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Artificial neural network modeling of water quality of the Yangtze River system: a case study in reaches crossing the city of Chongqing*

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Abstract: An effective approach for describing complicated water quality processes is very important for river water quality management. We built two artificial neural network (ANN) models, a feed-forward back-propagation (BP) model and a radial basis function (RBF) model, to simulate the water quality of the Yangtze and Jialing Rivers in reaches crossing the city of Chongqing, P. R. China. Our models used the historical monitoring data of biological oxygen demand, dissolved oxygen, ammonia, oil and volatile phenolic compounds. Comparison with the one-dimensional traditional water quality model suggest that both BP and RBF models are superior; their higher accuracy and better goodness-of-fit indicate that the ANN calculation of water quality agrees better with measurement. It is demonstrated that ANN modeling can be a tool for estimating the water quality of the Yangtze River. Of the two ANN models, the RBF model calculates with a smaller mean error, but a larger root mean square error. More effort to identify out the causes of these differences would help optimize the structures of neural network water-quality models.

Keywords: water quality modeling; Yangtze River; artificial neural network; back-propagation model; radial basis function model

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1 Introduction

The Yangtze River, the largest in P. R. China and the third longest in the world, flows through 10 provinces and autonomous regions of China. It finally enters the East China Sea after running 6 300 km across a catchment of 1.8×10^6 km^2 which covers one fifth of land area of P. R. China [1]. The Yangtze River provides drinking water for 500 million Chinese people and its watershed is home to approximately 40% of P. R. China's GDP (gross domestic product). Considering the great significance of water resource utilization and ecological environment protection in the Yangtze River basin, the environmental protection framework of the Yangtze River [1] was set up early in 1970s, which included a water quality monitoring program, water quality management, and pollution control planning. As the significant basic work of water quality management, where the core issue is the environmental capacity calculation and waste loadings allocation of the Yangtze River basin, water quality models showing the fate and transport of contaminants in the Yangtze River are useful tools.

Traditional mathematical modeling of water quality aims at explaining the fate of different pollutants in both water bodies and sediments with respect to advection, dispersion/diffusion and biogeochemical conversion through rough approximation of the real system [2]. This leads to large, comprehensive and often over-parameterized models difficult to identify

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and with many uncertainties [3]. New modeling approaches, such as non-linear description of water processes, have become popular due to their performance in characterizing complex water quality processes with high accuracy.

In contrast to the biogeochemical conversion process which is primarily considered in water quality modeling of small rivers, hydrological characteristics (advection, dispersion/diffusion, etc.) have been the focus of water quality modeling for the Yangtze River for decades. Two directions have attracted much attention: one is the application of advanced algorithms to solve the hydraulic partial differential equations under various boundary conditions of complexity; and the other aims to identify and calibrate parameters, especially those related to the advection and dispersion/diffusion process in water quality models. To date, there has not been a reported application of artificial neural network (ANN) models to the simulation of Yangtze River water quality. It is therefore worthwhile to try a new modeling approach based on artificial intelligence to simulate the water quality of the Yangtze River.

In this work, we established two one-dimensional (1D) ANN models to represent quantitatively the relationships among major contaminants in the reaches of the Yangtze River and the Jialing River (a tributary of the Yangtze) passing through the city of Chongqing in the upper Yangtze basin. We concentrated on deriving deterministic quantitative relationships among the constituents between different cross sections for the two rivers without complex description of biogeochemical conversion processes in a water column, and comparing the performance of different models.

2 Background and methods

2.1 Study site

Chongqing is a river-girdled city hemmed in between mountains, where an upper reach of the Yangtze River is joined by one of its major tributaries, the Jialing River. This study focused on the trunk streams of the Yangtze River and the Jialing River within the Chongqing Municipality. The length of Yangtze in the study area was 240.8 km from Yangshi in Jiangjin County to Huangcaoxia in Changshou District, flowing through 9 Chongqing Municipality districts. The maximum flow of the Yangtze through the Cuntan cross section was 85 700 m^3/s, and the average annual flow was 11 308 m^3/s [4]. The Jialing River travels 153.8 km in the Chongqing Municipality from Guanyinyan in Hechuan County to Daxigou in the Yuzhong District next to its confluence with the Yangtze at Chaotianmen. The maximum flow of the Jialing at Daxigou was 44 800 m^3/s and average annual flow was 2 120 m^3/s [4]. The Fujiang River is the largest tributary of the Jialing River. In the model, it was simplified as the largest point source of pollution into the Jialing. Fig. 1 shows a map of the study site and the cross sections to be calculated. Basic hydrological data of both rivers are shown in Table 1.

Besides the complex hydrological characteristics of the two rivers, sewage discharge in the study area was rather complicated. The two rivers especially were contaminated traveling through the urban area. Major pollutants came from point sources of industrial and municipal wastewater, added to by the pollution loads from their tributaries and also non-point sources from agriculture and urban runoff [4].

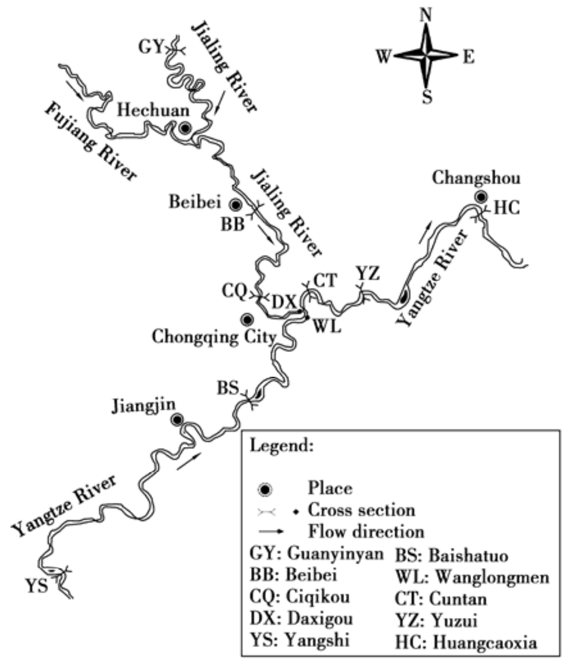

Fig. 1 Map of the study site

2.2 Data source

The Ministry of Water Resources and the State Environmental Protection Administration of P. R. China jointly initiated a long-term river water quality monitoring program for the Yangtze River basin in the 1970s. The water quality data of the Yangtze and the Jialing Rivers used in this study were sourced from the monitoring program in 1989 [4], before the start of the Three Gorges Dam (TGD) Project, which reflected the original hydrological characteristics of both rivers before the interruption of TGD.

Cross sections selected for the Yangtze River monitoring system in the city of Chongqing were at Yangshi, Baishatuo, Wanglongmen, Cuntan, Yuzui and Huangcaoxia, respectively; and those for the Jialing River system were at Guanyinyan, Beibei, Ciqikou and Daxigou (Fig. 1). Concentrations of major pollutants in the two rivers measured in February and August of 1989 were used as typical data of flood season and drought season (Table 1 [4]). Biochemical oxygen demand (BOD), dissolved oxygen (DO), ammonia (NH_3-N), oil and volatile phenolic compounds (Φ-OH) were selected as the water quality variables.

3 ANN modeling

3.1 ANN

The ANN architecture is a massive parallel distributed information-processing system that has certain performance characteristics resembling biological networks of the human brain [5]. Back-propagation (BP) is a type of ANN among the most researched and widely-used structures in hydrology and water-resource problems. It usually comprises three or more layers: an input layer, one or more hidden layers, and an output layer [6-7]. Each layer of BP neural networks is linked by weights that need to be determined through a learning algorithm [8]. The delta-bar-delta (DBD) algorithm is an effective learning algorithm with a self-adapted learning rate and has the advantages of minimizing convergence time and diminishing local extremum vibration in BP neural networks [8].

To obtain fast convergence and avoid local vibration when processing a large number of samples in BP neural networks, a radial basis function (RBF) neural network model was developed [6]. The RBF architecture is similar to that of the BP, but uses a Gaussian Kernel function and consists of only three layers (see Fig. 3) while the BP consists of three or more layers. The RBF neural networks, in theory, provide an effective method for the learning (training), not only showing good performance in convergence, but also avoiding over-fitting. The learning of RBF neural networks is 10^3 to 10^4 times faster than that of a simple BP algorithm. The number of hidden neurons critically affects the performance of RBF neural networks, however [8-10].

3.2 Configuration of neural network models

In this study, we built a BP-DBD neural network model and an RBF neural network model to simulate the water quality in different cross sections. Selection of indicative pollutants in water for both models followed the same procedure as in the traditional river-water-quality model in Ref. [4]. River flow, pollutant retention time, point and non-point pollutant loadings, and upstream pollutant concentration are the most important factors influencing the water quality from the upstream cross section to downstream. As a result, the objective of the neural network model is to establish the functional mapping relationship between upstream and downstream cross sections, which can be described as

$$(\mathrm{Sd}) = f[(\mathrm{Su}),(Q,L,B,t),(q,S)]\,, \tag{1}$$

where Sd is the output of the state variables of the model, i.e., the concentrations of DO, BOD, NH_3-N, Φ-OH and Oil, at downstream cross section; Su refers to the water quality at the upstream cross section, which is regarded as the initial boundary; Q, L, B and t are hydrological parameters of the system, with Q as the river flow in both flood season and drought season in 1989, L the length of the segment, B the average width of the water surface and t the average retention time of constituents; q and S are the pollutant loading forcing functions in the river, with q as the input flow of a tributary and S the overall pollutant loading, including point source and non-point source in the segment during the periods of concern. Structures for BP-DBD and RBF are shown in Figs. 2 and 3.

Table 1 Monitoring data of water quality (WQ) and hydraulic characteristics of the segments in the studied reaches of the Yangtze River and the Jialing River [4]

Period	River	Segment	WQ of upstream cross-section					WQ of downstream cross-section					Segment characteristics				Pollutant loadings in the segment					
			DO /(mg/L)	BOD /(mg/L)	NH_3-N /(mg/L)	Φ-OH /(mg/L)	Oil /(mg/L)	DO /(mg/L)	BOD /(mg/L)	NH_3-N /(mg/L)	Φ-OH /(mg/L)	Oil /(mg/L)	Q /(m^3/s)	L /km	B /km	T /h	q /(m^3/s)	DO /(g/(m d))	BOD /(g/(m d))	NH_3-N /(g/(m d))	Φ-OH /(g/(m d))	Oil /(g/(m d))
Drought Season	Yangtze	YS→BS	8.60	1.10	0.51	0.001	0.10	8.40	1.10	0.55	0.001	0.130	2 990	117.80	0.55	26.64	79.79	41.27	14.93	3.385	0.597 6	2.034
		BS→WL	8.40	1.10	0.55	0.001	0.13	8.50	1.20	0.57	0.002	0.110	3 069	42.00	0.30	14.64	4.92	4.54	109.13	24.393	10.250 0	1.726
		WL→CT	8.50	1.20	0.57	0.002	0.11	8.30	1.50	0.47	0.005	0.100	3 075	8.00	0.35	1.16	675.89	6 701.25	1 456.55	251.538	17.175 0	84.950
		CT→YZ	8.30	1.50	0.47	0.005	0.10	8.40	1.20	0.37	0.001	0.100	4 426	23.00	0.35	4.48	1.58	3.80	3.62	0.709	0.652 2	0.209
		YZ→HC*	8.40	1.20	0.37	0.001	0.10	8.50	1.50	0.36	0.002	0.120	4 428	50.00	0.35	14.77	54.29	48.67	45.50	13.530	2.264 0	1.428
	Jialing	GY→BB	9.30	0.90	0.03	0.001	0.11	9.00	1.60	0.19	0.001	0.040	323	91.80	0.15	34.09	347.53	194.28	45.22	10.932	1.128 5	3.922
		BB→CQ	9.00	1.60	0.19	0.001	0.04	8.70	1.30	0.27	0.001	0.100	671	47.00	0.20	25.62	e5.36	4.33	7.13	2.583	1.014 9	0.262
		CQ→DX	8.70	1.30	0.27	0.001	0.10	8.60	2.00	0.38	0.001	0.100	676	15.00	0.20	12.32	0.00	0.00	222.64	32.333	1.606 7	7.033
Flood Season	Yangtze	YS→BS	7.50	3.00	0.41	0.001	0.09	7.00	0.60	0.53	0.001	0.110	17 200	117.80	0.80	16.38	274.43	177.68	53.01	13.175	2.660 0	6.065
		BS→WL	7.00	0.60	0.53	0.001	0.11	7.40	0.80	0.44	0.001	0.030	17 474	42.00	0.70	7.84	14.71	19.14	129.95	21.912	10.386 0	10.862
		WL→CT	7.40	0.80	0.44	0.001	0.03	7.50	0.90	0.56	0.001	0.040	17 489	8.00	0.70	0.95	39.39	2 587.50	3 858.70	1 650.200	43.738 0	450.326
		CT→YZ	7.50	0.90	0.56	0.001	0.04	7.30	1.00	0.34	0.001	0.060	21 467	23.00	0.70	2.22	5.41	19.74	7.27	0.367	0.652 1	0.273
		YZ→HC*	7.30	1.00	0.34	0.001	0.06	7.20	0.90	0.37	0.001	0.100	21 743	50.00	0.80	6.89	189.89	218.54	83.40	22.482	2.824 0	8.598
	Jialing	GY→BB	7.20	0.80	0.37	0.002	0.02	6.80	1.40	0.35	0.002	0.030	1 990	91.80	0.40	18.66	1935.5	199.40	298.71	101.676	3.180 8	68.599
		BB→CQ	6.80	1.40	0.35	0.002	0.03	6.60	1.20	0.41	0.001	0.040	3 926	47.00	0.60	14.02	13.36	30.90	18.43	2.538	1.963 8	0.621
		CQ→DX*	6.60	1.20	0.41	0.001	0.04	6.40	1.30	0.49	0.003	0.050	3 939	15.00	0.50	7.84	0.00	0.00	228.30	32.680	1.606 7	7.033

Notes: Data sourced from the Scientific and Technical Report of the Water Pollution Control Planning of the Chongqing City Reach of Yangtze River and the Jialing River, 1992 [4]

YS, BS, WL, CT, YZ, HC, GY, BB, CQ and DX stand for the locations of cross sections at Yangshi, Baishatuo, Wanglongmen, Cuntan, Yuzui, Huangcaoxia, Guanyinyan, Beibei, Ciqikou and Daxigou, respectively; Q, L, B and T refer to the flow, the length and the width of the segment, and the hydraulic retention time of the pollutant in the segment; q is the input flow of tributaries in the segment, BOD the biochemical oxygen demand, DO the dissolved oxygen, NH_3-N the ammonia nitrogen, and Φ-OH the volatile phenolic compounds.

Data of asterisked segments were used in the validation of the neural network models but not in the parameter estimation.

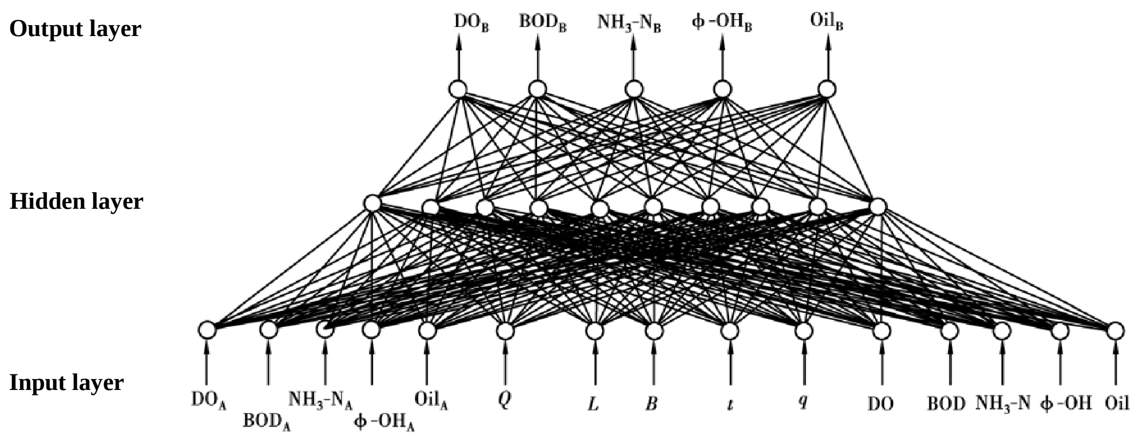

Fig. 2 Neural network model structure for BP-DBD (back probation–delta-bar-delta), where BOD is the biochemical oxygen demand; DO the dissolved oxygen; NH3-N, the concentration of ammonia nitrogen; Oil, the concentration of oils; and Φ-OH, the concentration of volatile phenolic compounds; the subscript A refers to the variables in the input layer and the subscript B, the variables in the output layer

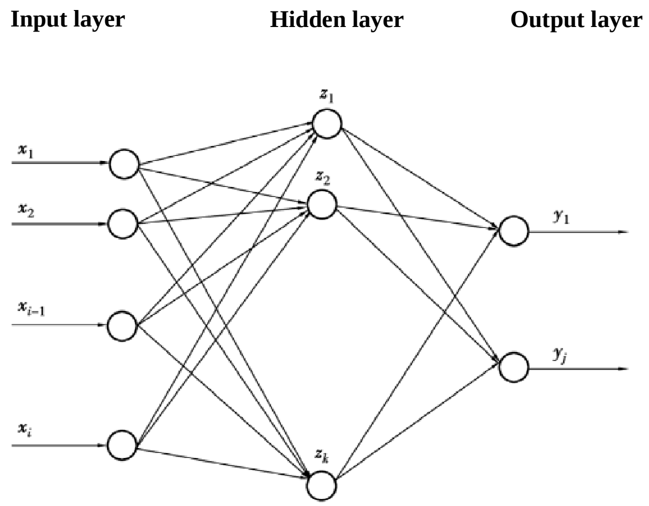

Fig. 3 Sketch of neural network model structure for radial basis function (RBF), where x_1, x_2, x_{i-1} and x_i are the variables in the input layer, y_1 and y_j are the variables in the output layer; and z_1, z_2 and z_k are the variables in the hidden layer

Several segments in the Yangtze and Jialing Rivers were defined for simplifying the complexity of the physical boundaries of natural water bodies. Each segment was assumed to be of the same physical characteristics, including hydraulic gradient and boundary condition, but in modeling was regarded as an independent unit, linking end-to-end in series to create a single spatial step during the calculation of water quality.

In this study, the target sections of the Yangtze and Jialing Rivers were divided into 5 and 3 segments, respectively, based on the water quality monitoring data. Water quality at the upstream cross section in a segment, hydrological characteristics and pollutant loadings between two neighboring cross sections of one segment were regarded as the input of the neural network model, and the output was the water quality at the downstream cross section of the segment (see Fig. 4). Sixteen groups of the water quality data samples and the hydrological characteristics in both flood season and drought season of the 8 segments are listed in Table 1. In these data samples, 3 groups were used for validation but not for training and parameter estimation, i.e., the data of the segment of the Yangtze River between Yangshi and Baishatuo in both flood and drought seasons and the data of the segment of the Jialing River between Ciqikou and Daxigou in the flood season, and the other 13 groups were used in the training for both BP-DBD and RBF neural network models.

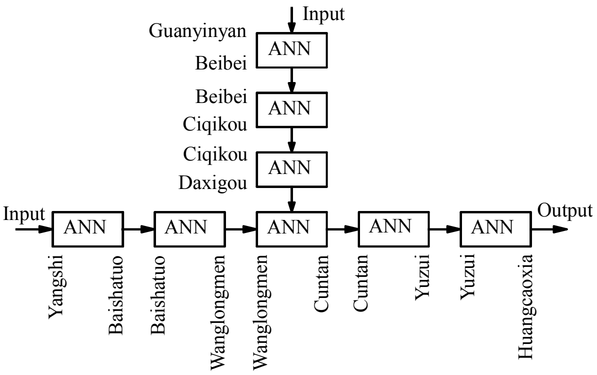

Fig. 4 Segmentation of the Yangtze between Yangshi and Huangcaoxia and of the Jialing between Guanyinyan and Daxigou in ANN (artificial neural network) modeling

3.3 Implementation and performance evaluation of the neural network models

Both the BP-DBD and RBF neural network models of the reaches of the Yangtze and the Jialing passing through the city of Chongqing were implemented using Matlab 6.0 (www.mathworks.com). In the BP-DBD model, the initial weight matrix, the threshold matrix of the neural network, and the momentum factors were all set to equal 0.1.

In the RBF neural network model, the number of neurons in the input layer was 15, the output layer had 5 neurons, and the initial number of neurons in the hidden layer was set at 9. The first 4 training samples in Table 1 were used as the centers for RBF. The initial parameter in normalization was set at 0.1, and maximum number of iterative times was 1 000, the learning accuracy was set at 0.001, and other parameters in the neural network were set according to the defaults in Function Newrb in the Matlab tool box for neural network models.

The simulation results of the BP-DBD and RBF neural networks were compared with traditional water quality modeling in Ref. [4]. Performance of these 3 models were evaluated by 3 efficiency parameters: correlative coefficient (R^2), the mean error (ME), i.e., the systematic difference between the estimated and measured data, and the measure of goodness-of-fit, root mean square error (RMSE) calculated by [11]

$$\mathrm{RMSE} = \sqrt{\frac{1}{MN}\sum_{m=1}^{M}\sum_{n=1}^{N}\left[\hat{Y}_{mn} - Y_{mn}\right]}, \tag{2}$$

where M is the number of estimated output; N is the number of samples; $\hat{Y}_{mn}$ is the m-th estimated output value of the n-th sample; Y_{mn} is the m-th actual output value of the n-th sample. The performance of a model is more precise with R^2, ME and RMSE closer to 1, 0 and 0, respectively.

4 Traditional water quality modeling

The 1D water quality model [4] was a steady state model. A modeled segment was regarded as a continuously stirred-tank reactor (CSTR), and the entire study site was regarded as a thoroughly mixed system of linked CSTRs. The state variables included 5 quality indicators: BOD, DO, NH_3-N, oil content and Φ-OH.

In the 1D steady state water quality model, we used the same monthly water-quality data and hydrological characteristics of the study site coming from the Sino-British science program: Water Pollution Control Planning of the Chongqing City Reach of Yangtze River and Jialing River performed in 1992 [4]. We set the attenuation rate at 0.1 for BOD and ammonia nitrogen, and at 0.001 for oil content and Φ-OH content based on previous research [4].

5 Results and discussion

5.1 Comparison of BP-DBD and RBF models with 1D traditional water quality model

Table 2 gives the final network characteristics of both BP-DBD and RBF neural network models, while Fig. 5 shows the performance efficiencies (i.e., R^2, ME and RMSE).

Table 2 Final network characteristics of the BP-DBD and RBF neural networks

Model	Number of neurons in a layer			Number of iterations
	Input	Hidden	Output	
BP-DBD	15	10	5	4 700
RBF	15	13	5	267

Among the BP-DBD, RBF and 1D traditional water quality models, the BP-DBD and RBF neural network models achieved higher accuracy and better correlative performance than the 1D tradition water quality model (Fig. 5). The ME and RMSE values of both BP-DBD and RBF neural network models for each of the 5 water quality indicators were smaller, especially those for NH_3-N, Oil and Φ-OH. The overall RMSEs of BP-DBD and RBF were also much smaller than the overall RMSE of 1D, with their values equal to 0.106 00, 0.121 24, and 0.243 62, respectively.

The traditional water quality model aims to describe the purification process of water. Nevertheless, when applied to large water bodies, the model delivers no discernible response to the pollutant loadings, leaving no clear “signal” with which to calibrate the model [12]. This was the case of the study reaches of the Yangtze and the Jialing Rivers, for which the responses of the model to the loadings of the foregoing mentioned five indicators were unclear, lacking DO depletion or “DO sag”. This potential impediment resulted in the poor performance of the traditional water quality model.

On the other hand, neural network models seek to build up black box models representing the potential relationship between water qualities of natural water bodies without considering the complex biochemical process in water. This modeling approach avoids error propagation and uncertainty generation in the model structure, parameter estimation and calibration in traditional water quality model. Therefore, higher accuracy and goodness-of-fit in a black box model can be expected.

5.2 Comparison between BP-DBD and RBF models

Both the BP-DBD and RBF neural network models performed well. The RBF neural network required fewer iterative times, however (Table 2). This is the primary advantage of an RBF neural network model, which is credited to the distinct functional framework of this type of network.

Both the BP-DBD and RBF models yielded high accuracy in the estimation of water quality at the downstream cross section of a segment. As the concentration of Φ-OH and oil were at a relatively low level in both drought and flood seasons, however, there remained no significant differences in the MEs of Φ-OH and oil between the BP-DBD and RBF neural networks. Nevertheless, for the other 3 indicators, DO, BOD and NH_3-N, the RBF neural network achieved a higher accuracy than the BP-DBD neural network model.

Both the neural networks model fitted well with the measured data in the form of R^2 and RMSE, though some differences remained. For both BOD and DO, the higher R value of the BP-DBD model, corresponding to the smaller RMSE, showed that BP-DBD model performed better than the RBF model in the estimation of DO and BOD (see Table 4 and Fig .4), whereas the results of the other 3 constituents were contrary. Although the differences between the performance of the BP-DBD and RBF models were small, the results remain interesting.

Moreover, evaluating the overall performance of both ANN models with RMSE calculated by Eq. (2), revealed that the goodness-of-fit of BP-DBD for the whole water quality model was better than that of RBF, seeing the smaller RMSE value of BP-DBD.

The performance of ANN models is sensitive to model structure (e.g., spreads for RBF), data inputs and ANN connective initial weight matrix [13]; all have the potential to contribute to differences in performance of the BP-DBD and RBF models. More effort is needed to identify which factor affects most the water quality simulation with a neural network approach.

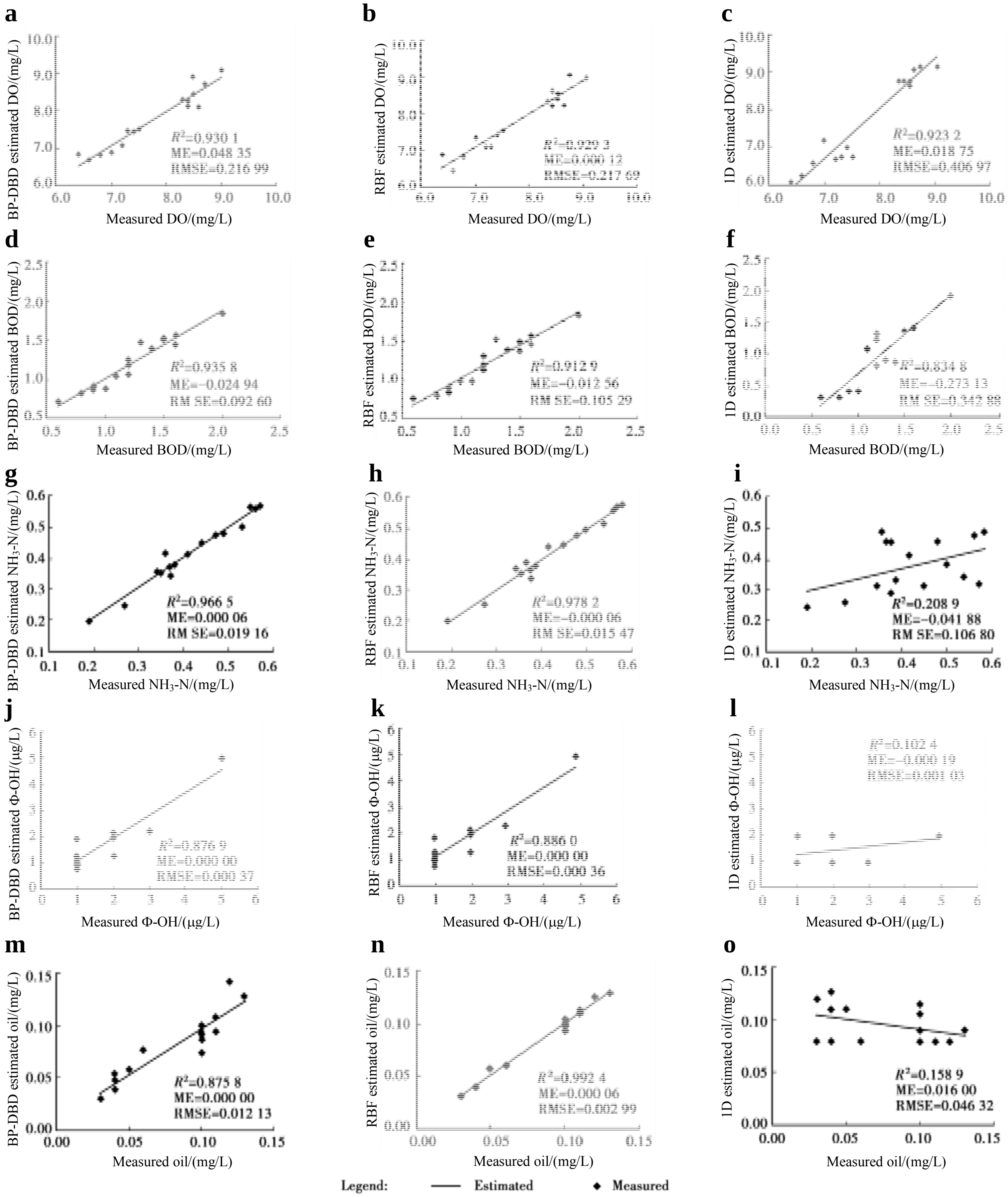

Fig. 5 Correlative coefficient (R^2), mean error (ME), and root mean square error (RMSE) of the BP-DBD (back-propagation delta-bar-delta) and RBF (radial basis function) neural networks and one-dimensional (1D) tradition water quality model for (a), (b) and (c) BOD (biochemical oxygen demand); (d), (e) and (f) DO (dissolved oxygen); (g), (h) and (i) NH_3-N (ammonia nitrogen); (j), (k) and (l) Φ-OH (volatile phenolic compounds); and (m), (n) and (o) oil

6 Conclusions

The BP-DBD neural network model and RBF neural network model established for simulating water quality of the reaches of the Yangtze and Jialing Rivers crossing Chongqing were proven to be advantageous over the 1D traditional water quality model for higher accuracy and better goodness-of-fit. Of the two ANN models, the RBF needed fewer iterations and achieved a higher accuracy. Nevertheless, the results for the R^2 and RMSE for individual quality indicators and the overall quality indicated that the RBF neural network model performed no better than the BP-DBD. More effort is needed to identify the factors that considerably affect the simulation of water quality based on neural network approaches.

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