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Risk assessment of water quality using Monte Carlo simulation and artificial neural network method

Yunchao Jiang [a,b], Zhongren Nan [a,b,*], Sucai Yang [c]

[a] College of Earth and Environmental Sciences, Lanzhou University, No. 222, Tianshui Road (South), Chengguan District, Lanzhou, Gansu Province, China
[b] Collaborative Innovation Centre for Arid Environments and Climate Change, Lanzhou University, No. 222, Tianshui Road (South), Chengguan District, Lanzhou, Gansu Province, China
[c] Enviromental Protection Research Institute of Light Industry, No. 27, West Third Ring North Road, Beijing, China

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ABSTRACT

There is always uncertainty in any water quality risk assessment. A Monte Carlo simulation (MCS) is regarded as a flexible, efficient method for characterizing such uncertainties. However, the required computational effort for MCS-based risk assessment is great, particularly when the number of random variables is large and the complicated water quality models have to be calculated by a computationally expensive numerical method, such as the finite element method (FEM). To address this issue, this paper presents an improved method that incorporates an artificial neural network (ANN) into the MCS to enhance the computational efficiency of conventional risk assessment. The conventional risk assessment uses the FEM to create multiple water quality models, which can be time consuming or cumbersome. In this paper, an ANN model was used as a substitute for the iterative FEM runs, and thus, the number of water quality models that must be calculated can be dramatically reduced. A case study on the chemical oxygen demand (COD) pollution risks in the Lanzhou section of the Yellow River in China was taken as a reference. Compared with the conventional risk assessment method, the ANN-MCS-based method can save much computational effort without a loss of accuracy. The results show that the proposed method in this paper is more applicable to assess water quality risks. Because the characteristics of this ANN-MCS-based technique are quite general, it is hoped that the technique can also be applied to other MCS-based uncertainty analysis in the environmental field.

1. Introduction

Typically, many of the processes associated with water pollution are uncertain in nature (Thomann, 1982). The most typical sources of uncertainty accounted for are the uncertainty in the initial state of the system, uncertainty in the model parameter estimates, uncertainty in the observed input disturbances and output responses, and uncertainty arising from unobserved input disturbances of the system (Beck, 1987). A Monte Carlo simulation is an effective method for characterizing risks and uncertainty in circumstances where a considerable amount of data that describe the system dynamics is available (Vose, 2000). The MCS is perhaps the most widely used probabilistic technique for propagating uncertainty in simple or complex models. There are numerous water-related programs that use Monte Carlo simulations. In particular, the DYNTOX model (USEPA, 1992), QUAL2K model (USEPA, 2006) and the complex BASINS modeling system (USEPA, 2007) all include a Monte Carlo simulation module for risk analysis. Additionally, there are many studies related to the practical application of an MCS for risk assessment (Harris and Jones, 2008; Lee et al., 2011; Weir et al., 2011; Lonati and Zanoni, 2012). It has been determined that the advantages of MCS-based risk assessment are due to their outputs providing more information, such as cumulative distribution functions and probability distribution functions. Distribution functions for risk assessment provide the range of risk and the probability associated with each value of risk.

The primary disadvantage of an MCS is the large computational effort that is generally necessary. When there are a large number of uncertainty sources, an MCS requires large storage capacities and long run times (Revelli and Ridolfi, 2004). The MCS is accomplished by running an existing model multiple times with different values for all uncertain parameters, which are randomly selected from the predetermined probability distributions. Exhaustive sampling of the inputs and parameters is achieved by running as many simulations as possible. A large number of numerical calculations of partial

* Corresponding author. College of Earth and Environmental Sciences, Lanzhou University, No. 222, Tianshui Road (South), Chengguan District, Lanzhou, Gansu Province, China. Tel.: +86 0931 8912574, +86 13038761559; fax: +86 0931 8912574.
E-mail address: submitpaper@yahoo.cn (Z. Nan).

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differential equations that represent a water quality model are therefore required. It is often necessary to use a computationally expensive numerical method, such as the finite element method (FEM) to solve the model. This process can be extremely time consuming and cumbersome, where many of the parameters and dimensions of the models are typically simplified; even the rivers are often approximated as channel flow in risk assessment practice so that the water quality model equation can be solved using simple analytic methods instead of complicated numerical methods. Thus, efficient sampling techniques must be sought to tackle the computational burden associated with the MCS. A variety of variance reduction techniques, such as Stratified Sampling (Helton and Davis, 2003; Cacuci and Ionescu-Bujor, 2004), Latin Hypercube Sampling (LHS) (Helton and Davis, 2003) and Line Sampling (LS) (Koutsourelakis et al., 2004) have been proposed to create a more efficient MCS method. These techniques can reduce the computation time to a certain extent; however, they still require a disproportionately large computational effort for treating practical problems.

An ANN is an information processing technique based on the way biological nervous systems, such as the human brain, process information (Adhikary and Mutsuyoshi, 2004). An ANN has the capability to respond to input stimuli, produce the corresponding response by learning from experience and reproduce/generalize the data during a recall process. Over the last few decades, an increasing number of articles have presented implementations of ANNs in environmental risk assessment (Lin et al., 2008; Dogan et al., 2009; He et al., 2011) and quality prediction (Gautam et al., 2008; Cho et al., 2011; Verney-Carron et al., 2012). In addition, several of the latest studies in environmental field examined the applicability of using an ANN in wastewater treatment process control and optimizations (Mjalli et al., 2007; Kulkarni and Chellam, 2010; Pendashteh et al., 2011). This distinct advantage of a trained ANN over the conventional computing paradigm, under the provision that the ANN can rapidly map a given input into the desired output quantities, leads to results that can be obtained in a few clock cycles, which thereby enhances the efficiency of the standard analysis approach compared with the conventional computational process. Most recently, ANNs have been used as a powerful tool to replace time-consuming procedures in engineering applications. Reliability analysis problems with imperfect performance functions require thousands or millions of performance functions to be calculated in an MCS. Lopes et al. (2010), Kingston et al. (2011), Lü et al. (2012) and their co-workers used ANNs to emulate the complex numerical analysis within an MCS for a reliability analysis of structures. Their studies proved that the accuracy and gains in the obtained computational efficiency when using an ANN-based MCS were satisfactory. ANNs have been termed as a universal approximator. Therefore, perhaps ANNs could be used to replace the time-consuming repeated FEM calculations in MCS-based risk assessments of water quality.

In the present study, a pragmatic procedure that combines an ANN model with an MCS-based risk assessment is proposed. The ANN model was used as a substitute to the iterative FEM calculations by approximating complicated input–output relationships of water quality models; thus, the number of FEM runs could be dramatically reduced without a loss of accuracy. Training and test data sets for the model were obtained from FEM calculations of the water quality model equation. The ANN model was then connected to the MCS to assess the water quality risk. The ANN-MC-based risk assessment method proposed in the paper was compared with the conventional MCS-based method in terms of computational cost and accuracy through a case study. The main purpose of this paper is to verify the application potential of ANN-MCS-based risk assessment methods, which has not been attempted previously by other researchers.

2. Methods

Water quality risk can be defined as the probability that the observed/predicted concentration value of a water quality indicator exceeds a regulatory limit. In general, the risk assessment of water quality encompasses four steps: developing a water quality model; selecting an appropriate probability distribution for each uncertain parameter of the model; running the simulation many times to obtain an acceptable variance in the combined results; and making a decision.

2.1. Water quality model

Here, water quality risk assessment begins with a classical, deterministic water quality model that predicts pollutants, which overlays probability theory in such a way that the exceedance probability of the water quality indicator can be obtained. If the degradation reaction of the pollutant is a first-order reaction, the water quality model equation is:

$$\frac{\partial C}{\partial t}+\frac{\partial(uC)}{\partial x}+\frac{\partial(\nu C)}{\partial y}+\frac{\partial(\omega C)}{\partial z}=E_x\frac{\partial^2 C}{\partial x^2}+E_y\frac{\partial^2 C}{\partial y^2}+E_z\frac{\partial^2 C}{\partial z^2}-K_1 C \qquad (1)$$

where C is the concentration of the pollutant (mg/L); t is the travel time (s); u, ν, ω are the longitudinal, lateral, and vertical advective velocities (m/s), respectively; E_x, E_y, E_z are the longitudinal, lateral, and vertical diffusion coefficients (m^2/s), respectively; K_1 is the first-order decay coefficient for a certain pollutant (day^{-1}); the x- and y-coordinates are in the horizontal plane, and the z-coordinate is in the vertical plane.

In most cases, numerical analysis methods (such as the FEM, finite difference method and finite volume element method) must be used to solve Eq. (1) because its analytical solutions can be derived only under specific conditions (e.g., a steady, uniform, turbulent open channel flow with constant discharge). Here, the FEM was used to solve the water quality model described by Eq. (1).

From Eq. (1), we know that parameters u, ν, ω, E_x, E_y, E_z, K_1 are the main factors that influence the pollutant concentration C. Thus, the probability distributions of C can more easily relate to water quality by defining these parameters in Eq. (1) as random variables. To ensure that the simulation results are reasonable and that the sample distributions are sufficient, we assumed that u, ν and ω follow a uniform distribution, $U(a, b)$. According to the study of Burn and McBean (1985), the parameter values E_x, E_y, E_z and K_1 in the water quality model are distributed symmetrically and can be simulated as a normal distribution, $N(\mu, \sigma)$. Details about the probability density functions and cumulative probability density functions of uniform distribution and normal distribution can be found in various statistics books.

2.2. MCS-based risk assessment

In an MCS-based risk assessment, discrete values of the input random variables (e.g., model parameters) are generated in a fashion consistent with their probability distributions, and the water quality model is calculated for each generated input set and also produces outputs in the form of a statistical distribution. The input variables are sampled independently in Matlab, and correlations among different parameters are not considered. The process is repeated many times to evaluate the water quality risk by determining whether the regulatory limits are exceeded.

The output from an MCS varies with the number of samples; that is, the larger the number of samples is, the greater the output accuracy. According to the Kolmogorov Smirnov Test, the number of

samples required for an MCS can be estimated using the following equation (Amstadter, 1971):

$$n \geq \lambda_\alpha^2 / D_n^2 \tag{2}$$

where n is the sample number of the random variable, α is the confidence level, λ_α is a constant and D_n is the maximum desired error of the random variable. More details on the relationship between n, α and λ_α can be seen in the work of Amstadter (1971).

In this paper, we pay attention to the water quality risk at certain locations, denoted as checkpoints. Checkpoints are important locations, such as water quality monitoring sections, intakes of drinking water sources and sewage outlets. The water quality risk of a certain checkpoint is defined as follows:

$$\text{risk}_i = n_i / N \times 100\% \tag{3}$$

where risk_i is the risk at checkpoint i; N is the total run number in the MCS and n_i is the number of times that the deserved/predicted values of the water quality indicator are beyond the regulatory limit (C^*) at checkpoint i.

As mentioned above, the mathematical formulation of the MCS-based risk assessment is relatively simple, where its accuracy is primarily limited by the computational time. The assessment method has the capability of handling practically every possible case regardless if its complexity; however, it has not received overwhelming acceptance due mainly to the excessive computational effort required. In this study, to improve the computational efficiency of the MCS-based assessment method, an ANN was incorporated into the MCS to reduce the computational cost. See below for a more detailed description of the procedure.

2.3. ANN-MCS-based risk assessment

The popularity of ANNs stems from its ability to identify relationships in numerical data through a mapping of the relationships between various input variables and one or more output variables (Goh and Kulhawy, 2005). In this work, the ANN was used to perform rapid and efficient risk assessments. This objective consists of the following tasks: (i) determining a suitable ANN architecture and training algorithm, (ii) selecting proper training and testing sets, and (iii) training/testing the neural network.

2.3.1. ANN architecture and training algorithm

Among the many neural network architectures, the three-layer feed forward back propagation network (BP) is a popular model and has already been successfully implemented on many occasions. Hornik et al. (1989, 1990) showed that the three-layer feed forward network with a single hidden layer and an appropriately smooth hidden layer activation function, such as BP, was capable of an arbitrarily accurate approximation to an arbitrary function and its derivatives. Here, BP was used to replace the time-consuming, repeated FEM calculations in the risk assessment of water quality.

A neural network consists of a set of interconnected individual neurons. The neurons are organized into several layers: the first layer is the input layer, which receives the input data; the final layer is the output layer, which produces the network output. The layers between the first and the last layers are the hidden layers, which process the data. The general structures of ANN models are well known and can be found in numerous publications (Hagan et al., 1996; Jiang, 2001). To use an ANN model to approximate data, a selected set of representative configuration values must be adjusted until the error function values between the ANN-predicted output values and the desired output values are minimized. The process is called training the ANN. For brevity, additional details about ANN models are not reported here; the interested reader may refer to the cited references and the copious literature in the field.

The number of neurons in the hidden layer is an extremely important parameter that determines the accuracy of ANN models. Fletcher and Goss (1993) suggested that the appropriate number of neurons in the hidden layer range from $(2n^{1/2} + m)$ to $(2n + 1)$, where n is the number of input neurons and m is the number of output neurons. Generally, the number of hidden layer neurons is determined by a trial-and-error process, and the model with the most accurate results will be used, which contains the most appropriate number of neurons in the hidden layers.

In the present study, the Levenberg–Marquardt (LM) algorithm was adopted for its efficiency in training networks. Compared with the standard gradient descent training method, the improved methods are generally several times faster. In addition, the algorithm produces smaller errors (Hagan et al., 1996).

2.3.2. Data preparation

In this work, the data set was divided into two subsets. These subsets consisted of (i) a training set to adjust the connection weights, to determine when to stop training and to optimize the network architecture and internal parameters (e.g., the number of hidden layer neurons, learning rate, etc.), and (ii) a test set to verify the generalization ability of the model over the range of data used for calibration.

To improve the convergence properties of the ANN model, all data were normalized into the range of [0,1] before the network was trained. The details can be found in EFECIT research and the development institute's work (2005) and numerous literature in the field. The training and testing sets consist of groups of corresponding random variables. The data selection determines the quality of the ANN predictions; thus, to achieve a valid ANN model, the training data should cover the full range of possible input variables. The training set was generated randomly to fall within a wide range: $\mu_x \pm 3\sigma_x$ with a normal distribution, where μ_x and σ_x are the mean value and standard deviation of the ith random variable, respectively. This procedure was done to fall within the range of $[a,b]$ with a uniform distribution, where a and b were the minimum and maximum of the ith random variable.

2.3.3. ANN-MCS-based risk assessment

The ANN was used to substitute repeated FEM calculations of the water quality model. A limited-size samples of input/output data sets was used to construct the ANN regression model. Generally, the range of samples size is dependent on the required simulation accuracy. The number of samples needs to be increased gradually from a smaller number, which is less than approximately one percent, even 0.5 percent of that of MCS sampling, until the errors between the ANN-predicted output values and the desired output values are small enough. Once the ANN model was built, it was used within the MCS runs to estimate the water quality risk in an insignificant amount of computational time. The procedure of the ANN-MCS-based risk assessment of water quality is presented in Fig. 1.

3. Case study

3.1. Study area

In this section, the accuracy and efficiency of the developed risk assessment method were tested using observed water quality data from the Lanzhou section of the Yellow River. The Lanzhou section has an area of approximately 85,000 km^2 and is located upstream of the Yellow River, the Mother River of China. This important river

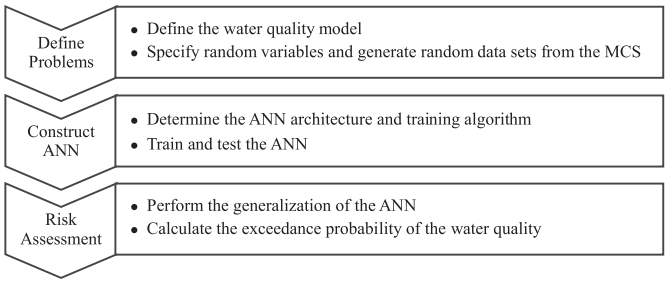

Fig. 1. Procedure of the ANN-MCS-based risk assessment of water quality the figure shows the contents, methods and steps of the ANN-MCS-based risk assessment of water quality.

supplies a considerable part of the water demand of the convergent area that contains a population of 4.97 million people. The Lanzhou section of the Yellow River contains the Lanzhou City and the Baiyin City, an industry center of West China, where many industries exist, and also several smaller towns and villages are near the river. Municipal and industrial wastewater from these population centers is mostly discharged to the Yellow River. The Lanzhou section is the main area to discharge organic pollutants in the Yellow River Basin, particularly COD. The overall length of the Lanzhou section of the Yellow River is 358.6 km. The studied river section has a length of 258 km, beginning from the Qingcheng Bridge down to the Jingyuan Bridge and then reaches the Wu fosi (Fig. 2).

COD was selected as the water quality indicator simulated because it is a main characteristic of pollution and there are existing data for the study area. All the data were supported by the local government. The mean yearly precipitation in the Lanzhou section is 200–400 mm, where the evaporation is quadruple that, and therefore, the pollution in the system is mainly caused by point loads. Thus, the impacts of diffuse sources were ignored in the paper.

The checkpoints mentioned here refer to the Jingyuan Bridge and Wu fosi, two water quality monitoring sections along the Lanzhou section of the Yellow River. The initial values were determined using the initial pollutant concentration C_0 at the upstream reach, the Qingcheng Bridge, and the pollutant concentrations C_q at the discharge outlets along the Lanzhou section of the Yellow River. Table 1 displays C_0at the Qingcheng Bridge and $C_q$at the five outlets (East drain, West drain, Jingyuan power plant, domestic sewage drain, Rare Earth Company).

3.2. Method application

In this section, it is shown how and why determining the COD risk assessment in a dry season for the Jingyuan Bridge with the ANN-MCS-based assessment method is more effective and convenient than the conditional MCS-based method.

All water quality models can be used in the developed ANN-MCS-based risk assessment procedure in this paper; however, the characteristics of the river and the available data will influence the

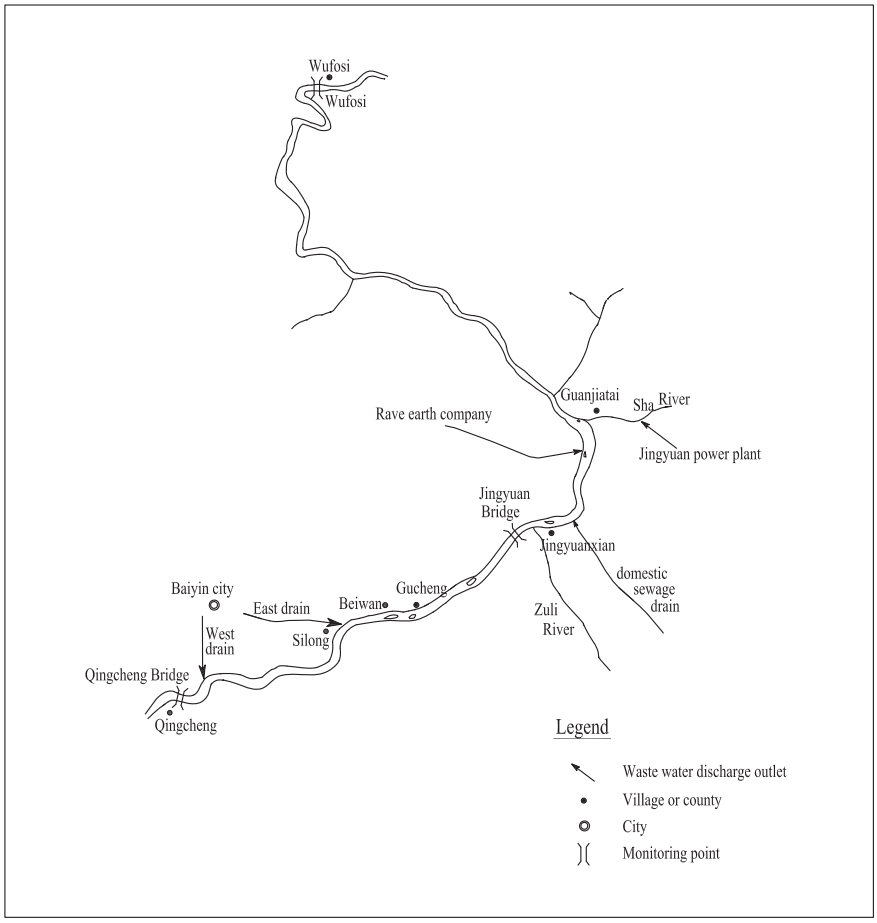

Fig. 2. Lanzhou section of the Yellow River the figure displays the water quality monitoring sections and the discharge outlets along the Lanzhou section of the Yellow River.

Table 1
C_0 at Qingcheng Bridge and C_q at the outlets.

Period	Water quality indicator	C_0 Qingcheng Bridge	East drain	West drain	C_q Jingyuan power plant	Domestic sewage drain	Rare Earth Company
Dry season	COD	13.3	126.0	354.0	50.0	626.0	1128.0

model selection. The average length, width and depth for the Lanzhou section of the Yellow River are approximately 358,000 m, 172 m and 2 m, respectively. The model can be simplified, where a one-dimensional river is simulated according to its characteristics; furthermore, the available information on the river section is extremely limited, which is a similar situation for many other waters in developing countries. Therefore, a one-dimensional water quality model was used in this study.

In this work, uncertainties of the model parameters were considered through the longitudinal advective velocity (u), longitudinal diffusion coefficient (E_x) and the first-order decay coefficient (K_1). All parameters were assumed to be uncorrelated, where their statistical parameters are listed in Table 2. The lateral, vertical velocities (ν and ω) and the diffusion coefficients (E_y and E_z) were neglected because a one-dimensional water quality model was used in this study.

A three-layer BP network was established to represent the iterative water quality model calculation with the FEM. The input layer contained three neurons, which correspond to three random parameters of the water quality model listed in Table 2. In the output layer, there is one neuron, which provides the simulation results (i.e., the COD concentrations). The optimum number of neurons in the hidden layer was 7, as determined by trial and error. Thus, the architecture for the ANN model was set as [3-7-1], and the training algorithm used was the Levenberg–Marquardt method. The network programming was performed in the computer software Matlab.

3.3. Results and discussion

To test the accuracy and efficiency of the ANN-MCS-based risk assessment, the ANN model was trained by increasing the number of training samples from the initial 10. The range of samples size is from 10 to 35. Table 3 shows the generalized results of the COD concentration after this increase. From the Table 3, it can be seen that increasing the number of training data sets affects the relative error (RE). When the number of training samples is increased to 25, the average absolute value of RE, $|\overline{\mathrm{RE}}|$, is 0.238%. The small errors indicate that 25 training samples is adequate to build an accurate ANN model, and the trained network can be used to generalize. Table 3 shows that the ANN model requires more training data sets to improve the accuracy of its approximation. However, using a large number of training data sets may result in little improvement in accuracy, and the required computational time to develop the training data sets will increase. Actually, from Table 3, it can be observed that the increase in the number of training data sets from 25 to 35 only results in a slight difference in the generalized COD results. Thus, the training data sets should only consist of 25 samples. The COD concentration values calculated using the FEM and the generalized results from the trained ANN with 25 training samples are given as electronic supplementary material. The training sets and test sets were all generated randomly.

To determine the performance of the ANN model used in this case, the correlation coefficient was used, which is defined as follows:

$$r^2 = \left[\sum_{i=1}^{n}(x_i-\overline{x})(y_i-\overline{y})\right]^2 \Big/ \sum_{i=1}^{n}(x_i-\overline{x})^2\sum_{i=1}^{n}(y_i-\overline{y})^2 \tag{4}$$

where x_i and x are the calculated and averaged COD concentration values determined with the FEM; y_i and y are those values generalized by the ANN model; and n denotes the number of ANN training data sets or test sets. The coefficient r^2represents the degree of correlation between the FEM calculated results and the ANN generalized results. As shown in Fig. 3, small generalization errors and good correlation ($r^2 = 0.9954$ for the training data and $r^2 = 0.9946$ for the test data) can be observed between the generalized results and the calculated results, which suggests that the ANN model can be used to represent the repeated calculation of water quality models with small deviations. If only inputting the basic random parameters, the network can generate an adequate, accurate value of the corresponding COD concentration.

The sample number of three random parameters shown in Table 2 required for the MCS was initially estimated using Eq. (2), where the maximum allowable error, D_n, was assumed to be ± 0.01 day^{-1} for the first-order decay coefficient K_1, ± 0.1 for the longitudinal diffusion coefficient E_x and ± 0.1 m/s for the longitudinal advective velocities u. A confidence level of 95% was selected. The application of Eq. (2) to the three random parameters indicated that a minimum sample size of 18,496 was required for K_1 and 185 samples for both E_x and u. The simulation requirement of K_1 was limiting, and therefore, the required number of MCS was 18,496.

Thus, all of the 18,496 samples of K_1, E_x and u were inputted into the established ANN model as input neurons. Then, the ANN produced 18,496 COD concentration values corresponding to the input variables accordingly. By analyzing these 18,496 results, the risks (i.e., the COD exceedance probability) can be calculated according to Eq. (3). When the regulatory limit of water quality was class III; with the COD concentration ($\leq$15.00 mg/L) in the Jingyuan Bridge, the risk beyond the limit obtained from ANN-MCS-based assessment method showed a better accuracy of 0.950 compared with that from the conventional MCS-based method of 0.947 as shown in Table 4.

As noted in the introduction, the reason for using an ANN model as a substitute to repeated FEM runs in water quality risk assessment is to reduce the number of numerical calculations. Thus, the

Table 2
Distributions of random parameters.

Parameter	Distribution
K_1	$N(0.091,0.002)$[a]
E_x	$N(1497,224.6)$[a]
u	$U(1.5,1.76)$[b]

[a] Normal distribution (mean, variation).
[b] Uniform distribution (minimum, maximum).

Table 3
Generalized results of COD.

Number of training samples	$\lvert\overline{\mathrm{RE}}\rvert$ (%)
10	1.2245
15	0.6831
20	0.2708
25	0.2380
35	0.2223

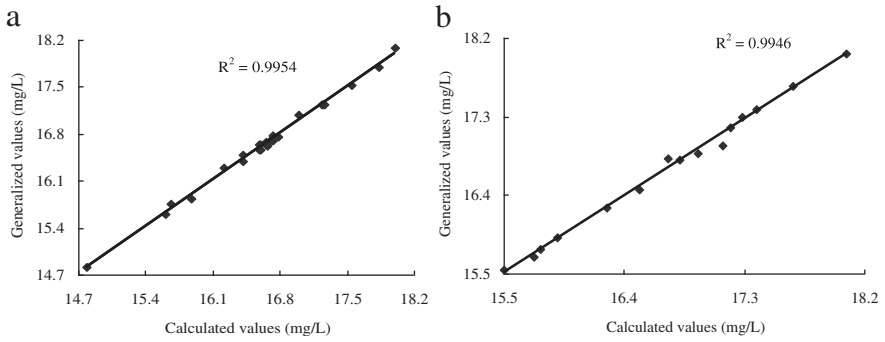

Fig. 3. Comparison between the ANN model and the FEM analysis using (a) training data and (b) test data the figure illustrates the generalization errors of the ANN and the degree of correlation between the generalized results of the ANN model and the FEM numerical analysis results using training data and test data of the ANN.

Table 4
Comparison of performances for the two different methods of risk assessment.

Risk assessment method	Numbers of simulations (NS)	The risk beyond the limit
MCS-based	18,496	0.947
ANN-MCS-based	25	0.950

criterion to measure the efficiency should be the number of FEM runs required to solve the water quality model equations. The number is normally equal to the number of training data sets needed for developing the ANN model. Hence, the number of training data sets for establishing an ANN model was used to measure the efficiency of the ANN-MCS-based risk assessment method in this study. Table 4 presents the performances of the different methods. A "true" value of the risk beyond the regulatory limit is also shown in Table 4 for reference (i.e., risk = 0.947), which was obtained using a large number of FEM runs (i.e., NS = 18,496). Examining the performances, it is clear that using the ANN model dramatically reduces by three orders of magnitude the number of runs compared with the tens of thousands of runs required by the conventional MCS-based risk assessment.

4. Conclusion

In this paper, a new and efficient ANN-MCS-based method for risk assessment is proposed by incorporating an ANN model into the time-consuming process of an MCS. The method could also be used for problems with complicated and highly non-linear performance functions or for problems with many basic random variables. Solving such problems is extremely difficult by conventional MCS because of either excessive computational cost or loss of accuracy. A case study of the COD pollution risk in the Lanzhou section of the Yellow River was taken as reference. It was demonstrated by the example that the ANN-MCS-based risk assessment of water quality can be effective both in terms of efficiency and accuracy. The advantage of the ANN model lies in its robustness and generality capability, which reduces the iterative number of FEM calculations within the MCS-based risk assessment by a large margin. Because using an ANN can practically eliminate any limitation of the sample size and lead to extremely accurate estimates of risk without any simplifying assumptions, it is possible to increase the MCS sample size to predict more accurately when the water environment is implicit and numerical analysis methods have to be adopted to solve the water quality model equations. Consequently, this ANN-MCS-based method is applicable to risk assessment and management of water quality and many complex, uncertain environmental problems.

Although the one-dimensional water quality model was used to simulate the outcome of pollution from the characteristics of the river with limited data in this study, the method proposed in the paper is independent of the risk analysis and treats the water quality model as a black box. Thus, any water quality models can be used to apply the proposed procedure.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.jenvman.2013.03.015.

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