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Optimization of desalination wastewater treatment unit performance; Experimental investigation accompanied with artificial neural network and adaptive neural fuzzy interferences modeling

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ABSTRACT

Almost high salinity effluent stream of desalination units is drained into the sea or dispersed on soil breaking the aqua salt concentration balance and also increase salt content of sea ecosystem or soil. So it is concerned with environmental engineering, corrosion engineering, control engineering, chemical engineering and etc. So zero discharge desalination (ZDD) plants have been proposed with a view of reaching salt and water instead of hazardous saline wastewater. Predicting wastewater pretreatment performance (effluent total hardness, CO₂ content and electrical conductivity) as the first step in ZDD plants is considered in this work both experimentally (on a pilot plant) and mathematically (modeling with artificial neural network and adaptive neuro fuzzy inference system). So, optimum operating conditions (150 cc $Al_2(SO_4)_2$ as coagulant, mixing rate in first pretreatment reactor= 110 rpm, 600 cc NaOH and 450 cc Na₂CO₂ as additives) are recognized, then optimal NN architecture (three layer feed forward back propagation network with 10 neurons in hidden layer, Levenberg-Marquardt algorithm is as network training function, tangent sigmoid transfer function) and also optimal ANFIS architecture (five layers with six neurons in two hidden layers, two Bell membership functions and four rules) are determined. The results confirm predictive modeling by ANN is most efficient comparing with ANFIS in prediction of performance. © 2014 Trade Science Inc. - INDIA

INTRODUCTION

Direct drainage of the concentrated brine wastewater of desalination units into sea, could cause salinity and thermal shocks to aqua environment as mentioned^[28]. But if the concentrated brine wastewater is pretreated in basic softening process, it can be used in order to production of salt and potable water. Total hardness which is caused by Mg²⁺ salts and Ca²⁺ salts, are removed and

KEYWORDS

Artificial neural network; Network optimization; Treatment of desalination wastewater; Zero discharge desalination; Adaptive neural fuzzy interference system.

production of Sodium Chloride becomes possible during pretreatment process^[10]. Usage of Sodium Carbonate and Sodium Hydroxide or Calcium Hydroxide in wastewater, vanishes the temporary and permanent hardness as Magnesium Hydroxide and Calcium Carbonate compounds. These particles are small and time is needed for the sedimentation as demonstrated^[32,38]. Required time for coagulation, flocculation and sedimentation steps will be short enough and also the turbidity of the product is

minimized By using mineral coagulants in special conditions. Determination of the optimized amounts of Sodium Carbonate, Sodium Hydroxide, suitable conditions of the pretreatment process, type and dosage of coagulant, have to be studied and evaluated to reach the higher yield and minimize total hardness.

Published papers in the field of pretreatment process of wastewater from a desalination unit are scarce in the literature and there is not enough information about this to predict the performance of pretreatment units. In the other hand wastewater pretreatment process is one of unit in zero discharge desalination plants. In recent years, neural networks have been used as a powerful modeling tool in various pretreatment processes to predict the unit performance; some features of previous studies are summarized in TABLE 1. These are obtained from TABLE 1;

- 1) Most popular form of neural network in use is feed forward neural network.
- 2) No record for modeling of pretreatment of desalination wastewater unit by neural network is found in the literature.
- 3) Back propagation algorithm is also efficient in prediction networks.

	Reference	Year	Model type	Application
1	Zvi Boger [5]	(1992)	Back propagation feed forward neural network	Wastewater Treatment Plant Operation
3	Spall et al.[33]	(1997)	Network model.	Wastewater quality predication system
4	Zhu et al. [47]	(1998)	Fuzzy systems and neural networks	Wastewater treatment
5	Tay et al. [35, 36]	(1999, 2000)	Fuzzy modeling, Back propagation neural network	Anaerobic biological wastewater pretreatment
6	Belanche et al. [3]	(2000)	Feed-forward net time-delay neural networks	Wastewater treatment plants
7	Gontarski et al.[14]	(2000)	Feed-forward back propagation neural network	Industrial treatment plant
8	Lee et al.[17]	(2002)	Hybrid neural network	Industrial waste water treatment
9	Timothy et al.[37]	(2003)	Kohonen Self-Organising Feature Maps (KSOFM) neural network	Municipal wastewater treatment plant
10	Zeng G.M. et al. [45]	(2003)	Back-propagation neural network	Paper mill wastewater treatment
11	Hamed et al. [15]	(2004)	Feed forward neural network	Waste water treatment plan
12	Onkal-Engin et al. [25]	(2005)	Artificial Neural Network (ANN) trained with a back-propagation algorithm	Biochemical Oxygen Demand (BOD) values of samples from wastewater treatment plant
13	Ozer Cinar [8]	(2005)	Kohonen self-organizing feature maps	Pelham wastewater biological oxygen demand (BOD), total suspended solids (TSS) and fecal coliform
14	Lee et al. [18]	(2005)	Feedforward back-propagation neural network	Cokes wastewater treatment plant
15	Cinar et al. [9]	(2006)	Cascade-forward back-propagation	Treating cheese whey wastewater
16	Chen et al. [6]	(2007)	Back propagation neural networks (BPN) algorithm	Wastewater Treatment Process
17	Majlli et al.[23]	(2007)	Back propagation, artificial neural network (ANN)	Wastewater treatment plants performance
18	Parthinban et al.[28]	(2007)	Feed-forward neural network	Starch wastewater treatment
19	Rangassamy et al. [31]	(2007)	Multi layer feed forward perceptron	Starch wastewater treatment
20	Macho'n et al. [19]	(2007)	Feed-forward neural network	Coke wastewater nitrification
21	Yu et al.[43]	(2008)	Back propagation artificial neural network models	Wastewater reuse applying ORP/pH monitoring

TABLE 1: Researchers' studies in modeling of pretreatment process of wastewater by neural network

	Reference	Year	Model type	Application
22	Torrecilla et al. [38, 39]	(2007, 2008)	Feed-forward back propagation neural network	Olive oil mill wastewater
23	Suh et al. [34]	(2009)	Back propagation learning algorithm	Scale activated-sludge wastewater treatment plant
24	Aber et al. [1]	(2009)	Feed forward back propagation network	Removal of Cr(VI) from synthetic and real wastewater
25	Mingzhi et al. [21]	(2009)	Fuzzy neural networks	Biofilm wastewater treatment Process
26	Mingzhi et al. [22]	(2009)	Feed-forward back propagation algorithm	Paper mill wastewater treatment
27	Purkait et al. [30]	(2009)	Feed-forward network	Leather plant effluent
28	Pai et al. [26]	(2009)	Neuron fuzzy inference system (ANFIS)	Hospital wastewater treatment plant effluent
29	Chen z. et al. [7]	(2009)	Back propagation neural network	Wastewater treatment and reuse in submarine cabin for long voyage
30	Sadrzadeh et al. [32]	(2009)	Feed-forward back propagation neural network	Pb2+ removal from wastewater using electrodialysis
31	Basha et al. [3]	(2010)	Feed-forward back propagation neural network	Chemical industry effluent
32	Fang et al. [13]	(2010)	Feed-forward back-propagation NN	Municipal wastewater treatment plant
33	Waewsak et al. [41]	(2010)	Neural-fuzzy control system, neural network with back propagation algorithm	Wastewater treatment and biogas production,
34	Nandi et al. [24]	(2010)	Back propagation-based multi-layer feed forward artificial neural network (ANN) model	Treatment of oily wastewater using low cost ceramic Membrane
35	Turan et al. [40]	(2011)	Feed forward back propagation network with	Cu(II) from industrial leach ate by pumice
36	. Silvia Curteanu et al. [10]	(2011)	Feed-forward back propagation neural network	Electrolysis process in wastewater treatment
37	Pendashteh et al [29]	(2011)	A feed-forward neural network trained by batch back propagation algorithm	Treating hyper saline oily wastewater
38	Pai et al. [27]	(2011)	Adaptive neuron fuzzy inference system (ANFIS)	Wastewater treatment plant of industrial Park
39	Bhatti et al. [4]	(2011)	RSM and ANN modeling	Removal of copper from synthetic wastewater

Although, ANFIS is a powerful modeling tool to predict the performance of nonlinear process, but this has not been considered as much as artificial neural network.

This work focused on the prediction of performance of one step in zero discharge desalination plant which is desalination waste water pretreatment. The goal of this step is softening high salinity wastewater from a petrochemical desalination plant and preparing it to produce salt and water instead of drainage into sea. So, natural salt concentration of sea and soil doesn't be increased by desalination wastewater. This subject can be interesting as a view of sciences related to corrosion, control, environmental, chemical and etc sciences. Both experimental work and modeling are applied to opti-

CHEMICAL TECHNOLOGY An Indian Journal mize the performance prediction of pretreatment process.

Modeling is done by ANN and ANFIS which are powerful adaptive models in prediction and optimization of processes, based on experimental data.

MATERIALS AND METHOD

Optimum amounts of each coagulant, and also the type of mixture and the best speed of the first pretreatment reactor are investigated experimentally. Three commercial mineral coagulants, Aluminum Sulfate, $Al_2(SO_4)_3$, Ferric Sulfate, $Fe_2(SO_4)$ and Ferric Chloride, $FeCl_3$, are used in the pretreatment process

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of concentrated brine wastewater. Moreover in softening process Sodium Carbonate and Sodium Hydroxide must be added to the brine wastewater. So the appropriate fraction of these additives to coagulant is considered. Experiments are held in two PVC series tanks equipped by adjustable agitator. Optimum values of speed, coagulant and additives are gained when total hardness of produced wastewater reaches to minimum amount. Figure 1 shows this setup.



Figure 1 : Basic structure of an two layer neural network model, (IW (input weights), LW (layer weights), 10 neuron, 3 input, 1 target and two transition function)

Optimum results of experiments are used in an ANN program and also in ANFIS program to train and simulate networks for predicting the amounts of total hardness, CO_2 content and electrical conductivity.

Practical desalination unit of mobin petrochemical complex

Mobin petrochemical complex is located in south of Iran and works as a utility unit for whole petrochemical companies. Five MED practical desalination units in Mobin petrochemical complex provide the water supply. About $1030^{ton}/_{hr}$ flow rate of sea water is fed to each of desalination unit although each unit has designed for $1100^{ton}/_{hr}$ of sea water. About 28% of the feed is produced as sweet water and high saline water is drained to the sea as brine wastewater. So, the total flow rate of brine wastewater is $3700^{ton}/_{hr}$, approximately. Salinity of the brine wastewater is 54500ppm and the to-

 TABLE 2 : The properties of Wastewater before treatment

 process

Composition	Unit	Brine outlet line
Ca++	ppm as CaCO ₃	14616.3
Mg++	ppm as CaCO ₃	36080
Total hardness	ppm as CaCO ₃	50696.3
Fe++	ppm	Trace
Ba++	ppm	Trace
SO ₄	g/l	5.25
HCO ₃ -	g/l	0.185
Salinity	ppm	54500
Silica	ppm	0.1
Specific Gravity at 15 c		1.04
pН		8.2
Viscosity (Kinematic)	Mm2/s	0.7
TSS	g/l	Trace
Total Dissolved Solids	g/l	63.8
Conductivity	ms/cm	77100

tal hardness is about 50696.3 ppm as $CaCO_3$. Some of specifications of brine wastewater are in TABLE 2.

Artificial neural network

Artificial neural network (ANN) has been adopted in many areas of science. Neural networks are adjusted, or trained, so that a particular input leads to a specific target output as demonstrated^[36]. The term backpropagation refers to the manner in which the gradient is computed for nonlinear multilayer network as mentioned^[2,3,9] and is commonly used in many ANN

applications as demonstrated^[22,29,41].

Structure of a multi layers neural network model is shown in Figure 2. In this work Back propagation feed forward type is selected to be optimized. This neural network consists of two layers (hidden and output), neurons in hidden layer, network training functions and layer's learning function. Experimental input data are normalized and then divided into training (40%), testing (30%) and validation data (30%).

Optimization of this network includes finding appropriate network training function among Levenberg-Marquardt back propagation, *trainlm*, Gradient descent with momentum back propagation, *traingdm* and BFGS quasi-Newton back propagation, *trainbfg*, network architecture using hyperbolic tangent sigmoid transfer function, *tansig*, Log-sigmoid transfer function, *logsig* and Linear transfer function, *purelin*, in each layer of network and determining optimum number of neurons in hidden layer using trial- and- error approach. A number of steps are during the model development process which is shown schematically in Figure 3.

Reasonable results are obtained when the *rmse* is small and the validation and test correlation coefficient gets close to one. Since the used transfer function in the hidden layer is sigmoid, all samples must be normalized. So any samples (X_i) from the training, validation and test sets are scaled to a new value (X_{newi}) as follows:

$$Y = (X - X_{mean}) \times \left(\frac{Y_{std}}{X_{std}}\right) + Y_{mean}$$
(1)

Where X_{mean} and Y_{mean} are mean values of each row of input and each row of output, X_{std} and Y_{std} are standard deviation for each row of input and each row of output, respectively.

Training aims at estimating the parameters (*IWij*, *LW_j*, b_j , and b_2) by minimizing an error function, such as the root mean square error (RMSE) which is expressed as:

$$RMSE = \left(\frac{\sum_{i=0}^{i=N} (Ytar_i - Yout_i)^2}{N}\right)^{0.5}$$
(2)

Where data is the number of data points and targets are experimental outputs and output shows program results. Also correlation coefficient (R) and mean abso-





Figure 2 : Steps of the neural network model development process



Figure 3: Experimental apparatus

lute error (*MAE*) are two statistical criteria which are employed to show the modeling performance and described as:

$$MAE = \frac{\sum_{i=1}^{N} |(Ytar_i - Yout_i)|}{N}$$
(3)

$$R = \frac{\sum_{i=1}^{N} (Ytar_i - \overline{Ytar}) (Yout_i - \overline{Yout})}{\sqrt{\sum_{i=1}^{N} (Ytar_i - \overline{Ytar})^2 \sum_{i=1}^{N} (Yout_i - \overline{Yout})^2}}$$
(4)

Fuzzy interference system

Experiments show that there are various variables affect on TH, EC and CO_2 content and nonlinear relations between desalination effluent wastewater indices

and characteristics of pretreatment effluent stream. Fuzzy system is a powerful tool to predict outputs in nonlinear systems fast and precisely. Neuro-fuzzy inference system (ANFIS) using a given input/output data set. This function constructs a fuzzy inference system (FIS) whose membership function (MFs) parameters are adjusted using either a BP algorithm alone or in combination with a least squares type of method. This adjustment allows the fuzzy systems to learn from the data they are modeling. The process of fuzzy inference involves Membership

TABLE 3 : Categories of experiments are done in this study

Parameters	unit	Value
Mixing rate in first pretreatment reactor	rpm	50, 70, 90, 120, 140, 160, 180, 200, 220
Coagulant (Al ₂ (SO ₄) ₃ , FeCl ₃ , Fe ₂ (SO ₄) ₃)	cc	10, 20, 30, 40, 50, 70, 110, 150, 115, 130, 140, 100, 85, 160, 180
NaOH/4000 cc coagulant		1.5, 3, 4
Na ₂ CO ₃ /4000 cc coagulant		1,2, 3

TABLE 4 : Experimental data for Al₂ (SO₄)₃. (Mixing rate in coagulation step= 70 rpm; mixing rate in flocculation step=50 rpm; wastewater sample=4lit)

Run	NaOH cc	Na ₂ CO ₃	Al ₂ (SO ₄) ₃	Wastewater nH	Temperature C	Total Alkalinity ppm as CaCO3	Total Hardness	Clarified water PH	CO ₂ ppm as CaCO3	EC μΏ/cm
1	150	100	100	8.99	19.6	933.3333	5100	9.9	0.267265	62921.35
2	40	30	10	8.93	19.5	1200	6573.3333	10.4	0.108664	71161.05
3	15	20	10	8.4	19	3333.333	7140	10.65	0.16974	73408.24
4	15	10	10	8.6	19.1	3466.667	7933.333	10.8	0.124973	75655.43
5	150	200	100	9.14	19.5	1600	4306.667	10.4	0.778081	71910.11
6	160	120	40	8.99	19.8	1733.333	4533.333	10.75	0.070111	68164.79
7	60	80	40	8.99	19.6	933.333	4873.333	9.44	0.770799	73408.23
8	60	40	40	8.93	19.8	333.333	5893.333	9.39	0.308875	73408.24
9	225	150	150	8.84	19.9	666.6667	3740	10.1	0.120452	68164.79
10	225	300	150	8.81	19.7	1200	1773.3333	10.55	0.076928	666666.7
11	600	450	150	8.82	19.7	2133.33	453.33	11.44	0.00374	62921.30
12	400	300	100	7.7	20	2933.3333	2040	11.99	0.004748	65168.54
13	127.5	85	85	8.6	18	933.333	2720	10.4	0.084517	66666.67
14	127.5	170	85	8.7	17.8	800	2606.667	10.4	0.072443	65917.6
15	340	255	85	8.57	18	1066.667	2266.667	10.75	0.043145	64423.22
16	560	420	140	8.12	19.2	2366.66	643.333	9.52	0.076231	62353.21
17	80	60	20	8.23	19.5	1133.333	6014.6667	10.6	0.058623	70362.61
18	200	150	50	8.88	18.9	1566.6667	3566.666	10.32	0.031562	63223.44
19	280	210	70	8.69	19.42	1233.333	3055.3333	11	0.099532	66022.05
20	440	330	110	9.45	18.6	2766.6667	1856	11.2	0.084123	63223.44
21	460	345	115	9.42	19.94	2526.333	1243.6667	10.36	0.083175	63012.11
22	520	390	130	8.54	18.68	2166.6667	755	11.33	0.063213	63112.23
23	640	480	160	8.88	17.9	2033.333	575.2223	9.68	0.075845	60123.01
24	720	540	180	8.65	18.5	1800	721.333	10.2	0.0469523	59754.21

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Functions, Logical Operations, and If-Then Rules. A network type structure is similar to that of a neural network, which leads inputs through input membership functions and associated parameters, and then through output membership functions and associated parameters to outputs, can be used to interpret the input/output map.

RESULTS AND DISCUSSION

Experimental results

Total hardness removal of effluent stream from desalination unit is conveyed in two pretreatment reactors. Major parameters which decrease the amount of TH, CO₂ content and EC are mixer speed in first pretreatment step, type of coagulant and amount of coagulant. Also, experiments performed to find the optimum ratio of Sodium Carbonate to coagulant and Sodium Hydroxide to coagulant and these ratios are investigated by experiments. 405 experiments are done for three mineral coagulants and TABLE 3 summarizes types of experiments also TABLE 4 shows some obtained data for $Al_2(SO_4)_3$ just in 70 rpm mixing rate of first pretreatment reactor. Results are visualized in Figure 4 and Figure 5.



Mixing rate of first reactor(rpm)



Data analyzing reveals that decreasing total hardness, eliminating ions effectively so electrical conductivity decreases, it seems when appropriate amounts of NaOH, Na₂CO₃ and coagulant are used, HCO3⁻ is consumed to form sediments so TH and CO₂ content decrease and consequently EC decreases. Figure 4 visualizes that $Al_2(SO_4)_3$ is the most effective coagulant comparing with $Fe_2(SO_4)$ and $FeCl_3$. Also total hardness minimizes when mixing rate in first



Figure 5 : Influence of amounts of NaOH and Na₂CO₃ on TH

pretreatment reactor is 70 rpm. Mixing rate in the first pretreatment reactor causes direct effect on coagulation step, it must be adjusted in such value to improve breaking connections in coagulant compound and also improve proper ions conjunctions to perform coagulation.

Using $Al_2(SO_4)_3$ as coagulant, optimum values of NaOH and Na₂CO₃ which are added into the solution are considered in Figure 5.

Optimum characteristics resulted in these experiments to meet minimum levels of TH, CO_2 content and EC are as followed.

- a) Mixing rate in the first pretreatment reactor is equal to 70 rpm, lower mixing rate doesn't make enough turbulences in the solution to breaks connections while higher mixing rate than 70 rpm refuses forming effective connections to coagulate so prevent sedimentation.
- b) Effective type of coagulant is $Al_2(SO_4)_3$
- c) 150 cc of coagulant is added to 4000 cc of wastewater.
- d) Ratio of NaOH to coagulant is equal to 4 and for Na₂CO₃ is equal to 3.
- e) Decreasing TH leads decreasing CO₂ content and also decreasing EC so monitoring TH can be criteria to predict EC value and CO₂ content of effluent wastewater. These are important to control corrosion damages.

So optimum data (influent values and effluent values) are carried out to optimize the artificial neural network,

TABLE 5 : Experimental data is	s used to optimize neural network
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Parameter	Unit	Value
Type of coagulant		$Al_2(SO_4)_3$
Amount of coagulant in each 4000 cc of wastewater	00	10, 20, 30, 40, 50, 70, 110, 150, 115, 130, 140,
sample	ll	100, 85, 160, 180
Amount of NaOH in each 1000 cc of wastewater sample	CC	40, 80, 120, 160, 200 280, 440, 600, 460, 520,
A mount of reach note of waste water sample		560, 400, 340, 640, 720
Amount of NA ₂ CO ₃ in each 1000 cc of wastewater	CC	30, 60, 90, 120, 150 210, 330, 450, 345, 390,
sample	cc	420, 300, 255, 480, 540
Mixing rate in coagulation step	rpm	70

this is explained in next section. TABLE 5 shows data that is used to optimize the artificial neural network.

Neural network modeling results

In this case study, gained experimental data are normalized and randomized and then divided into training (40%), testing (30%) and validation data (30%). First the effect of each input on each output is monitored by training networks. Then 12 different types of neural network are created and verified then the optimal performance is revealed by

- a) Minimum rmse.
- Factor of correlation coefficient, R², gets close to one.

Sensitivity analyzing

Three layers network with 10 neurons in hidden layer and *tansig* transfer function and *trainlm* training function is trained to investigate sensitivity analyzing.

TABLE 6 shows the sensitivity of each output variables to inputs, each input shows the same effect and has highest effect on TH. For CO₂ content $R^2_{NaOH} = R^2_{Na2CO3}$ (1)> R^2_{AL2} (0.9997) is visualized and for

A	BL	Æ	5:	Sensit	ivity	analyzing	
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		(1) NaOH	(2) Na ₂ CO ₃	(3) Alum	1;2	1;2;3
TU	R2	1	1	1	0.9996	0.99988
п	rmse	0.0024	0.0078	0.0053	0.0210	0.0339
EC	R2	0.9998	0.9998	0.9996	0.999	0.999
EC	rmse	0.0132	0.0170	0.0190	0.0456	0.0298
CO2	R2	1	1	0.9994	0.9966	0.9968
	rmse	0.0021	0.0046	0.0229	0.0567	0.00587

EC, $R^2_{NaOH} = R^2_{Na2CO3} (0.9998) > R^2_{AL2 (SO4)3} (0.9996)$ is obtained. Higher amount of R^2 indicate higher sensitivity.

The effect of additives on each output also investi-

gated by the same network and concluded that R^2 _{TH}(0.9996) > $R^2_{CO2 \text{ content}}$ (0.999) > R^2_{EC} (0.9966). Also, effects of three influent indices on each efflu-

Also, effects of three influent indices on each effluent parameter are shown in TABLE 6 and again this is shown that they predict TH, precisely. So predicting TH values of effluent stream is dependent strongly on three influent indices and experimental results also indicate this.

Network optimization

According to the contributed algorithm the optimum architecture and training function of neural network is determined.

- 1) A multi layers feed forward back propagation network with three neurons in input layer and three neurons in output layer is used.
- 2) Three training functions are examined for faster optimization and *trainlm* finds better optima and decreases value of *rmse* much more rapidly with time than *traingdm* and *trainbfg* functions. TABLE 7 shows the performance of the training functions according to the amount of *rmse*.
- 3) Using *trailm* with fixed number of neurons in hidden layer, three possible transfer functions in hidden layer and output layer are analyzed in five types of networks architectures. TABLE 8 shows that *tansig* function in both hidden and output layer has minimum *rmse* and maximum R².
- 4) The last step in network optimization is fixing the number of neurons in hidden layer to reach lowest *rmse* and also gain proper performance without time consumption. TABLE 9 contains results of modeling of 6 types of neural networks.

Figure 6 and Figure 7 show a comparison between calculated and experimental values of the output variable (TH) for test and validation sets, using the optimized neural network model with number of hidden layer

Neuron in hidden layer	Network training function	Hidden transfer function	Output transfer function	RMSE	R ²
10	traingdm	Tansig	tansig	8.54×10^{-8}	0.93211
10	Trainbfg	Tansig	tansig	2.25×10^{-14}	0.88614
10	Trainlm	Tansig	tansig	9.23×10^{-11}	0.99791

TABLE 7 : Performance of network training functions

TABLE 8 : Architecture of neural network

Neuron in hidden layer	Network training function	Hidden transfer function	Output transfer function	RMSE	R ²
10	trainlm	Tansig	tansig	9.23×10^{-11}	0.99791
10	trainlm	Logsig	logsig	0.1220798	0.91262
10	trainlm	Tansig	logsig	0.1320765	0.87387
10	trainlm	Tansig	purelin	5.15×10^{-7}	0.97362
10	trainlm	Logsig	purelin	3.21×10 ⁻⁸	0.99002

TABLE 9 : Optimization of number of neurons in hidden layer

Neuron in hidden layer	Network training function	Hidden transfer function	Output transfer function	RMSE	\mathbf{R}^2
8	trainlm	Tansig	tansig	1×10^{-8}	0.99510
10	trainlm	Tansig	tansig	9.23×10^{-11}	0.99791
12	trainlm	Tansig	tansig	1.31×10^{-11}	0.95988
15	trainlm	Tansig	tansig	2.46×10^{-10}	0.99641
18	trainlm	Tansig	tansig	3.602×10^{-6}	0.99456
20	trainlm	Tansig	tansig	1.10×10^{-7}	0.99320





Figure 6 : Comparison of the experimental test data with those predicted via neural network modeling

equal to ten, respectively. Obviously, calculated data tracks experimental ones very well and correlation coefficient, R^2 , is close enough to one. Figure 8 shows CO_2 experimental values and the precise prediction of optimized network for CO_2 content. Also, Figure 9 and

Figure 7 : Comparison of the experimental validation data with those predicted via neural network modeling

Figure 10 compare experimental and predicted values of EC and TH, respectively.

The suitable architecture for prediction of effluent performance is determined to consist of a hidden layer with 10 neurons with *tansig* transfer function. Also *trainlm* shows the best performance in this investiga-

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Figure 9 : Predicted EC data versus experimental



Figure 10 : Predicted CO₂ content vs. experimental



Figure 11 : Comparison between TH prediction data by ANFIS1 and experimental data



Figure 12 : Comparison between predicted CO₂ content by ANFIS1 and experimental data

tion when initial data divided into 40% (training), 30% (testing) and 30% (validating). TABLE 10 reports *Weight* and *Bias* values which are obtained with the optimized neural network.

Fuzzy interference results

TABLE 11 shows types of ANFIS models which are examined to predict treatment unit effluent qualities. Number of layers and MFs and rules are determined for optimal model.

Statistics criteria which are used to show the model

TABLE 10 : Matrices of weights, IW: weights between input and hidden layers; LW: weights between hidden and output layers

IW					
Variable			Diag	Neuron	LW
NaOH	Na2(CO3)	Al2(SO4)3	- Blas		
-1.3345	2.6985	-0.4639	2.9339	1	-1.2281
-0.1190	3.2331	-0.6928	1.5836	2	-1.8267
-1.3486	0.5628	0.4592	4.0818	3	6.2114
1.3974	1.3603	2.2730	5.1039	4	-2.8053
-0.8324	1.9868	-2.1414	-1.2313	5	0.2601
-0.8403	-1.8547	-3.7155	2.6674	6	1.0171
0.7875	-0.6412	-3.3781	2.6697	7	-0.8059
-0.7134	-2.5426	-2.0331	-2.8525	8	-0.8042
-0.6422	-1.7614	2.3629	-2.2570	9	0.0424
0.1735	-1.4767	2.6963	2.8603	10	-0.8283
	· · · · · · · · · · · · · · · · · · ·			bias	-0.9125
	Var NaOH -1.3345 -0.1190 -1.3486 1.3974 -0.8324 -0.8403 0.7875 -0.7134 -0.6422 0.1735	IW Variable NaOH Na2(CO3) -1.3345 2.6985 -0.1190 3.2331 -1.3486 0.5628 1.3974 1.3603 -0.8324 1.9868 -0.8403 -1.8547 0.7875 -0.6412 -0.7134 -2.5426 -0.6422 -1.7614 0.1735 -1.4767	IW Variable NaOH Na2(CO3) Al2(SO4)3 -1.3345 2.6985 -0.4639 -0.1190 3.2331 -0.6928 -1.3486 0.5628 0.4592 1.3974 1.3603 2.2730 -0.8324 1.9868 -2.1414 -0.8403 -1.8547 -3.7155 0.7875 -0.6412 -3.3781 -0.7134 -2.5426 -2.0331 -0.6422 -1.7614 2.3629 0.1735 -1.4767 2.6963	IW Variable Bias NaOH Na2(CO3) Al2(SO4)3 -1.3345 2.6985 -0.4639 2.9339 -0.1190 3.2331 -0.6928 1.5836 -1.3486 0.5628 0.4592 4.0818 1.3974 1.3603 2.2730 5.1039 -0.8324 1.9868 -2.1414 -1.2313 -0.8403 -1.8547 -3.7155 2.6674 0.7875 -0.6412 -3.3781 2.6697 -0.7134 -2.5426 -2.0331 -2.8525 -0.6422 -1.7614 2.3629 -2.2570 0.1735 -1.4767 2.6963 2.8603	IW Bias Neuron NaOH Na2(CO3) Al2(SO43) Bias Neuron -1.3345 2.6985 -0.4639 2.9339 1 -0.1190 3.2331 -0.6928 1.5836 2 -1.3486 0.5628 0.4592 4.0818 3 1.3974 1.3603 2.2730 5.1039 4 -0.8324 1.9868 -2.1414 -1.2313 5 -0.8403 -1.8547 -3.7155 2.6674 6 0.7875 -0.6412 -3.3781 2.6697 7 -0.7134 -2.5426 -2.0331 -2.8525 8 -0.6422 -1.7614 2.3629 -2.2570 9 0.1735 -1.4767 2.6963 2.8603 10

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TABLE 11 : Architecture of ANFIS models

Item	1	2	3	4	5	6
Basic structure						
No. of total layers	5	5	5	5	3	3
No. of input and output layers	3	3	3	3	2	2
No. of nodes in hidden layers	6	6	6	6	6	6
No. of nodes in input layer	4	4	4	4	4	4
No. of neurons in output layer	3	3	3	3	3	3
MFs	Bell	Bell	Gaussian	Gaussian	Gaussian	Bell
No. of MFs	2	4	2	4	2	4
No. of fuzzy rules	2 ²	4 ²	2^2	4^{2}	2^{2}	4^{2}

Effluent indices	Statistical criteria	1	2	3	4	5	6
TH	R	0.9669	0.9593	0.9664	0.9447	0.9072	0.9195
	MAE	0.0473	0.0572	0.0583	0.0599	0.0726	0.0626
	RMSE	0.0332	0.0358	0.0372	0.0396	0.0446	0.0416
CO2	R	0.9860	0.9800	0.9771	0.9773	0.8695	0.8999
	MAE	0.01321	0.0142	0.0181	0.0210	0.1103	0.1030
	RMSE	0.2216	0.2235	0.2241	0.2258	0.2363	0.2213
EC	R	0.7969	0.7424	0.7152	0.7011	0.5869	0.6690
	MAE	0.0412	0.0441	0.0487	0.0511	0.1320	0.1011
	RMSE	0.0946	0.0944	0.0924	0.0954	0.1912	0.1506





Figure 13 : Comparison between predicted EC by ANFIS1 and experimental data

performance are reported in TABLE 12. Comparison between criteria for ANFIS 3 and ANFIS 5 also between NAFIS 2 and ANFIS 6 concludes increasing numbers of hidden layers increases the accuracy of ANFIS prediction so amounts of *mae* and *rmse* between experimental data and model results gets lowest. Also Bell membership function acts better than Gaussian and increases amount of correlation coefficient. Comparing obtained results between ANFIS1 and ANFIS2 shows increasing membership rules doesn't show posi-

CHEMICAL TECHNOLOGY An Indian Journal tive effect in predicting precisely. Finally ANFIS1 is selected as an optimal model to predict treatment performance.

Figure 11 shows ANFIS1 results versus experimental amounts of TH and indicates the excellent agreement, Figure 12 shows comparison between ANFIS1 predicted values of CO_2 content and experimental data and they show somehow a good agreement. Good agreement is obtained between experimental amounts of EC and predicted ones shown in Figure 13.

CONCLUSIONS

The influence of the main parameters of the pretreatment process on the final values of total hardness is evaluated experimentally. On the other hand, the predictions of the main system outputs of a treated waste as a function of initial characteristics (optimized amount of NaOH to coagulant, Na₂CO₃ to coagulant and Al₂ (SO₄)₃), are performed using neural networks. According to this investigation bellow results are obtained:

1) The best of coagulant is $Al_2(SO_4)_3$ and the best mix-

ing rate in first pretreatment reactor is 70 rpm, lower speed can't break coagulant connections properly and higher speed can't make effective collision to form sediments and remove total hardness.

- 2) This is beneficial to use amounts of additives considering the amount of coagulant so the optimum value for NaOH to coagulant and Na_2CO_3 to coagulant is 4 and 3, respectively.
- 3) In optimum operating conditions, total hardness decreases to 453.33 ppm as CaCO₃, Also electrical conductivity and CO₂ content reaches minimum levels and 62921.3 and 0.00374, respectively.
- 4) The optimized Multilayer neural network consists of tangent sigmoid transfer function in hidden layer, and also in output layer. The number of optimized neurons is 10 in the hidden layer and Levenberg-Marquardt algorithm as network training function. Obtained mean squared error is 9.61×10⁻⁶ and correlation coefficient is 0.99791 so this neural network modeling could give excellent agreement with experimental results.
- 5) The optimized Multilayer ANFIS consists of five layers with six neurons in two hidden layers, two *Bell* type membership functions with four rules.
- 6) Optimized ANN predictions are more precise than optimized ANFIS results. ANN shows lower *rmse* with experimental data.
- 7) The optimized neural network can be used to predict the efficiency of pretreatment process of desalination effluent, generally.
- 8) Predictions of optimized neural network can be applied for optimization purposes for pretreatment units and also for forecasting performance of zero discharge desalination plants.
- 9) Results are applicable for control engineers, corrosion engineers and process engineers, chemical and environmental engineers.

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