

Regional optimal allocation for reducing waste loads via artificial neural network and particle swarm optimization: a case study of ammonia nitrogen in Harbin, northeast China

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ABSTRACT

Cutting external waste loads can improve water quality. Allocation for reducing waste loads should consider changing variables, such as river flows and pollutant emissions. A particle swarm optimization (PSO) method and coupling artificial neural network (ANN) models have been applied to optimize reduction rates of ammonia nitrogen (NH₃-N) loads from sewage outlets in Harbin, northeast China. For the planned water quality functional section (WQFS), the NH₃-N concentration is related to emitted pollutant loads and can be well predicted by ANN linkage models. Further, NH₃-N load reduction rates of all outlets are optimized by PSO with the water quality standard target. The highest NH₃-N concentrations occur in January and February, a typical low-flow period in Harbin. The results delivered optimum NH₃-N reduction rates for the five outlets, for January and February 2011. All predicted NH₃-N concentrations after the reduction meet the water quality standard. The results indicate that the outlet with the highest NH₃-N load has the biggest reduction rate in each WQFS, and outlets in the WQFS with higher background NH₃-N concentrations need to cut more NH₃-N loads. Decision-makers should not only focus on the outlet with the highest NH₃-N emission load, but also ensure that the NH₃-N concentration of upper WQFS meets the water quality goal.

Key words | ammonia nitrogen, artificial neural network, particle swarm optimization, waste load control, water quality management

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INTRODUCTION

Surface water pollution has been a serious problem due to rapid industrial development, population growth and urbanization in the last decades in China (Yang *et al.* 2008). The main solution to this problem is to reduce external waste loads and to limit untreated direct discharges from point or non-point sources. Many studies indicate that water quality management practices can significantly improve water quality (Maeda *et al.* 2010; Zhao *et al.* 2014).

The Ministry of Environmental Protection of the People's Republic of China is primarily applying a total maximum loads control strategy (TMLCS) to allocate waste loads. The aim of TMLCS is to limit the maximum amount of pollutants in a water quality functional section (WQFS), resulting in water quality that can meet the national standard (Chang & Wang 2010). In the TMLCS, assimilative capacity of receiving river water is simply obtained from river flow multiplied by the water quality

standard (i.e., numerical concentration standard). Low flow is commonly used to evaluate the assimilative capacity, and the TMLCS supposes pollutant discharge is uniform all the time. Consequently, water quality violations often arise when more pollutants are discharged into rivers in low-flow periods (Kim *et al.* 2008), although the total pollutant load has achieved the TMLCS goal within the planned year (Zhao *et al.* 2011). Thus, the allocation for cutting waste loads should be considered and designed dynamically, based on the changing assimilative capacity of river water, to meet the water quality standard.

Like allocation of waste loads, the allocation for cutting waste loads to river water is also a critical issue. Many researchers have studied the allocation strategy, such as equal proportion allocation, economic contribution allocation (Deng *et al.* 2011), programming model (Xie *et al.* 2011) and analytic hierarchy process method (Bottero *et al.*

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2011). However, these approaches suffer from experts' subjective preferences and may not produce objective results for loads reduction allocation because they are focused on economic factors rather than on the relationship between waste loads and water quality. Water quality models have played an important role in linking pollution sources and water quality, whereas mechanism models, such as WASP (Water Quality Analysis Simulation Program) (US EPA 2013) and MIKE (DHI 2013), usually need significant amounts of complicated hydraulic and hydrological parameters and they are difficult to calibrate. Compared with them, artificial neural networks (ANNs) have been proposed as an efficient data-driven tool for environmental modeling in recent years (May & Sivakumar 2009; He *et al.* 2011), mainly because of their capability to treat nonlinear and complicated environmental problems. Kuo *et al.* (2006) used ANN models to simulate the behavior of nutrient loads into reservoirs. The authors proved that the ANN model could successfully predict pollutant concentration in the water body, based on watershed waste loads data.

Allocating the reduction of waste loads is essentially an optimization project. Therefore, the particle swarm optimization (PSO) method is an important branch of stochastic techniques to explore the problem space for searching the optimization (Kennedy & Eberhart 1995). The population-based evolutionary PSO method had stable convergence and can generate a robust solution within a shorter calculation time in comparison with other stochastic methods (Afshar 2012). Moreover, the significant advantage was solving nonlinear and highly complex problems without gradient techniques (Ho *et al.* 2006). The PSO method has been applied successfully to management problems with a searching optimal strategy by several researchers (e.g., Mategaonkar & Eldho 2012). Therefore, the adoption of PSO for dynamic water quality management, which demanded a fast, stable, robust solution, appeared to be appropriate and effective for optimizing the allocation for reducing waste loads.

Harbin City is the capital of the Heilongjiang Province. The Songhua River flows across the downtown of Harbin City and merges with two tributaries (i.e., the Ashen River and the Hulan River) in the Harbin region (Figure 1). In this area, precipitation is concentrated from June to September, accounting for 85% of annual rainfall. The annual mean temperature is 5–10 °C and the temperature is positively correlated with river flows (Figure S1(b), available online at <http://www.iwaponline.com/wst/070/348.pdf>). A thick ice layer and low temperature lead to high NH₃-N concentrations in the icebound period, which usually lasts for 4 months. Harbin has been facing the fact that the

concentrations of ammonia nitrogen (NH₃-N) in most WQFSs were found to highly exceed their permitted national water quality standard in winter months (Figure S2, available online at <http://www.iwaponline.com/wst/070/348.pdf>).

The mean values in Table S1 (available online at <http://www.iwaponline.com/wst/070/348.pdf>) show that pollution sources discharge excess pollutant, resulting in the mean value of NH₃-N concentrations violating their water quality standard grades in most stations. One part of the NH₃-N loads came from point sources, such as industries, and sewage treatment plants in Harbin City; another part were from non-point sources, like livestock, land disposal of waste and agriculture activities. Thus, an optimal allocation method for cutting NH₃-N loads is developed in this paper. The method covers the PSO loop procedure and the ANN linkage model between NH₃-N loads and water quality. Using the output of this method, we expect to provide some constructive suggestions to decision-makers for controlling NH₃-N loads in the Harbin region.

METHODS

Artificial neural network

In this research, ANN models include a three-layer feed-forward system trained with a back propagation algorithm. This is introduced in the Supplementary information, available online at <http://www.iwaponline.com/wst/070/348.pdf>. ANN models are trained with 1–15 hidden nodes and the model with the least MSE value is chosen as the optimum model. The target goal MSE and the maximum epochs of all ANN models are set to 10⁻⁵ and 1,000, respectively. Training stops when any of the two conditions occur.

ANN variables and data collection

Two input variables were selected for ANN models. One is the NH₃-N concentration at the beginning of the objective WQFSs, which interprets the natural background value of NH₃-N concentration in this WQFS. Another represents the external NH₃-N loads to this WQFS. The output variable of ANN is NH₃-N concentration at the end of the objective WQFS. The ANN variables are shown in Table 1.

The 7 year (2005–2011) monthly NH₃-N concentration (mg/L) data, including five sewage outlets and three monitoring stations, were collected by the Environmental Monitoring Center of Harbin City. For a sewage outlet, the monthly NH₃-N load (LC, g/s) is calculated by multiplying

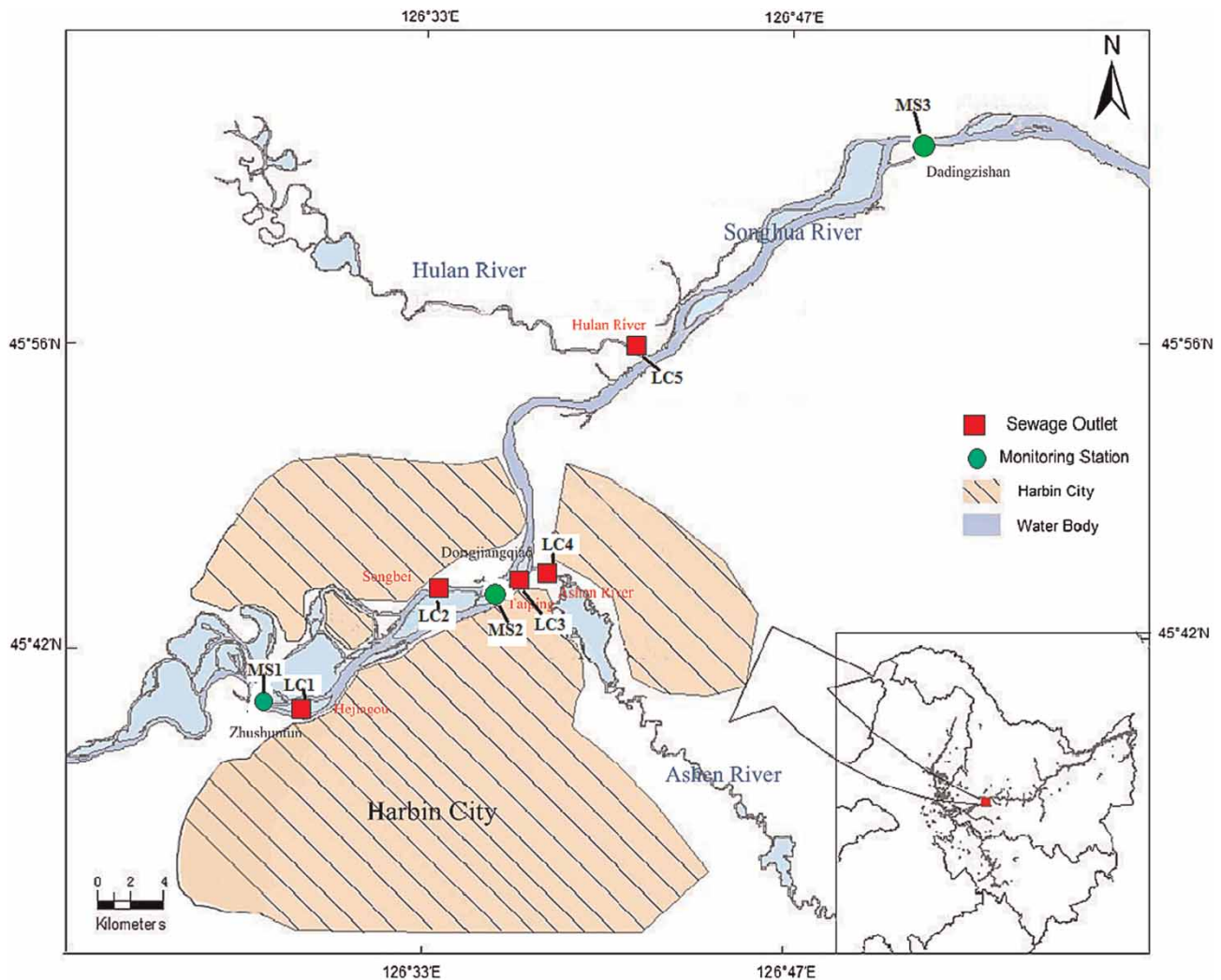


Figure 1 | Map and location of the Songhua River, Harbin region, indicating the monitoring stations and the outlets.

Table 1 | The input and output variables of ANN models

Functional section	Variable ^a	Symbol	
WQFS1	Input	NH ₃ -N concentration of Zhushuntun station	MS1
	Output	NH ₃ -N loads from Hejiagou outlet	LC1
		NH ₃ -N loads from Songbei outlet	LC2
WQFS2	Input	NH ₃ -N concentration of Dongjiangqiao station	MS2
		NH ₃ -N loads from Taiping outlet	LC3
		NH ₃ -N loads from Ashen River	LC4
		NH ₃ -N loads from Hulan River	LC5
	Output	NH ₃ -N concentration of Dadingzishan station	MS3

^aThe output data corresponding to the input variables belong to the same water sample, thus measured at the same time, *t*, and space.

its monthly NH₃-N concentration and its monthly average emission flow. The basic statistics of the previously mentioned variables are presented in Table S1. In addition, the field data are divided into training and testing subsets for each WQFS. Two subsets include 60 (for years 2005–2009) and 24 (for years 2010–2011) samples, respectively.

Modeling performance evaluation

Nash–Sutcliffe efficiency (NSE) and root mean squared error proportional (RMSEP) are used to evaluate the accuracy of the bootstrap neural networks. The NSE (Equation (1)) has a statistical character to measure the difference between the predictions and the mean of observations (Nash & Sutcliffe 1970). The value of NSE ranges from $-\infty$ to 1, in which the value closer to 1 represents a better fit of the model. The

RMSEP (Equation (2)) provides statistical information about the effects of root mean square error on observations. The values of RMSEP vary from 0 to $+\infty$ and lower value indicates a higher accuracy. In this paper, the forecasting is considered satisfactory if the NSE is not less than 0.5 as well as the RMSEP being not more than 0.4

$$\text{NSE} = 1 - \frac{\sum_{i=1}^N (t_i - y_i)^2}{\sum_{i=1}^N (t_i - \bar{t}_i)^2} \quad (1)$$

$$\text{RMSEP} = \frac{1}{\bar{t}_i} \sqrt{\frac{\sum_{i=1}^N (t_i - y_i)^2}{N}} \quad (2)$$

where t_i and y_i are the i th observations and predictions, respectively; \bar{t}_i is the mean of the observations; N is the number of observations in testing sets.

Optimization procedures

Objective function

To ensure the water quality target, the main constraint considered is that the value of $\text{NH}_3\text{-N}$ concentration must be smaller than that of the expected water quality standard. The objective function is the minimum of sum of the waste load reduction rate, which means the minimum treatment level or investment. For each WQFS, the goal of the minimum cost is summarized as

$$\text{Minimum } Z = \sum_{i=1}^n r_i \quad (3)$$

subject to

$$\text{MS}_t^{\text{out}} = f_{\text{ANN}}(\text{LC}_{i,t}(1 - r_{i,t})) \forall i, t \quad (4)$$

$$\text{MS}_t^{\text{out}} \leq \text{MS}^{\text{Grade}} \forall t \quad (5)$$

$$0 \leq r_i \leq 1 \forall i \quad (6)$$

where Z represents the total investment; r_i is the waste load reduction rate of the i th sewage outlet; $\text{LC}_{i,t}$ is the waste load of i th sewage outlet in the t th month; MS_t^{out} is the predicted $\text{NH}_3\text{-N}$ concentration of the ANN model in the t th month; MS^{Grade} is the planned value of water quality standard in this WQFS; n is the total number of the sewage outlets. For example, n is 2 for WQFS1 and 3 for WQFS2.

In the above equations, Equation (3) is the target function for optimization. Equation (4) is the input–output constraint supported by ANN models. Equation (5) is the main constraint for controlling water quality. Equation (6) is the constraint for technique or economic investment, with the assumption that the investment is linear with the waste load cutting rate.

Particle swarm optimization

The PSO algorithm is shown in the Supplementary information (available online at <http://www.iwaponline.com/wst/070/348.pdf>). In velocity change Equation (S4), the inertia weight w regulates the balance of local and global search ability. Larger w facilitates the global search while a small one enhances the local search; so there would be much better performance by reducing w (Equation (7)) (Ko et al. 2007, 2009)

$$w(t) = w_{\min} + \left(\frac{\text{iter}_{\max} - t}{\text{iter}_{\max}} \right)^a (w_{\max} - w_{\min}) \quad (7)$$

where t is the current iteration; iter_{\max} is the maximum iteration; a is the learning rate; w_{\max} and w_{\min} are the maximum and minimum inertia weight.

Based on previous research (Ko et al. 2007; Vasumathi & Moorthi 2012), the other important parameters such as size of swarm, maximum velocity, maximum iteration and acceleration constants are shown in Table S2 (available online at <http://www.iwaponline.com/wst/070/348.pdf>).

Optimizing the objective

The proposed ANN models, deployed as the forecasting module, were embedded in the PSO procedure to generate the optimal reduction rates for waste loads (see Figure 2).

For managing a WQFS in month Tm , the optimizing procedure executes as follows:

- (1) Train and validate the ANN models to predict the objective $\text{NH}_3\text{-N}$ concentration. Calibrated ANN models will be proposed.
- (2) Forecast the objective $\text{NH}_3\text{-N}$ concentration with all crucial variables of the month Tm . Waste loads should be reduced if the MS^{out} is greater than the MS^{Grade} .
- (3) Generate the particles randomly and test for their respective fitness by calculating Equation (3) in the PSO procedure. The lower the objective function value is, the higher is the fitness.

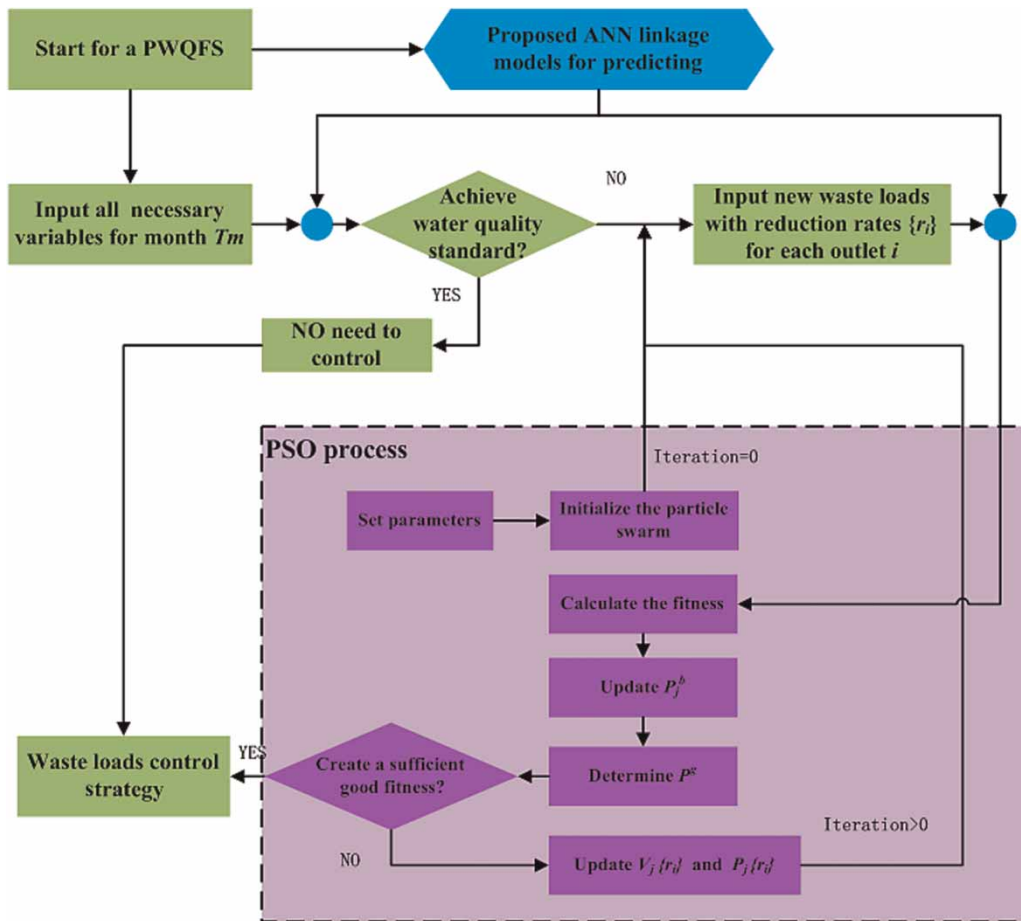


Figure 2 | Flowchart of the ANN-PSO procedure for optimizing the objective. The PSO searches the optimal reduction scheme while the predicted water quality by ANN can meet the planned standard.

- (4) Repeat the following steps until a sufficiently good fitness has been created.

For each particle j :

- Change the ANN input variables of waste loads from LC_i to new $LC_i(1-r_i)$ based on the current position $P_j \{r_i\}$.
 - Predict the objective $\text{NH}_3\text{-N}$ concentration using the step (1) ANN. Go to the step (c) if the MS^{out} is smaller than the MS^{Grade} .
 - Calculate the fitness according to Equation (3).
 - Update particle's best position P_j^b .
 - Determine the global best position P^g .
 - Calculate particle's new velocity $V_j \{r_i\}$ according to Equation (S4).
 - Calculate particle's newfound position $P_j \{r_i\}$ according to Equation (S5).
- (5) Output and record the optimal reduction rates combination strategy (P^g).

RESULTS AND DISCUSSION

ANN linkage models

The RMSEP < 0.4 and NSE > 0.5 for the best ANN models were fulfilled (see Table S3, available online at <http://www.iwaponline.com/wst/070/348.pdf>), suggesting the two ANN models were satisfactory for the two WQFSs. Figure 3 reveals that an acceptable agreement between the observations and the predictions has been achieved. However, some predictions for WQFS2 were underestimated (Figure 3(b)), especially in low-flow months (i.e., from January to March). Tiwari & Chatterjee (2010) found a similar underestimate by ANN, and they explained it as a systematic shift. However, larger underestimates are seen from May to July in 2010, which can be attributed to the $\text{NH}_3\text{-N}$ loads from non-point sources in WQFS2. There was abundant precipitation from May to July in 2010 and there are large areas of farmland along the river in downstream WQFS2. It is

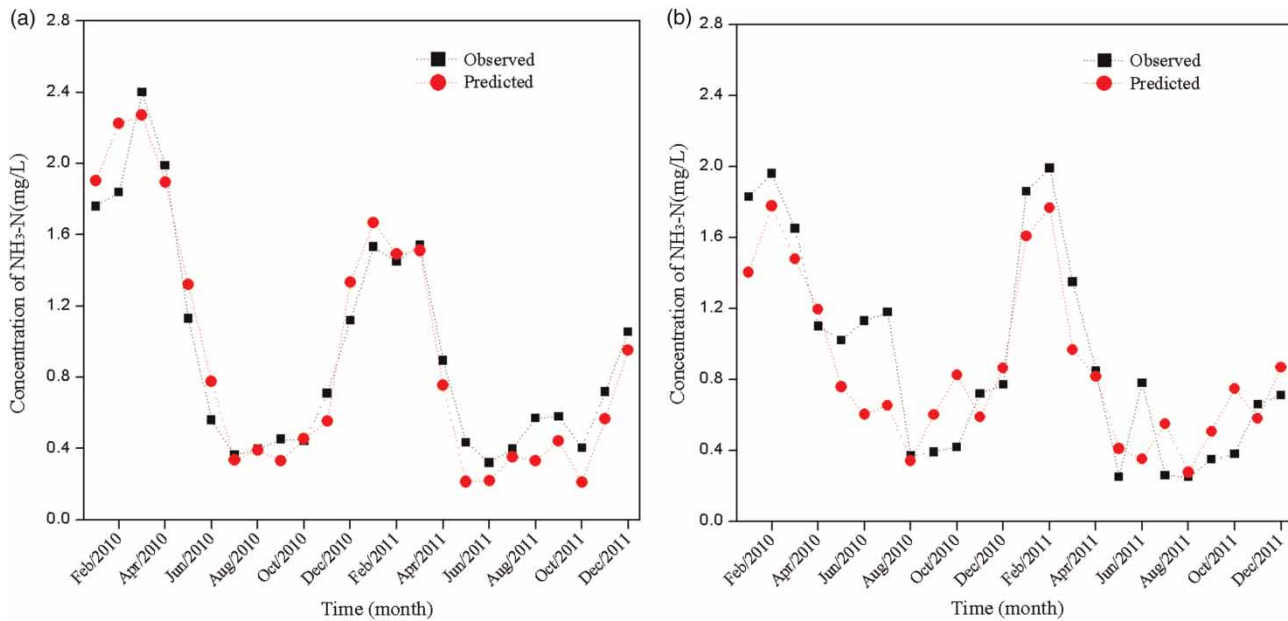


Figure 3 | Comparison of the ANN model predicted and observed $\text{NH}_3\text{-N}$ concentrations for (a) WQFS1 and (b) WQFS2.

inevitable that extra loads from the non-point source are brought into the river by the precipitation in this period.

Note that oscillation of data-driven models may lead to noteworthy mistakes, such as the phenomenon that the predicted $\text{NH}_3\text{-N}$ concentration increases when reducing the input $\text{NH}_3\text{-N}$ loads. Considering the stability of the proposed ANN model, the same r_i , from 0 to 0.9, is assigned to all sewage outlets and the model output is analyzed. Figure S3 (available online at <http://www.iwaponline.com/wst/070/348.pdf>) presents the predicted $\text{NH}_3\text{-N}$ concentration with different reduction coefficient r_i for all sewage outlets. The predictions of three typical-period months are all decreasing when increasing r_i and the output is stable in 2011. It indicates that the ANN approach can successfully link the controlled (i.e., $\text{NH}_3\text{-N}$ loads) and objective variables (i.e., $\text{NH}_3\text{-N}$ concentration). Also, we have to point out that the $\text{NH}_3\text{-N}$ loads are all assumed to be from point sources in this study; so ANN would be available if the loads from non-point or diffuse pollution sources could be handled as input variables of ANN models.

Optimum reduction rate for meeting water quality standard

The optimization procedure was executed for 12 months in 2011. In WQFS1, the LC1 and LC2 ought to be reduced only if the predicted MS2 was bigger than 1.0 mg/L. The water quality from MS2 severely violated the Grade III

water quality standard. Figures 4(a) and 4(b) show the optimum $\text{NH}_3\text{-N}$ load reduction rates scheme P^g by PSO in January and February. It is shown that the optimal initialized reduction rates combination P^g for LC1 and LC2 is randomly formed as $P^g(1) = \{P_1^g = 0.8439, P_2^g = 0.5208\}$. The PSO converges initial particles through N iterations, directed by the goal of achieving better fit. Then it finds the near-optimum $\text{NH}_3\text{-N}$ load reduction rates systematically and finally obtains the convergence at iteration $t=22$ (Figure 4(a)) with the predicted 0.9978 mg/L of the MS2. The optimum scheme $P^g(22) = \{P_1^g = 0.8915, P_2^g = 0.0567\}$ means the respective 89.15 and 5.67% $\text{NH}_3\text{-N}$ loads of the Hejiagou and the Songbei should be reduced or allocated to other months. Similarly, the optimum $\text{NH}_3\text{-N}$ load reduction rates combination for February is $P^g(30) = \{P_1^g = 0.3722, P_2^g = 0.0743\}$ (Figure 4(b)). The results illustrate that the PSO method can generate a stable solution.

Further, MS3 in WQFS2 is required to meet the Grade IV water quality standard. As seen in Figure 4(c), at iteration $t=26$, the particles clustered together to the optimum scheme $P^g(26) = \{P_1^g = 0.3733, P_2^g = 0.0164, P_3^g = 0.9250\}$, suggesting that the optimum $\text{NH}_3\text{-N}$ load reduction rates of the Taiping, Ashen River and Hulan River are 37.33%, 1.64% and 92.50%, respectively in January. Similarly, the optimum for February is $P^g(18) = \{P_1^g = 0.1873, P_2^g = 0.3184, P_3^g = 0.7381\}$ (Figure 4(d)).

$\text{NH}_3\text{-N}$ concentrations will meet the planned water quality goals in 2011 (Figure S4, available online at

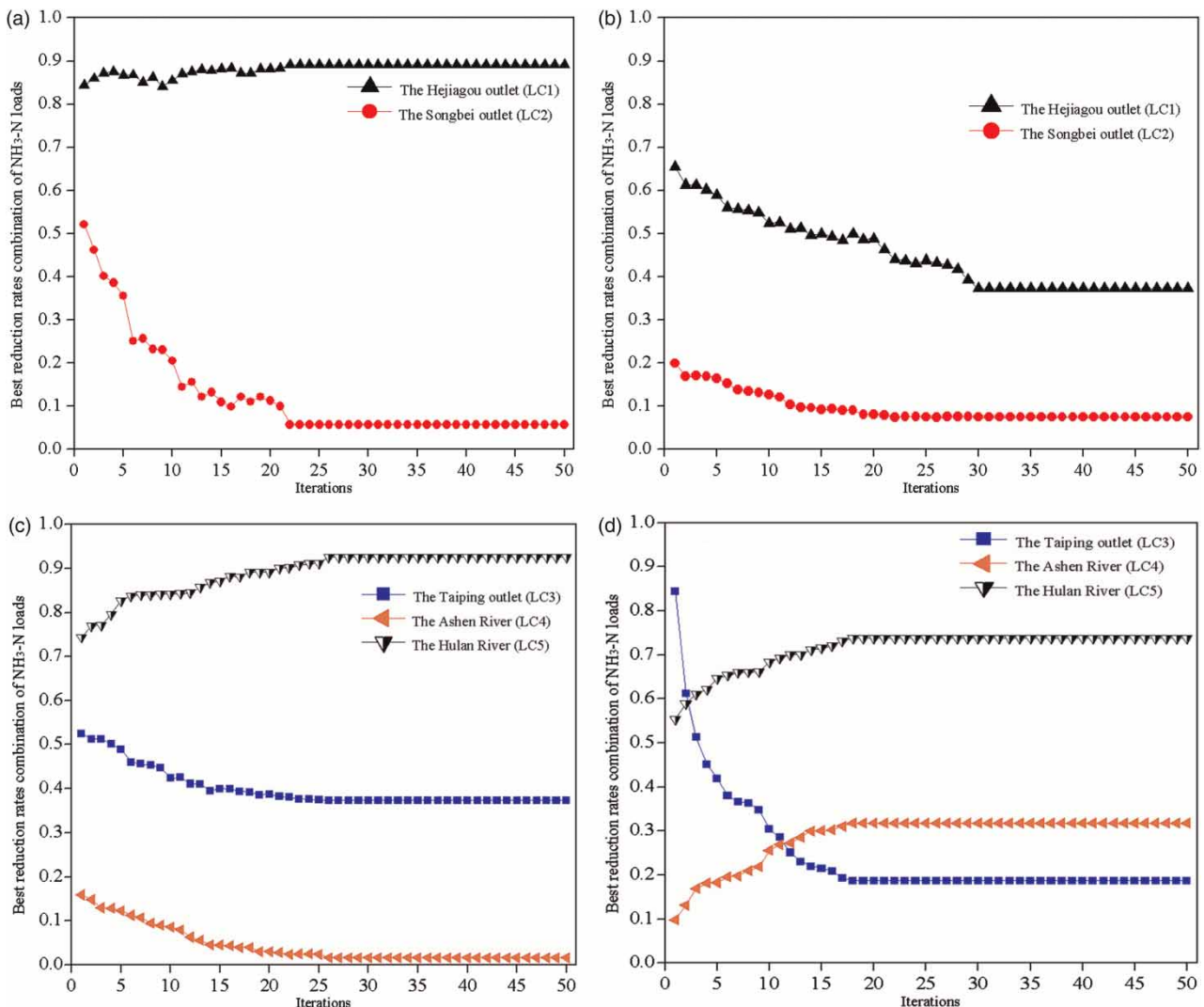


Figure 4 | The optimum $\text{NH}_3\text{-N}$ load reduction rates scheme during PSO iterations for (a) WQFS1 in January, (b) WQFS1 in February, (c) WQFS2 in January and (d) WQFS2 in February in 2011.

<http://www.iwaponline.com/wst/070/348.pdf>) if the above-suggested reduction rates of $\text{NH}_3\text{-N}$ loads could be implemented. Optimum combinations of $\text{NH}_3\text{-N}$ reduction rates in each month are different, implying that this ANN-PSO method contains comprehensive monthly changes, such as the properties of the outlets and the river (e.g., flow rate and temperature). In terms of the PSO approach, the random particles at iteration $t = 1$ can affect the convergence speed. However, different initialized random particles still cluster together to the nearly identical combination $P^g(\text{best})$, which demonstrates that the PSO is effective at optimizing loads reduction rates and it is stable to converge. Meanwhile, all new predicted $\text{NH}_3\text{-N}$ concentrations at all iterations can reach the planned water quality standard grade. Thus, these $P^g(t)$ before the convergence can be alternatively chosen as

additional reduction schemes for decision-makers, because sometimes the $P^g(\text{best})$ is not easy to implement due to economic or technical limitations. The main purpose of discharge management is to control pollutant loads into river sections to ensure water quality meets the targeted goals. Thus, although the relation between reduction rate and its investment is actually nonlinear, the results of this ANN-PSO method can guide decision-makers to assess how much waste loads should be reduced or reallocated under different hydrological conditions.

Monthly $\text{NH}_3\text{-N}$ discharge management in Harbin region

According to ANN predictions and the monitoring data of Harbin region, the $\text{NH}_3\text{-N}$ concentrations often

exceed the permitted national water quality standard in a low-flow period, that is, January and February in 2011. The mean flows of the winter months are much smaller than those of other months and low flow leads to the high $\text{NH}_3\text{-N}$ concentration (see Figure S1). In addition, low water temperature and a thick surface ice layer also decelerate the degradation of ammonia nitrogen in winter. Low water temperature decreases the activities of nitrite bacteria in river water, and the thick ice layer can reduce photosynthesis, so reducing the dissolved oxygen and air reaeration, indirectly decreasing the oxidation of $\text{NH}_3\text{-N}$.

Compared with the equal rate strategy, this ANN-PSO method achieves a more reasonable reduction rates scheme (Table 2). Reduction loads of ANN-PSO are smaller than the equal rate strategy, except for Hejiagou outlet (LC1) and Hulan River (LC5). These sites present the highest emission loads, suggesting that the decision-makers ought to focus on them primarily. In addition, due to the large flow of the Songhua River, the total $\text{NH}_3\text{-N}$ load reduction rates are bigger in this WQFS when the background $\text{NH}_3\text{-N}$ concentration is higher. The predicted MS2 values are smaller than 1.0 mg/L from April to November in WQFS1 and the MS3 values are less than 1.5 mg/L in WQFS2 from March to December (Figure S4), mainly because of the lower background concentration levels and the excellent self-purification capacity in these months. Hence, based on the ANN-PSO results, the $\text{NH}_3\text{-N}$ concentration of the nearest upriver WQFS should be ensured to meet its goal, which is very important for monthly discharge management in the Harbin area.

Table 2 | Comparison of the ANN-PSO method and equal rate strategy (Equal) for $\text{NH}_3\text{-N}$ reduction loads allocation: an example for January and February 2011

	January			February		
	Load (g/s)	ANN-PSO (%)	Equal (%)	Load (g/s)	ANN-PSO (%)	Equal (%)
WQMS1 ^a	1.19 (mg/L)			1.11 (mg/L)		
LC1	39.84	89.15	79.00	83.95	37.22	35.00
LC2	16.25	5.67	79.00	16.08	7.43	35.00
WQMS2 ^a	1.62 (mg/L)			1.77 (mg/L)		
LC3	1.74	37.33	66.00	1.66	18.73	69.00
LC4	56.97	1.64	66.00	92.5	31.84	69.00
LC5	108.16	92.50	66.00	208.32	73.81	69.00

^aHere is the observed $\text{NH}_3\text{-N}$ concentration.

CONCLUSIONS

The optimization of discharge management will lead to better river water quality and reduced economic investment. A PSO method, coupling ANN models, has been applied to optimize the reduction rates of ammonia nitrogen ($\text{NH}_3\text{-N}$) loads from sewage outlets of Harbin, northeast China. In planned WQFS, the $\text{NH}_3\text{-N}$ concentrations in different months are linked with their emission loads and well predicted by ANN models. Then the $\text{NH}_3\text{-N}$ loads of all outlets can be optimized by PSO according to a targeted water quality standard.

This hybrid ANN-PSO method is effective to obtain many $P^g(t)$ before the convergence, which can be alternatively chosen as additional reduction schemes for decision-makers, because sometimes the $P^g(\text{best})$ is not easy to implement due to economic or technical limitations. Analogously, this ANN-PSO methodology can also be applied to other pollutants, like chemical oxygen demand, after successful construction of linkage models. In fact, the allocation task of wastewater discharge contains many more components, such as marginal utility. Thus, it is necessary to study these specific economic factors in the future.

The highest $\text{NH}_3\text{-N}$ concentrations occur in January and February, a typical low-flow period in Harbin. The results delivered optimum $\text{NH}_3\text{-N}$ reduction rates for the five outlets, for January and February of 2011. All predicted $\text{NH}_3\text{-N}$ concentrations after the reduction meet the water quality standard. The results indicate that the outlet with the highest $\text{NH}_3\text{-N}$ load has the biggest reduction rate in each WQFS and the outlets in the WQFS with higher background $\text{NH}_3\text{-N}$ concentrations need to cut more $\text{NH}_3\text{-N}$ loads. Decision-makers should focus not only on the outlet with the highest $\text{NH}_3\text{-N}$ emission load, but also on the need to ensure that the $\text{NH}_3\text{-N}$ concentration of the nearest upriver WQFS meets the water quality goal.

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