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Multiobjective ideal design of ANFIS for modeling and optimization of disinfectant substance consumed in water treatment

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ABSTRACT

Water is a component that makes up about 60%–70% of the adult human body weight and is the basic ingredient for life after oxygen. Satisfactory and high quality water is essential for human life. Nowadays in water treatment, disinfection is considered as one of the main methods for chemical water treatment. Currently the use of chlorine for disinfection is the most common method in the world including Iran because of low cost and high germicidal power in water distribution networks and good residual effect. Dosage of chlorine is different depending on the circumstances of inlet raw water including pH, temperature, and amount of suspended solids and the injection of chemicals such as preliminary chlorine, coagulant (aluminum sulfate), and coagulant assistant (polyelectrolyte). Free residual chlorine is used to disinfect water sources and water transfer lines to the houses of citizens. In this paper, adaptive neuro-fuzzy inference system (ANFIS) was used to optimize the amount of injected secondary chlorine in clear water. For modeling, exploitation data are divided into two categories (training and testing). Eventually, the results of modeling were compared with experimental data that demonstrates fine data compliance, as correlation coefficient in neuro-fuzzy inference network was 0.95 for training data, and 0.93 for testing data.

Keywords: Water treatment; Unit operation; Chlorination; Neural networks; Modeling; Optimization; ANFIS

1. Introduction

Nowadays, improving the environmental health of a community is directly related to the quality and quantity of water consumed by the community. By increase in consumption of water in industry, and public consumption, need for more water treatment is necessary, and in case of availability of enough water, considering water quality and sanitation before delivery to the consumer, even in the last consumer unit also, has a special significance. Water chlorination before consumption is a necessary process for water treatment, and the last try to destroy pathogenic agents, the diseases transmitted through water is prevented or reduced as much as possible; and the susceptibility to such diseases is reduced at a rate of 40%–100% [1]. However, controlled use of chlorine and its derivatives for water disinfection is also effective in flavor and odor control. The use of chlorine, however, presents many advantages but disadvantages as well. Chlorine produces compounds known as tri-Halton in combination with organic materials in water that these compounds are carcinogenic. Chlorine contact with skin and hair causes allergy, hair loss, and other troubles, and inhalation of chlorine in pool or bathrooms is harmful for human lungs. Therefore, free residual chlorine is important to determine needed chlorine [2]. Chlorine dosage is different depending on the conditions of raw water including pH, temperature, suspended solids, and injecting chemicals, including preliminary chlorine, coagulant (aluminum sulfate), and coagulant assistant (polyelectrolyte).

In recent years, modeling and optimization have received great importance in most areas. Optimization allows us to have a better understanding about the needed system and predict system behavior as well. In this article, adaptive

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neuro-fuzzy inference system (ANFIS) is used to predict chlorine consumed in treatment. In modeling, obtaining a non-linear relationship between input and output is the most important part that in classical way is often expensive and time-consuming and has little flexibility against sudden changes [3]; thus, researchers decided to use neuro-fuzzy networks to solve these problems [4] that we will have a brief review on history of neuro-fuzzy systems.

Phase theory was first introduced by Loftizadeh in 1968 [5]. He introduced ideas of fuzzy algorithms in 1968 [6], decision-making in a fuzzy environment in 1970, and fuzzy orderings in 1971 [7]. In 1973, he published another article called "Outline of a new approach to the analysis of complex systems and decision processes" [8]. This article built the basis of fuzzy control. In this paper, the ideas of linguistic variables using if-then rules were introduced to formulate human knowledge. In 1975, Mamdani and Assilian [9] determined a primary framework for the fuzzy controller and applied it in a steam engine. They discovered that construction of the fuzzy controller is simple and works well. In 1980, Sugeno began to build the first Japanese use of phase called Fuji water purification system. Success of the fuzzy systems in Japan made researchers in America and Europe surprise. In February 1992, the first IEEE International Conference in fuzzy systems was held in San Diego. In 2013, modeling and optimization of polyelectrolyte dosage with variable suspended solids, temperature, PH, conductivity, turbidity, and color of raw water were conducted using GMDH neural networks and MOGA by Daghbandan et al. [10].

In this study, modeling was conducted with six inputs including: PH, temperature, suspended solids, and also the amount of chemical injection containing Preliminary chlorine, coagulant (aluminum sulfate), and coagulant assistant (polyelectrolyte) that the effect of input parameters on the consumed chlorine was studied. To ensure the accuracy of the proposed approach toward behavior of experimental data, correlation coefficient and root mean square error (RMSE) were used, which points out error of provided G model compared with experimental data.

2. Data collection

Clean output water from treatment plants is one of the highly important parameters with regard to the inlet water to treatment plant from natural sources like rivers. Chlorine dosage depends on parameters such as temperature, suspended solids, PH, amount of coagulant injection, and preliminary chlorine [11]. A schematic diagram of experimental plant is shown in Fig. 1. Raw water is supplied from bed of river and surface waters, and a screen filter is installed to remove debris that might cause problems with pumps. In order to provide proper height of raw water, a pumping station where multiple centrifugal pumps are installed is considered. Output water from primary pumping station enters to divider of primary sedimentation ponds. In this unit, chemicals (polyelectrolyte) are added to water in order to accelerate the settling process; and copper sulfate and lime milk are used to control the growth of rooted aquatic plants. In the primary sedimentation, after mixing with chemicals, the raw water is directed to several circular ponds, and then in the next stage, after injecting aluminum oxide as coagulant and polyelectrolyte as coagulant assistant into water, it first enters to coagulation and flocculation unit and then settling basin. After coagulation, filtration is used to remove suspended solids in the liquid, which is the last stage of treatment to remove suspended solids in the water. In water filtration output, disinfectants (secondary chlorine) are used to destroy or deactivate the pathogenic microorganisms (pathogens) including bacteria, seaweeds, viruses, etc. In Guilan water treatment plant, chlorine disinfection is performed in divider unit (primary chlorination) to reduce microorganisms and convert ammonia and nitrite of raw water to nitrate, but secondary chlorination is performed for complete elimination of residual pollution and keeping water healthy and clear.

Required data for modeling was collected from Guilan tapping unit of water treatment plant found in Rasht, from June 2013 to August 2014 over 15 months. The lower and upper bounds of the data are shown in Table 1. To collect operating unit data, hourly sampling was carried out, and residual chlorine in water was measured after filtering (gained from preliminary chlorination) using *N*,*N*-diethyl-*p*-phenylenediamine indicator kits, which if necessary, required chlorine for secondary disinfection is determined experimentally or by using trial and error, and injection is performed that the water quality is not uniform due to human mistake and the inaccuracy of the amount of injected chlorine.

Therefore, from this data with details of the raw water and coagulant injection rate corresponding to the chlorine time

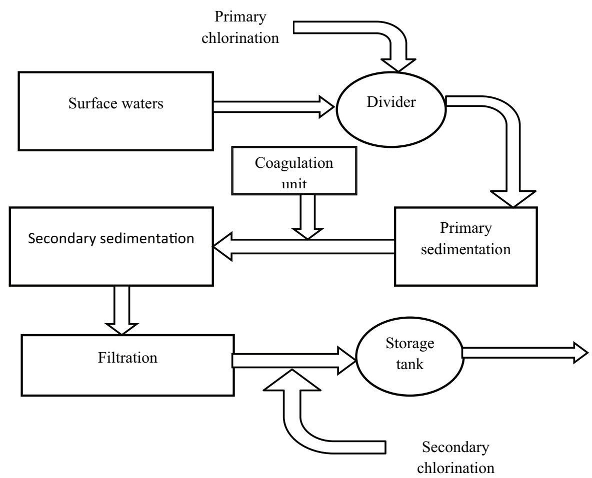

Fig. 1. Water treatment stages in treatment plant.

Table 1
Range of collected data from tapping unit

Inputs	Minimum	Maximum
Suspended particles (ppm)	1	765
Primary chlorine (ppm)	1.55	8.86
PH	6.7	8.5
Temperature (°C)	1.7	27.9
Polyelectrolyte (ppm)	0.0678	1.0611
Aluminum sulfate (ppm)	5.58	39.89
Secondary chlorine (ppm)	0.22	4.87

measurement, because of the high number of data series, a limited number of data were chosen at different times of day and every day of year to be an acceptable sample in which 900 data series were collected (Table 2).

The results of this experiment were used to provide a non-linear model to predict disinfectants [11]. The model consists of six parameters as input and one output that is amount of secondary chlorine consumption.

3. ANFIS theory

Artificial neural networks information in parallel structures and the memory is of a distributed and inherently associative form that has a certain executive function from the biological structure of the human brain network. In this system, process is performed in nodes called neurons, and information can be transmitted by the connections between nodes, and an activation function is used to transform inputs into outputs [12]. Fuzzy theory was introduced by Prof. Loftizadeh in 1965 in an article called "fuzzy sets". Fuzzy systems are based on knowledge or rules. Heart of a fuzzy system is a base of knowledge that is composed from fuzzy if-then rules that has the following form in Sugeno fuzzy model [13].

$$R_j : \text{ if } x_1 \text{ is } A_{j1} \text{ and } x_2 \text{ is } A_{j2} \text{ and } \ldots \text{ And } x_n \text{ is } A_{jn} \text{ then } y = f_j\left(x_1, x, \ldots, x_n\right) \tag{1}$$

In Eq. (1), R_j is the rule label; A_{jn} is fuzzy set in introduction; N is the number of rules in the fuzzy database; and y is a non-fuzzy function in the resulting inference system. Fuzzy set is a theory to action in conditions of uncertainty. This theory can formulate many imprecise and ambiguous systems, and provide area for inferring and control. Neuro-fuzzy inference system is an adaptation of network learning algorithms and fuzzy that is used in non-linear mapping between input and output variables, and also, because of combining expressive power of fuzzy logic and numerical calculations, a neural network is powerful and accurate in the process [13–15].

A fuzzy set A in X, which is referred to as universe of discourse, is defined as a set of ordered pairs:

$$A = \left\{\left(x, \mu_A\left(x\right)\right) lx \in X\right\} \tag{2}$$

According to Fig. 2, X includes independent variables such as: temperature (T), suspended solids (SS), PH, the amount of coagulant injection (alum and poly), and primary chlorine. $\mu_A(x)$ is called membership function (MF) for the fuzzy set A, which ranges between 0 and 1. There are some well-known parameterized MFs including triangular MFs, trapezoidal MFs, and Gaussian MFs. MFs can either be defined by an expert or be learnt from data [16]. For simplicity, it is assumed that the fuzzy inference includes two inputs (x and y) and one output (z). For first-order Sugeno fuzzy model, a set of rules with two If-Then rules can be expressed as follows:

$$\text{Rule 1: if } x \text{ is } A1 \text{ AND } y \text{ is } B1, \text{Then} \quad f_1 = p_1x + q_1y + r_1 \tag{3}$$

$$\text{Rule 2: if } x \text{ is } A2 \text{ AND } y \text{ is } B2, \text{Then} \quad f_2 = p_2x + q_2y + r_2 \tag{4}$$

Fig. 3 is a view of ANFIS structure where nodes in each layer have an identical node function.

ANFIS has five layers. In the first layer, to each variable, two or more MFs are assigned, which is better to be equal. In the second layer, by multiplying input values of each node with one another (T-norm) and weight of laws (W) are achieved that the number of weights is equal to the number of variables in the number of MFs. In the third layer, calculations of relative weight of rules and normalization are done:

$$\overline{w}_i = \frac{w}{\sum_{i=1}^{N} w_i} \qquad i = 1,2\ldots \tag{5}$$

In the fourth layer, for each condition, based on written conditions, a linear function is considered that operation on input signals can be obtained in this layer that for Sugeno fuzzy systems, the linear function is shown as follows:

$$F\left(x\right) = a_0 + a_1x_1 + a_2x_2 + \ldots + a_nx_n \tag{6}$$

And the last network output layer aims to minimize the difference between obtained and actual output of the network [11]:

$$f = \Sigma_i \overline{w}_i f_i \tag{7}$$

Table 2
Sample of experimental data including obtained input and output from operation unit of water treatment plant

Test No.	Model inputs						Model output
	Suspended solids (ppm)	Injected chlorine into the divider	PH	Temperature (°C)	Polyelectrolyte (ppm)	Aluminum sulfate (ppm)	Secondary chlorine consumption (ppm)
1	25	3.54	8.1	24.5	0.119	11.17	1.77
2	22	3.54	8.1	23	0.119	11.17	1.77
–	–	–	–	–	–	–	–
–	–	–	–	–	–	–	–
899	30	2.65	8.1	13.2	0.119	10.37	0.554
900	559	2.65	8.1	13.1	0.183	17.55	0.664

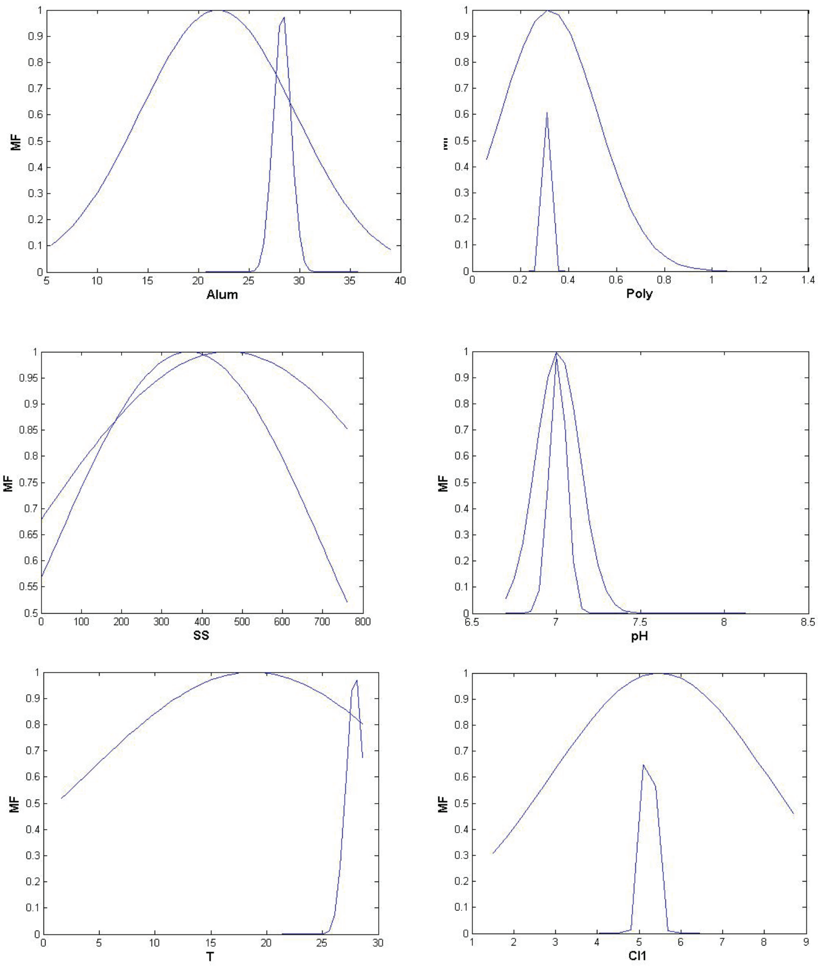

Fig. 2. Membership functions developed by genetic algorithm or two objective functions for the consumption of consumed secondary disinfectant.

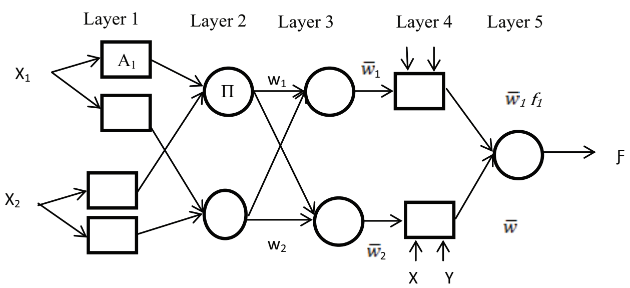

Fig. 3. ANFIS structure.

4. Modeling and analysis

In this study, neuro-fuzzy inference system is used to predict the optimum amount of used chlorine after coagulant stage. Gaussian function is used for input variables.

$$\text{MF} = \frac{\left(X - C\right)^2}{2\delta^2} \tag{8}$$

In this MF, X is input variable; C and δ are non-linear parameters of Gaussian function. These parameters are determined by the genetic algorithm, so the obtained model has the lowest error. The purpose of modeling is to find a relationship between input and output, and increase the accuracy in modeling using ANFIS, so the effects of six input variables on output of the experiment are considered. Input parameters include temperature, suspended particles, PH, primary chlorine, amount of aluminum sulfate, and polyelectrolyte.

In this modeling, for better network training, laboratory data were divided into two categories (70% for training and 30% for testing). To assess accuracy of the model and error calculation, mean squared error (MSE; Eq. (9)), mean absolute error (MAE; Eq. (10)), RMSE (Eq. (11)), and regression (R^2; Eq. (12)) relations were used [17].

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}\left(Y_{(i,\exp)} - Y_{(i,\text{model})}\right)^2 \tag{9}$$

$$\text{MAE} = \frac{1}{n}\left|\sum_{i=1}^{n} Y_{i,\exp} - Y_{i,\text{model}}\right| \tag{10}$$

$$\text{RMSE} = \left[\frac{\sum_{i=1}^{n} \left(Y_{i,\exp} - Y_{i,\text{model}} \right)^2}{n} \right]^{0.5} \tag{11}$$

$$R^2 = 1 - \left[\frac{\sum_{i=1}^{n} \left(Y_{i,\exp} - Y_{i,\text{model}} \right)^2}{\sum_{i=1}^{n} \left(Y_{i,\exp} \right)^2} \right] \tag{12}$$

The data include 900 series of data. First, to create model, 70% of data were used; then the rest of them were used to test the model.

In order to investigate the connection, type, and the orientation between two variables, "Pearson correlation coefficient", which is also referred to as "moment correlation coefficient" or "zero-order correlation coefficient", is applicable [18]. This coefficient measures the linear relationship between two random variables.

$$r = \frac{n\left(\sum xy\right) - \left(\sum x\right)\left(\sum y\right)}{\sqrt{\left[n\left(\sum x^2\right) - \left(\sum x\right)^2 \right]\left[n\left(\sum y^2\right) - \left(\sum y\right)^2 \right]}} \tag{13}$$

Pearson correlation coefficient varies between –1 and 1. If $r = 1$ indicates a direct relationship between two variables, a direct or positive relationship means that if one of the variables increase (decrease), the other one also increases (decreases).

Regarding to the lack of equation providing by ANFIS network, a model is utilized by using a polynomial, which gives a non-linear equation that is defined as follows [19]:

$$f_i = a_0 + \sum_{i=1}^{N} a_i X_i \tag{14}$$

$$A = \begin{bmatrix} 1 & X_{1,1} & X_{2,1} & X_{N,1} \\ 1 & X_{2,1} & X_{2,2} & X_{N,2} \\ 1 & .. & .. & .. \\ 1 & X_{1,M} & X_{2,M} & X_{N,M} \end{bmatrix} \tag{15}$$

The following equation is used to obtain the above equation constants:

$$a = \left(A_i^T A_i \right)^{-1} A_i^T Y_{i,\exp} \tag{16}$$

where $Y_{i,\exp}$ is the consumption rate of disinfectants; X_i is the input variables; A is the input matrix; and $a$is the coefficients matrix.

5. Results and discussion

After obtaining the proposed model, results of the model were compared with experimental results. As can be seen in Fig. 5, the results of the model are in good agreement with the obtained results in operation unit of water treatment plant.

Genetic algorithm is used to create optimum chromosome in which an initial population is considered for optimization, and new chromosomes are produced with mutation probability functions and the new chromosome crossover.

Chromosome with lowest experimental and training error is selected as the top chromosome that is shown by Pareto curve in Fig. 4 [20]. Considering the graph, point A has

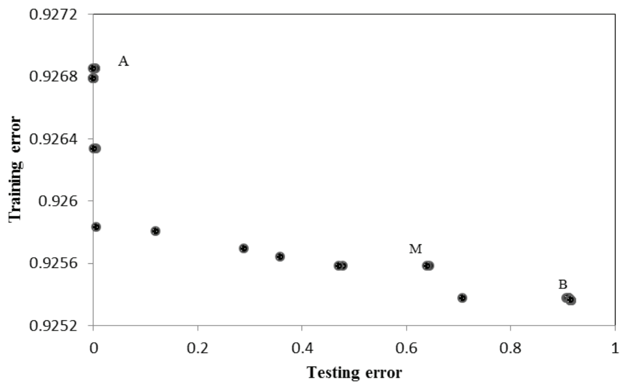

Fig. 4. Pareto points of training and testing errors of ANFIS model.

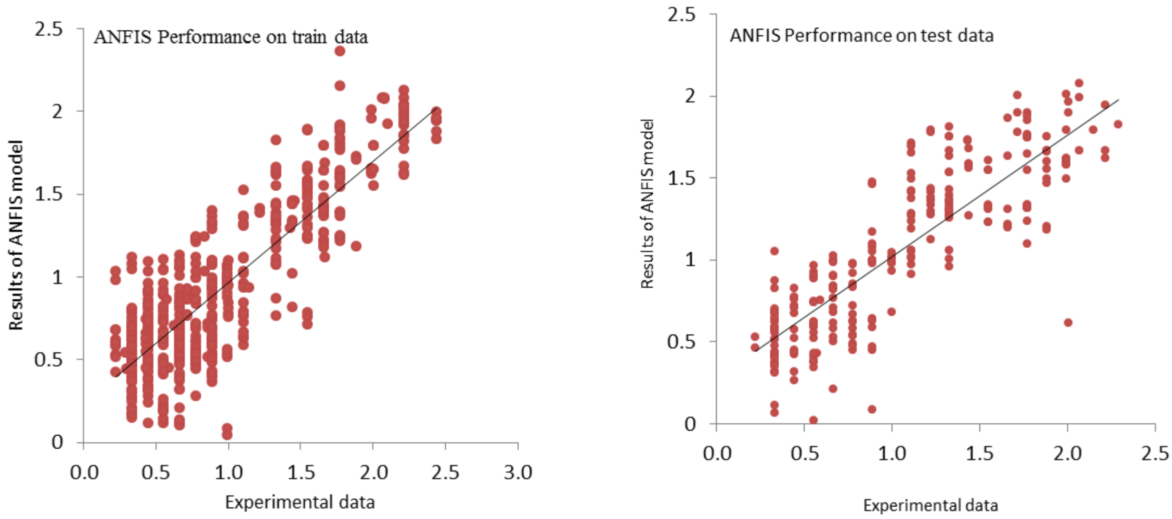

Fig. 5. Comparison of actual and modeled output in ANFIS modeling.

the greatest training error and the least experimental error. In this paper, the purpose is to optimize the training and experimental error that point M is the optimum due to the high correlation coefficient point. Genetic stage parameters are shown in Table 4.

According to Table 4, number of MFs of 2 was considered for each data in this model. By conducted surveys, it was determined that to make the symmetrical program structure, the number of MFs for all entries should be similar. Initially the MF of 1 was considered that the results had great difference with experimental data. Because of high volume calculations and runtime, the possibility of running the program with the MFs of 3 and more is not possible.

Process modeling was conducted using a polynomial equation of utilization data that includes 900 series of data. The model was consisted of six effective parameters as input and an output parameter that is the consumed chlorine. The obtained results from this model are presented in Fig. 6.

Table 3
Pearson coefficient of operation data for consumed secondary chlorine

p valve	Secondary chlorine
Suspended solids	–0.246
Injected chlorine into the divider	0.789
pH	–0.111
Temperature (°C)	0.79
Polyelectrolyte (ppm)	–0.166
Aluminum sulfate	–0.233

Table 4
Structural parameters of ANFIS model

Initial population	200	Number of membership functions (MFs)	2	Mutation probability	0.1
Number of repetitions	500	Number of fuzzy rules	64	Graft probability	0.96

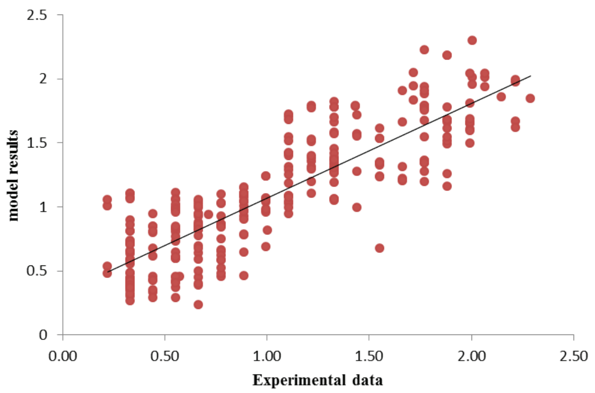

Fig. 6. Real output vs. modeled output for polynomial model of secondary disinfectant consumption.

In order to predict coagulant consumption in exploitation unit, constants of the provided equation are given in Table 5.

In Table 5, a_0 is a constant value of equation, and a_1–a_6 are suspended solids, preliminary chlorine, PH, temperature, aluminum sulfate coagulant, and coagulant assistant, respectively.

In this paper, modeling of secondary chlorine consumption after filtration step was carried out using ANFIS and polynomial models. According to Table 6 after the modeling and prediction of secondary chlorine consumption, it was observed that the proposed model is in a good agreement with gained values from operation unit of water treatment plant. First, variables in the model were examined individually and then were used in combination for modeling that the results are listed in Table 6 and the analysis is mentioned in results section. Because of the high number of modeling cases, models that had a better result were brought in table.

According to the results of Table 6, for the training data, correlation coefficient was equal to 0.95, and RMSE was 0.28; and for testing data, correlation coefficient was equal to 0.93, and RMSE was 0.32. This estimate shows the effectiveness of the proposed model in anticipation of disinfectant consumption. This model can be a good alternative for traditional methods of calculating chlorine consumption that were costly and associated with a large error. ANFIS can estimate the needed parameters with high accuracy. Also, they do not need complex mathematical formula and can be well applied to estimate needed parameters in a short time, if we choose the correct model of training and right network training. As the number of used data in network increase, better network training is carried out. By checking the obtained model, it was found that by increasing the chlorine injected into the divider, the secondary chlorine consumption is reduced; by increasing in water temperature, the effect of disinfection is increased; and also, by increasing PH, the effect of disinfection is decreased that causes an increase in the chlorine consumption. By increasing suspended solids, due to the less contact possibility of chlorine with microorganisms, the effect of disinfectants decreases that causes coagulants consumption that causes an increase in the secondary chlorine consumption. Eventually, temperature, chlorine dosage injected into the divider, PH, and suspended solids have the greatest effect on the secondary chlorine in water. Using the obtained model reduces operator intervention, and as a result, human error is decreased. As is clear from Table 2, the amount of injected secondary chlorine in treatment is much more than

Table 5
Coefficients of provided polynomial for the prediction of consumed chlorine in exploitation unit

Disinfectant type	Chlorine
Parameters of polynomial model	
a_0	2.384
a_1	8.314×10^{-5}
a_2	0.286
a_3	–0.373
a_4	0.05057
a_5	–0.3247
a_6	0.00525

Table 6
ANFIS and polynomial model results for training, testing, and total data

Type of model		Input combinations	MF	Number of MF	Training set				Testing set			
					MAE (ppm)	MSE	RMSE (ppm)	R^2	MAE (ppm)	MSE	RMSE (ppm)	R^2
ANFIS method	1	T	Gauss*	2	0.262	0.110	0.332	0.66	0.318	0.144	0.379	0.4
	2	SS	Gauss*	2	0.467	0.305	0.552	0.16	0.515	0.341	0.584	0.16
	3	Cl1	Gauss*	2	0.261	0.106	0.326	0.43	0.303	0.159	0.399	0.46
	4	SS Cl1	Gauss*	3	0.277	0.122	0.349	0.64	0.237	0.095	0.307	0.58
	5	pH T	Gauss*	2	0.221	0.076	0.276	0.64	0.249	0.107	0.327	0.59
	6	T Alum	Gauss*	2	0.259	0.101	0.318	0.67	0.270	0.113	0.336	0.51
	7	SS Cl1 pH	Gauss*	2	0.280	0.126	0.354	0.79	0.256	0.103	0.321	0.7
	8	pH T poly alum	Gauss*	2	0.194	0.063	0.250	0.88	0.262	0.117	0.343	0.76
	9	pH T poly alum Cl1 SS	Gauss*		0.236	0.103	0.321	0.95	0.234	0.082	0.286	0.93
Polynomial equation	–	–	–	–	0.897	1.028	1.014	0.88	1.086	1.437	1.199	0.84

the required amount, and because some of chlorine should be considered as residual chlorine to prevent water from pollution on the route of transmission.

6. Summary and conclusion

Due to the fact that artificial intelligence (AI) provides an effective tool for many complicated engineering problems in various fields, in this study, AI-based techniques of ANFIS were employed for prediction of consumed disinfectant in various operating conditions [16]. In this paper, a model was presented using neuro-fuzzy network, which indicated the relation between temperatures, suspended particles, PH, injected chlorine into the divider, and consumed coagulants with chlorine after secondary sedimentation.

Coagulant consumption increases by increasing coagulant and PH due to improper formation of large and stable coagulum that this issue causes the chlorine waste in excess coagulants of water. Furthermore, increasing pH reduces the chlorine germicidal power. The antimicrobial effect of chlorine in acidic conditions is more than alkaline conditions; even in an acidic environment, less contact time is required. Considering Fig. 2, in higher temperatures, chlorine absorption rate increases non-linearly, and activity of microorganisms becomes more. Therefore, more of them are destroyed in contact with chlorine. So, more chlorine should be injected at lower temperatures. By increasing the suspended particles, coagulant consumption increases that causes an increase in consumed chlorine.

According to the model results and Tables 3 and 6, the sensitivity of consumed secondary chlorine to temperature and injected chlorine dosage into the divider was higher.

And also, Table 6 shows that ANFIS network has less errors and more coefficients of determination in comparison with polynomial model. So, ANFIS model has an optimal performance.

This study can be used to optimize the consumed chlorine in water treatment plants and also for making other parts of the treatment plant like coagulation unit smarter. In this paper, due to impossibility of creating experimental conditions in the laboratory, the data were used from the operation unit where there was no possibility to check the variables individually because of the stability of the process and lack of control over the amount of variables.

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