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RESEARCH PAPER

Establishment of Relationship Between Coagulant and Chlorine Dose Using Artificial Neural Network

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Abstract

Multiple treatment phases are involved in a water treatment plant (WTP), but coagulation and disinfection are the most crucial for producing safe and clear water. Determining the optimal coagulant and chlorine doses in the laboratory is time-consuming and poses a significant challenge in water treatment. To streamline this process, artificial neural network (ANN) models have been developed to predict the chlorine dose based on the coagulant dose. Studies comparing various ANN models indicate that the radial basis function neural network (RBFNN) model provides excellent predictions (R = 0.999). In modeling with radial basis function neural networks (RBFNN) and generalized regression neural networks (GRNN), the spread factor was varied from 0.1 to 15 to achieve a stable and accurate model with high predictive accuracy. Employing soft computing models to define the coagulant and chlorine doses has proven highly beneficial for the management of WTPs, significantly enhancing the efficiency and accuracy of dosing predictions.

Keywords Chlorine dose · RBFNN · Neural network (ANN) · GRNN · Water treatment plant · Water quality

Abbreviations

ANN	Artificial neural networks
ANFIS	Adaptive neural fuzzy inference system
BFGS	Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm
BR	Bayesian regularization
BOD	Bio-chemical oxygen demand
COD	Chemical oxygen demand
CFNN	Cascade feed forward neural network
CDNN	Coagulant dose neural network
CCDNN	Coagulant and chlorine dose neural network
CGB	Conjugate gradient back propagation
CFNNWQ1	Cascade feed forward neural network water quality model using Levenberg–Marquardt training algorithm
CFNNWQ2	Cascade feed forward neural network water quality model using Bayesian regularization training algorithm
CFNNCD1	Cascade feed forward neural network coagulant dose model using Levenberg–Marquardt training algorithm
CFNNCD2	Cascade feed forward neural network coagulant dose model using Bayesian regularization training algorithm
DO	Dissolved oxygen
DOM	Dissolved organic meter
ELM-RBF	Extreme learning machine with radial basis neural network
FFNN	Feed forward neural network
FFNNWQ1	Feed forward neural network water quality model using Levenberg–Marquardt training algorithm
FFNNWQ2	Feed forward neural network water quality model using Bayesian Regularization training algorithm

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FFNNCD1	Feed forward neural network coagulant dose model using Levenberg–Marquardt training algorithm
FFNNCD2	Feed forward neural network coagulant dose model using Bayesian regularization training algorithm
FWMPM	Fuzzy weighting multiple predictive model
GUI	Graphical user interface
GA-LP	Genetic algorithm–linear programing
GRNN	Generalized regression neural networks
GD	Gradient descent
GDM	Gradient descent with momentum
GCF	Conjugate gradient back propagation with fletcher-powell
GP	Genetic programming
LM	Levenberg–Marquardt
LFOM	Linear flow orifice meter
LCDC	Linear chemical dose controller
MAE	Mean absolute error
MPN	Most probable number
MLR	Multiple linear regression
MMPC	Multiple model predictive control
MSE	Mean square error
OSS	One step secant
PAC	Poly aluminum chloride
PCMC	Pimpri Chinchwad Municipal Corporation
RBFNN	Radial basis function neural network
RCNN	Residual chlorine neural network
RP	Resilient back propagation
RMSE	Root mean square error
R^2	Coefficient of determination
SS	Suspended solids
SF	Spread factor
TDS	Total dissolved solids
TSS	Total suspended solids
TP	Total phosphorus
VLRGD	Variable learning rate gradient descent
WQNN	Water quality neural network
WTP	Water treatment plant
WWTP	Wastewater treatment plant
WDN	Water distribution network
WQI	Water quality index

1 Introduction

In water treatment plants (WTP), a multitude of phases are encompassed; however, among them, coagulation and disinfection stand out as pivotal stages responsible for generating water that is both safe and clear (Gibbs et al. 2006; Guan-De et al. 2008; Kim and Parnichkun 2017; Hebati et al. 2017). As an economical, efficient bactericidal agent with minimal residuals, chlorine is widely utilized for disinfection purposes (Lee et al. 2004; Bello et al. 2014; Librantz et al. 2018). The effectiveness of the chlorination process depends up on three critical factors such as water turbidity, pH levels, and the quantity of chlorine introduced (Zhang et al. 2011). Turbidity holds a significant role in both coagulation and disinfection, facilitating particle settlement and offering a protective shield against microorganisms (Bowden et al. 2006; Wadkar et al. 2021a, b, c; Wang et al. 2023). Attempting to represent the complex, nonlinear relationship between turbidity, chlorination, and coagulation with a linear mathematical model presents a significant challenge (Constans et al. 2003; Wu and Lo 2010; Liu et al. 2018; Kote and Wadkar 2019; Bobadilla et al. 2019). Hence, it becomes essential to ascertain the association between chlorine and coagulant dosages. Despite the feasibility of predicting chlorine dosing through coagulant concentrations at a WTP, there is a current scarcity of published literature addressing these issues. To bridge this existing gap, the present study is centered on the development of multiple artificial neural network (ANN) models aimed at establishing the intricate correlation between coagulant and chlorine doses. The testing and comparison of diverse ANN models and training algorithms (Asnaashari et al. 2014; Ayvaz et al. 2015; Abba et al. 2017; Amali et al. 2018; Reilly et al. 2018; Narges et al. 2021) are of paramount importance in order to pinpoint a network capable of achieving satisfactory outcomes within a reasonable timeframe. Each model is subjected to numerous training iterations, and the evaluation of the most adept model is grounded in its performance (Bekkari and Zeddouri 2019). Turbidity plays is a vital role in coagulation and disinfection as it responsible for settlement of particles and provide shields to microorganisms. It is difficult to describe the nonlinear behavior of turbidity in relation to chlorination and coagulation by means of a linear mathematical model. Determination of the relationship between chlorine dose and coagulant dose is therefore necessary. Application of soft computing model for defining dose of coagulant and dose of chlorine are inextricably linked at a WTP will be highly beneficial for WTP Managers. In this study, numbers of ANN models for establishment of relationship between Coagulant and Chlorine Dose are developed. It is necessary to test and compare various ANN and training algorithms in order to develop a network that can perform satisfactorily in a reasonable amount of time. Each model is trained many times and the best performance is evaluated. While chlorine dose prediction using coagulant concentrations at a WTP is possible, as there is no published literature on interrelation ship between coagulant and chlorine dose at WTP. Every model underwent repeated training sessions, with the optimal performance being assessed.

Table 1 Performance indices of CCDNN1 models during testing period

Type of ANN Model	SF/Training algorithm	Error statistics			Standard statistics			
		R	MSE	MAE	$\bar{x}$ (1.954)	σ (0.171)	γ1 (2.53)	γ2 (12.39)
RBFNN1	0.1	0.753	0.018	0.077	1.962	0.120	−2.438	12.287
	1	0.504	0.033	0.113	1.926	0.180	−2.023	15.283
	5	0.285	0.040	0.133	1.916	0.200	−2.058	13.280
	10	0.443	0.617	0.647	1.890	0.786	0.374	2.183
	15	0.421	0.631	0.661	1.913	0.795	0.414	2.147
GRNN1	0.1	0.554	0.534	0.584	1.885	0.731	0.352	2.431
	1	0.451	0.611	0.642	1.888	0.782	0.401	2.177
	5	0.424	0.633	0.663	1.980	0.796	0.506	2.134
	10	0.385	0.660	0.699	1.929	0.812	0.593	2.073
	15	0.342	0.684	0.720	1.888	0.827	0.619	2.024
FFNN	LM	0.427	0.628	0.651	1.903	0.792	0.392	2.181
	BR	0.400	0.648	0.646	1.910	0.803	0.473	2.288
	BFG	0.396	0.649	0.672	1.9064	0.805	0.386	2.298
	RP	0.384	0.655	0.677	1.8063	0.809	0.475	2.100
	CGF	0.398	0.657	0.684	1.8038	0.810	0.406	2.191
	CGM	0.302	0.715	0.702	1.921	0.844	0.516	2.171
	OSS	0.197	0.763	0.753	1.908	0.873	0.403	2.258
CFNN	LM	0.407	0.640	0.654	1.962	0.800	0.463	2.249
	BR	0.411	0.638	0.665	1.934	0.799	0.449	2.147
	BFG	0.219	0.731	0.742	1.879	0.855	0.6351	1.980
	RP	0.237	0.724	0.732	1.914	0.851	0.631	1.978
	CGF	0.256	0.717	0.731	1.862	0.847	0.623	1.983
	CGM	0.373	0.665	0.689	1.880	0.815	0.586	2.088
	OSS	0.405	0.642	0.666	1.985	0.801	0.452	2.165

2 Material

The water treatment plant located in Sant Tukaram Nagar, Pimpri Chinchwad, Pune, Maharashtra, India. the area having the widespread coordinates of 18° 37′ 33.88″ N latitude and 73° 48′ 43.77″ E longitude. The WTP pull out 428 MLD water from Khadakwasla dam. After the treatment, water is distributed to entire Sant Tukaram Nagar Pimpri Chinchwad, Pune. Daily around 180 lpcd water supplied.

3 Methodology

For CCDNN modeling, 1849 data samples of input variables (Turbidity of the outlet water, residual chlorine, and coagulant dose) and target variable (chlorine dose) collected from WTP. The variables examined in this study are inextricably linked to the coagulation and chlorination processes. Data were collected from the plant laboratory during four years for inlet and outlet water quality daily (2012–2016). MATLAB version 16 was used to develop ANN models. ANN models such as RBFNN, FFNN, CFNN and GRNN have been developed with trial run that allows modification of the input variables, hidden nodes, training function, the spread factor (SF). It is always a difficult task to create an optimal number of hidden nodes in ANN applications. The optimum number of nodes in each layer is not possible precisely and easily. In this study, information of both input and output nodes is used for building hidden neurons in a hidden layer. The training and test data are divided between 75:30 and 80:20 respectively during development of the ANN models. Training functions that are diverse, such as Bayesian Regularization (BR),

Levenberg–Marquardt (LM), Resilient Back Propagation (RP), BFGS Quasi-Newton (BFG), One-Step Secant (OSS) Conjugated Gradient Back Propagation (CGB), Cluster–Powell (CGF), Gradient Back Propagation (VLRB) are used. It was reported that the RBFNN and the GRNN models have the best test performance respectively with the SF of 1 and 0.1. Thus, RBFNN and GRNN models ranging from 0.1 to 15 have been tested in this study. Standard statistics (JK), a standard deviation (L), skewness (M1), kurtosis (M2) and error statistics like regression coefficient (R), mean square error (MSE) and mean absolute error are used to quantify the percentage performance of these ANN models (MAE).

For its highest R and lowest MSE and MAE values, the best performing ANN model is chosen. In addition, standard statistics, time series plots and scatter plots are checked for the mapping with the observed series. For the best model in each category, GUIs for chlorine prediction and coagulant dosage were developed.

4 Result and Discussion

4.1 Neural Network Model for Coagulant and Chlorine Dose 1

Sixteen models are developed for the coagulant and chlorine dose neural network 1 (CCDNN1) model. In order to establish the optimal networks, coagulant dose as input parameter and chlorine dose as output parameter are examined with various training functions and ANN (Heddam et al. 2011; Cuesta et al. 2014; Chandwani et al. 2016; Haghiri et al. 2017). On the basis of numerous performance criteria, the behaviour of ANNs is evaluated which is shown in Table 1. For ANN prediction with FFNN and CFNN, different training function were tried with varying hidden nodes from 15 to 90 and for RBFNN and GRNN the value of SF varies from 0.1 to 20 during training to achieve best performing network. It is observed during training period that minimum MSE = 0.019, and minimum MAE = 0.078 whereas maximum value of R = 0.753 is found. Similarly, standard statistics σ = 0.137 to 0.873, γ1 = -2.058 to 0.635, and γ2 = 1.978 to 15.718. During training, it is observed that as SF value decreases in GRNN and RBFNN models, the values of R increases and values of MSE decreases. On the other hand, prediction is highly comparable by RBFNN 1 model with SF = 0.1. Similarly, it is observed during testing period, minimum MSE = 0.014, and minimum MAE = 0.068 whereas maximum value of R = 0.715 is found. Similarly, standard statistics such as σ = 0.12 to 0.608, γ1 = -2.461 to-0.762, and γ2 = 3.184 to 12.287.

Prediction accuracy is higher for the RBFNN1 model with SF = 0.1 obtained. Further performance measures of all models are compared and observed that all the models resulted in poor performance, only RBFNN1 model produce a good result (R = 0.72). Figure 1. shows the plot of observed and predicted series of best FFNN, CFNN, RBFNN, and GRNN model during testing period.

4.2 Neural Network Model for Coagulant and Chlorine Dose 2

In coagulant and chlorine dose neural network 2 (CCDNN2) model, sixteen models are developed for the coagulant and chlorine dose neural network 2 (CCDNN1) model. In order to establish the optimal networks, coagulant dose and

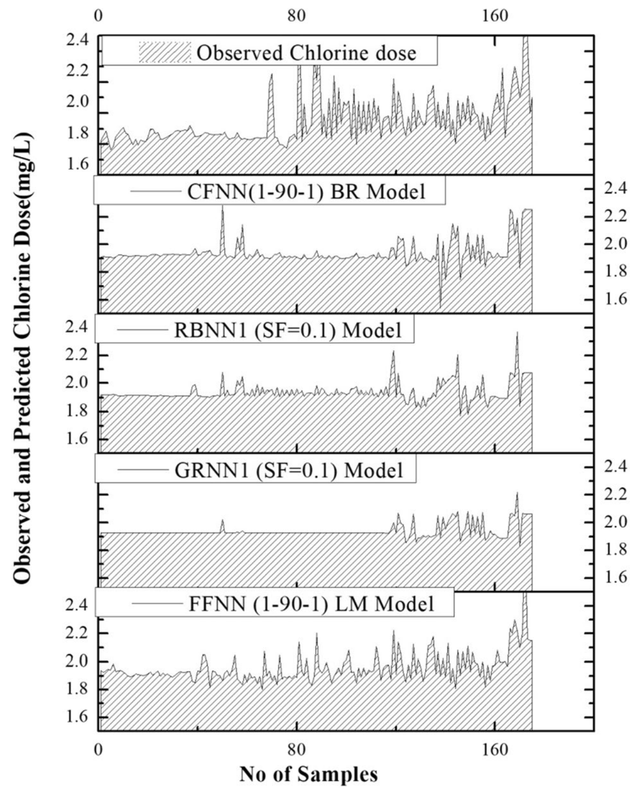

Fig. 1 Comparison of best CCDNN1 models during testing period

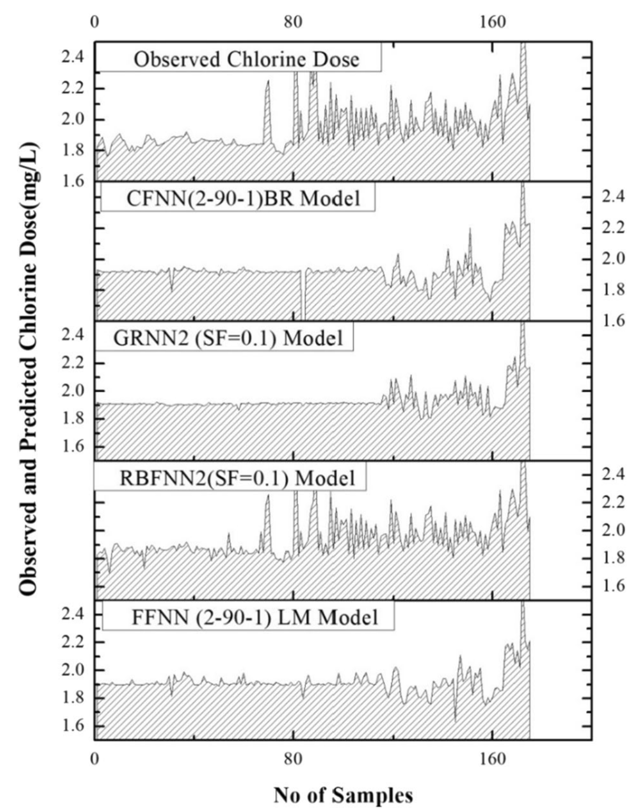

Fig. 2 Comparison of best CCDNN2 models during testing period

Table 2 Performance indices of CCDNN3 models during testing period

Type of ANN model	SF/Training algorithm	Error statistics			Standard statistics			
		R	MSE	MAE	$\bar{x}$ (1.954)	σ (0.171)	γ1 (2.53)	γ2 (12.39)
RBFNN3	0.1	0.999	0.001	0.009	1.953	0.026	1.032	21.046
	1	0.812	0.01	0.047	1.949	0.1	−3.014	20.019
	5	0.012	1.069	0.298	1.853	1.005	−10.24	15.45
	10	−0.175	0.091	0.272	1.782	0.181	−2.265	12.225
	15	−0.237	0.181	0.391	1.771	0.22	−1.608	7.813
GRNN3	0.1	0.477	0.023	0.099	1.91	0.151	−2.324	11.231
	1	0.053	0.051	0.199	1.851	0.138	−3.786	28.395
	5	0.053	0.051	0.199	1.851	0.138	−3.786	28.395
	10	0.246	0.028	0.113	1.894	0.166	−2.539	12.257
	15	0.053	0.051	0.199	1.852	0.138	−3.786	28.395
FFNN	LM	0.444	0.025	0.1	1.911	0.154	−1.963	10.019
	BR	0.271	0.037	0.108	1.867	0.188	−3.107	20.4
	BFG	0.392	1.028	0.982	1.889	0.519	−1.922	6.269
	RP	0.349	0.046	0.145	1.901	0.184	−1.337	6.873
	CGF	0.407	0.033	0.119	1.918	0.166	−1.122	8.197
	CGB	0.239	0.063	0.177	1.889	0.192	−1.035	5.309
	OSS	0.262	0.037	0.117	1.899	0.186	−2.306	11.735
CFNN	LM	0.277	0.125	0.324	1.878	0.193	−2.178	10.786
	BR	0.314	0.099	0.287	1.898	0.182	−2.263	12.078
	BFG	0.32	0.143	0.344	1.888	0.212	−1.681	8.283
	RP	0.249	0.074	0.187	1.889	0.234	−1.003	4.76
	CGF	0.433	0.035	0.124	1.896	0.164	−1.133	8.628
	CGB	0.378	0.041	0.135	1.898	0.194	−0.51	9.123
	OSS	0.376	0.052	0.157	1.882	0.19	−1.136	9.387

residual chlorine as input parameter and chlorine dose as output parameter are examined with various training functions and ANN [46–55]. On the basis of numerous performance criteria, the behaviour of ANNs is evaluated. It is observed that during training period, MSE = 0.002 to 0.028, and MAE = 0.013 to 0.104 whereas R varies from 0.197 to 0.978. Similarly, standard statistics such as σ = 0.044 to 0.184, γ1 = −2.713 to −4.286 and γ2 = 19.83 to 62.15 Prediction accuracy is higher for the RBFNN2 model with SF = 0.1 obtained. Similarly, it is observed during testing period that minimum MSE = 0.001, and minimum MAE = 0.015 whereas maximum value of R = 0.97 is found. Similarly, standard statistics such as σ = 0.036 to 0.128, γ1 = −1.713 to −8.717 and γ2 = 17.667 to 89.15. It is seen from results of training and testing period that RBFNN2 model with SF = 0.1 resulted consistently better than FFNN, CFNN and GRNN models. Figure 2 shows the plot of observed and predicted series of best FFNN, CFNN, RBFNN, and GRNN model during testing period.

4.3 Neural Network Model for Coagulant and Chlorine Dose 3

In coagulant and chlorine dose neural network 3 (CCDNN3) model, sixteen models were developed. In order to establish the optimal networks, turbidity of the outlet water, residual chlorine, and coagulant dose as input parameter and chlorine dose as output parameter are examined with FFNN, CFNN, RBFNN, and GRNN. The developed models were tested to get an appropriate network that provided satisfactory performance. The important performance indices of all ANN model are displayed in Table 2, indicating standard statistics and error statistics during testing period. From Table 2, it has been observed that during testing period, standard statistics for example σ (Min) = 0.026, γ1 (Max) = 1.032 and γ2 (Min) = 5.309. Similarly, error statistics such MSE (min) = 0.001, and MAE (min) = 0.009 whereas maximum value of R = 0.99 is found. In RBFNN and GRNN models as SF increases prediction efficiency decreased. In the RBFNN model, however, there is clear superiority in prediction with SF = 0.1. Figure 3 shows a comparison of the best CCDNN3

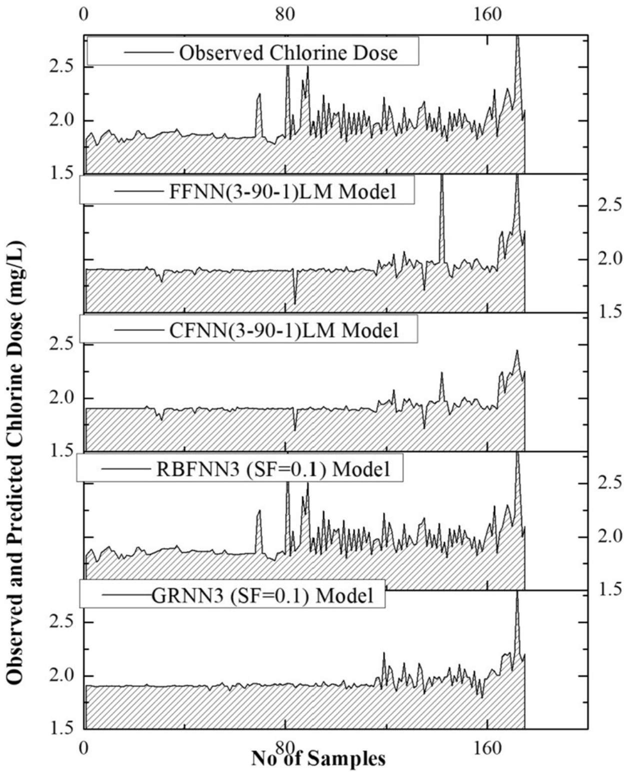

Fig. 3 Comparison of best CCDNN3 models during testing period

models in the test period, where plot of RBFNN3 almost coincides with the plot of observed values. Compared to all other ANN models, RBFNN3 model with SF 0.1 produced the highest R. It is found that the prediction efficiency has increased in RBFNN and GRNN models, with a decrease in SF value. Furthermore, compared to all other training algorithms, FFNN and CFNN models with BR training function produced good prediction. These models, however, are less efficient.

RBFNN models, on the other hand, have a noticeable advantage in prediction. It also demonstrates that models with three inputs perform better than models with various input variations to the networks. Tables 3 show a summary of standard statistics for the best RBFNN models in Class I, II, and III during the training and testing period. Standard statistics for all ANN models were evaluated and displayed in Table 3 during the training and testing periods. During training and testing, RBFNN 3 model exhibited least σ and γ2. Most of the best ANN models produced a positive kurtosis, where heavier tails are associated with a higher peak. The σ (least) of the RBFNN 3 model suggests that the data points tend to be close to the set' s predicted value; whereas the σ (Max) of the RBFNN 1 model indicates that data points are dispersed throughout a larger range of values.

The results of model simulation indicate that the lower the absolute value of γ1 (1.032), and the larger the γ2 (21.046) lies with RBFNN3 models, which indicate higher the accuracy of the prediction. Compared to other ANN models from Class I, II, and III, the RBFNN3 model performed the best with MSE = 0.001 and R = 0.999 over the testing period shown in Fig. 4a. Time series plot and scatter plots of RBFNN3 model during the testing period is shown in Fig. 4b, c respectively. The observed and predicted chlorine dose series is seen to closely map indicating the best model. Due to better non-linear approximation, RBFNN model showed excellent predictive results.

In most developing countries, the chlorine dose in a WTP is usually calculated by the operator's knowledge, while the coagulant dose is measured by a jar test (Kennedy et al. 2015; Wang et al. 2017). Laboratory analysis is usually used to determine the coagulant and chlorine dosage, which takes a long time in WTP. As a result, at WTP, a link between chlorine dose and coagulant dose must be established. Operators of WTP will be able to use the developed relationship to select the optimum dose.

Similarly, relation between chlorine dose and coagulant dose, which is quite simplified by various nth degree expressions as shown in Eq. 1, 2 and 3.

$$y = -0.00046 \times z + 1.6 \tag{1}$$

$$y = 3.5 \times 10^{-6} \times z^2 - 0.001 \times z + 1.9 \tag{2}$$

$$y = -3.5 \times 10^{-8} \times z^3 + 1.4 \times 10^{-5} \times z^2 - 0.0017 \times z + 1.9 \tag{3}$$

where y = chlorine dose and z = coagulant dose in mg/L.

Table 3 Standard statistics of RBFNN models during the training and testing period

ANN model	Training period				Testing period			
	$\bar{x}$	σ	γ1	γ2	$\bar{x}$	σ	γ1	γ2
Observed values	1.909	0.2088	2.0978	12.314	1.954	0.171	2.533	12.390
RBFNN1 SF = 0.1	1.910	0.137	− 1.967	15.718	1.962	0.120	− 2.438	12.287
RBFNN2 SF = 0.1	1.910	0.044	− 4.286	62.155	1.954	0.036	− 1.713	17.667
RBFNN3 SF = 0.1	1.910	0.026	3.027	98.898	1.953	0.026	2.032	21.046

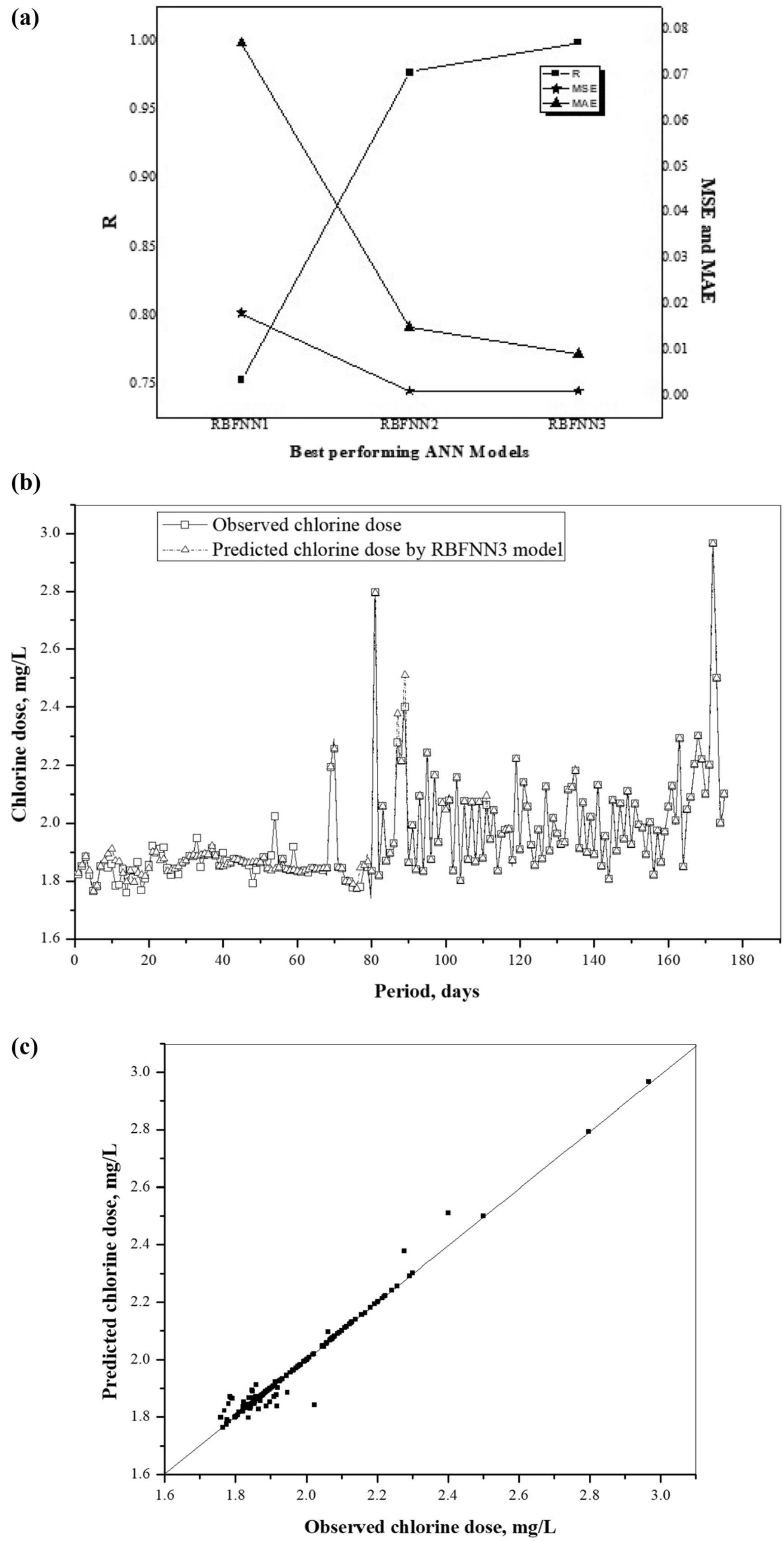

Fig. 4 **a** Error statistics of RBFNN models during testing period. **b**Time series of RBFNN3 model during testing period, **c**scatter plot of RBFNN3 model during testing period

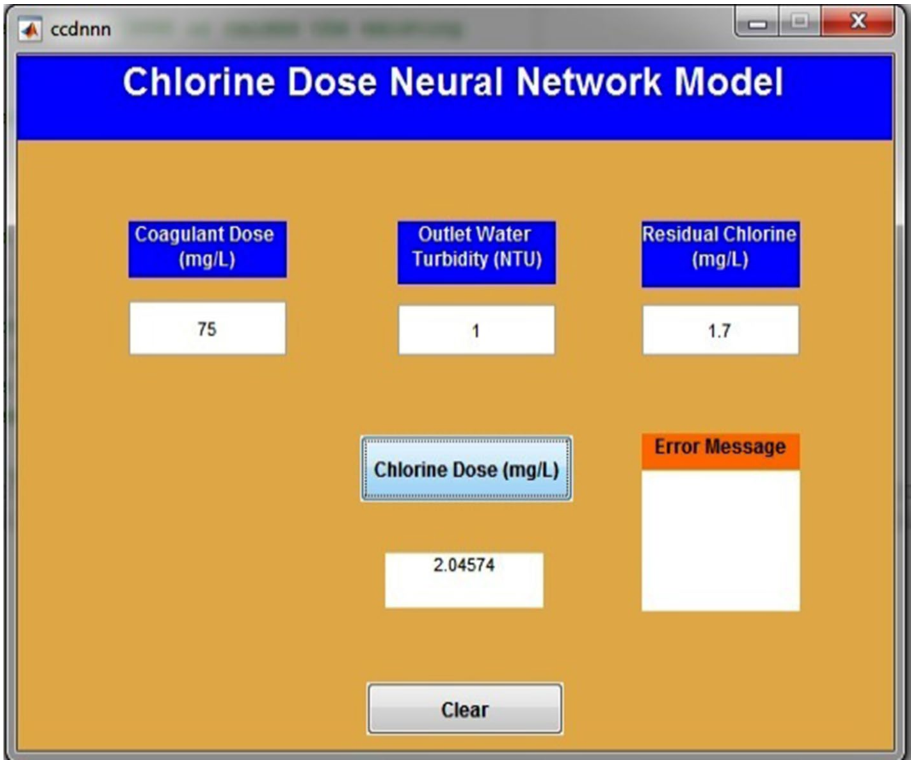

Fig. 5 Screen shot of GUI for CCDNN (RBNN3 (SF = 0.1)) model

5 Development of Graphical User Interface

In order to transfer the modelling knowledge to the field, GUI software has been developed. The developed GUI will provide a useful tool to plant operators and managers for deciding required chlorine and coagulant dose. GUIs for prediction chlorine dose in WTP was developed using the best model. The GUI was developed in MATLAB software. Determination of chlorine dose is an essential aspect in WTP. It decides the concentration of residual chlorine in the outgoing water of WTP. In India, most of WTP operators provide higher chlorine dose for maintaining a high level of residual chlorine in WDN. The more chlorine consumption creates many health problems, hence there is need to apply optimum chlorine dose. The GUI will be useful for the determination of chlorine dose at WTP.

1. Run the CCDNN model.
2. Enter the value of coagulant dose applied at WTP in mg/L.
3. Enter the value of outlet water turbidity (NTU).
4. Entre the value of desirable residual chlorine at the outlet of WTP so that minimum residual chlorine maintained at the end of WDN.
5. After entering all data, click on ' Chlorine Dose' button.
6. Within few seconds, chlorine dose value will be displayed in output window (Fig. 5).

Developed GUIs was definitely helpful for WTP operators and managers to plan the short term and long-term activities.

6 Conclusion

Soft computing, through the use of ANNs plays a crucial role in the prediction and interpretation of coagulant and chlorine doses in water treatment plants. By handling uncertainties, modeling non-linear relationships, integrating diverse data sources, optimizing model parameters, and enhancing interpretability, soft computing provides a powerful toolkit for improving water treatment processes. This results in more accurate, reliable, and actionable dose predictions, ultimately leading to better water quality and more efficient treatment operations. Numbers of CCDNN models are developed for prediction of chlorine dose. The input parameters viz., Turbidity of the outlet water, residual chlorine, and coagulant dose are used for ANN modeling. The selected input parameters are closely related to the chlorination and coagulation process. Prediction efficiency of RBFNN and GRNN models reduces as SF rises. In RBFNN and GRNN models prediction efficiency decreases as SF increases. In the RBFNN model, however, there is clear superiority in prediction, with SF ranging from 0.1 to 1. Such relationships are useful for deciding optimum chlorine dose or coagulant dose. It is also found that the range of chlorine dose is less as compared to the coagulant dose. The relation between them is developed by CCDNN model in which chlorine dose predicted with the help of coagulant dose showed R = 0.99 by RBFNN.

Declarations

Conflict of interest The authors declare that there are no any conflicts of interest.

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