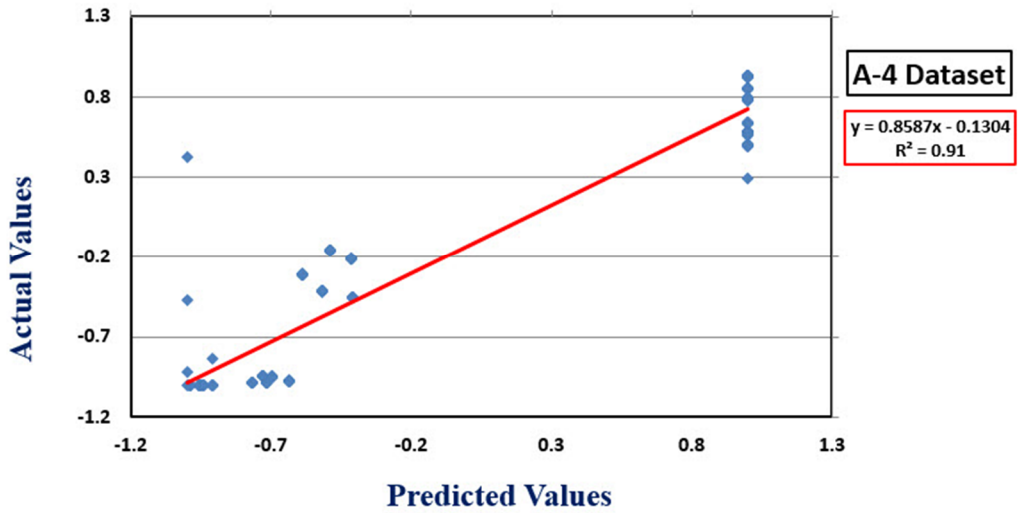

Figure 7. Predicted values versus actual values for A-4.

As mentioned earlier, in this work, to develop the models, each model was run via different control parameters to gain the optimum results. In addition, the best equations obtained for dataset were also compared based on their performance indices. According to the results in Tables 1 and 2 and Figures 4-7, the following remarks can be made:

- In comparison with the statistical results of the dataset, the results obtained shows that Eq. (2) can be selected as the best predictive model among the other statistical models with the determination coefficient = 0.84 in A-4.
- Different models were developed using PSO-ANN with a range of control parameters. As it can be seen, the performance indices for the four datasets describe their high capability for predicting the process of adsorption of pollutants. Although all the proposed models and datasets have proper results, A-4 obtained the maximum value of performance indices among the other datasets according to Table 2 and Figure 7 with the determination coefficient = 0.91.
- Comparing the optimized PSO-ANN models with the statistical models, it was shown that the PSO-ANN method could provide a higher performance capability for evaluating the process of adsorption of pollutants.

Thus it can be concluded that in this case study, the proposed hybrid model is suitable for evaluating the process of adsorption of pollutants from industrial wastewaters. It is worth noting that this model is only applicable in this case and should not be used directly in other similar cases because this modelling depends on some other factors such as the number of datasets (output- input) and the definition of control parameters.

3. Conclusions

The adsorption of pollutants for different contact times (T), pH values, adsorbent weights (m), and solution concentrations (ppm) were analyzed in four dataset groups. The predictive adsorption models were developed using the multiple regression analysis. Validation of the models was carried out by considering the determination coefficient, t-test, F-test, and plots of observed adsorption values versus estimated adsorption values. The results obtained showed that two models including the contact time and solution concentration were good for predicting the pollutant adsorption from industrial wastewaters. The determination coefficient of these models were 0.84 and 0.74, respectively. In the proposed hybrid approach, a pollutant adsorption assessment was carried out using PSO-ANN, which was found to be a powerful tool for identifying the environmental complex problems. This work demonstrates that the PSO-ANN technique is a reliable system modeling technique for predicting pollutant adsorption from industrial wastewaters. The results of performance indices showed that the coefficients of determination (R^2) for the A-1, A-2, A-3, and A-4 data groups were 0.65, 0.70, 0.77, and 0.91, respectively. It was concluded that the best performance indices belonged to the A-4 group of data by R^2 of 0.91. Such studies can be used to better manage the industrial wastewaters in order to diminish the environmental effects. In the future research works, a sensitivity analysis can also be used to investigate the use of other kinds of artificial

intelligence (AI) approaches and performance indicators.

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کاربرد روش‌های رگرسیون غیرخطی و پردازش نرم در مدل‌سازی فرآیند جذب آلاینده از پساب‌های صنعتی

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چکیده:

فرآیند جذب آلاینده از پساب‌های صنعتی یک مسئله چند متغیره است. فاکتورهای زیادی از جمله زمان تماس (t)، pH، وزن جاذب و غلظت محلول (ppm) بر فرآیند جذب تأثیرگذار هستند. هدف اصلی این پژوهش مدل‌سازی و ارزیابی فرآیند جذب آلاینده از پساب‌های صنعتی با استفاده از روش‌های رگرسیون غیرخطی و محاسبات هوشمند است. به منظور رسیدن به هدف تعداد ۵۴ نمونه از پساب صنعتی که توسط مؤسسه تکنولوژی و علوم رنگ تولید شده است، مطالعه شد. بر پایه شرایط انجام آزمایش‌ها، داده‌ها به چهار گروه (A-1، A-2، A-3 و A-4) تقسیم شدند و برای هر گروه یک مدل رگرسیون غیرخطی ایجاد شد. نتایج آماری به دست آمده نشان داد که دو مدل ساخته شده برای گروه‌های A-3 و A-4 با ضریب R^2 به ترتیب ۰/۸۴ و ۰/۷۴ بهترین مدل‌ها هستند. در این مدل‌ها پارامترهای زمان تماس و غلظت محلول به عنوان مهم‌ترین پارامترهای مؤثر شناخته شدند. اعتبارسنجی مدل‌ها توسط آزمون‌های t و F انجام شد. در ادامه مدل ترکیبی شبکه عصبی مصنوعی (ANN) و بهینه‌سازی ازدحام ذرات (PSO) برای مدل‌سازی فرآیند جذب آلاینده از داده‌های مورد مطالعه ساخته شد. بر اساس این مدل ترکیبی شاخص کارایی برآورد شد. نتایج این مدل بیان کرد که بهترین مقدار این شاخص متعلق به داده‌های گروه A-4 با ضریب R^2 برابر با ۰/۹۱ است. به طور کلی نتایج این تحقیق نشان داد که روش‌های رگرسیون غیرخطی و مدل ترکیبی PSO-ANN ابزارهای مفیدی برای مدل‌سازی فرآیند جذب آلاینده از پساب‌های صنعتی هستند.

کلمات کلیدی: رگرسیون غیرخطی، محاسبات هوشمند، پساب، مدل‌سازی، آلاینده.