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Research Article

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New Artificial Intelligence Modeling for the Photocatalytic Removal of C.I. Acid Yellow 23 in Wastwater

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Abstract

This paper proposes two methods to predict the efficiency of photochemical removal of AY23 by UV/Ag-TiO_2 process. In this work the potential of the particle swarm optimization (PSO) and imperialist competitive algorithm (ICA) modeling approaches are presented to forecast the photocatalytic removal of AY23 in the presence of Ag-TiO_2 nanoparticles prepared under desired conditions. To validate the techniques, a total of 100 data are used that randomly splitted in two parts, 80 samples for the training the models and 20 for testing of the models. Experimental results on datasets show that ICA approach is better than PSO approach. Remarkable analysis results reveal that AY23 initial concentration is the most significant factors that influence on the AY23 removal efficiency.

Keywords : Nanoparticles; Ag-TiO_2; C. I. Acid Yellow 23; Particle swarm optimization; Imperialist competitive algorithm.

1 Introduction

THe developed countries are facing a serious problem of water pollution caused by dyes. Synthetic dyes are the significant water contaminants and industrial pollutants [10, 17]. dyes are used by various industries for coloring their products. These extremely colored ingredients when released with wastewater in the water bodies stop the reoxygenation scope of the obtaining water and cut-off sunlight, thereby upsetting biological activity in aquatic life. Azo dyes, the greatest class of synthetic dyes utilized in the food industries, are specified by the appearance of one or more azo bonds (-N=N-) at par with one or more aromatic systems, it may also carry sulfonic acid groups. Numerous studies reveal that these dyes are toxic or carcinogenic. If the mentioned colorants come into contact with definite drugs inside the human body they are able to cause alergic and asthmatic reactions among people who are sensitive [4].

Several real-world problems from operations research as well as management science are severely complicated in nature and very difficult to resolve by traditional optimization methods. From 1960 there has been an increasing tend for solving such types of complex optimization problems. The simulation of natural evolutionary processes related to human beings outcomes in stochastic optimization methodologies termed as evolutionary algorithms (EAs) which perform superiorly when compared with traditional optimization techniques that are implemented to tackle real-world problems. EAs often implicate metaheuristic optimization algorithms such as PSO as well as ICA.

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PSO is a searching algorithm, that is utilized for searching large and non-linear spaces where the investigated knowledge is lagged and conventional optimization methodologies are not of use [5, 8, 9]. It is a strong evolutionary algorithm having the global optimization capability. The method is initially designed and generated by Kennedy and Eberhart [16]. PSO is a current heuristic methodology where its mechanics are influenced by the swarming or collaborative nature of biological populations.
In order to evaluate as well as to locate the superior candidates for a task, the ICA is considered to be a very efficient methodology [18, 22]. This algorithm impart less mathematical needs, also it does not need very accurate stated mathematical models. ICA is a novel global research scheme influenced by the socio-political process of Imperialistic competition. Similar to other evolutionary types, the ICA begins with an initial population. Population individuals which are termed as country considered to be of two types namely colonies as well as imperialists that all together form some empires [2].
In the current work, the evaluations of the algorithms PSO as well as ICA are demonstrated for predicting the eradication of C.I. Acid Yellow 23 (AY23) by UV/Ag-TiO_2 process. In the earlier work, Ag nanoparticles on TiO_2 powders are developed by using a simple sol-gel route [10]. This work is on the basis of a real-life multi-stage case having 100 data set extracted via statistical design related to the study, whereas four parameters to be mentioned as initial concentration of dye, UV light intensity, initial dosage of nano Ag-TiO_2 as well as irradiation time are utilized as the input variables and eradication of AY23 as output variable. In order to construct the models, an artificial neural network (ANN) is implemented where PSO as well as ICA are utilized for training it. The comparisons among two training algorithms validates that the ICA can be selected as most efficient algorithm. This is one of the primary efforts in implementing the PSO as well as ICA schemes for the eradication of AY23 in water by utilizing UV/Ag-TiO_2 process.

2 Materials and methods

2.1 Materials

Tetraisoprpylorthotitanate $Ti(OC_3H_7)_4$, methanol (MeOH) as well as silver nitrate ($AgNO_3$) are extracted from Merck (Germany) and utilized without any additional purifications. Acid Yellow 23 is brought from Acros (USA) and utilized without additional purification. Fig. 1 displays the chemical structure of this dye. Deionized water is employed throughout the proceedings.

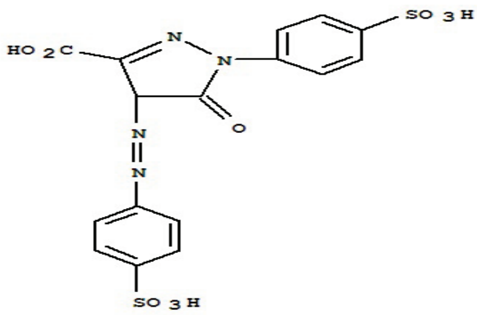

Figure 1: Chemical structure.

2.2 Ultrasonic bath (T 460/H)

All experiments are processed in a batch photoreactor. The radiation source is a low pressure mercury UV lamp (30 W, UV-C, λ_{max}=254 nm, manufactured by Philips, Holland), that is kept above a batch photoreactor of 0.5 L volume. The incident UV light intensity is computed by utilizing a UV-IR meter (Leybold Co. Ltd., Japan). In each experiment, a known amount of TiO_2 is summed up to 500 mL of the solution, also a magnetic stirrer is utilized for achieving a homogeneous mixture.

2.3 Photocatalytic experiments

The ultrasonic bath Elma (GmbH) is utilized with the operating frequency of 35 KHz as well as a rate output power of 170 W. The bath has the dimensions of 240 mm×137 mm × 100 mm. The total internal body is built from stainless steel.

2.4 Analytical method

In the existence of Ag-TiO_2 as photocatalyst, AY23 is utilized as pollutant. Sample solutions are sonicated before irradiation for 5 min. At known irradiation time intervals, the samples (5 mL) are removed, and hence analysis is carried out by UV-V which is spectrophotometer (Ultrospec 2000, Biotech Pharmacia, England) at 428 nm. A linear correlation is laid down between the AY23 concentration and the absorbance in the range 0-50 mg/L having a correlation coefficient $R^2 = 0.9981$. The Eq. (2.1) is utilized in order to compute the photocatalytic eradication effectiveness of $(R, \%)$ which is used in the experiments mentioned as

$$R = \left(\frac{C_0 - C_t}{C_0}\right) \times 100, \tag{2.1}$$

where, C_0 (mg/L) as well as C_t (mg/L) are initial concentration of AY23, also the concentration of AY23 at time t.

2.5 Particle swarm optimization method

PSO methodology is a case of successful implementation of the philosophy related to the bounded rationality as well as decentralized decision-making for solving the global optimization problems [3]. In PSO, a set of arbitrarily produced agents (called particles) generate in the design space towards the optimal solution via a number of iterations. Every particle demonstrates a candidate solution related to the optimization problem. The location of a particle is effected by the superior location visited by itself (i.e. its own experience) as well as the location of the superior particle in its total population. The excellent location which is extracted considered as the global best particle. The performance of each particle (i.e. how near the particle is from the global optimum) is computed by employing a fitness function which changes based on the optimization problem [6].
The process of PSO is actuated by utilizing a group of arbitrarily dispersed particles allotted to some random velocities. The particles fly in the d-dimensional problem space, bonded with each others, also in the final phase it approaches to a global optimum field. The movement of particles in the search space is at par with the flying experience related to the individual as well as its nearby particles in the swarm population (swarm intelligence). assume the ith particle in the swarm are at $x_{id}(t)$ which are moving with a velocity $v_{id}(t)$. Therefore, the position as well as velocity related to the particle in the next iteration can be $x_{id}(t+1)$ and $v_{id}(t+1)$, respectively, that is demonstrated in Fig. 2, also it can be illustrated mathematically as mentioned below [7]:

$$v_{id}(t+1) = w.v_{id}(t)+c_1.r_1[p_{id}(t)-x_{id}(t)]+c_2.r_2[g_d(t)-x_{id}(t)], \tag{2.2}$$

$$x_{id}(t+1) = x_{id}(t).v_{id}(t+1). \tag{2.3}$$

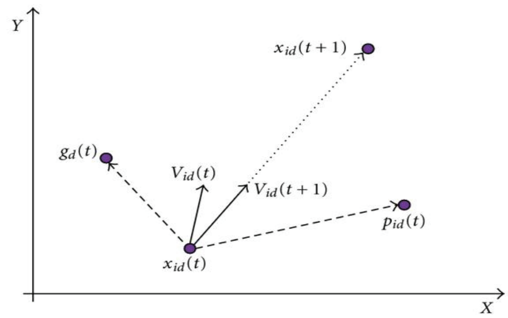

Figure 2: Position and velocity are upgraded to ith particle in the swarm.

In the above relation, parameter w is termed to be as inertia constant which holds a balance between the local and global search. c_1 as well as c_2 are termed to be as acceleration constants. r_1 as well as r_2 are termed to be two independently produced random numbers that are uniformly distributed in the interval [-1,1]. $p_{id}(t)$ demonstrates coordinates having the best location found out by the ith particle (local optima), while the coordinates of superior location is found out by the entire swarm (global optima) which are saved in $g_d(t)$. Here, the capability of the suggested technique to forecast the eradication of AY23 in water by utilizing the set of four operational variables termed as estimators is proved. The total process of PSO is illustrated as a flowchart which is shown in Fig. 3.

2.6 Imperialist competitive algorithm method

The utilization of ICA in order to resolve various types of optimization problems is growing

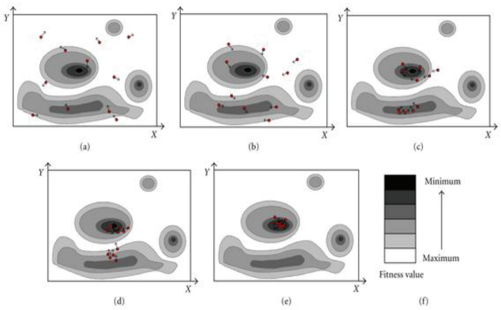

Figure 3: Flowchart of PSO algorithm.

rapidly. The ICA is suggested by Atashpaz et al. [2]. This technique is a novel socio-politically motivated global search scheme that is currently induced in order to deal with various optimization tasks. In [19], this algorithm is utilized to detect the optimized weights of ANN. ICA has major performances to be mentioned as rapid convergence and superior global minimum attaintment. The algorithm begins with choosing some arbitrary candidate solutions in the search space. These candidate solutions are termed as countries. The strength of each country is stated by the cost function related to the problem. Among these primary countries, few of them are chosen as imperialist on the basis of their strength, also it makes colonies by arbitrarily taking control of minimal strong countries. Every imperialist attempts to provide power to their Imperial by improvising their colonies. This process in final phase will lead the search towards the global optima.

In optimization problems the ultimate intention is to extract an optimal solution at par with the variables related to the problem. Therefore in these problems an array of variables are generated which are needed to be optimized. In ICA, the term country is utilized for this array. In an N_{var}dimensional optimization problem, a country is demonstrated by $1 \times N_{var}$ array. This array is stated as below:

$$Country = [p_1, p_2, ..., p_{N_{var}}],$$

where $Pj : j = 1, 2, ..., N_{var}$ are termed as the variables that need to be optimized.

The cost of a country is determined by analysing the cost function at the variables $(p_1, p_2, ..., p_{N_{var}})$. Hence

$$Cost = f(Country) = f(p_1, p_2, ..., p_{N_{var}}).$$

To begin the optimization algorithm, initial countries of size $N_{Country}$ is generated. We choose N_{imp} of the most strong countries to develop the empires. The remaining N_{col} of the primary countries will be the colonies, each of which tends to an empire. To develop the initial empires, the colonies are arbitrarily divided among imperialists on the basis of their strength. The initial number of colonies related to an empire must be directly proportional to its strength. In order to divide the colonies between imperialists proportionally, the normalized cost of an imperialist by $C_n = c_n - maxc_i$ is stated, where c_n is termed as the cost of nth imperialist as well as C_n is its normalized cost. The initial empires are depicted in Fig. 4.

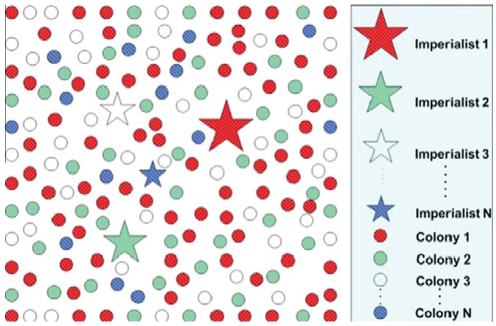

Figure 4: Generating the initial empire.

As displayed in this figure, powerful empires have higher colonies in comparison with weaker ones [2]. The normalized power of an imperialist is stated by

$$p_n = |\frac{C_n}{\sum_{j=1}^{N_{imp}} C_j}|. \tag{2.4}$$

After dividing the colonies in the midst of the imperialists, these colonies tend toward their related imperialist countries. Fig. 5 demonstrates this movement.

On the basis of this concept, each colony moves toward the imperialist by X units, also it reaches its novel position.

$$X \sim U(0, \beta \times d), \tag{2.5}$$

where β is termed as a number greater than 1, also d is termed as the distance in the midst of the colony and the imperialist state. $\beta > 1$ makes the colonies to get nearer to the imperialist state from both sides. In order to increment the capability of searching more area around the imperialist, an

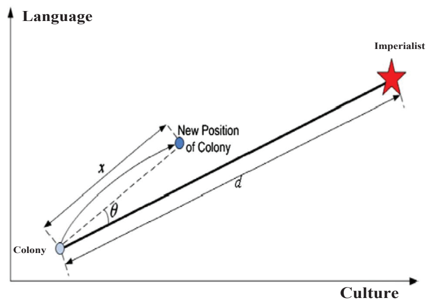

Figure 5: Moving colonies toward their relevant imperialist.

arbitrary amount of deviation is summed up to the direction of movement. Here, ICA model is initiated to forecast the eradication of AY23 in water by utilizing the set of four operational variables termed as estimators. The flowchart of this algorithm process is displayed in Fig. 7.

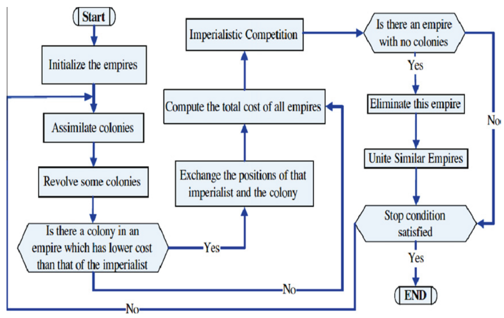

Figure 6: Flowchart of the imperialist competitive algorithm.

2.7 The dataset

As discussed previously, this study attempts to generate artificial intelligence concept on the basis of predictive model for eradication of AY23 in water by utilizing a set of chosen variables termed as the estimators. Dataset which are utilized to generate the PSO as well as ICA models in this research work is conveyed by the authors via laboratory studies performed under statistical experimental design. four parameters to be mentioned as initial concentration of dye, UV light intensity, initial dosage of nano Ag-TiO_2 as well as irradiation time are selected as the input variables and eradication of AY23 as output variable. The range of variables which are discussed is summarized in Table 1. Out of the 100 data sets extracted via statistical design related to the study, 80 are utilized in order to train the models, also the remaining 20 that were not included in the training, are demonstrated in order to test the models.

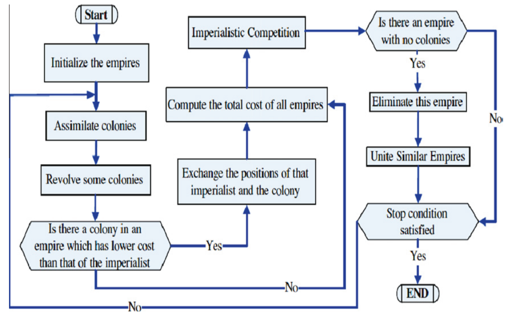

Figure 7: Flowchart of the imperialist competitive algorithm.

3 Result Analysis

Among intelligent methodologies, artificial intelligence has became more popular in different areas [11, 12, 13, 14]. PSO as well as ICA are a class of the artificial intelligence methodologies that have the superior performance in the literature. In order to analyze the performance of PSO as well as ICA methodologies for eradicating AY23 in water, we extract their mean square error (MSE). MSE is calculated from the model predicted and actual measured values related to the response variable, as follows

$$MSE = 1/N \sum_{j=1}^{N} (A_j - Y_j)^2, \qquad (3.6)$$

where, A_j as well as Y_j are the model predicted and measured values of the response variable, respectively, also N is total number of data points. Here various numbers of neurons are tested from 2 to 16, in the hidden layer. Each topology is repeated six times in order to avoid arbitrary correlation because of the arbitrary initialization of the weights. Fig. 8A as well as Fig. 8B portray the relation among the network error and the number of neurons in the hidden layer in PSO as well as ICA models respectively. It can be noticed that the performance of the network is stabilized after addition of an adequate number of hidden units only about six, eight and seven in PSO and ICA models respectively. The network with additional

Table 1: Range of studied variables.

Variable	Range
layer	
$Ag\text{-}TiO_2$ initial dosage (g/L)	0.01-0.05
AY23 initial concentration (mg/L)	5-60
UV light intensity (W/m^2)	0-60
Irradiation time (min)	0-60
Output layer	
Removal of AY23 (%)	0-100

Table 2: Performance statistics of the PSO and ICA models.

Model	Sub-set	MSE	RMSE	E_f	A_f	R^2
PSO	Training	0.02048	0.14313	0.97562	0.97998	0.96907
	Validation	0.02227	0.14924	0.95301	0.95224	0.93895
ICA	Training	0.01585	0.12589	1.00561	0.99001	1.01021
	Validation	0.01240	0.11135	1.00985	0.98992	1.03387

Table 3: Matrices of weights by PSO as training algorithm. W1: weights between input and hidden layers, W2: weights between hidden and output layers.

W1						W2	
Neuron	$[Ag\text{-}TiO_2]_0$	$[AY23]_0$	UV light	Time	Bias	Neuron	weight
2	-0.558	-0.697	0.999	-0.979	-0.558	2	-0.558
3	-0.697	0.989	-0.310	-0.999	-0.697	3	-0.697
4	-0.188	-0.968	0.826	-0.830	-0.188	4	-0.188
5	-0.171	-0.990	0.856	-0.655	-0.171	5	-0.171
6	-0.535	-0.958	0.605	0.976	-0.535	6	-0.535
7	-0.468	-0.578	-0.894	0.483	0.457	7	0.657
8	0.754	-0.963	-0.854	-0.991	-0.323	8	-0.776
						Bias	-0.558

Table 4: Matrices of weights by ICA as training algorithm. W1: weights between input and hidden layers, W2: weights between hidden and output layers.

W1						W2	
Neuron	$[Ag\text{-}TiO_2]_0$	$[AY23]_0$	UV light	Time	Bias	Neuron	weight
2	-0.843	0.735	-0.218	-0.992	-0.843	2	-0.843
3	0.272	0.872	-0.985	0.991	0.272	3	0.272
4	0.272	0.985	-0.291	0.928	0.272	4	0.272
5	0.328	0.999	-0.967	0.963	0.328	5	0.328
6	-0.584	0.755	-0.621	-0.981	0.352	6	0.467
7	0.646	0.998	-0.605	-0.758	0.646	7	-0.866
						Bias	-0.843

neurons in the hidden layer is barred from converging efficiently.

For the training as well as the validation sets, the model predicted and experimentally measured values of the eradication of AY23 in water are portrayed in Fig. 9 as well as Fig. 10 respectively. It is visible that the outcomes extracted from the ICA model are in proper phase with the corresponding experimental outcomes, both for the training (Fig. 9A) and the validation sets (Fig. 10A). Adequately high and nearly comparable values associated with the coefficient

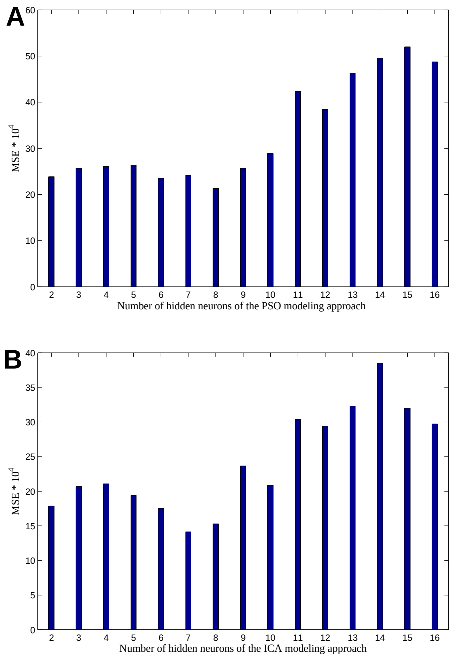

Figure 8: Influence of the number of neurons in the hidden layer based on the performance of (A) PSO and (B) ICA modeling schemes.

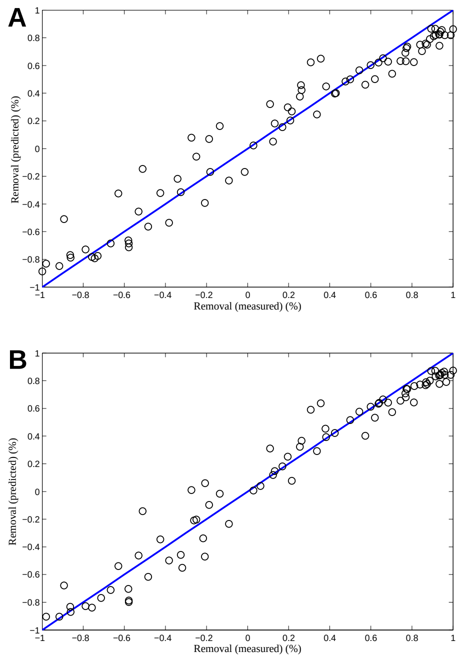

Figure 9: Plot of the measured and predicted eradication of AY23 in water by (A) PSO, (B) ICA models in training set.

of determination (R^2) in the midst of the predicted as well as the measured levels of AY23 eradication which are generated by using these models for both the training and validation sets authenticate the adequacy of the two modeling concepts for AY23 eradication prediction. The R^2 value of more than 0.8 among two groups shows that the two data are remarkably interconnected [21]. Also, low MSE by PSO as well as ICA models considering both training and validation sets elaborate superior generalization and predictive capabilities of the two modeling concepts regarding to the given data set. Whatsoever, from the interconnection in the midst of the measured and the predicted values associated with the response variable, both in the training as well as validation set (Table 2), it can be seen that the ICA model outperforms in comparison with the PSO model. The ANN which is utilized in this work supplies the weights mentioned in Table 3 and Table 4 by PSO as well as ICA as training algorithms, respectively. The weights are coefficients in the midst of the artificial neurons, that are analogous to synapse strengths among the axons as well as dendrites in real biological neurons. Hence, each weight determines that which proportion of the incoming signal can be transferred into the neuron's body [20].

The weight matrix can be utilized for approximating the relative significance of the different input variables on the output variables. An equation relied on the partitioning of connection weights is suggested as below [1, 15]:

$$I_j = \frac{\sum_{m=1}^{m=N_h}\left((|W_{jm}^{ih}|/\sum_{k=1}^{N_i}|W_{km}^{ih}|)\times|W_{mn}^{ho}|\right)}{\sum_{k=1}^{k=N_i}\{\sum_{m=1}^{m=N_h}(|W_{km}^{ih}|/\sum_{k=1}^{N_i}|W_{km}^{ih}|)\times|W_{mn}^{ho}|\}}, \tag{3.7}$$

where, I_j is termed as the relative significance of the jth input variable on the output variable, Ws are termed as connection weights, N_i and N_h are the numbers of input as well as hidden neurons, respectively, the superscripts 'i', 'h' and 'o' signifies input, hidden as well as output layers, respectively, also subscripts 'k', 'm' and 'n' signifies input, hidden as well as output neurons, respectively.

The relative significance of input variables on the AY23 eradicate effectiveness is displayed in Table 5. It is clear that, all of the variables include powerful influences on the AY23 eradication efficiency. However, the influence of AY23 initial concentration is higher in comparison with others. Hence, none of the variables which are researched in this work could have been avoided in the current analysis.

Table 5: Relative importance (%) of input variables on AY23 removal efficiency.

Input variable	Importance (%)
Ag-TiO_2 initial dosage (g/L)	10
AY23 initial concentration (mg/L)	40
UV light intensity (W/m^2)	30
Time (min)	20

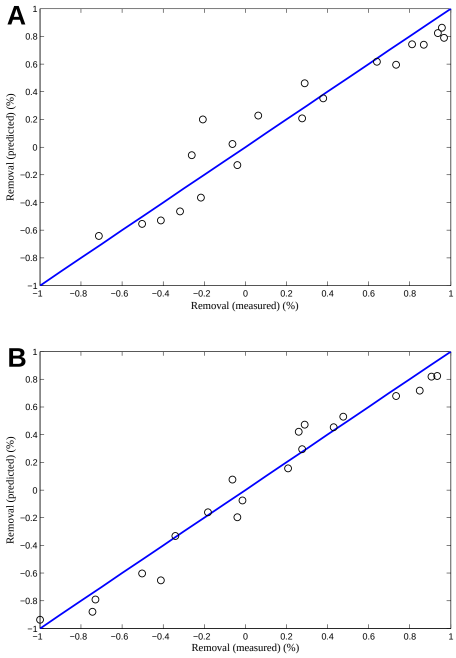

Figure 10: Plot of the measured and predicted eradication of AY23 in water by (A) PSO, (B) ICA models in validation set.

4 Conclusions

In this research work, two new methods termed as PSO as well as ICA are suggested in order to forecast the effectiveness of photochemical eradication of AY23 by utilizing UV/Ag-TiO2 process. The methods are exhaustively tested on 100 data set extracted from the literature. The primary concentration of dye, UV light intensity, initial dosage of nano Ag-TiO_2 as well as irradiation time are utilized as the predictor variables. Experiments on data sets prove the efficiency of the models. The mean square error is minimum only about eight neurons in the hidden layer in PSO model as well as seven neurons in the hidden layer in ICA model. The calculation experiments signifies that ICA method generates the best overall outcomes in comparison with PSO methods. Sensitivity analysis outcomes suggest that AY23 initial concentration is the most valuable factor that effects on the AY23 eradication efficiency. As the upliftment of artificial intelligent methodologies are suffered highly because of the shortage of training methodologies, hence our methods fill this emptiness and it will lead to several novel applications.

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