J. Inst. Eng. India Ser. A (January–March 2014) 95(1):29–38
DOI 10.1007/s40030-014-0064-0

ORIGINAL CONTRIBUTION

Modelling Dissolved Pollutants in Krishna River Using Adaptive Neuro Fuzzy Inference Systems

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Received: 13 June 2012 / Accepted: 26 March 2014 / Published online: 16 May 2014

Abstract Water quality models are used to describe the discharge concentration relationships in the river. Number of models exists to simulate the pollutant loads in a river, of which some of them are based on simple cause effect relationships and others on highly sophisticated physical and mathematical approaches that require extensive data inputs. Fuzzy rule based modeling extensively used in other disciplines, is attempted in the present study for modeling water quality with respect of dissolved pollutants in Krishna river flowing in Southern part of India. Adaptive Neuro Fuzzy Inference Systems (ANFIS), a recent development in the area of neuro-computing, based on the concept of fuzzy sets is used to model highly non-linear relationships and are capable of adaptive learning. This paper presents the results of the application of ANFIS for modeling dissolved pollutants in the Krishna River. The application and validation of the models is carried out using water quality and flow data obtained from the monitoring stations on the river. The results indicate that the models are quite successful in simulating the physical processes of the relationships between discharge and concentrations.

Keywords Non-point pollution · Indirect approaches · Water quality modeling · Pollutant loads · Fuzzy inference systems

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Introduction

Discharge—concentration relationships generally are used for water quality studies in the river basins. Traditionally, this task has been accomplished using methods ranging from those that are based on empirical relationships to those that are based on cause-effect relationships. In using models that are based on cause-effect relationships, rigorous mathematical equations are often used to describe the physical, chemical and biological processes. Solutions of such models often require vast data and it is often necessary to estimate input parameters specific to the basin being modeled. In many instances (especially in large river basins), a large number of hydrological parameters are involved and there is no unique way of estimating them. However, they are to be determined subjectively, based on the judgment and the effect is normally manifested in the model output. Hence, these deterministic models, which require large quantity of data in terms of model parameters, have limited applicability in basins where there are data constraints. Therefore, models which are easy to handle and have minimum data requirement are often sought to solve problems where data availability is limited and is difficult to obtain data by experimental investigations and monitoring, which would be very expensive and cumbersome [14].

Recently mathematical models using fuzzy variables rather than numerical variables are encroaching into water quality related studies. In water quality modeling, there are many domains which can be best characterized by linguistic terms rather than directly, by numbers. For instance, a modeler in a particular domain will employ terms such as large flows and low flows to describe the discharge conditions in a river. The problem faced, then, is how to deal with what has been described—imprecision, uncertainty and in particular linguistic terms that cannot be defined exactly. A fuzzy rule based modeling is qualitative modeling approach by which one can describe the system behavior using a natural language [1]. By utilizing fuzzy logic based approach in modeling cause-effect, relationships are described verbally rather than using governing physical relationships. However, in this approach, some of the causes that are considered for physically based models are omitted and some of the causes not considered for in those physical models (because of nature of generalization or unavailability of known relationships) can be included. The researchers have demonstrated the applicability of fuzzy rule based approaches in hydrological modeling [2–5]. It has been reported earlier the use of artificial neural networks as a viable means of forecasting water quality parameters in River Murray, South Australia [6].

The purpose of this work is to report the results of water quality modeling study based on fuzzy rule based approach (ANFIS). An attempt is made to model discharge—concentration relationships of conservative dissolved pollutants in the river.

A Review of ANFIS

The concepts of fuzzy logic introduced by Zadeh in 1964 can be used to model problems of uncertainty and imprecision. A Fuzzy Inference System (FIS) is a popular computing frame work based on concepts of fuzzy logic. Adaptive Neuro-Fuzzy Inference System (ANFIS) incorporated the concepts of neural network learning in FIS. ANFIS model has the capability of approximating any non-linear function and thus is considered as universal approximator [7]. ANFIS models are being employed in wide variety of applications of modeling, decision making, signal processing and control. The basic concepts and features of ANFIS are described in the following sections.

Fuzzy Logic

Zadeh introduced fuzzy sets in 1964 as an approach to handling vagueness or uncertainty and, in particular, linguistic variables. Classical set theory allows for an object to be either a member of the set or excluded from the set. Fuzzy sets differ from classical sets in that they allow for an object to be a partial member of a set [8]. Fuzzy sets are defined by a membership function. For any fuzzy set A, the function $\mu_A(x)$ represents the membership function for which μ indicates the degree of membership that x, of the universal set X, belongs to set A and is, usually, expressed as a number between 0 and 1:

$$0 < \mu_{\mathrm{A}}(\mathrm{x}) < 1 \tag{1}$$

Fuzzy sets can either be discrete or continuous. Fuzzy sets allow us to represent vague concepts expressed in natural language. The representation depends not only on the concept, but also on the context in which it is used. Several fuzzy sets representing linguistic concepts such as low, medium, high and so on are often employed to define states of a variable. Such a variable is usually called a Fuzzy variable. Membership functions can have any shape. Trapezoidal, triangular, bell shaped functions are commonly used to represent membership functions.

Adaptive Neuro-Fuzzy Inference System (ANFIS)

Various types of models are reported in literature for different categories of neuro-fuzzy integration. During the past few years, integration of neural networks and fuzzy logic has emerged as one of the most active and fruitful areas of research in the fields of fuzzy logic and neural networks. Several paradigms of neural fuzzy modeling are available in the literature, such as fuzzy inference networks [9], fuzzy aggregation networks [10], neural network driven fuzzy reasoning [11], fuzzy modeling networks [12] and ANFIS [13]. The concepts of Adaptive Neuro Fuzzy Inference system (ANFIS) proposed by the researchers are discussed in various literature [13]. Among the various NFS based models proposed in literature, ANFIS is popular and has potential applications in a wide variety of engineering problems. ANFIS, proposed by the literatures is based on the first-order Sugeno fuzzy model [13]. The neural network paradigm used is a multi-layer feed-forward back propagation network.

For simplicity, let the fuzzy inference system under consideration be assumed to have two inputs, x and y, and one output z as presented in Fig. 1. For a first-order Sugeno fuzzy model, a typical rule set with two fuzzy if then rules can be expressed as,

In the ANFIS, nodes in the same layer have similar functions as described below. The output of node i in layer l is denoted as O_{li}.

Layer 1: Every node in this layer is an adaptive node with a node output defined as,

$$O_{1,i} = \mu_A(x) \quad \text{for } i = 1, 2 \tag{2}$$

$$O_{1,i} = \mu_{Bi-2}(y) \quad \text{for } i = 3, 4 \tag{3}$$

where x (or y) is the input to the node; and A_i (or B_{i-2}) is fuzzy set associated with this node.

Layer 2: Every node in this layer is a fixed node labeled **Π**, which multiplies the incoming signals and outputs the product. For instance

$$O_{2,i} = w_i = \mu_{Ai}(x) \times \mu_{Bi}(y), \quad i = 1, 2 \tag{4}$$

Each node output represents the firing strength of a rule.

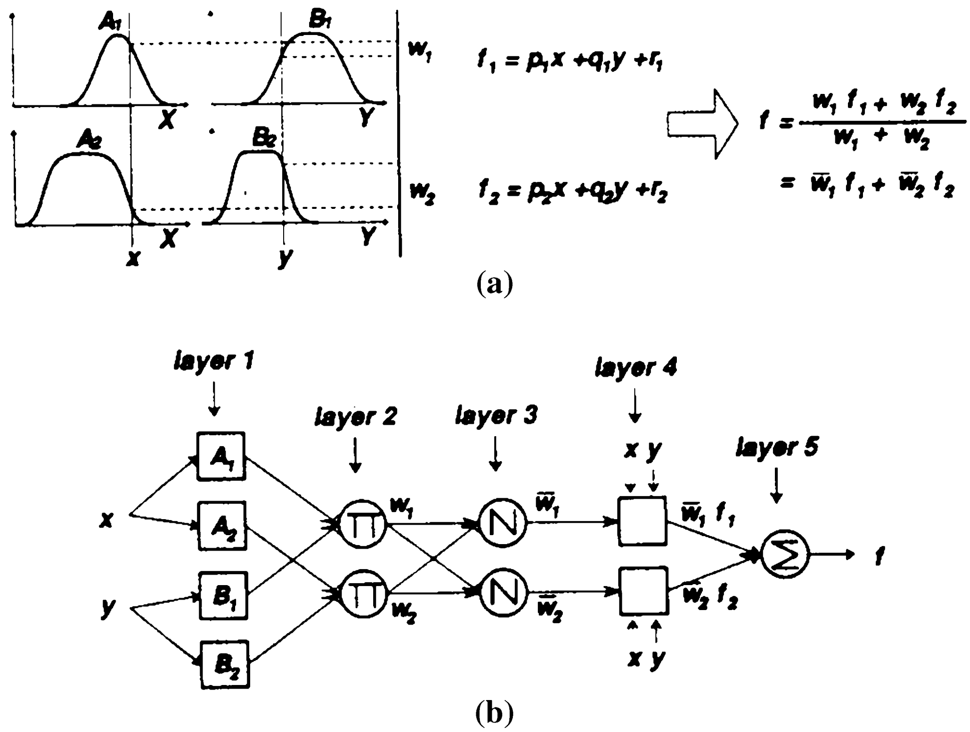


Fig. 1 First order Sugeno Fuzzy model and ANFIS network [13]. Rule 1: If x is A, and y is B, then $f_1 = p_1x + q_1y + r_1$, Rule 2: If x is A_2 and y is B_2 then $f_2 = p_2x + l_2y + r_2$

Layer 3: Every node in this layer is a fixed node labeled **N**. The ith node calculates the ratio of ith rule's firing strength to the sum of all rules' firing strengths.

$$O_{3,i} = W_i = \frac{w_i}{w_1 + w_2}, \quad i = 1, 2 \tag{5}$$

Layer 4: Every node in this layer is an adaptive node with a node function

$$O_{4,i} = \boldsymbol{W}_i f_i = \boldsymbol{W}_i(p_i x + q_i y + r_i) \tag{6}$$

where $\boldsymbol{W}_i$ is output of layer 3 and $\{p_i, q_i, r_i\}$ is the parameter set.

Layer 5: The single node in this layer is fixed node labeled $\sum$, which computes the overall output as the summation of the incoming signals

$$O_{5.1} - = \text{ overall output } = \sum_i Wif_i = \frac{\sum_i wif_i}{\sum w_i} \tag{7}$$

Thus, an ANFIS network is functionally equivalent to a Sugeno fuzzy model. This network can easily be extended to a Sugeno fuzzy model with multiple inputs and rules.

The output f of a ANFIS network shown in Fig. 1 can be written as:

$$\begin{aligned} \mathrm{f} &= \frac{w_1}{w_1 + w_2}\mathrm{f}_1 + \frac{w_2}{w_1 + w_2}\mathrm{f}_2 \\ &= \boldsymbol{W}_1 f_1 + \boldsymbol{W}_2 f_2 \\ &= (\boldsymbol{W}_1 x)p_1 + (\boldsymbol{W}_1 y)q_1 + (\boldsymbol{W}_1)\, r_1 + (\boldsymbol{W}_2 x)p_2 \\ &\quad + (\boldsymbol{W}_2 y)q_2 + (\boldsymbol{W}_2)r_2 \end{aligned} \tag{8}$$

where p_1, q_1, r_1, p_1, q_2 and r_2 are the parameters of the model.

From Eq. (7), it is observed that the output is linear in the parameters p_1, q_1, r_1, p_2, q_2 and r_2, which are known as consequent parameters.

The nodes in layer 1 are adaptive nodes with a node function given by Eq. (1). The output, $O_{1,i}$. Of node i in this layer is the membership grade of a fuzzy set A (=A_1, A_2, B_1 or B_2) and it specifies the degree to which the given input x (or y) satisfies the quantifier A. The membership function for A can be any appropriate parameterized membership function. If generalized bell function is used, the membership function is given by,

$$\mu_{\mathrm{Ai}} = (\mathrm{x}) = \frac{1}{1 + \left|\frac{x - c_i}{a_i}\right|^{2b_i}} \tag{9}$$

where $\{a_i, b_i, c_i\}$ is the parameter set. These parameters are referred as premise parameters. The output of the network f is obviously non-linear in premise parameters. Thus the set of total parameters S can be partitioned into two subsets: a set of premise (non linear) parameters S_1 and a set of consequent (linear) parameters S_2.

The researchers have shown that ANFIS has unlimited approximation power for matching any non linear function arbitrarily well, provided the number of rules is not restricted [7]. Some researchers have proposed a hybrid learning algorithm for training ANFIS [13]. The learning takes place in two stages. In the forward pass of the hybrid learning algorithm, functional signals go forward till layer 4 and the consequent parameters are identified by the least squares estimate. In the backward pass, the error rates propagate backward and the premise parameters are updated by the gradient descent, similar to back propagation algorithm.

Description of the Study Area

Krishna is one of the major rivers of peninsular India along with the Godavari and Kaveri Rivers. The Krishna originates as a small stream in the Western Ghats and traverses eastwards 25 km through the rocky terrains of the Deccan traps. Finally it drains into Bay of Bengal with two major dams at Srisailam and Nagarjuna Sagar. The Deccan traps are considered to be the second most extensive geological formation of the peninsular India, next only to Archean igneous—metamorphic province in south India. The lithology of the upper river basin is almost entirely tholeiitic basalts, with scattered alkaline/saline soils, laterites and calcareous tutas. Down the basin in Karnataka and Andhra Pradesh, the basin includes granites, ganitoids, green stones, schists, amphibolites and gneisses.

The river Krishna drains an area of 258,948 km^2, which is nearly 8 % of the total geo-graphical area of the country. The total population in the basin as per 1991 causes has been estimated as 60.78 million. The river and its tributaries flow through different terrain having varied land use activities, soil conditions, vegetation and agricultural practices. The water potential of the River Krishna and its tributaries are mainly used for drinking, industries, irrigation and power generation. The average annual rainfall in the river basin is about 780 mm. About 90 % of the rainfall occurs during the wet season (June–October) and during the rest of the year (dry season) there is very little rainfall with no regular pattern. Typical tropical climate prevails in the basin for better part of the year. For practical considerations two seasons: dry (December–May) and wet (June–November) seasons exist in the area. The predominant soils in the area are sandy loams and loams. The study area presented in Fig. 2, in particular is part of the Krishna River reach between two monitoring stations: Pondugala (upstream, No. 7 in the Fig. 2) and Wadenapalle (downstream, No. 5 in the Fig. 2). The river reach between the monitoring stations is approximately 80 km long along the river. In addition to other districts, major parts of Nalgonda and Guntur districts drain into this part of the Krishna river reach in Andhra Pradesh.

Results and Discussions

The river water quality data for the years 1989–1994 is used for training the ANFIS model and water quality for the years 1994–1997 is used for testing of the developed models. The normalized data is used for modeling and testing purpose. Normalization is performed by dividing loads and discharges by the corresponding maximum value recorded during 1989–1994.

Discharge in the river is considered as fuzzy set A. During the monsoon season the discharges vary largely between 1,000 and 5,000 m^3/s, and hence discharge is classified into two fuzzy classes, namely low and high. Generalized bell function given in Eq. 8 is used as membership function. The ANFIS models developed take two inputs, discharge in the river in present time interval and in the previous time interval, and one output, the concentration of the pollutant being modeled. The pollutant load at any time is influenced by the load already existing and what is contributed additionally to that of the previous load. Thus each ANFIS model has four fuzzy if then rules with 12 premise parameters and twelve consequent parameters. Training of the ANFIS models is done with water quality data of the monsoon season for 5 years. The results of training in terms of '*r*' and RMSE indicate the success of the application of ANFIS models for that particular water quality parameter.

The pollutant concentrations/loads in the river depend on the rainfall and catchment characteristics and thus the runoff contribution from the drainage basin. The runoff in turn influences the discharge and hence the load of the pollutant. In utilizing fuzzy-rule based classification of flows, the modeling approach helps in establishing relationship between discharge and pollutant load, which is quite different from conventional water quality modeling approaches. The researchers have shown that ANFIS has the ability to model non-linear relationship through FUZZY—IF–THEN rules [7]. ANFIS was proved to be better than Artificial Neural Network (ANN) models in mapping the input—output relationship. Hence, an attempt is made in this study to use ANFIS to model complex relation between discharge and pollutant loads.

The parameters ANFIS models developed for prediction of pollutant loads are presented in Table 1. The pictorial representation of results is presented in Figs. 3, 4, 5, 6, 7, 8, 9, 10, and 11. The results describe the models with respect to the model architecture, parameters of the model, fuzzy rules and applicability of the models. For each water quality parameter considering the four fuzzy rules (Low–Low, Low–High, High–Low and High–High), the twelve consequent model parameters are determined with the training data and presented in Table 1. Time series plots (Figs. 3a 4a, 5a, 6a, 7a, 8a, 9a, 10a, and 11a) for testing data are of great use in finding the applicability of the models for the water quality parameters under question. The influence of previous load on the present pollutant load is not similar for the pollutants and the pictures presented

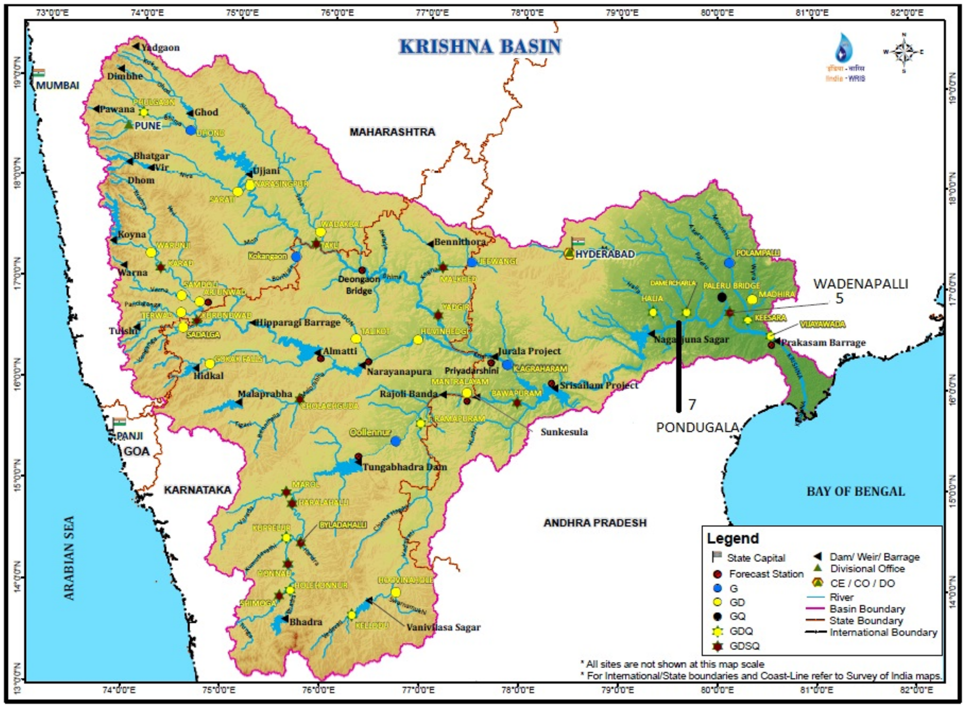


Fig. 2 Location of monitoring stations in the basin

(Figs. 3b 4b, 5b, 6b, 7b, 8b, 9b, 10b, and 11b) indicate the variations for different water quality parameters.

The major dissolved cations (positively charged species dissolved in water) in the river water are sodium (Na), calcium (Ca), and magnesium (Mg). The major anions (negatively charged species) are sulfate (SO_4), chloride (Cl), and bicarbonate (HCO_3). Although most of the cations and anions exist as individual ions dissolved in the river water (as Na^+, Ca^{2+}, Mg^{2+}, $SO_4{}^{2-}$, Cl^-, and $HCO_3{}^-$), substantial concentrations of selected ions are associated with one another (particularly calcium, magnesium, and sulfate which form the dissolved ion pairs $CaSO_4$ and $MgSO_4$). The formation of other ion pairs with sodium and bicarbonates is also quite possible. In lieu of the above discussion, time series plot for sodium, calcium, magnesium, bicarbonates, chlorides and sulpahtes (Figs. 3a, 4a, 5a, 6a, 7a, 8a) indicated good applicability of the ANFIS models in describing the relation between flow and pollutant load. The concentration of dissolved silica, which is reported as SiO_2, is usually in the range 10–24 mg/L in Krishna River water. Essentially all of the silica dissolved in the river water occurs as undissociated silicic acid (H_4SiO_4). Time series plots of silica (Fig. 11a) indicated good applicability of the models. Time series plots for Nitrates (Fig. 9a) did not follow the actual loads closely indicating that the limitation of the model. This is perhaps due to the fact that the formation of nitrate—N in the river takes a long time. With the limited data that was available the developed model for Phosphorous could not explain the relation between flow and load. Hence, the time series plots for phosphorous (Fig. 10 a) were spread all over with out any pattern.

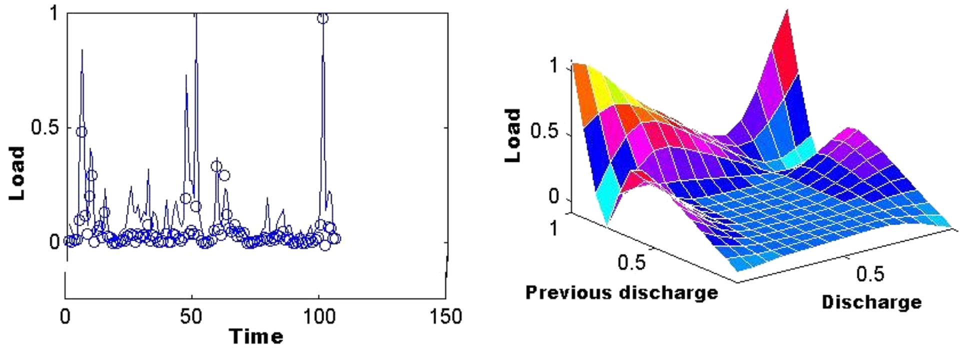
The correlation coefficients (r) and root mean squared Error (RMSE) for training and testing are presented in Table 2. The correlation coefficients between observed and predicted loads during testing phase is observed to be very close to that obtained during training phase for water quality parameters, namely, magnesium, bicarbonates and chlorides. The correlation coefficient for sodium, calcium, sulphates, nitrates and silicates is comparatively lower in testing phase. However, the correlation coefficients obtained for these water quality parameters in both training and testing phases is reasonably satisfactory indicating the applicability of ANFIS model. The correlation coefficients for phosphates both in training and testing phases are very low indicating that the inability of ANFIS to model phosphate loads. The possible reason for this perhaps may be due to trace level phosphate concentrations and hence, very low loads for considerable period of time. The RMSE values presented in Table 2 indicate the errors in computations using the models. For all the parameters except for phosphates the error is small representing good applicability of the developed ANFIS models.

The load variations corresponding to the four rules for the river discharge in the present and previous time intervals (L–L, L–H, H–L and H–H) are presented in Figs. 3b 4b, 5b, 6b, 7b, 8b, 9b, 10b, and 11b. The results presented in the 3-D plots represent a particular possible flow condition during the wet season (low = 1000 m^3/s and high = 5000 m^3/s). However, there can be several such

Table 1 Parameters of ANFIS models

Parameter	Rule	Discharge (X_1)	Previous discharge (X_2)	$Z = pX_1 + qX_2 + r$		
				p	q	R
Sodium	1	Low	Low	−0.19	1.52	−0.03
	2	Low	High	0.98	11.40	−10.29
	3	High	Low	0.32	−1.46	0.06
	4	High	High	−3.31	−10.52	11.42
Calcium	1	Low	Low	−2.39	0.13	−1.81
	2	Low	High	7.09	−0.23	15.86
	3	High	Low	0.07	2.22	2.89
	4	High	High	0.16	2.14	−9.34
Magnesium	1	Low	Low	−0.14	0.63	0.11
	2	Low	High	−1.27	13.40	−9.24
	3	High	Low	0.15	0.93	−0.18
	4	High	High	−0.30	−84.70	65.85
Bicarbonates	1	Low	Low	−3.13	−1.73	−10.04
	2	Low	High	4.98	−18.33	21.35
	3	High	Low	0.01	1.03	0.28
	4	High	High	−0.01	1.47	−0.57
Chlorides	1	Low	Low	2.38	−0.29	0.66
	2	Low	High	−7.44	1.75	−1.93
	3	High	Low	2.90	1.66	−3.47
	4	High	High	−8.48	−0.29	10.16
Sulphates	1	Low	Low	1.43	0.53	0.47
	2	Low	High	2.86	7.23	−4.18
	3	High	Low	1.84	0.41	−2.04
	4	High	High	4.08	−5.89	0.39
Nitrates	1	Low	Low	−0.97	−0.46	1.95
	2	Low	High	1.41	3.87	−2.95
	3	High	Low	−22.75	22.38	−8.28
	4	High	High	27.36	−50.24	17.91
Phosphates	1	Low	Low	0.25	2.58	4.09
	2	Low	High	−1.19	10.52	−11.37
	3	High	Low	7.50	3.077	2.39
	4	High	High	−16.03	21.25	−10.52
Silicates	1	Low	Low	−95.68	29.74	15.09
	2	Low	High	182.10	20.90	−41.15
	3	High	Low	0.033	10.43	3.76
	4	High	High	0.05	13.54	−13.29

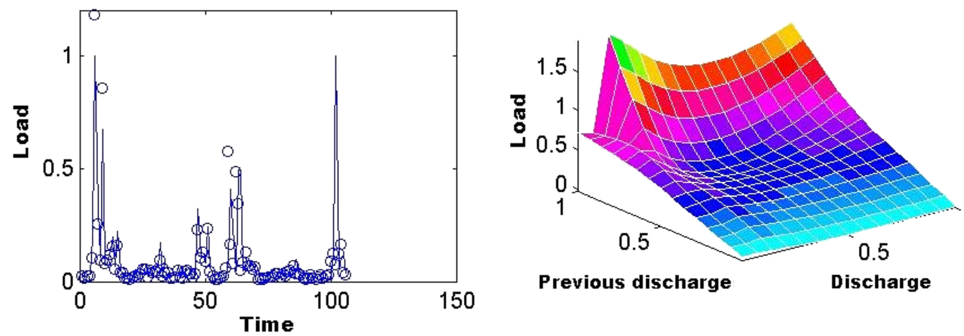
combinations possible in the real situation and hence, the influence varies depending on the flow variations. In general, the influence of low–low and low–high conditions is not considerable on loading pattern. For most part of the wet season the flow conditions are low–low (as flow fluctuates between 1000 m^3/s and about 1500 m^3/s) and this condition indicates lower loading conditions. As the low–low condition is perhaps partial continuation of the earlier flow conditions the influence on load is not significant. Significant effect of the condition low–high (rising stage) is not indicated in the results, as a high of 5,000 m^3/s is reached after considerable period of low–low conditions. This is possibly due to mixing and dilution being dominant in the initial rising stage of the flow. Considerable increases in loading pattern are observed for high–high conditions (at peak flow conditions) in the river. The influence of previous high flow on present high flow represents a real situation similar to doubling the pollutant loads and hence, for all the pollutants the loads at peak flow conditions are quite high. However, the results for high–



(a) Load time series – Testing

(b) Variation of load

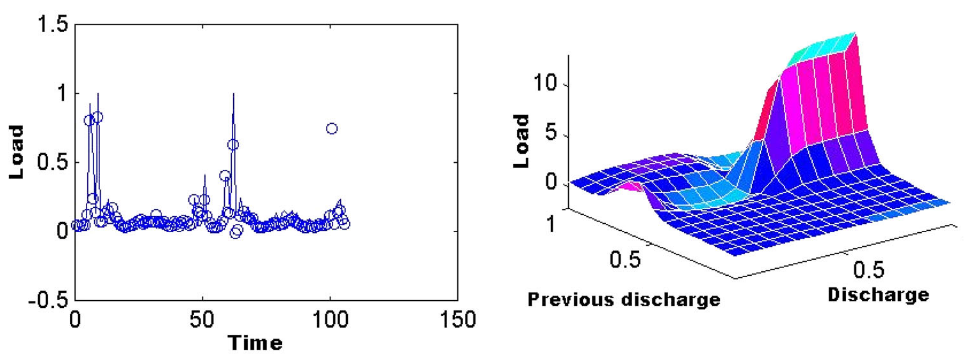
Fig. 3 Results of ANFIS model for sodium. **a** Load time series—testing, **b** variation of loads



(a) Load time series – Testing

(b) Variation of load

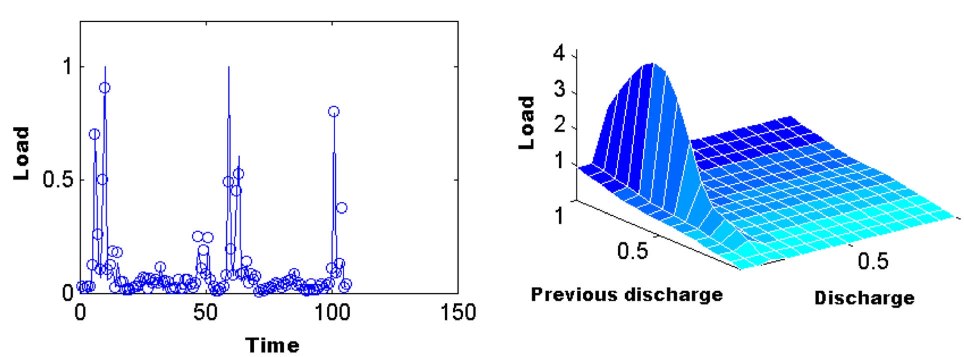
Fig. 4 Results of ANFIS model for calcium. **a** Load time series—testing, **b** Variation of loads



(a) Load time series – Testing

(b) Variation of load

Fig. 5 Results of ANFIS model for magnesium. **a** Load time series—testing, **b** variation of loads

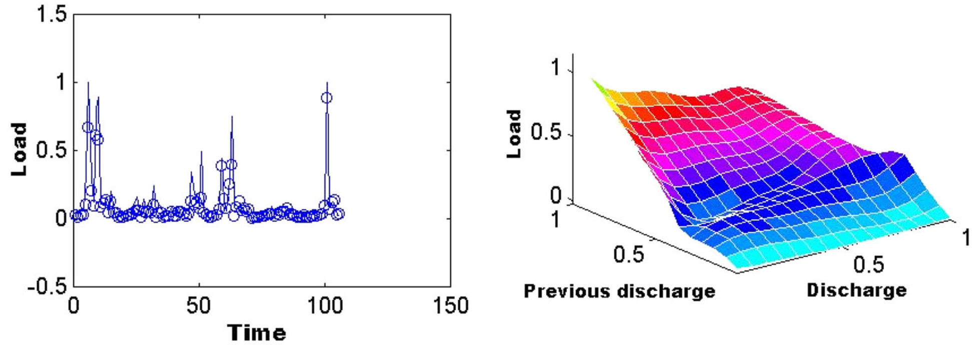


(a) Load time series – Testing

(b) Variation of load

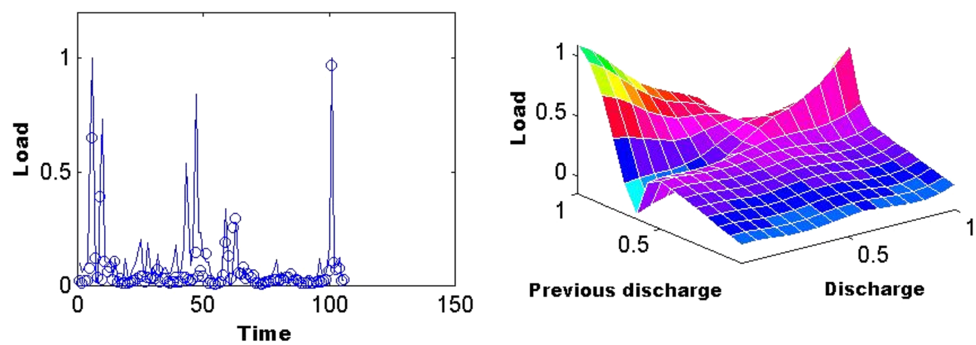
Fig. 6 Results of ANFIS model for bicarbonates. **a** Load time series—testing, **b** variation of loads

Fig. 7 Results of ANFIS model for chlorides. **a** Load time series—testing, **b** variation of loads



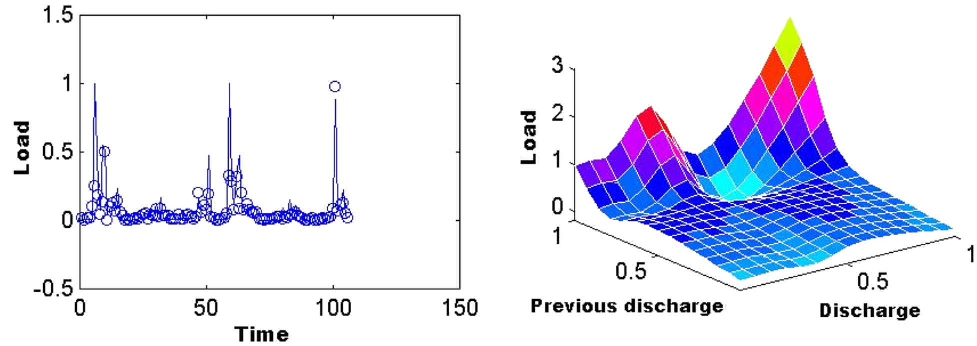
(a) Load time series – Testing **(b)** Variation of load

Fig. 8 Results of ANFIS model for sulphates. **a** Load time series—testing, **b** variation of loads



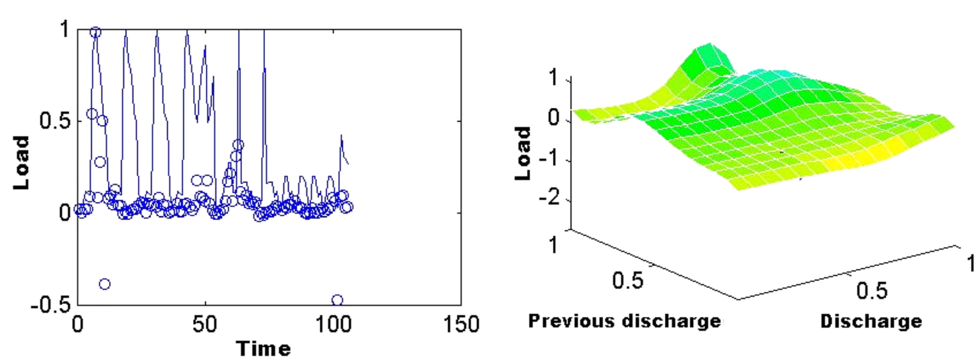
(a) Load time series – Testing **(b)** Variation of load

Fig. 9 Results of ANFIS model for nitrates. **a** Load time series—testing, **b** variation of loads



(a) Load time series – Testing **(b)** Variation of load

Fig. 10 Results of ANFIS model for phosphates. **a** Load time series—testing, **b** variation of loads



(a) Load time series – Testing **(b)** Variation of load

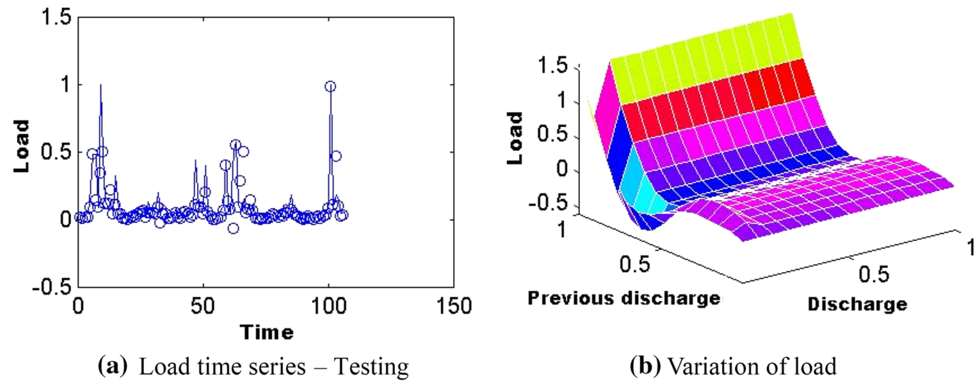


Fig. 11 Results of ANFIS model for silicates. **a** Load time series—testing, **b** variation of loads

Table 2 Validation results of ANFIS models

Parameter	r (training)	r (testing)	RMSE (training)	RMSE (testing)
Sodium	0.98	0.79	0.03	0.14
Calcium	0.99	0.69	0.02	0.13
Magnesium	0.94	0.84	0.06	0.09
Bicarbonates	0.99	0.94	0.03	0.06
Chlorides	0.99	0.95	0.04	0.08
Sulphates	0.99	0.72	0.02	0.14
Nitrates	0.93	0.65	0.05	0.12
Phosphates	0.55	0.30	0.16	0.40
Silicates	0.80	0.76	0.11	0.12

low (falling stage of the river) conditions continue to indicate the influence of previous flow on the present loading conditions. The overall trends represent some delayed effect on loads during the peak flow conditions and during the falling stage of the river after the peak flow. Such trends are possible once or twice in a year during the wet season as such peaks occur once or twice a year.

Conclusion

The modeling approach presented in this paper uses fuzzy inference system to establish the relationships between loads and discharge in the river. Generalized ANFIS models successfully explained the variation in loads for different flow conditions in the river. The peak flow and falling stage conditions indicated the influence of previous flow on the load due to delayed effect in the river reach under study. The correlation coefficients in the range of 0.6–0.9 and low RMSE indicate suitability of the models to the study area. The results presented in this paper clearly indicate that ANFIS approach can be used for forecasting non-conservative dissolved pollutants generally found in river waters. However, the greatest difficulty in using these models can be the inputs used to drive the model. This data driven approach is suggested for situations where model inputs are available. If the model inputs are carefully determined, the size of the network and training time can be reduced. As mathematical relationship between the cause and effect is not necessary in ANFIS models, rule arguments include unknown relationships which are not possible in conceptual models.

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