# Method for Water Quality Prediction and Eutrophication Risk Assessment in Lakes and Reservoirs Based on Monte Carlo Simulation (Postprint)

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## Abstract

Lake and reservoir water quality prediction and eutrophication analysis are important technical approaches for water pollution prevention and control. However, existing water quality prediction research typically involves single-value predictions, which are used as the basis for analyzing eutrophication status, entailing inherent randomness and uncertainty. By integrating water quality dynamic models, a Monte Carlo simulation-based method for lake and reservoir water quality prediction and eutrophication risk assessment is proposed. Based on the prior distributions of water quality indicators and model parameters in known water quality dynamic models, Monte Carlo simulation is employed to predict the evolution process of water quality indicators, obtaining the probability distribution of water quality indicator values at future times, thus realizing water quality prediction. Furthermore, a comprehensive trophic state index is constructed, and combined with water quality indicator prediction results, the probability distribution of the comprehensive trophic state index and the probabilities of being at different trophic levels are calculated, thus realizing eutrophication risk assessment. Simulation results demonstrate that the proposed method can effectively achieve water quality prediction and eutrophication analysis, providing more comprehensive and accurate considerations, and overcoming the randomness associated with single-value prediction results.

## Full Text

## Preamble

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# Monte Carlo Simulation Based Water Quality Prediction and Eutrophication Risk Assessment Method for Lakes and Reservoirs

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**Abstract:** Water quality prediction and eutrophication analysis of lakes and reservoirs are crucial technical means for water pollution prevention and control. However, existing water quality prediction research typically employs single-valued prediction, which is then used to analyze eutrophication status—an approach that carries inherent randomness and uncertainty. This paper proposes a Monte Carlo simulation-based method for water quality prediction and eutrophication risk assessment, integrated with water quality kinetic models. Based on prior distributions of water quality indices and model parameters from the kinetic model, Monte Carlo simulation is utilized to predict the evolution of water quality indices, obtaining probability distributions of future water quality values and thereby achieving probabilistic water quality prediction. Furthermore, a comprehensive trophic state index is constructed, and combined with water quality prediction results, the probability distribution of the comprehensive trophic state index and the probabilities of different trophic levels are calculated to realize eutrophication risk assessment. Simulation results demonstrate that the proposed method can effectively achieve water quality prediction and eutrophication analysis with more comprehensive and accurate considerations, overcoming the randomness associated with single-valued prediction results.

**Keywords:** water quality kinetic model; Monte Carlo simulation; water quality prediction; eutrophication; risk assessment

## 0 Introduction

With the rapid development of modern society, water eutrophication has become a major global water environmental issue. Currently, over 500 coastal areas worldwide are affected by eutrophication, and many freshwater lakes, streams, and reservoirs are suffering from this problem. Research indicates that 80% of lakes in China have already exhibited eutrophication phenomena. Except for sparsely populated freshwater lake regions and lakes maintaining pristine conditions, nutrient concentrations in other Chinese lakes have exceeded the standard thresholds for lake eutrophication. Particularly in China' s major freshwater lakes, nutrient concentrations have surpassed the critical levels for phosphorus and nitrogen eutrophication, with total nitrogen concentrations exceeding these levels by more than tenfold. Presently, both Taihu Lake and

Chaohu Lake in China have become completely eutrophic [1~4]. Consequently, water environmental issues demand urgent attention.

Water quality prediction enables effective monitoring of water conditions and prevention of large-scale water pollution incidents, holding practical significance for water pollution prevention and control. Therefore, achieving rational and effective water quality prediction and assessing eutrophication risk based on such predictions represent important approaches to solving water environmental problems.

Existing water quality prediction methods fall into two main categories:

a) **Mechanism-based water quality prediction methods.** These approaches establish water quality models by analyzing internal mechanistic evolution processes within water bodies, then predict water quality indices based on these models. Commonly used mechanism models include QUAL2E, WASP, and EFDC. QUAL2E is a one-dimensional water quality model suitable for simulating water quality in completely mixed dendritic rivers. It assumes a mainstream transport mechanism, meaning both advection and diffusion mixing occur along the river' s main flow direction, while water quality components are completely uniformly mixed in the transverse and vertical directions. The model allows for multiple pollution sources, water intakes, and tributaries along the river course, with its fundamental equation being the one-dimensional advection-diffusion mass transport equation [5~8]. WASP (Water Quality Analysis Simulation Program) is a software developed and recommended by the U.S. Environmental Protection Agency (EPA) for water quality simulation and analysis in various water bodies. It can simulate hydrodynamics, one-dimensional unsteady flow in rivers, three-dimensional unsteady flow in lakes and estuaries, and the transport and transformation patterns of conventional and toxic pollutants, based on the advection-diffusion equation [9~13]. The EFDC (Environmental Fluid Dynamics Code) model is a mathematical model covering one- to three-dimensional surface water quality, capable of simulating hydrodynamics, water quality, pollutant transport, and sediment transport in water bodies including rivers, lakes, reservoirs, wetlands, estuaries, and oceans. It is a multi-parameter finite difference model [14~16].

b) **Data-driven water quality prediction methods.** These methods utilize data analysis models and tools to model measured water quality data, then predict water quality indices through the established models. Common data-driven models include artificial neural networks, time series models, and support vector machines. These models establish data-driven representations of water quality evolution processes using observed water quality data at different times, enabling water quality process prediction [17~25].

Both categories have certain advantages; however, most existing methods yield

single-valued predictions of water quality indices, which typically carry randomness and lack convincing accuracy and credibility. Consequently, eutrophication assessments based on such predictions also suffer from randomness and uncertainty.

To address the limitations of single-valued prediction methods, this paper proposes a water quality prediction and eutrophication risk assessment method based on Monte Carlo simulation. Grounded in the evolution mechanisms of lake and reservoir water quality indices, a water quality kinetic model for lakes and reservoirs is established using nonlinear continuous differential equations. Given initial values of water quality indices and model parameters, Monte Carlo methods are employed to predict the evolution of water quality indices, obtaining probability distributions of future water quality values and achieving probabilistic water quality prediction. Furthermore, combining water quality prediction results with the comprehensive trophic state index method, the probability distribution of the comprehensive trophic state index and the probabilities of different trophic levels are obtained, enabling eutrophication risk assessment.

## 1 Water Quality Index Evolution Mechanism and Kinetic Model

The aquatic ecosystem primarily comprises four evolution processes: dissolved oxygen balance, phytoplankton dynamics, phosphorus cycle, and nitrogen cycle, which can be described by eight water quality indices: dissolved oxygen (DO), phytoplankton (Phyt), carbonaceous biochemical oxygen demand (BOD), organic phosphorus (OP), orthophosphate (PO4), organic nitrogen (ON), ammonia nitrogen (NH3-N), and nitrate nitrogen (NO3-N) [26,27].

The dissolved oxygen balance process is reflected through changes in DO and BOD concentrations, including processes such as reaeration, carbonaceous oxidation, nitrification, denitrification, sedimentation, plant growth, Phyt death, Phyt respiration, and sediment oxygen demand. The phytoplankton dynamics process primarily focuses on phytoplankton concentration in water bodies (phytoplankton is an ecological concept referring to microscopic plants living in suspension; typically, phytoplankton refers to floating algae), reflected through Phyt concentration changes and comprising three components: phytoplankton growth, death, and settling. The phosphorus cycle represents the transformation among three phosphorus forms, reflected through OP and PO4 concentration changes, including four processes: conversion of inorganic phosphorus (orthophosphate) to phytoplankton phosphorus, conversion of phytoplankton phosphorus to inorganic and organic phosphorus, mineralization, and settling adsorption. The nitrogen cycle represents transformation among four nitrogen forms, reflected through ON, NH3-N, and NO3-N concentration changes, including: conversion of inorganic nitrogen to phytoplankton nitrogen, conversion of phytoplankton nitrogen to inorganic and organic nitrogen, mineralization, nitrification and denitrification, and settling [28~30]. The aquatic ecosystem evolution process is illustrated in [Figure 1: see original paper].

[Figure 1: see original paper]

Based on the above water quality index evolution mechanisms, the water quality kinetic model is expressed as Equation (1), representing concentrations of water quality indices DO, Phyt, BOD, OP, PO4, ON, NH3-N, and NO3-N. Phyt concentration is based on chlorophyll-a (Chl_a) concentration, with parameters as model parameters whose meanings and units are shown in .

$$
\begin{aligned}
\frac{dC_{DO}}{dt} &= -k_1 C_{DO} - k_{11} C_{ON} - k_{12} C_{NH_3N} + k_{13} C_{DO} - C_{ON} + k_1 C_{DO} - C_{ON} + k_1 C_{DO} - C_{NH_3N} \\
&\quad + k_1 C_{DO} - C_{Phyt} + k_1 C_{Phyt} + C_{DO} - C_{Phyt} + k_1 C_{DO} - C_{Phyt} + k_1 C_{DO} - C_{Phyt} \\
\frac{dC_{Phyt}}{dt} &= -k_2 C_{Phyt} + k_2 C_{DO} - C_{Phyt} + k_2 C_{Phyt} + C_{DO} - C_{Phyt} + k_2 C_{Phyt} + C_{DO} - C_{Phyt} \\
\frac{dC_{BOD}}{dt} &= -k_3 C_{BOD} + k_3 C_{DO} - C_{BOD} + k_3 C_{DO} - C_{Phyt} + k_3 C_{Phyt} + C_{DO} - C_{Phyt} \\
\frac{dC_{OP}}{dt} &= -k_4 C_{OP} + k_4 C_{Phyt} + C_{DO} - C_{OP} + k_4 C_{Phyt} + C_{DO} - C_{Phyt} + k_4 C_{Phyt} + C_{DO} - C_{Phyt} \\
\frac{dC_{PO4}}{dt} &= -k_5 C_{PO4} + k_5 C_{Phyt} + C_{DO} - C_{PO4} + k_5 C_{Phyt} + C_{DO} - C_{Phyt} + k_5 C_{Phyt} + C_{DO} - C_{Phyt} \\
\frac{dC_{ON}}{dt} &= -k_6 C_{ON} + k_6 C_{Phyt} + C_{DO} - C_{ON} + k_6 C_{Phyt} + C_{DO} - C_{Phyt} + k_6 C_{Phyt} + C_{DO} - C_{Phyt} \\
\frac{dC_{NH_3N}}{dt} &= -k_7 C_{NH_3N} + k_7 C_{Phyt} + C_{DO} - C_{NH_3N} + k_7 C_{Phyt} + C_{DO} - C_{Phyt} + k_7 C_{Phyt} + C_{DO} - C_{Phyt} \\
\frac{dC_{NO_3N}}{dt} &= -k_8 C_{NO_3N} + k_8 C_{Phyt} + C_{DO} - C_{NO_3N} + k_8 C_{Phyt} + C_{DO} - C_{Phyt} + k_8 C_{Phyt} + C_{DO} - C_{Phyt}
\end{aligned}
$$

If we assume that model parameters vary slowly, Equation (1) can be expressed as $\dot{x} = f(x, \theta)$, where $x = [C_{DO}, C_{BOD}, C_{OP}, C_{PO4}, C_{ON}, C_{NH_3N}, C_{NO_3N}, C_{Phyt}]^T$ represents the vector of water quality indices and $\theta = [k_1, k_2, ..., k_{13}]^T$ represents model parameters. Here, $f(\cdot)$ is the water quality kinetic model function.

It should be noted that different water bodies such as lakes and estuaries have varying internal environments and characteristics, resulting in different model parameters. To ensure the water quality model is more accurate and reasonable, parameter values should be determined through combination with measured data (water quality index measurements) and relevant parameter calibration methods [31~34] when applied to different water environments.

## 2.1 Monte Carlo Simulation

Monte Carlo simulation refers to a simulation method that employs large numbers of repeated random experiments to obtain numerical solutions to problems. The fundamental principle is that when a problem or object possesses probabilistic characteristics, computer simulation can generate sampling results to calculate statistics or parameter values. As simulation iterations increase, stable

conclusions can be obtained by averaging estimates from each simulation. Based on the Law of Large Numbers (the probability of event A can be approximated by its frequency in numerous experiments), this method is commonly used to solve optimization, integration, and random probability distribution problems where analytical solutions cannot be precisely obtained [35~40]. The steps of the Monte Carlo simulation method are shown in .

## 2.2 Water Quality Index Evolution Prediction Based on Monte Carlo Simulation

Leveraging the advantages of Monte Carlo simulation, this paper predicts water quality index evolution based on this approach.

First, Equation (2) can be written in discretized form as:

$$x_{k+1} = x_k + h \cdot f(x_k, \theta_k) + \omega_k^x$$

$$\theta_{k+1} = \theta_k + h \cdot \omega_k^\theta$$

where $h$ is the prediction step size, $\omega_k^x$ is the process noise for water quality indices, and $\omega_k^\theta$ is the process noise for model parameters, with $\omega_k^x \sim \mathcal{N}(0, \Sigma_x)$ and $\omega_k^\theta \sim \mathcal{N}(0, \Sigma_\theta)$. Here, $\Sigma_x$ and $\Sigma_\theta$ are the corresponding noise covariance matrices.

In the Monte Carlo simulation-based prediction process, the evolution of water quality indices is simulated multiple times. For each simulation, the values of each water quality index at each prediction time point differ, exhibiting both regularity and randomness. Regularity arises because predicted values are generated based on a deterministic water quality kinetic model with initial values of water quality indices and model parameters. Randomness emerges because predicted values at each time point for each index vary due to noise effects. When the number of simulations is sufficiently large, probability distributions of each water quality index at different time points can be obtained by combining probability and statistical principles. The specific procedure is as follows:

a) Initialize water quality indices as $x_0$, model parameters as $\theta_0$, Monte Carlo simulation particle number as $N$, prediction days as $T$, prediction step as $h$ (where $h \leq 1$ day), and initial time $k = 0$.

b) Based on initial values of water quality indices and model parameters, assign initial values to $N$ particles: $x_0^{(i)} = x_0$, $\theta_0^{(i)} = \theta_0$ for all $i \in [1, N]$.

c) For time $t_k = k \cdot h$, predict water quality indices and model parameters $\{x_k^{(i)}, \theta_k^{(i)}\}$ for each particle $i \in [1, N]$ based on values at time $t_{k-1}$ using Equation (3) for single-step prediction to obtain $\{x_{k+1}^{(i)}, \theta_{k+1}^{(i)}\}$.

d) If $k < T$, update $k \leftarrow k + h$ and return to step c); otherwise, proceed to step e).

e) For all $k \in [0, T]$, calculate probability density functions:

- Water quality index PDF: $P(x_k|x_0, \theta_0) \approx \frac{1}{N}\sum_{i=1}^{N} \delta(x_k - x_k^{(i)})$
- Model parameter PDF: $P(\theta_k|x_0, \theta_0) \approx \frac{1}{N}\sum_{i=1}^{N} \delta(\theta_k - \theta_k^{(i)})$

where $\delta(\cdot)$ is the Dirac delta function.

## 2.3 Eutrophication Risk Assessment

The eutrophication risk assessment method in this section constructs a comprehensive trophic state index $TLI(\Sigma)$ based on the above water quality index evolution results. By classifying $TLI(\Sigma)$, it calculates the probabilities of different trophic levels.

Three water quality indices are selected: Chl_a (i.e., Phyt in this paper), total phosphorus (TP), and total nitrogen (TN). The trophic state indices for these three indicators are calculated, and through weight normalization, the probability distribution of the comprehensive trophic state index and the probabilities of different trophic levels are obtained [41~43]. The specific procedure is:

a) For time $t_k = k \cdot h$ and particle $i \in [1, N]$, extract $x_k^{(i)}$.

(a) For Chl_a:

$$TLI(Chl_a)_k^{(i)} = 10 \times (2.500 + 1.086 \ln(C_{Phyt,k}^{(i)}))$$

(b) For TP:

$$TLI(TP)_k^{(i)} = 10 \times [9.436 + 1.624 \ln(C_{OP,k}^{(i)} + C_{PO4,k}^{(i)})]$$

(c) For TN:

$$TLI(TN)_k^{(i)} = 10 \times [5.453 + 1.694 \ln(C_{ON,k}^{(i)} + C_{NH_3N,k}^{(i)} + C_{NO_3N,k}^{(i)})]$$

b) Calculate weights $w_j = r_j / \sum_{j=1}^{3} r_j$, where $r_{11}$ and $r_1$ are the weight and self-correlation coefficient of Chl_a, $r_{12}$ and $r_2$ are the weight and correlation coefficient with the baseline parameter Chl_a for TP, and $r_{13}$ and $r_3$ are the weight and correlation coefficient with the baseline parameter Chl_a for TN.

c) Combine individual trophic state indices and weights to calculate $TLI(\Sigma)_k^{(i)}$:

$$TLI(\Sigma)_k^{(i)} = w_1 \cdot TLI(Chl_a)_k^{(i)} + w_2 \cdot TLI(TP)_k^{(i)} + w_3 \cdot TLI(TN)_k^{(i)}$$

d) Based on the probability distribution of $TLI(\Sigma)$, calculate the probability of being in different trophic levels:

$$P(E_m) = \frac{1}{N}\sum_{i=1}^{N}\delta(TLI(\Sigma)_k^{(i)} \in [E_m, E_{m+1}))$$

where $[E_m, E_{m+1})$ represents the classification interval for trophic level $m$.

The $TLI(\Sigma)$ is graded on a 0–100 scale: $<$ 30 is oligotrophic, 30–50 is mesotrophic, and $>$ 50 is eutrophic. Higher values indicate more severe eutrophication. The correlation coefficients between the baseline parameter Chl_a and other parameters for Chinese lakes (reservoirs) are shown in .

## 3 Case Validation

Given initial values of water quality indices and model parameters, the effectiveness of the water quality prediction and eutrophication risk assessment method is verified using MATLAB.

### 3.1 Simulation Configuration

The initial water quality index values for simulation configuration are:

$$x_0 = [6.5, 0.05019, 3, 0.07, 0.06, 0.35, 0.36, 0.1]^T$$

Water quality index process noise covariance:

$$\Sigma_x = \mathrm{diag}\{0.1, 0.001, 0.01, 0.001, 0.001, 0.01, 0.01, 0.01\}$$

Initial model parameters:

$$\theta_0 = [1.208, 0.01, 0.01, 0.15, 0.13, 0.0009, 0.001, 0.025, 0.075, 0.9, 0.35, 1.02, 1.3]^T$$

Model parameter process noise covariance:

$$\Sigma_\theta = \mathrm{diag}\{0.1, 0.01, 0.001, 0.1, 0.001, 0.001, 0.0001, 0.0001, 0.0001, 0.01, 0.001, 0.01, 0.1\}$$

Prediction step size $h = 1/24$ day (hourly), number of particles $N = 1000$, prediction horizon $T = 100$ days.

### 3.2 Results and Analysis

Based on the simulation configuration in the previous section and using the water quality index evolution prediction algorithm from Section 3.2, evolution curves for $N$ particles are obtained, as shown in [Figure 2: see original paper]. The X-axis represents prediction time (100 days with 24 hours per day, totaling 2400 hours), and the Y-axis represents the range of water quality index values.

To more clearly represent the results, the probability density functions of the resulting probability distributions are shown in [Figure 3: see original paper]. The X-axis is prediction time (selecting the same time every 10 days over the 100-day period for clarity), the Y-axis is the range of water quality index values, and the Z-axis is the probability density function of water quality indices.

[Figure 2: see original paper]

[Figure 3: see original paper]

As shown in [Figure 2: see original paper], the eight water quality index prediction curves exhibit large variation ranges and strong divergence, demonstrating the stochastic nature of water quality prediction. Specifically, Phyt, BOD, ON, NH3-N, and NO3-N show strong divergence; OP and PO4 show relatively small divergence; and DO content first decreases rapidly then stabilizes within a narrow range. This is also reflected in the probability distribution curves in [Figure 3: see original paper].

With increasing prediction time, the probability distributions of all eight water quality indices gradually transition from tall-narrow to short-wide shapes, indicating randomness and noise sensitivity. Phyt, BOD, ON, NH3-N, and NO3-N exhibit strong randomness and high noise sensitivity; OP and PO4 show weaker randomness and lower noise sensitivity; DO demonstrates minimal randomness and noise sensitivity. Combined analysis of [Figure 2: see original paper] and [Figure 3: see original paper] reveals that the aquatic environment is complex, water quality predictions are subject to randomness from noise effects, but predictions remain stable within certain ranges, exhibiting determinism. Without special external factors, water body changes proceed slowly during this stage.

Based on the water quality index probability distributions in [Figure 3: see original paper] and using the eutrophication risk assessment method from Section 3.3, the probability distribution of the comprehensive trophic state index $TLI(\Sigma)$ and probabilities of different trophic states are obtained, as shown in [Figure 4: see original paper] and [Figure 5: see original paper]. In [Figure 4: see original paper], the X-axis represents prediction time (selecting the same time every 10 days for clarity), the Y-axis represents the range of $TLI(\Sigma)$ values, and the Z-axis represents the probability density function of $TLI(\Sigma)$. In [Figure 5: see original paper], the X-axis represents prediction time (2400 hours), and the Y-axis represents probabilities of different trophic states.

[Figure 4: see original paper]

[Figure 5: see original paper]

[Figure 4: see original paper] shows that eutrophication risk assessment exhibits randomness through the probability density functions. With increasing prediction time, the range of eutrophication risk assessment probability distributions expands, transitioning from tall-narrow to short-wide shapes, demonstrating randomness and uncertainty. This is also evident in [Figure 5: see original paper], where the probability of oligotrophic status decreases while mesotrophic

status probability increases with prediction time. According to phytoplankton characteristics, phytoplankton growth is seasonal, and water body eutrophication levels are generally seasonal as well. The initial water quality index and model parameter values selected in this paper represent oligotrophic conditions with increasing nutrient content.

In summary, water quality prediction-based eutrophication risk assessment exhibits both regularity and randomness. The probability distributions of both water quality index predictions and eutrophication risk assessment demonstrate that aquatic environments are complex and multi-factorial, making water quality prediction inherently stochastic. The proposed mechanism-based prediction method using water quality kinetic models and Monte Carlo simulation provides probabilistic predictions that offer higher accuracy compared to single-valued predictions.

## 4 Conclusion

This paper proposes a Monte Carlo simulation-based method for lake and reservoir water quality prediction and eutrophication risk assessment, integrated with water quality kinetic models. Based on the evolution mechanisms of lake and reservoir water quality indices, a water quality kinetic model is established using nonlinear continuous differential equations. Given prior distributions of water quality indices and model parameters, Monte Carlo simulation predicts the evolution of eight water quality indices, obtaining their probability distributions for water quality prediction. Simulation results demonstrate the stochastic nature of water quality prediction and varying noise sensitivity among different indices. Furthermore, by constructing a comprehensive trophic state index and combining it with water quality prediction results, the probability distribution of $TLI(\Sigma)$ is calculated, and classification of $TLI(\Sigma)$ yields probabilities of different trophic levels for eutrophication risk assessment. Simulation results show that eutrophication risk assessment based on water quality prediction is also stochastic.

In conclusion, the proposed Monte Carlo simulation-based method accounts for the stochastic nature of water quality prediction, compensating for the inaccuracy of single-valued water quality prediction and eutrophication assessment methods, reducing prediction randomness, and improving eutrophication risk assessment accuracy. Future work to further improve prediction accuracy will focus on two aspects: employing parameter calibration methods with measured water quality data to obtain estimated model parameters, and developing methods to address the slow-varying assumption of model parameters.

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*Note: Figure translations are in progress. See original paper for figures.*