

## Article

# Simulation of Chlorophyll a Concentration in Donghu Lake Assisted by Environmental Factors Based on Optimized SVM and Data Assimilation

Xiaodong Tang <sup>1</sup> and Mutao Huang <sup>2,\*</sup>

<sup>1</sup> School of Civil and Hydraulic Engineering, Huazhong University of Science and Technology, Wuhan 430074, China; d201780886@hust.edu.cn

<sup>2</sup> School of Electrical and Electronic Engineering, Huazhong University of Science and Technology, Wuhan 430074, China

\* Correspondence: huangmutao@hust.edu.cn

**Abstract:** Lake eutrophication is a global water environmental problem and has become a research focus nowadays. Chlorophyll a concentration is an important index in terms of evaluating lake eutrophication. The aim of this study was to build an effective and universal empirical model for simulation of chlorophyll a concentration in Donghu Lake. On the basis of the relationship between chlorophyll a concentration and dissolved oxygen (DO), water temperature (T), total nitrogen (TN), and total phosphorus (TP), models for simulating chlorophyll a concentration were built by using simulated annealing (SA), genetic algorithm (GA), artificial bee colony (ABC), and particle swarm optimization (PSO) to optimize parameters of support vector machine (SVM). Moreover, a collaborative mode (Col-SVM model) was built by introducing data assimilation, and meanwhile, accuracy and universality of the model were studied. Modeling results showed that the application of optimization algorithms and data assimilation improved the performance of modeling based on SVM. Model simulation results demonstrated that the Col-SVM model has high accuracy, decent stability, and good simulation effect; the root mean square error (RMSE), mean absolute percentage error (MAPE), Nash–Sutcliffe efficiency coefficient (NSE), bias, and mean relative error (MRE) between simulated values and observed values were 10.07  $\mu\text{g/L}$ , 0.31, 0.96,  $-0.050$ , and 0.15, respectively. In addition, model universality analysis results revealed that the Col-SVM model has good universality and can be used to simulate the chlorophyll a concentration of Donghu Lake at different times. Overall, we have built an effective and universal simulation model of chlorophyll a concentration that provides a new idea and method for chlorophyll a concentration modeling.

**Keywords:** chlorophyll a concentration; support vector machine; optimization algorithm; data assimilation; Donghu Lake



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## 1. Introduction

Lake eutrophication is a global water environmental problem [1,2]. Chlorophyll a concentration, as an important index of phytoplankton biomass as well as eutrophication, is of great significance for the study of primary productivity, eutrophication, and algal bloom [3,4]. Therefore, it is necessary to explore rapid and accurate methods to monitor chlorophyll a concentration [5].

The traditional in situ monitoring method is usually used as a method to acquire data as it is time-consuming, cumbersome, and of great space-time limitation [6]. Another category of chlorophyll a monitoring is modeling and simulation, which includes remote sensing inversion based on the special optical properties of chlorophyll a and water quality numerical modeling based on the formation mechanism of eutrophication. With the rapid development and wide application of remote sensing technology, remote sensing inversion

has gradually developed into an indispensable method for chlorophyll *a* monitoring because it is timely, widely covered, and costs relatively little [7,8]. Using in situ chlorophyll *a* concentration data and various satellite images such as Landsat 8 [9], MODIS [10], and Sentinel-2A [11], remote sensing inversion models have been built that are based on back propagation neural network (BPNN) [12], support vector machine (SVM) [13], extreme learning machine (ELM) [14], and artificial neural network (ANN) [15], and these models have good performance and high accuracy in simulating chlorophyll *a* concentration of inland water. However, remote sensing inversion has some limitations in monitoring chlorophyll *a* in lakes. Bad weather and a longer revisit cycle limit the images acquisition and application in time series analysis [16,17]. In addition, remote sensing of medium to small lakes requires moderate ( $\approx 300$  m) to high (10–30 m) spatial resolution sensors, and the resolution of commonly used and easily available satellite images usually cannot meet the requirements for water quality inversion of a small lake [18,19]. In addition, the inversion model has poor universality and it is only applicable to a specific area as the inland water body has different characteristics of regionality and seasonality [20,21]. Consequently, although there are many studies on the inversion of chlorophyll *a* concentration in Donghu Lake, there is no universally applicable model so far. Eutrophication is a water pollution phenomenon wherein large quantities of nutrition material such as nitrogen and phosphorus enter the water body, causing the rapid reproduction of algae and other phytoplankton, the decline of dissolved oxygen, the deterioration of water quality, and the destruction of the water ecosystem [22–24]. Water quality numerical modeling takes into consideration the complex physical, chemical, and ecological changes of water quality components during the formation of eutrophication, and therefore it can comprehensively and dynamically simulate the migration and transformation of water quality components as well as predict the change rule and development trend [25–27]. At present, the worldwide used water quality numerical models include WASP [28,29], EFDC [30,31], Delft3D [32,33], FVCOM [34,35], and MIKE [36,37]. However, adequate data and essential information needs to be collected to realize water quality numerical modeling and simulation of chlorophyll *a* concentration in lakes. In addition, the modeling process needs to input adequate files and appropriate parameters; the calibration of model parameters is cumbersome, and the operation of model system is complex. When lacking high-resolution satellite images and adequate data, we need to explore a new and effective method to monitor the concentration of chlorophyll *a* in lakes.

The factors leading to eutrophication differ from one lake to another as a variable environment [38]. However, lake eutrophication is mainly caused by excessive nutrient runoff to the lake [39]. There are many factors affecting the growth and reproduction of algae, such as light, temperature, pH, transparency, and nutrients [40,41]. At the same time, the rapid growth of algae will lead to some changes in lake water quality, such as the increase in chlorophyll *a* concentration and the decrease in transparency and dissolved oxygen (DO) [42]. Therefore, chlorophyll *a* concentration in water has a specific biochemical relationship with light, water temperature (T), total nitrogen (TN), total phosphorus (TP), and other physical or chemical environmental factors [43]. Nevertheless, the relationship has rarely been used to establish empirical models to simulate chlorophyll *a* concentration in lakes. Different from water quality numerical models, empirical models do not need to consider the complex formation mechanism of eutrophication, while it constructs the numerical relationship to realize simulation and prediction based on observed data and the machine learning algorithm.

SVM is a widely used machine learning algorithm that has advantages in solving nonlinear fitting and small sample learning problems [44,45]. Thus, it can be chosen as the method to explore the modeling of chlorophyll *a* concentration in Donghu Lake. Zhang et al. developed an SVM model for the chlorophyll *a* estimation of Donghu Lake using in situ chlorophyll *a* concentration data and synchronous Landsat 8 Operational Land Imager (OLI) images [46]. However, kernel function, kernel function parameters, and penalty factor have a great impact on the fitting effect of a SVM model [47]. Therefore, it is

necessary to select the appropriate kernel function and to use the optimization algorithm to optimize the parameters in a SVM model. Furthermore, due to the observation error of observed data and the systematic error of an empirical model, there are uncertainties in the modeling process and error between simulated values of the model and the actual value [48]. Data assimilation is an effective method for dynamic modeling that fuses different observation data into a model to modify the initial conditions, model parameters, and state variables, so as to improve the model prediction value, make it closer to the objective truth value, and reduce the uncertainty of model [49,50]. The introduction of data assimilation can integrate the advantages of different models and data, avoid the uncertainty of single model, and improve model accuracy.

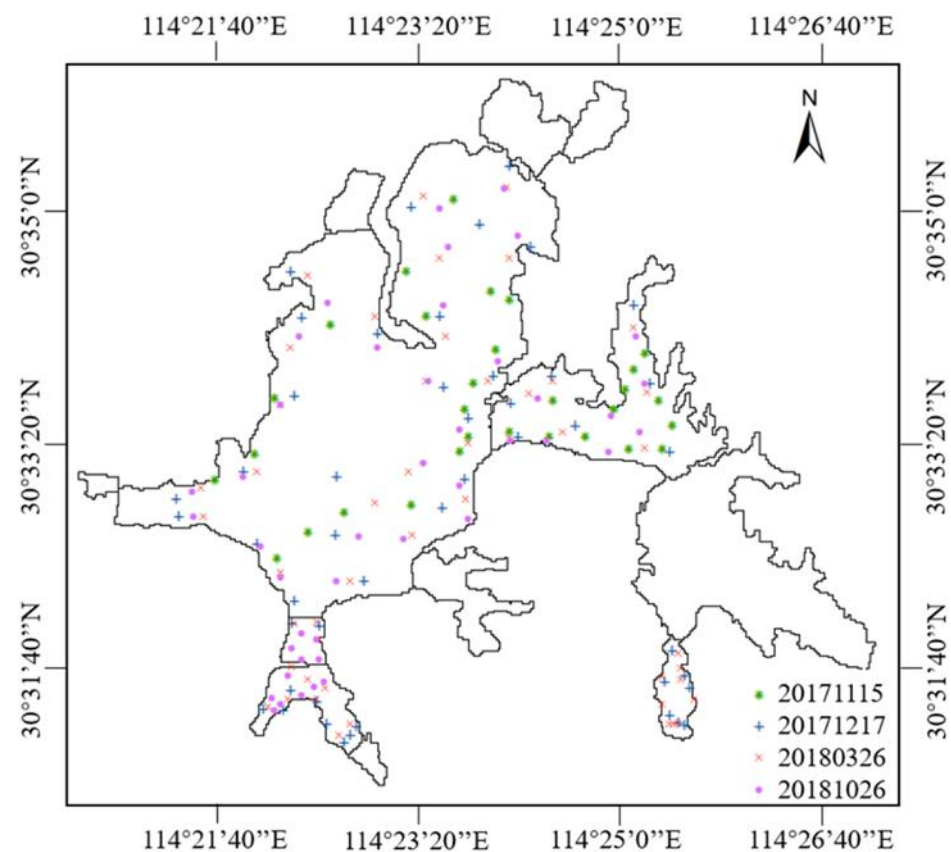
The main objective in this study is to build an effective and universal empirical model based on the relationship between chlorophyll a concentration and environmental factors and use it to simulate the chlorophyll a concentration in Donghu Lake. To improve the accuracy of the model, a variety of optimization algorithms and data assimilation are introduced into the modeling process. The contributions of this work are presented as follows: (a) multiple optimization algorithms are used to optimize parameters of the SVM, and empirical models for chlorophyll a concentration simulation are built on the basis of the relationship between chlorophyll a concentration and environmental factors (DO, T, TN, TP); (b) a collaborative model (Col-SVM model) is constructed to simulate chlorophyll a concentration that is based on SVM models and data assimilation; (c) the accuracy and universality of the Col-SVM model are analyzed and verified, proving that the Col-SVM model has high accuracy as well as good stability and can be used to simulate the chlorophyll a concentration of Donghu Lake at different times.

## 2. Materials and Methods

### 2.1. Study Area

Donghu Lake (30°22′–30°40′ N, 114°09′–114°39′ E) is located in the northeast of Wuhan, Hubei Province. It is a typical shallow lake in the middle reaches of the Yangtze River, covering an area of 32 km<sup>2</sup> and having a mean depth of 2.16 m with a maximum depth of 4.66 m [51]. Donghu Lake is one of the largest urban lakes in China, being mainly composed of Guozheng Lake, Tangling Lake, Miaohu Lake, Tuanhu Lake, Houhu Lake, and Shuiguo Lake. The average annual water temperature is 16.7 °C, the annual potential evaporation is 1269.6 mm, and the average annual precipitation is 1180 mm. The precipitation is concentrated from April to July, accounting for about 60% of the annual precipitation [52].

Sampling points were set up in Donghu Lake on 15 November 2017 (20171115), 17 December 2017 (20171217), 26 March 2018 (20180326), and 26 October 2018 (20181026). The sampling points were presented in Figure 1, and the water samples were taken from 0.5 m underwater at every sampling point. DO and T of each water sample were measured on site by a portable water quality detector, and TN and TP were detected by spectrophotometry with water samples sent to a laboratory.



**Figure 1.** Distribution of sampling points in Donghu Lake.

## 2.2. Support Vector Machine and Optimization Algorithms

### 2.2.1. Support Vector Machine (SVM)

SVM was proposed by Cortes and Vapnik in 1995 [53]. It can be used for classification [54,55], as well as regression [56,57]. When used for regression modeling, it has advantages in establishing models to solve small-sample, nonlinear, and multidimensional problems [58,59]. In addition, the selection of kernel function, the optimization of penalty parameter, and the kernel parameter determine the applicability and accuracy of the algorithm. The principle of SVM is discussed as follows [60,61]:

Suppose there is a training sample  $D = \{(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)\}$ , the regression model  $f(x) = \omega^T x + b$  can meet the condition that the maximum deviation between  $f(x)$  and  $y$  is below  $\epsilon$  for any  $x$ , where  $\omega$  and  $b$  are the model parameters to be determined, and  $\epsilon$  is the tolerable deviation. Then, the optimization target of SVM can be formalized as

$$\min_{\omega, b} \frac{1}{2} \|\omega\|^2 + C \sum_{i=1}^m l_{\epsilon}(f(x_i) - y_i) \quad (1)$$

where  $\frac{1}{2} \|\omega\|^2$  refers to the measurement of function flatness,  $C$  is the regularization constant,  $l_{\epsilon}$  is  $\epsilon$ -insensitive loss function, and  $l_{\epsilon}$  can be expressed as

$$l_{\epsilon}(z) = \begin{cases} 0, & \text{if } |z| \leq \epsilon \\ |z| - \epsilon, & \text{otherwise} \end{cases} \quad (2)$$

By introducing relaxation variables  $\xi_i$  and  $\hat{\xi}_i$ , Formula (1) is transformed into

$$\begin{aligned} \min_{\omega, b, \xi_i, \hat{\xi}_i} \quad & \frac{1}{2} \|\omega\|^2 + C \sum_{i=1}^m (\xi_i + \hat{\xi}_i) \\ \text{s.t.} \quad & f(x_i) - y_i \leq \epsilon + \xi_i \\ & y_i - f(x_i) \leq \epsilon + \hat{\xi}_i \\ & \xi_i \geq 0, \hat{\xi}_i \geq 0, i = 1, 2, \dots, m \end{aligned} \quad (3)$$

By introducing Lagrange multiplier  $\mu_i \geq 0, \hat{\mu}_i \geq 0, \alpha \geq 0, \hat{\alpha} \geq 0$ , Lagrange function is obtained:

$$\begin{aligned} L(\omega, b, \alpha, \hat{\alpha}, \xi, \hat{\xi}, \mu, \hat{\mu}) = & \frac{1}{2} \|\omega\|^2 + C \sum_{i=1}^m (\xi_i + \hat{\xi}_i) - \sum_{i=1}^m \mu_i \xi_i - \sum_{i=1}^m \hat{\mu}_i \hat{\xi}_i \\ & + \sum_{i=1}^m \alpha_i (f(x_i) - y_i - \epsilon - \xi_i) + \sum_{i=1}^m \hat{\alpha}_i (y_i - f(x_i) - \epsilon - \hat{\xi}_i) \end{aligned} \quad (4)$$

At the same time, satisfying the Karush–Kuhn–Tucker (KKT) conditions, the regression model of SVM can be obtained as

$$f(x) = \sum_{i=1}^m (\hat{\alpha}_i - \alpha_i) \kappa(x_i^T x) + b \quad (5)$$

where  $\kappa(x_i^T x) = \Phi(x_i)^T \Phi(x_i)$  is the kernel function. The sample that can meet the formula  $\hat{\alpha}_i - \alpha_i \neq 0$  is the support vector of SVM. The selection of kernel function and related parameters in the support vector machine has a great influence on the accuracy of the model.

### 2.2.2. Simulated Annealing (SA)

SA is a random optimization algorithm based on Monte Carlo iterative solution strategy. It was first proposed by N. Metropolis in 1953 [62], and it was successfully introduced into the field of combinatorial optimization by S. Kirkpatrick in 1983 [63]. It has few dependences on problem information, strong universality, and flexibility, and can effectively solve the problem of local optimal solution [64].

### 2.2.3. Genetic Algorithm (GA)

GA is an algorithm for searching the optimal solution by simulating the genetic mechanism and biological evolution. It was first proposed by John Holland in the 1970s [65]. R. H. Hollstien first used the genetic algorithm for function optimization [66]. It encodes the individuals of practical problems and obtains the optimal solution through a series of operations such as selection, crossover, and mutation. GA has high optimization efficiency, being able to prevent the optimization result from falling into the local optimal solution; at the same time, it has good stability.

### 2.2.4. Artificial Bee Colony (ABC)

ABC is a swarm intelligence optimization algorithm that was proposed by Karaboga in 2005 [67], being a global optimization algorithm based on swarm intelligence inspired by bees' behavior of searching for food sources [68]. It has the ability to get out of a local minimum and can be efficiently used for multivariable, multimodal function optimization [69]. In addition, it has fewer control parameters compared to other algorithms and has been successfully implemented for solving complex nonlinear optimization problems and engineering problems with high dimensionality [70].

### 2.2.5. Particle Swarm Optimization (PSO)

PSO is a swarm intelligence optimization algorithm based on bird feeding behavior. It was proposed by Eberhart and Kennedy in 1995 [71]. As a parallel global optimization algorithm, PSO has the advantages of simple structure, easy implementation, few parameters, and strong global ability [72].

## 2.3. Modeling and Simulation

### 2.3.1. Data Pre-Processing

The observed data obtained from four batches of water samples were processed to construct datasets named 20171115, 20171217, 20180326, and 20181026. The data of 43 sampling points on 26 March 2018 were randomly divided into two parts: the data of 28 sampling points were used to build the training dataset, and the data of 15 sampling points were used to build the testing dataset. Chlorophyll a was determined as the output layer and other water quality indexes as the input layer of the model. Mapminmax function was used in MATLAB software to normalize the training dataset and testing dataset.

### 2.3.2. Modeling

Radial basis function (RBF) was selected as the kernel function, and the chlorophyll a concentration simulation model was built on the basis of the training dataset and SVM. In addition, the model for which the penalty coefficient  $C$  and kernel parameter  $\gamma$  were not optimized in the modeling process was named as the SVM model, and it was used as the control group. At the same time, SA, GA, ABC, and PSO were used to optimize the SVM parameters (the penalty coefficient  $C$  and kernel parameter  $\gamma$ ). The optimal parameters of the SVM model were obtained through multiple training, and then the SA-SVM model, GA-SVM model, ABC-SVM model, and PSO-SVM model were built. In addition, the error between the simulated and observed values of chlorophyll a concentration in the training process was calculated and analyzed. According to the environmental factor data of the testing dataset, the SVM model, SA-SVM model, GA-SVM model, ABC-SVM model, and PSO-SVM model were used to simulate chlorophyll a concentration. Simulated values were compared with observed values to analyze the accuracy of each model.

The idea of classical data assimilation was to generate an optimal analysis value through the optimization algorithm under the condition of considering the background error and observation error, so that it can more accurately express and describe the real state variable. Model operator, observation operator, error estimation operator, and optimal algorithm are the constituent elements of data assimilation. The goal of data assimilation is to produce the optimal analysis value by optimizing the objective function. The objective function can be expressed as

$$J(x_a) = [H(x_a) - y_o]^T R^{-1} [H(x_a) - y_o] + (x_a - x_b)^T B^{-1} (x_a - x_b) \quad (6)$$

where  $J$  is the objective function;  $x_a$  is analysis value;  $H$  is observation operator, its function is to transform state variables into observation variables;  $y_o$  is the observed value;  $R$  is the observed error covariance matrix;  $B$  is the background error covariance matrix; and  $x_b$  is the background value. On the basis of the idea of data assimilation, the objective function of multi model collaborative simulation can be transformed into

$$J(x_a) = \sum_{i=1}^n (x_a - x_i)^T R_i^{-1} (x_a - x_i) \quad (7)$$

where  $J(\ )$  is the objective function,  $x_a$  is analysis values,  $n$  is the number of models,  $x_i$  is simulated values of different models, and  $R_i$  is the simulated error of different models. By calculating the gradient of Equation (7) and making it equal to 0, the optimal analysis value  $x_a$  can be obtained. The expression is

$$x_a = \sum_{i=1}^n K_i x_i \quad (8)$$

$$K_i = \frac{R_i^{-1}}{\sum_{i=1}^n R_i^{-1}} \quad (9)$$



where  $K_i$  is the weight of simulated values of different models, and  $R_i$  is the simulated error of different models. In this study, the root mean square error (RMSE) was used to describe the simulated error of different models.

According to simulated values and error of each model, the data assimilation method was introduced to construct the collaborative model and it was named the Col-SVM model.

### 2.3.3. Simulation and Model Analysis

Relative error (RE), absolute relative error (ARE), mean relative error (MRE), root mean square error (RMSE), mean absolute percentage error (MAPE), determination coefficient (R), Nash–Sutcliffe efficiency coefficient (NSE), and bias between simulated values and the true values were chosen as evaluation criteria to analyze the performance of the model. Generally, the observed value is used to represent the real value.

RE and ARE measure the error between simulated value and observed value from single group data, while MRE, RMSE, and MAPE measure the overall error between simulated values and observed values from the whole dataset. The smaller the values of RE, ARE, MRE, RMSE, and MAPE, the higher the model accuracy. R measures the linear relationship between the two variables; the absolute value of R is less than or equal to 1, where  $R < 0$  represents negative correlation and  $R > 0$  represents positive correlation. The larger the absolute value of R, the greater the correlation. NSE evaluates the accuracy of the model by comparing simulated values with the mean value of observed values. The closer the NSE value is to 0, the closer simulated value is to the mean value of observed values, and the model accuracy is poor. The closer the NSE value is to 1, the better the accuracy of the model. Bias reflects the error between the output of the model on the sample and the real value, that is, the smaller the bias, the smaller the deviation between the predicted value and the real value, and the higher the fitting degree of the model.

To analyze and evaluate the accuracy of the Col-SVM model, environmental factor data in the dataset 20180326 was used for the Col-SVM model to simulate the chlorophyll a concentration in Donghu Lake, and the error between simulated values and observed values was calculated. Furthermore, simulated values and observed values of chlorophyll a concentration were interpolated by Kriging interpolation method in ArcMap 10.2 software to obtain the chlorophyll a concentration distribution map of the whole Donghu Lake, and the differences between two distribution maps were compared to analyze the accuracy of the Col-SVM model.

The Col-SVM model was used to simulate the chlorophyll a concentration in Donghu Lake at four different times; the simulation results were analyzed, and the error between simulated values and observed values were compared to study the universality at different times.

## 3. Results and Discussion

### 3.1. Data and Datasets

Due to the vast water area of Donghu Lake and the limited sampling conditions, the amount of effective water sample data for the four times was different after excluding invalid data. In addition, the valid data constructed four datasets. Each dataset included five indexes: DO, T, TN, TP, and chlorophyll a concentration. The comparison of chlorophyll a concentration in the four datasets is shown in Table 1.

**Table 1.** The comparison of chlorophyll a concentration in four datasets.

Dataset	Number of Sampling Points	Minimum ( $\mu\text{g/L}$ )	Maximum ( $\mu\text{g/L}$ )	Average Value ( $\mu\text{g/L}$ )
20171115	29	6.91	50.65	23.00
20171217	42	5.25	157.72	49.00
20180326	43	3.57	162.29	44.77
20181026	43	17.46	140.93	57.25

Although the sampling time and sampling point location of the four sampling were different, the chlorophyll a concentration in Donghu Lake had an increasing trend only from the analysis of the chlorophyll a concentration average value.

The dataset of 20180326 was selected for modeling, being randomly divided into the training dataset and testing dataset. The comparison of chlorophyll a concentration in the two datasets is shown in Table 2.

**Table 2.** The comparison of chlorophyll a concentration in datasets for modeling.

Dataset	Number of Sampling Points	Minimum ( $\mu\text{g/L}$ )	Maximum ( $\mu\text{g/L}$ )	Average Value ( $\mu\text{g/L}$ )
Training dataset	28	3.71	159.49	48.37
Testing dataset	15	3.57	162.29	38.06

### 3.2. Parameter Optimization and Modeling

Using the 20180326 dataset, empirical models for chlorophyll a concentration simulation assisted by environmental factors was built on the basis of SVM. When modeling, RBF was selected as the kernel function, and RMSE between simulated values and observed values was selected as the fitness function. To improve the performance of empirical models, the penalty coefficient  $C$  and kernel parameter  $\gamma$  of SVM were optimized by SA, GA, ABC, and PSO. The optimized  $C$  and  $\gamma$  were obtained by optimization; then, the SA-SVM model, GA-SVM model, ABC-SVM model, and PSO-SVM model were built. At the same time, an empirical model named SVM model was built as the control group. The  $C$  and  $\gamma$  of each model are shown in Table 3.

**Table 3.** The comparison of model parameters.

Model	$C$	$\gamma$
SVM model	55.82	0.02047
SA-SVM model	15.27	0.5561
GA-SVM model	14.67	0.5959
ABC-SVM model	11.29	0.5316
PSO-SVM model	0.84	0.1890

As we can see from Table 3, the optimization of these optimization algorithms changed the parameters of SVM greatly in comparison with the control group. After optimization, the parameters of the SA-SVM model, GA-SVM model, and ABC-SVM model were close, while the parameters of the PSO-SVM model varied greatly compared with the SVM model; at the same time, they also had a large difference from the parameters of the other three optimized models.

The SA-SVM model, GA-SVM model, ABC-SVM model, and PSO-SVM model were used to simulate the chlorophyll a concentration. The RMSE, MAPE, NSE, and bias between simulated values and observed values of chlorophyll a concentration were calculated to compare and analyze the modeling performance of each model both in the training process and testing process. The error comparison of each model in the modeling process is shown in Table 4.

**Table 4.** The modeling error comparison of each model.

Model	RMSE ( $\mu\text{g/L}$ )	MAPE	NSE	Bias
SVM model	20.64	0.5180	0.8397	−0.06823
SA-SVM model	11.11	0.1702	0.9536	−0.02846
GA-SVM model	10.88	0.1673	0.9555	−0.02978
ABC-SVM model	11.93	0.1714	0.9465	−0.02605
PSO-SVM model	20.52	0.4727	0.8413	−0.06613



Through the modeling error comparison in Table 4, we see that RMSE and MAPE of four optimized models were all smaller than the SVM model, both in the training and testing process; in other words, the accuracy of empirical models is improved after the SVM parameters have been optimized. Among these models, the RMSE and MAPE of the GA-SVM model both in the training and testing processes were the smallest, which indicates that the GA-SVM model had the highest accuracy and the most stable performance. Furthermore, RMSE and MAPE of four optimized models were reduced in both training and testing processes compared with the SVM model, but those of the PSO-SVM model were not reduced by much. Combined with the result in that the parameters of the PSO-SVM model had a large difference from those of the other three optimized models, it illustrates that optimization of SVM parameters by PSO fell into local optimal value and that the optimized  $C$  and  $\gamma$  of the PSO-SVM model were not optimal.

The RMSE in the training process was selected to describe the simulated error of each model. Chlorophyll *a* concentration simulated values can be obtained by the simulation of the SVM model, SA-SVM model, GA-SVM model, ABC-SVM model, and PSO-SVM model on the basis of the environmental factor data in the testing dataset. According to the simulated error and simulated values of each model, the Col-SVM model can be built by introducing the data assimilation method. Six models were used to simulate the chlorophyll *a* concentration on the basis of the data of environmental factors in the testing dataset. The testing result comparison of each model is shown in Figure 2.

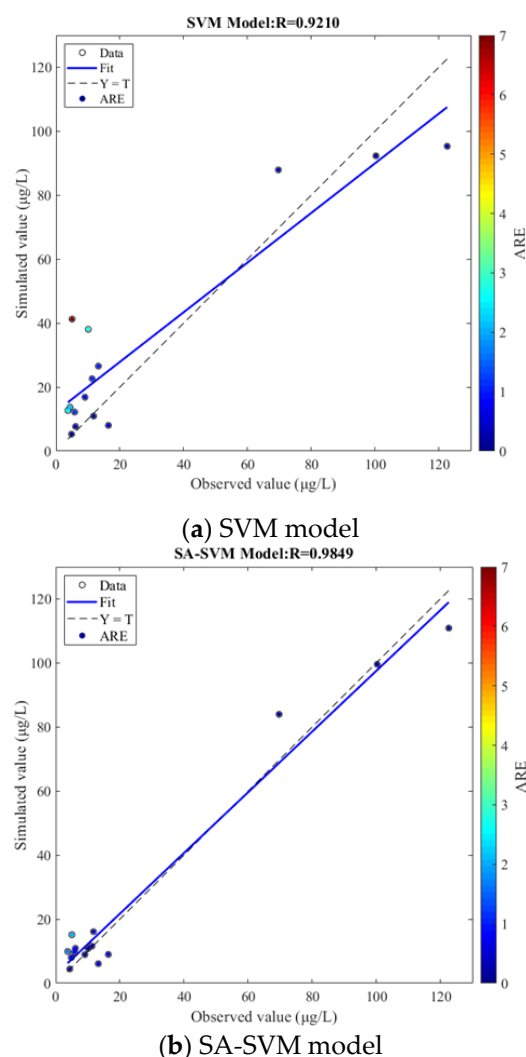
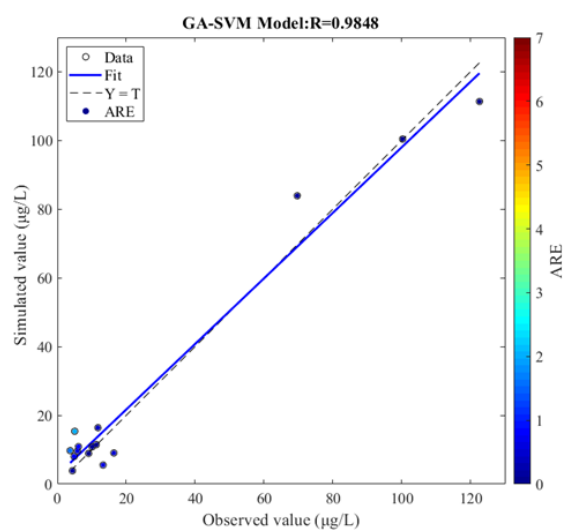
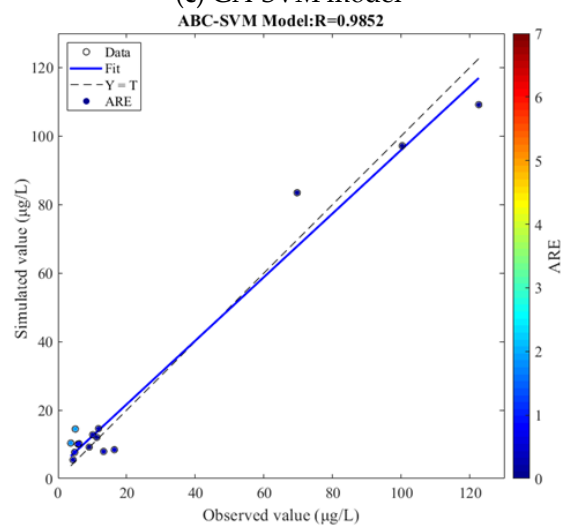


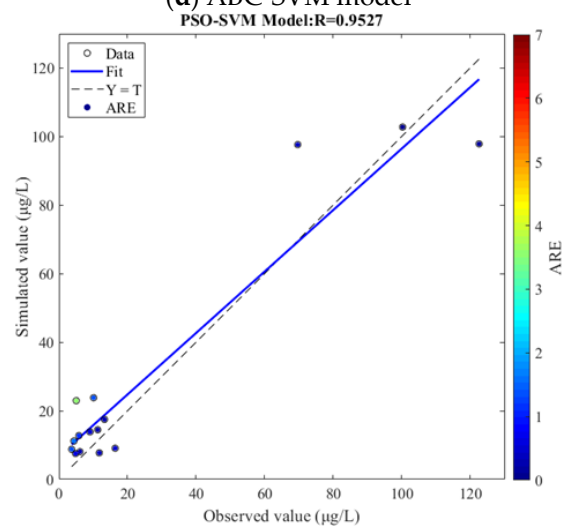
Figure 2. Cont.



(c) GA-SVM model

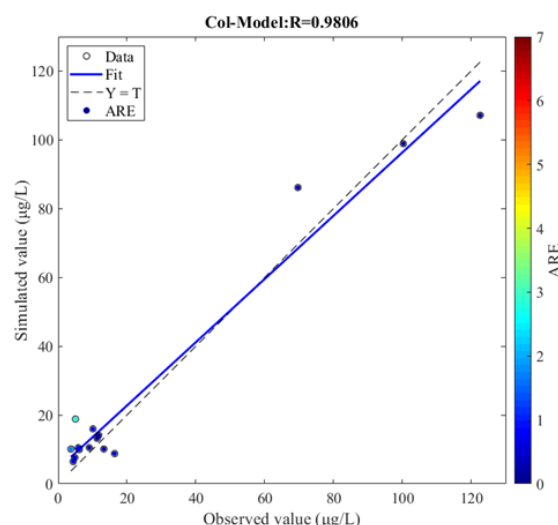


(d) ABC-SVM model



(e) PSO-SVM model

Figure 2. Cont.



(f) Col-SVM model

**Figure 2.** The testing results comparison of each model.

The results of linear regression analysis between simulated and observed values of chlorophyll a concentration in Figure 2 show that the Rs of each model were 0.9210, 0.9849, 0.9848, 0.9852, 0.9527, and 0.9806. All the Rs were larger than 0.92 in the analysis results of the five models, proving that it is feasible and effective to establish an empirical model based on SVM assisted by environmental factors for chlorophyll a concentration simulation. With the use of optimization algorithms, R of linear regression analysis was improved, and the coincidence degree between regression fitting line (Fit) and reference line ( $Y = T$ ) was enhanced. At the same time, ARE of sampling points was reduced, and sampling points were relatively closer to the regression fitting line compared with the control group. Furthermore, the analysis results of the Col-SVM model showed that the coincidence degree between Fit and  $Y = T$  was high, and the R can reach 0.9806, which was increased by 0.0596 compared with the SVM model. In addition, only a few sampling points deviated from the regression fitting line, and the ARE of all points did not exceed 1.8, except one point with a small observed value. Given all of this, the application of optimization algorithms and data assimilation improved the performance of empirical modeling, and the Col-SVM model showed a good effect on the simulation of chlorophyll a concentration in the testing process.

### 3.3. Simulation and Accuracy Comparison

On the basis of the environmental factors data in the 20180326 dataset, the SVM model, SA-SVM model, GA-SVM model, ABC-SVM model, PSO-SVM model, and Col-SVM model were used to simulate the chlorophyll a concentration, and the error between simulated values of each model and observed values was analyzed to compare the simulation performance of each model. RMSE, MAPE, NSE, and bias between simulated values and observed values were chosen as evaluation criteria to analyze the simulation effect and accuracy of each model. The simulation error comparison of each model is shown in Table 5.

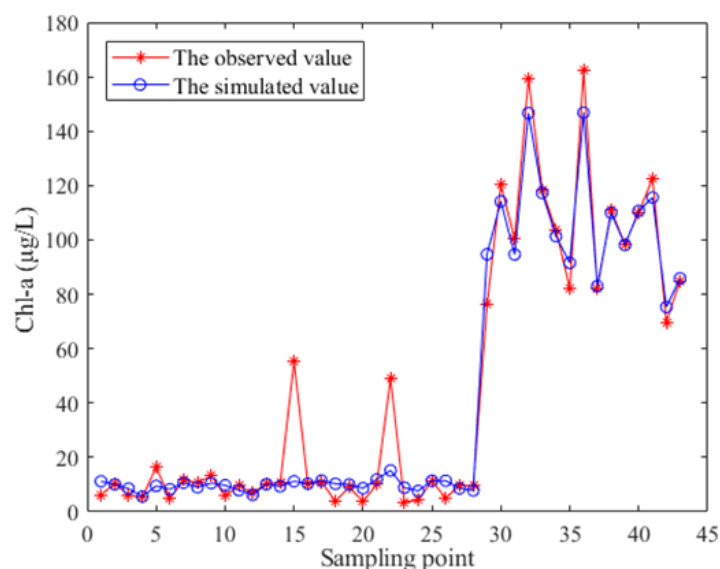
**Table 5.** The simulation error comparison of each model.

Model	RMSE ( $\mu\text{g/L}$ )	MAPE	NSE	Bias
SVM model	19.09	0.8477	0.7725	−0.02226
SA-SVM model	9.78	0.9600	0.2878	−0.01188
GA-SVM model	9.61	0.9614	0.2885	−0.01275
ABC-SVM model	10.40	0.9548	0.2913	−0.01101
PSO-SVM model	18.11	0.8630	0.6271	−0.00221

Table 5 shows that when the SVM model was directly used to simulate chlorophyll a concentration, there was an obvious error between simulated values and observed values, and the RMSE of SVM model reached 19.09  $\mu\text{g/L}$ . Due to the application of optimization algorithms and data assimilation in the SVM model, the RMSE between observed and simulated values of the empirical models was all reduced, showing that the simulation effect of the model on chlorophyll a concentration was improved with the application of optimization algorithms and data assimilation. Among all the optimized models, the RMSE reduction of GA-SVM model was the most, which was decreased by 9.48  $\mu\text{g/L}$ , and that of PSO-SVM model was the least, which was decreased by 0.98  $\mu\text{g/L}$  compared with the SVM model. For the Col-SVM model, its RMSE, MAPE, NSE, and bias were 10.07  $\mu\text{g/L}$ , 0.3132, 0.9577, and  $-0.0502$ , respectively, and its RMSE decreased by 9.02  $\mu\text{g/L}$  and MAPE decreased by 0.5345 compared with the SVM model. What is more, the Col-SVM model had the smallest MAPE and the largest NSE, and its NSE was closest to 1 among all the models. In other words, the error between simulated values and observed values was small, the Col-SVM model simulation accuracy was high, and the stability was good. This was because the Col-SVM model integrates the advantages of each SVM model through data assimilation, which ensures the stability of the model output. Taken together, the simulation error analysis result indicates that the application of optimization algorithms is useful in improving the performance of modeling based on SVM and environmental factors; in addition, GA has the best improvement effect. Moreover, data assimilation can not only improve the simulation effect, but also enhance the stability of the model.

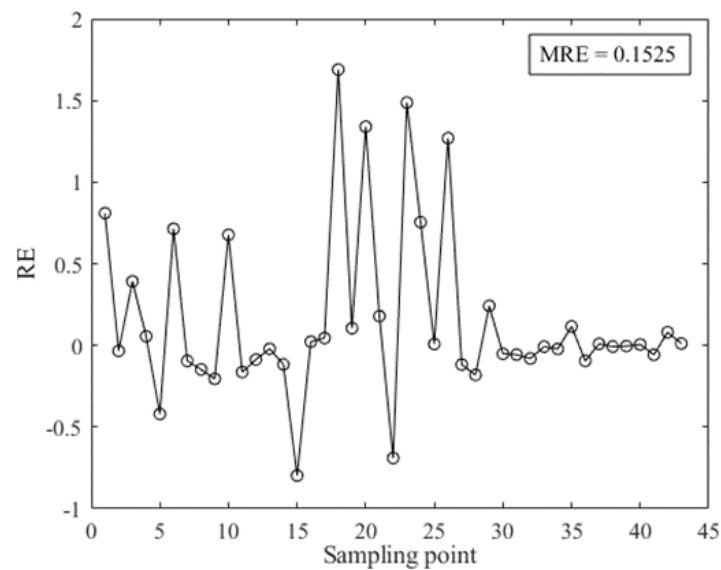
### 3.4. The Performance Analysis of the Col-SVM Model

To intuitively show the simulation accuracy of the Col-SVM model, comparison between the chlorophyll a concentration simulated values of the Col-SVM model and observed values at each sampling point was made; moreover, the error at each sampling point was analyzed by means of a chart. The comparison and analysis between simulated values of the Col-SVM model and observed values at each sampling point is shown in Figure 3.



(a) Comparison of simulation results

Figure 3. Cont.

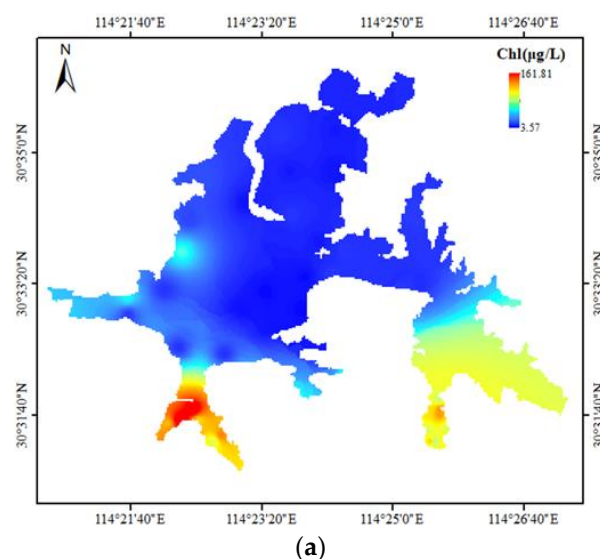


(b) Comparison of simulation error

**Figure 3.** The performance comparison and analysis of the Col-SVM model at each sampling point.

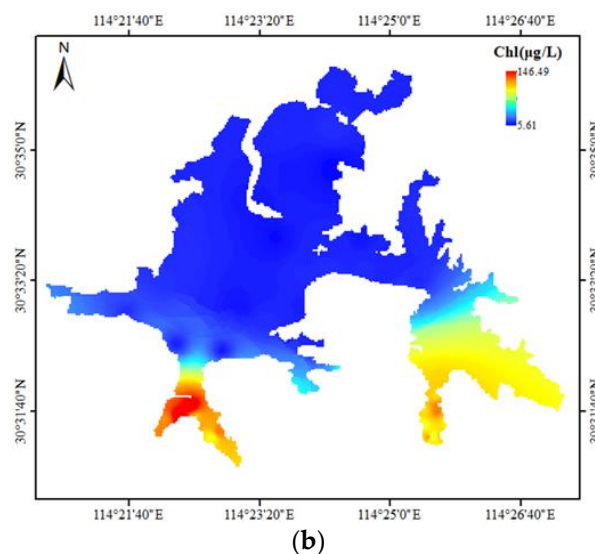
As shown in Figure 3a, simulated values of the Col-SVM model generally coincided with observed values, and simulated values of very few sampling points had obvious deviation from observed values. Figure 3b shows that relative error between simulated values and observed values at sampling points was mainly between  $-1$  and  $1$ , and most of them were between  $-0.5$  and  $0.5$ . In addition, MRE of simulation results was  $0.1525$ . Briefly, the error between simulated values and observed values was not large, and the Col-SVM model had high accuracy and a good simulation effect for chlorophyll a concentration.

To monitor the overall chlorophyll a concentration of Donghu Lake, it is necessary to convert the known chlorophyll a concentration at sampling points into the chlorophyll a concentration distribution map of the whole lake. The chlorophyll a concentration distribution maps of the whole Donghu Lake were obtained by the spatial interpolation method according to the Col-SVM model simulated values and observed values of chlorophyll a concentration, and they are shown in Figure 4. The simulation effect of the Col-SVM model can be comprehensively analyzed by comparing the differences between the two distribution maps.



(a)

**Figure 4.** Cont.



**Figure 4.** The comparison of chlorophyll a concentration distribution map in Donghu Lake. (a) Chlorophyll a concentration distribution map based on observed values. (b) Chlorophyll a concentration distribution map based on simulated values.

It is shown in Figure 4 that the chlorophyll a concentration distribution map based on observed values (a) and simulated values (b) were basically the same. Specifically, distribution of chlorophyll a concentration in the whole Donghu Lake varied greatly, and the areas with high chlorophyll a concentration were distributed in the south and southeast of Donghu Lake on 26 March 2018. Donghu Lake, as one of the largest urban lakes in China, has a vast area of water, but it has been divided into many sub lakes due to human intervention, the water fluidity is poor, and the material transfer and exchange between the sub lakes is slow. Guozheng Lake and Tangling Lake, which are located at the north of Donghu Lake, are the two largest sub lakes of Donghu Lake. They have a large water area and are connected with the Yangtze River and Shahu Lake. Therefore, the water body is flowing, and the pollutants in the water body are easy to diffuse, transfer, transform, and degrade. In addition, the two sub lakes are mainly surrounded by urban communities and natural scenic spots with strict pollution control and good ecological environment protection. As a result, the water quality is good, the eutrophication is not serious, and chlorophyll a concentration is not high. On the contrary, the area of other sub lakes is relatively small, and they have less connection with the external waters; the water flow is slow, and so is the material transfer and transformation. At the same time, most of these sub lakes are long and narrow in shape and have long shorelines around which are many residents, universities, markets, and farmland; as a result, a large amount of domestic sewage and irrigation wastewater containing nutrients are produced around it and are discharged into the water body of these lakes. From this, the concentration of nutrients such as nitrogen and phosphorus in local water bodies becomes extraordinarily high, resulting in water eutrophication and high chlorophyll a concentration. Generally, the simulation result of the Col-SVM model is basically consistent with the actual situation of Donghu Lake. However, there are some differences between Figure 4a,b. First, the concentration ranges of chlorophyll a in the two distribution maps were different. The maximum value in Figure 4a was greater than that in Figure 4b, and the minimum value in Figure 4a is smaller than that in Figure 4b. In addition, there were some differences in the distribution of chlorophyll a concentration in local waters in the two maps. For example, it is shown in Figure 4a that chlorophyll a concentration in Shuiguo Lake and the northwest of Guozheng Lake was higher than that in other waters of Guozheng lake. In the southeast sub lake of Donghu Lake, the chlorophyll a concentration of Miaohu Lake, Houhu Lake, and Yujia Lake increased successively as a whole. However, these differences were not reflected in Figure 4b. The difference between the two distribution maps shows that there were



some small errors in the simulation results of chlorophyll a concentration in Donghu Lake. In conclusion, the Col-SVM model shows a good effect on the simulation of chlorophyll a concentration in Donghu Lake, reflecting the real overall distribution of chlorophyll a concentration in Donghu Lake, but the local simulation effect was poor.

The universality of the Col-SVM model to simulate chlorophyll a concentration of Donghu Lake in the time dimension was verified by using the Col-SVM model and different datasets to simulate chlorophyll a concentration and comparing the error between simulated values and observed values at different times. The comparison between simulated values of the Col-SVM model and observed values of chlorophyll a concentration at different times is shown in Figure 5.

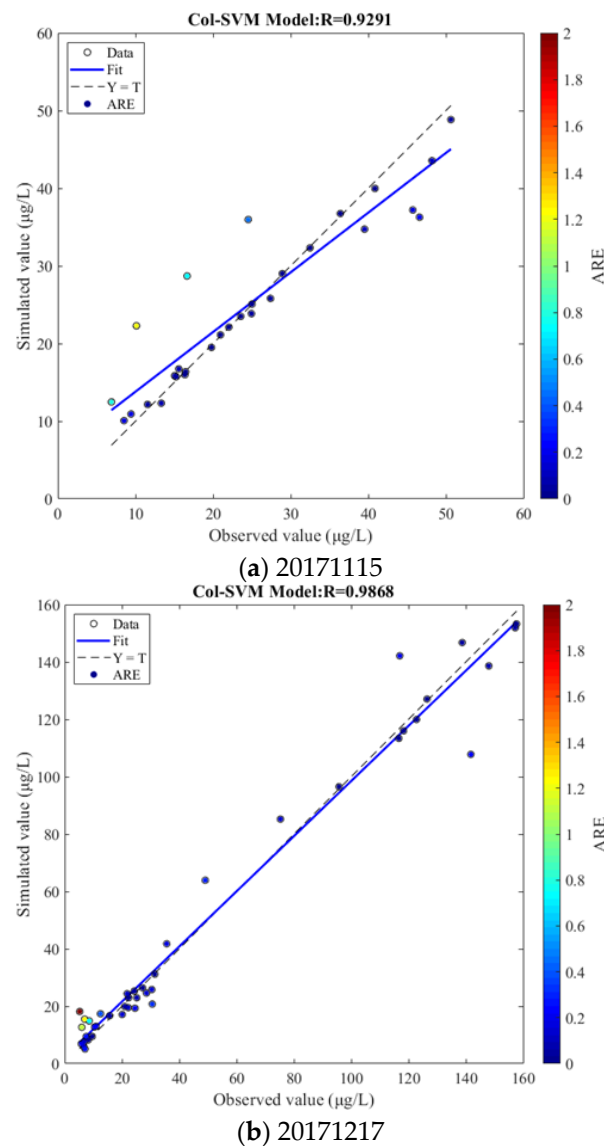
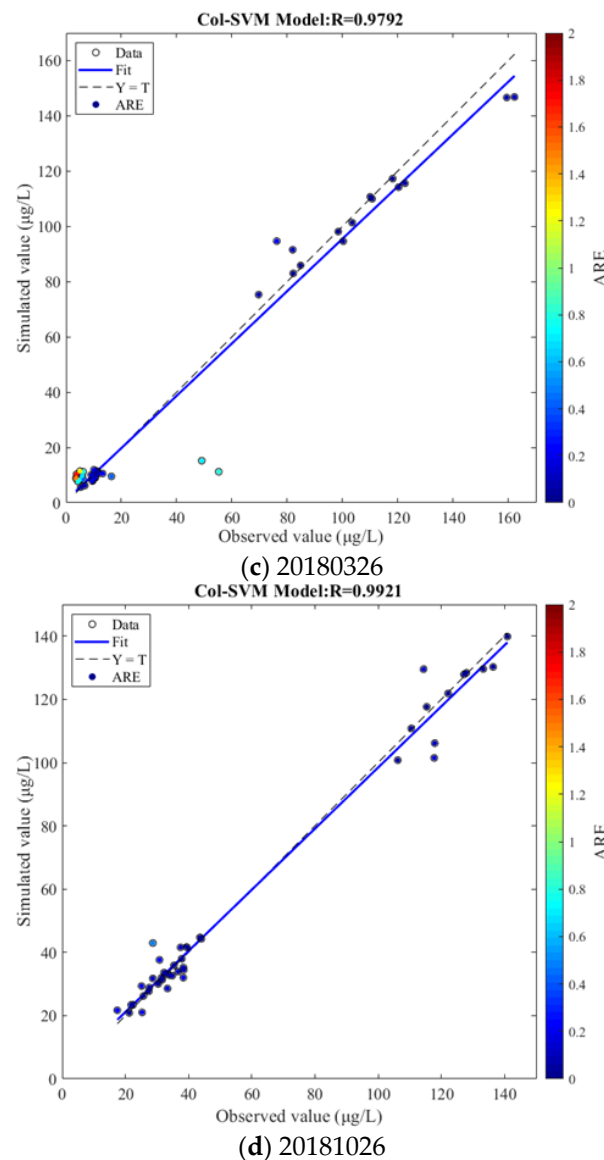


Figure 5. Cont.



**Figure 5.** The simulation results at four different times.

Figure 5 shows the comparison between simulated values and observed values of chlorophyll a concentration at different times, and the results demonstrated that R between simulated values and observed values of chlorophyll a concentration in four different time can reach 0.9291, 0.9868, 0.9792, and 0.9921, and that the determination coefficient between simulated values and observed values of chlorophyll a concentration at four different times all exceeded 0.92, indicating that the ABC-SVM model has good universality. At the same time, it can be found that when the chlorophyll a concentration was low, the simulated values were closer to the observed values, and the simulation effect of the ABC-SVM model was better. When the chlorophyll a concentration was too high, there was a large deviation between the simulation result and the observed values in some sampling points. In general, the difference was not large between simulated values and observed values of chlorophyll a concentration in four time periods, and only a few sampling points had obvious errors. In sum, the Col-SVM model has a good universality in the time dimension and can be used to simulate the chlorophyll a concentration in Donghu Lake at different times.

#### 4. Conclusions

In this study, we used SA, GA, ABC, and PSO to optimize the penalty coefficient C and kernel parameter  $\gamma$  of SVM and built SVM models for chlorophyll a concentration

simulation assisted by environmental factors. SVM models (SVM model, SA-SVM model, GA-SVM model, ABC-SVM model, PSO-SVM model) were used to construct the Col-SVM model collaboratively by the introduced data assimilation method. These empirical models were used to simulate the chlorophyll a concentration in Donghu Lake, and the simulation effect of the models was compared and analyzed. The modeling results show that the application of optimization algorithms improved the performance of modeling based on SVM and GA had the best improvement effect. In addition, data assimilation can not only improve the simulation effect, but it can also enhance the stability of the model. The Col-SVM model had good performance in simulating the concentration of chlorophyll a in Donghu Lake, and RMSE, MAPE, NSE, bias, and MRE between simulated values and observed values were 10.07  $\mu\text{g/L}$ , 0.3132, 0.9577,  $-0.0502$ , and 0.1525, respectively. Furthermore, R between simulated values and observed values of chlorophyll a concentration at four different times all exceeded 0.92, and Col-SVM model had a good universality in the time dimension and was able to be used to simulate the chlorophyll a concentration in Donghu Lake at different times. In conclusion, the Col-SVM model is a simple and effective empirical model for simulation of chlorophyll a concentration in Donghu Lake.

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