Research on multi-parameter stepwise coupling inversion method for marine integrated element water quality model based on data-driven and genetic calculation

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In this method, there are two inversion phases step by step, namely, preliminary inversion and precise inversion. Preliminary inversion is implemented by coupling data-driven model with Marine Integrated Element Water Quality Model (MIEWQM), to determine the relationship between the multi-parameter and the pollution concentration values in gauge stations. Field data are inputted the relationship to obtain the initial values of multi-parameter matching. MIEWQM is embedded into Genetic Algorithms (GAs) to search global multi-parameter optimal values in the precise inversion. Preliminary inversion provides the initial values of multi-parameter matching to the precise inversion for shortening the value-taking range of population in GAs. Case studies in Bohai Bay, China. An "identical twin experiment" method and a practical application with Dissolved Inorganic Nitrogen (DIN) are used to verify the present method.

[**Keywords:** marine integrated element water quality model, data-driven model, genetic algorithms, multi-parameter matching, stepwise coupling, inversion]

Introduction

The development of an effective parameter inversion method for water quality model play an important role in simulating both the long-term prediction of global climate feedback and the short-term forecast of the quality changes of basin-scale water[1].

To resolve this inverse problem mentioned above, many methods have been developed. Trial and error[2] is a widely used technique for model calibration[3]. It has advantage of simple and easy to perform. However, the accuracy of the model completely depends on subjective experience, a local optima is obtained from this method usually. For the inverse problem of multi-parameter and strong nonlinearity, uncertainty tremendously exists in this method.

With the abundance of satellite data, data assimilation methods with the adjoint technique have recently been developed. Lawson et al. (1996, 1995) [4, 5] introduced the adjoint method for data assimilation of marine ecosystem model,

the Lagrange operator is used to construct the adjoint equation, resulting in the successful estimation of the model parameter. Vallino (2000)[6] measured the capability of various data assimilation methods with incorporating mesocosm experiment data and the numerical instability of the adjoint approach. Model parameters are not constant but may vary in space and time due to different plankton taxonomic compositions and different external impact factors over a large domain. It has been proved that the temporal and spatial variations of the model parameters had more influence on the state variable than the improvement accuracy of the physical model by some studies[7-12]. However, adjoint equations are as complicated as water quality model equations, both water quality model equations and adjoint equations need to be calculated in each iterative process. How to raise the computation efficiency is the key difficulty for this method [13].

Following the development of the soft computing techniques, it has been applied to resolve the inverse problem popularly. Liu et al. (2007)[14] employed GAs method for calibrating the PIT model in the Windrush catchment. Same method is used by Tang et al. (2010)[15] for model parameter identification of river network. Simulated annealing algorithm is applied to estimate the parameters of river water quality model[16]. The strengths of these techniques include the fast convergence speed and global optimization.

Present study is to develop a more practical and precise technique to inverse the multi-parameter of marine water quality model. An outline of the procedure is as follows. As the value-taking range of population, the initial values of multi-parameter matching are inversed by a data-driven model[17] based on an Artificial Neural Network (ANN). Coupled with marine water quality model, GAs is employed for the precise inversion of multi-parameter. Based on the Osaka Daigaku Estuary Model (ODEM)[18], a MIEWQM is developed to simulate the marine

water quality in involved areas.

Materials and Methods
Numerical models
Data-driven model

Unlike knowledge-driven models (i.e., physically based models), data-driven models rely purely on the limited knowledge of the modeling process and the input and output data to describe the characteristics of the system. The model makes abstractions and generalizations of the process, and often plays a complementary role to the physically based model. Data-driven models can be implemented with ANNs, expert systems, fuzzy logic concepts, rule induction, and machine learning systems. The fundamental expression of the data-driven model is as follows:

$$\left(y_1, \cdots, y_i, \cdots y_m\right) = F\left(x_1, \cdots, x_i, \cdots x_n\right) \quad (1)$$

$\left(x_1, \cdots, x_i, \cdots x_n\right)$ and $\left(y_1, \cdots, y_i, \cdots y_m\right)$ are

the input and output variables, respectively, where m is the number of output variables, n is the number of input variables, and F is the objective function that needs to be dug by the model. In this paper, the results of ANN are used for the fitting of F.

BPNN

After McCulloch and Pitts (1943)[19] introduced the concept of an artificial neural network, numerous models have been developed. The BPNN proposed by Rumelhart et al. (1986)[20] has solved the hidden layer of learning difficulty in multi-layer networks and became the most commonly used model among all ANNs. The key point is the discovery of the error in the back propagation technique. In the learning process of the BPNN, the interconnection weights are adjusted from the back layers to the front layers to minimize the output error. The merit of the BPNN is that it can approach any nonlinear continuous function after being trained[21]. Several numerical details of the BPNN are described in the following section.

Data normalization

All of the data of input and output layers are normalized on a range from 0 to 1 by Eqs. (2):

$$\bar{Y}_{gi} = \frac{Y_{gi} - Y_{g\min}}{Y_{g\max} - Y_{g\min}} \qquad (2)$$

where $\bar{Y}_{gi}$ is the value of the data after normalization, Y_{gi} is the value of the data before normalization, $Y_{g\max}$ is the maximum of all data, and $Y_{g\min}$ is the minimum of all data.

To consider the nonlinearity, the sigmoid transfer function is used:

$$s(x) = 1 \Big/ 1 + e^{-x+\theta} \qquad (3)$$

where θ is the threshold value of hidden neurons.

Learning rate η and appended momentum

The efficiency and speed of convergence of the BPNN learning algorithm are affected by the learning rate η and the appended momentum (L&A). L&A are the control parameters of the BPNN training algorithms, which is responsible for controlling the step size when weights are iteratively adjusted. A low L&A leads to a slow learning of the network. A high L&A causes the weights and objective function to diverge, so learning is nil. The value of L&A depends on whether the time series changes frequently. If the time series changes frequently, the value of L&A should be increased. L&A ranges from 0 to 1, the learning rate is set to 0.05, and the appended momentum is 0.5 in the present research after testing.

Error function

The root mean squared error (RMSE) is used to evaluate the accuracy of prediction and is defined as follows:

$$RMSE = \sqrt{\sum_{i=1}^{n} (\eta_i^o - \eta_i^p)^2 \Big/ n} \qquad (4)$$

The correlation coefficient (CC) is computed using Eqs. (5)–(7).

$$CC = \frac{\sum_{i=1}^{n} \left(\eta_i^o - \bar{\eta}^o\right)\left(\eta_i^p - \bar{\eta}^p\right)}{\sqrt{\sum_{i=1}^{n} \left(\eta_i^o - \bar{\eta}^o\right)^2 \sum_{i=1}^{n} \left(\eta_i^p - \bar{\eta}^p\right)^2}} \qquad (5)$$

$$\bar{\eta}^o = \frac{\sum_{i=1}^{n} \eta_i^o}{n} \qquad (6)$$

$$\bar{\eta}^p = \frac{\sum_{i=1}^{n} \eta_i^p}{n} \qquad (7)$$

where CC is the correlation coefficient, η^o is the field data, η^p is the simulated data, and n is the number of data.

Structure of the BPNN

The structure of the neural network, including the number of hidden layers and neurons, is determined by the complexity of the problem to be solved. Although the increase in the number of hidden layers and neurons can reflect the complexity of the problem and decrease the number of iteration steps, it is not useful in increasing precision and may lead to over-fitness. Therefore, throughout the course of this research, one hidden layer is chosen.

The number of neurons for the hidden layer can be calculated using the following formula:

$$NH = \frac{NI + NO}{2} \qquad (8)$$

where NH is the number of neurons in the hidden layer, NI is the number of neurons in the input layer, and NO is the number of neurons in the output layer. Detailed information can be found in the work of Li et al. (2007)[22] and Liang et al. (2008)[23].

GAs

The genetic algorithm is a global random search method. The optimal solution could be obtained by the biological process of selection, crossover and mutation.

Encoding

In the progress of GAs, the first key problem is to decide the parameter encoding problem of design parameter. In this study, real coding is chosen because multi-parameter exist in water quality model. Real encoding GAs has been also introduced to a wide variety of applications in recent years. All genes in a chromosome used in real encoding GAs are real numbers. It is more suitable to directly represent genes as real values for most of real optimization problems during genetic operations. Because the procedures of binary encoding for a real number may suffer for the loss of precision depending on the number of the used bits, and it will be very complicated and difficult to implement if the numerical values are large. For the real encoding GAs, the length of chromosomes becomes much shorter than the one by using the binary encoding. This implies that the program for such algorithms can be easily performed.

Fitness calculation

As global search algorithm, GAs searches the global optimal solution through fitness of individual computed by the fitness function and doesn't use the external information input. The fitness function is the key step influencing the algorithm converge velocity and optimal solution resolved. Commonly the fitness function is converted by the objective function. Objective function is defined as RMSE and converted to the fitness function in this paper.

Selection method in evolution

This operator selects chromosomes in the population for reproduction. The fitter the chromosome, the more times it is likely to be selected to reproduce. A common selection method in GAs is fitness proportionate selection, in which the number of times an individual is expected to reproduce is equal to its fitness divided by the average of finesses in the population. (This is equivalent to what biologists call "viability selection.")

A simple method of implementing fitness proportionate selection is "roulette wheel sampling", which is conceptually equivalent to giving each individual a slice of a circular roulette wheel equal in area to the individual's fitness. The roulette wheel is spun, the ball comes to rest on one wedge shaped slice, and the corresponding individual is selected.

Crossover

Crossover is one of the main genetic operators, in which two chromosomes are selected as parents whose mating results in two new chromosomes called offsprings for the next generation. The performance of GAs heavily depends on the performance of the crossover operator used in GAs.

In real encoding GAs, one of the most commonly used crossover operator is arithmetic crossover in which the offsprings are obtained through the following equations by a certain crossover rate:

$$Os1 = \omega \times Pa1 + (1-\omega) \times Pa2 \qquad (9)$$

$$Os2 = \omega \times Pa2 + (1-\omega) \times Pa1 \qquad (10)$$

Where ω is a random parameter range from –0.25 to 1.25, Os and Pa is the offspring and parent respectively.

Mutation

Mutation is a background operator which produces spontaneous random changes in various chromosomes. A simple way to achieve mutation would be to alter the value of one or more genes. Mutation serves the crucial role of exploration of search space and generation of sufficient variety in the chromosomes being used in GAs.

In real encoding GAs, the mutation is done through the following equation by a certain mutation rate:

$$X = X' + \Delta(t, y) \qquad (11)$$

$$\Delta(t, y) = y \times \left(1 - r^{\left(1 - t/T\right)^b} \right) \qquad (12)$$

Where X is mutated gene, X' is original gene, t is current generation, T is maximum generation, r is a random parameter range from 0 to 1, b is a system parameter, y is defined as:

$$y = \begin{cases} X' - LD & i = 0 \\ UD - X' & i = 1 \end{cases} \qquad (13)$$

Where LD is the minimum of gene, UD is the maximum of gene, i is a random parameter equal to 0 or 1.

Results and Discussion

Marine Integrated Element Water Quality Model (MIEWQM),

A water quality model is a fundamental simulating tool for regional water environmental management. Moreover, a water quality model attempts to explain underlying physical-biochemical processes. There are many water quality models that can retrieve entitative ocean conditions with great precision. Complex models that include sufficient details of physical-biochemical processes have become possible due to the rapid increase of computing capability. However, excessive complexity inevitably leads to numerous uncertainties and problems in the interpretation of the dynamics process of the model[24]. ODEM, developed by Nakatuji et al. (2001)[18], is employed as a water quality simulating tool to validate the multi-parameter stepwise coupling optimization inversion method. ODEM has been used not only for water quality modeling but for coastal waters studies as well. The sensitive model's parameters are not constant but may vary in space and time due to different plankton taxonomic compositions over a large domain. Therefore, the split-domain and period parameter evaluation method, named MIEWQM, is presented in this model.
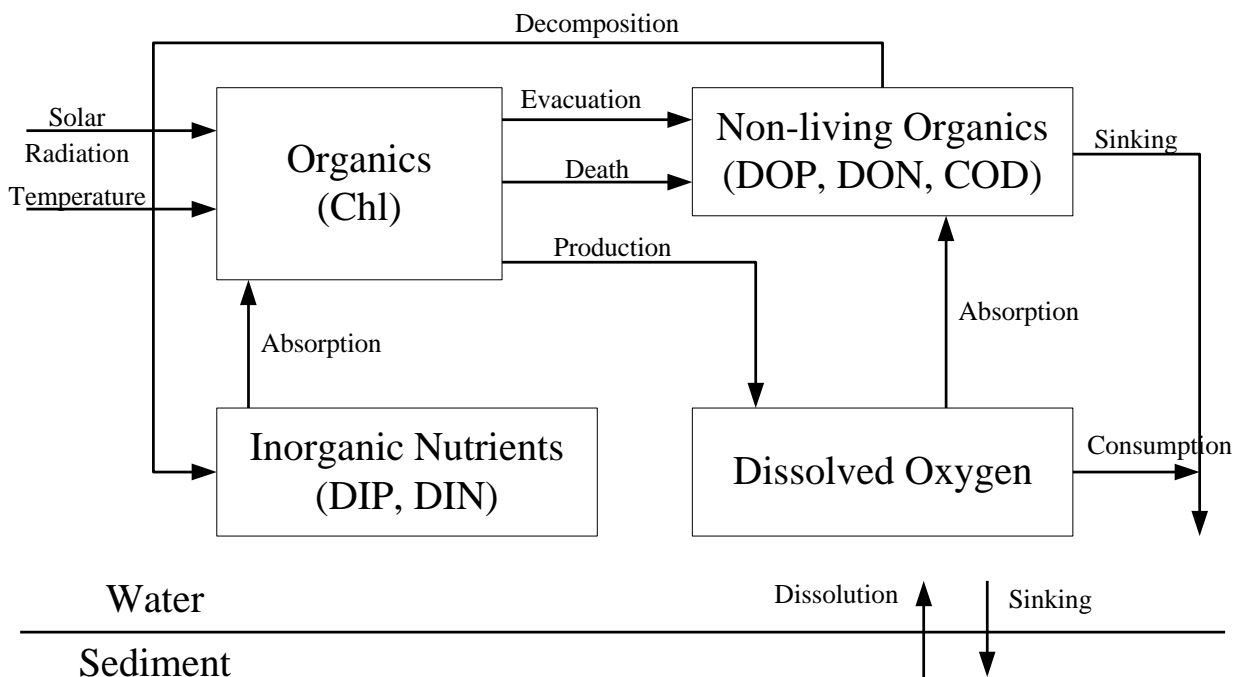

Fig. 1—Schematic diagram of matter circulation in ODEM

Figure 1 shows the schematic diagram of matter circulation in ODEM. The main processes in the model follow. Phytoplankton releases nonliving organics (e.g., organic nitrogen, organic phosphorus, and chemical oxygen demand) and dissolves oxygen by evacuation, death, and production. The parts of nonliving organics sink into the sediment with detritus, and others decompose into inorganic nutrients combined with dissolved oxygen. Phytoplankton growth is controlled by inorganic nutrients, temperature, and solar radiation.

Multi-parameter stepwise coupling optimization inversion method

Inversion method

A new technique that automatically combines a data-driven model and GAs with a MIEWQM was developed. In the technique, the water quality model repeats a series of designed computations. Subsequently, a data set that contains the corresponding relationship between the values of the model parameters $[(x_1, \cdots, x_i, \cdots x_n)$ in Eqs. (1)] and the values of gauge stations for pollution (state variables) $[(y_1, \cdots, y_i, \cdots y_m)$ in Eqs. (1)] is stored. The task of the data-driven model is to find the relationship [F in Eqs. (1)] between $(x_1, \cdots, x_i, \cdots x_n)$ and $(y_1, \cdots, y_i, \cdots y_m)$. After the field data are transferred into the model, the initial values of multi-parameter matching are obtained for the initial population in GAs. The optimal multi-parameter solution is obtained by the genetic calculation with the coupling of GAs and MIEWQM.

Figure 2 describes the process of multi-parameter stepwise coupling inversion method. The sequence is one through eighteen. The MIEWQM is coupled with data-driven model and GAs for preliminary and precise inversion respectively. There are two modules in the preliminary inversion, namely, water quality simulation module and preliminary inversion module. The computation of the designed cases is executed by the water quality simulation module. The preliminary inversion module is responsible for the analysis of water quality simulation results, as well as the initial values of multi-parameter matching. The precise inversion has water quality simulation module, judgment and output module and genetic calculation module. Water quality simulation module is applied for simulating each chromosome. The judgment and output module calculate the fitness of all chromosomes and judge the end conditions of program. If the end conditions are not satisfied, genetic calculation module is used to produce a new population. The initial values of multi-parameter matching are the key link of preliminary and precise inversion.

The detailed procedure of the technique is as follows.

Detailed inversion procedure

Preliminary inversion of multi-parameter matching by data-driven model

Step 1: Choice of control variables

There are various parameters in the water quality model that react differently with one another. If all forms are included, the computation cost will be excessive, and uncertainty increases[25]. Therefore, sensitive model parameters have been analyzed in order to select the control variables[26].

Step 2: Case computation by the water quality model

In water quality numerical models, the governing equations have to be discretized into the computation domain. Initial guess values for all control variables are assumed, and their corresponding ranges are set. If the number of control variables is m, and n values are taken for one control variable, there are as many as

$$\prod_{i=m} \left[C_n^1 \right]_i = n^m$$ designed cases. All designed

cases are individually computed by ODEM. The results of pollution concentration serve as output and are stored for the data-driven model.
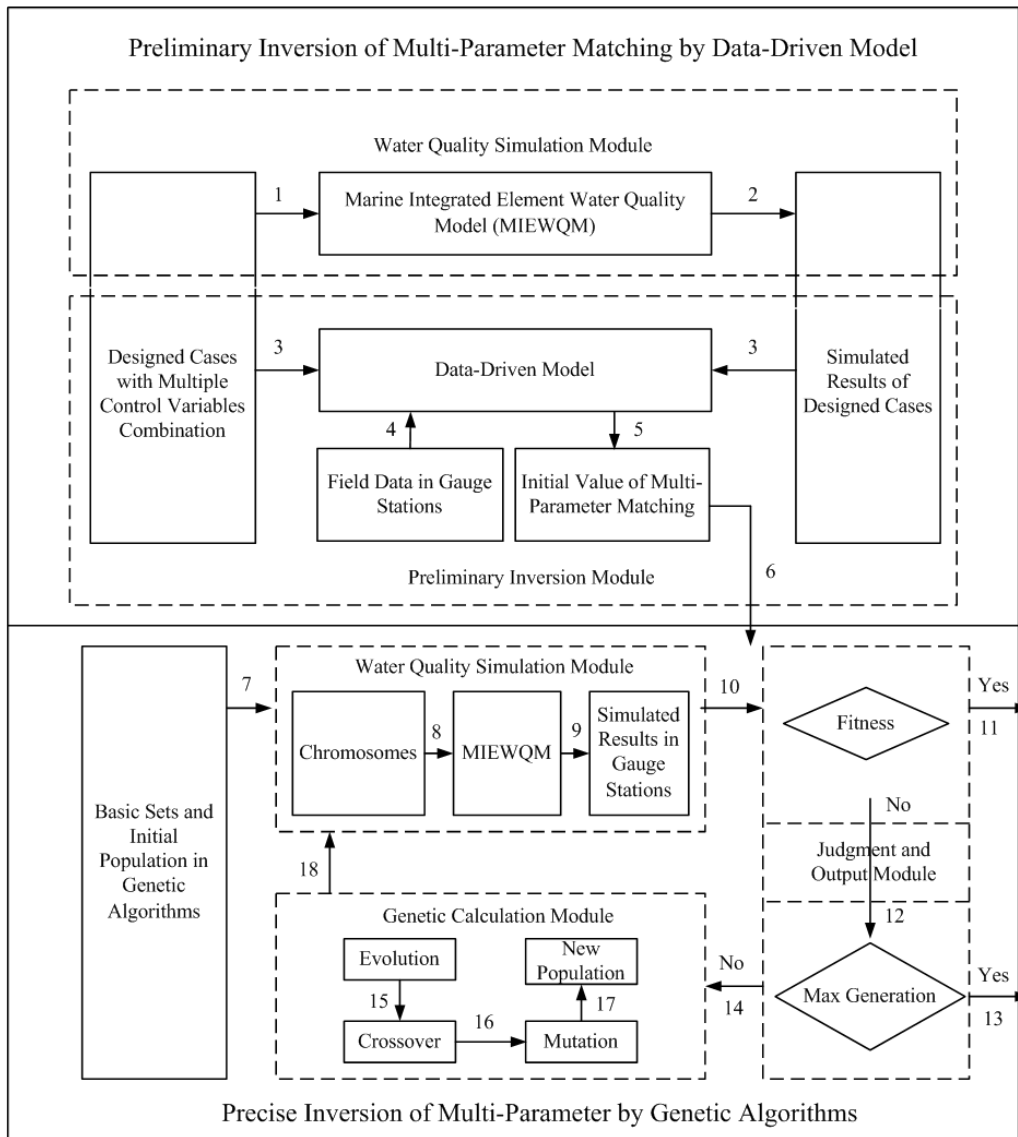
Fig. 2—Diagram of multi-parameter inversion of MIEWQM using stepwise coupling method

Step 3: Model parameters' preliminary inversion by the data-driven model

The results of pollution concentrations in gauge stations and the values of their corresponding parameters are inputted into the data-driven model in Fig. 3. After the training, the relationship between the gauge stations and the model parameters is generalized.

The field data in gauge stations are inputted into the relationship above and initial values of multi-parameter matching are obtained.

Precise inversion of multi-parameter by GAs

Step 4 Determination of population value range

The multi-parameter value-taking ranges are

obtained by expanding the initial values of the multi-parameter matching in step 3. This range smaller than that in step 3 (Figure 4) was taken as the constraining condition of the population in GAs.

For each parameter, (namely the gene), the r values within the value-taking range are selected randomly to obtain the r chromosomes for composing the multi-parameter solution population ($m \times r$).

Step 5 Water quality calculations

The MIEWQM is used to perform numerical calculations for each chromosome (total r times) in the population. The results of pollution concentration in gauge stations are output and

stored for the fitness calculation.

Step 6 Fitness calculations, judgment and output

The RMSE function is adopted to evaluate the fitness of all chromosomes in Eqs. (4).

If the set allowable error is satisfied, the calculation program will be skipped and the best chromosome (namely the optimal solution of multi-parameter) will be output. However, if the set allowable error is not satisfied, the program will move to the generation judgment. If the maximum generation is satisfied, the calculation program will be skipped and all chromosomes will be output. If the maximum generation is not satisfied, the program will continue the following calculation.

Step 7 Genetic calculation

Under the conditions that the allowable error and the maximum generations are not satisfied for current populations, evolution, crossover and mutation in genetic calculation module are performed to obtain new filial generation and new population. The new population is input into MIEWQM in step 5 for loop computing until the allowable error or maximum generation conditions are satisfied.

In Figure 3, a three-layer neural network is designed to inverse the model parameters. The input layer is the pollution concentrations in the gauge stations in each element, and the output layer is the model parameters.
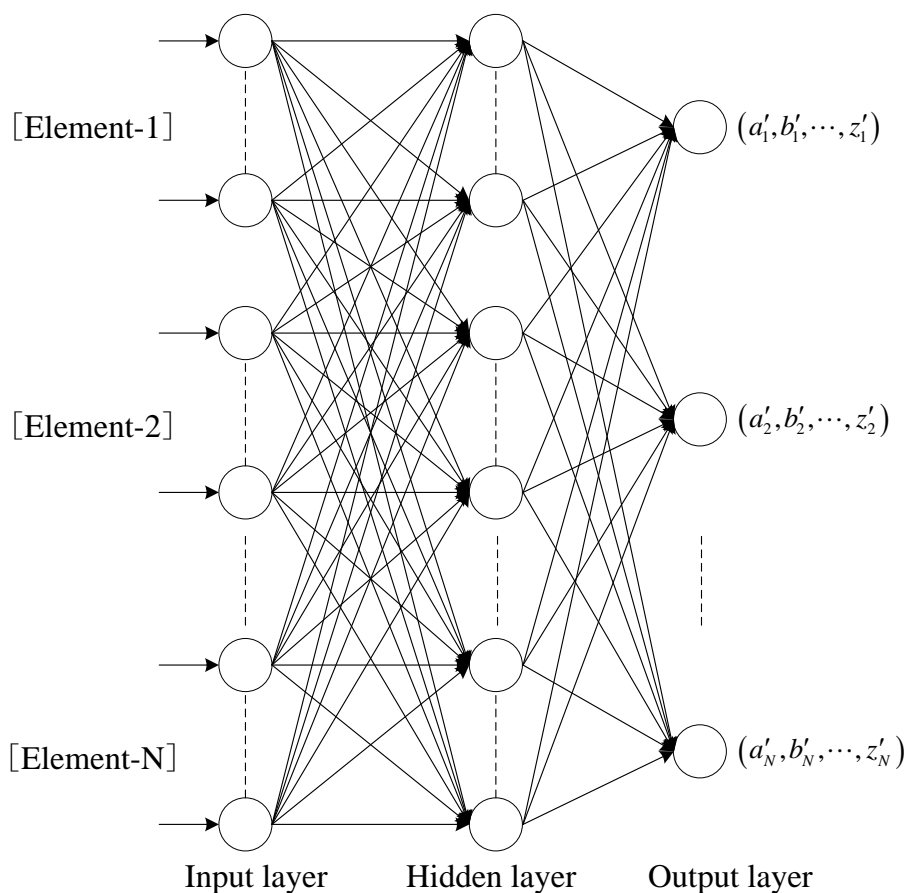

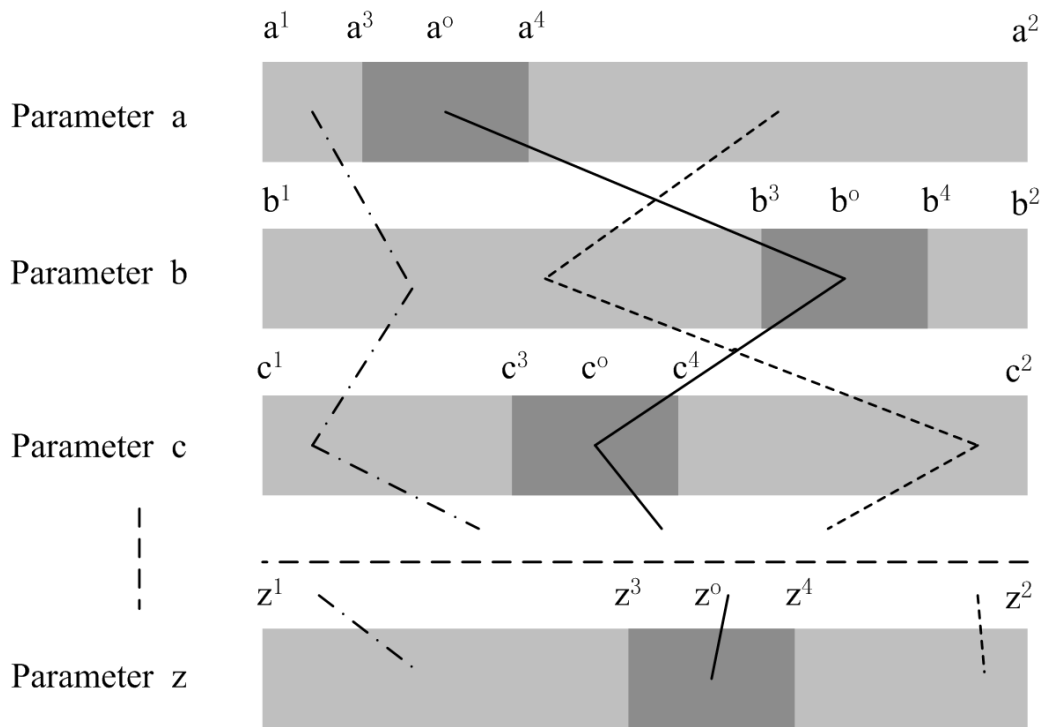Fig. 3—Network diagram of multi-parameter matching inversion using data-driven model

Fig. 4—Diagram of multi-parameter values in the process of stepwise coupling method

Figure 4 illustrates different multi-parameter value-taking range in the preliminary and precise inversion. Superscripts 1 and 2 represent the minimum and maximum values of the parameter, whereas the dotted line, dashed line and straight line represent multiple matching relations of the parameters. Superscript 0 represents the initial values of multi-parameter matching obtained by data-driven model in the preliminary inversion, which is taken as the benchmark and expanded to the value-taking range for the population of GAs, namely, superscripts 3 and 4.

Case studies

Research marine domain

Case tests were carried out in Bohai Bay in Fig. 5. It's one of the three largest bays in the Bohai Sea. The bay is located in western Bohai Sea and an area of 15 900 km^2, occupying approximately 1/5 of the Bohai Sea area. Bohai Bay is a shallow inlet concaved to the west in arc shape. The landform of the seabed inclines from the top of the bay to the center of the Bohai Sea, with slope of no more than 0.2%. The average water depth is 12.5 m.

In the numerical simulation, the area was discretized as 0.5 km×0.5 km horizontally and 10 levels in depth. To save on computational time and improve accuracy, the level thickness was varied (i.e., non-uniform) according to water depth. The level thickness was 2m×1, 3m×4 and 4m×5, from top to bottom, respectively. The model time step is 30 s. The surface height along the open boundary is given by interpolating the results between B1 and B2, and the hydrodynamic boundary conditions are provided by the Bohai Sea tide model[27-28]. The whole bay is divided into five elements. There are four gauge stations inside.

Method calibration by twin experiment

In this paper, the purported "identical twin experiment" method[25] is used to verify the efficiency of the present inversion method firstly. DIN is considered as the state variable. The coefficient of variation is computed by the Monte Carlo method[26] to validate the sensitivity of the model parameters. The state variable and its sensitive parameters are listed in Table 1.
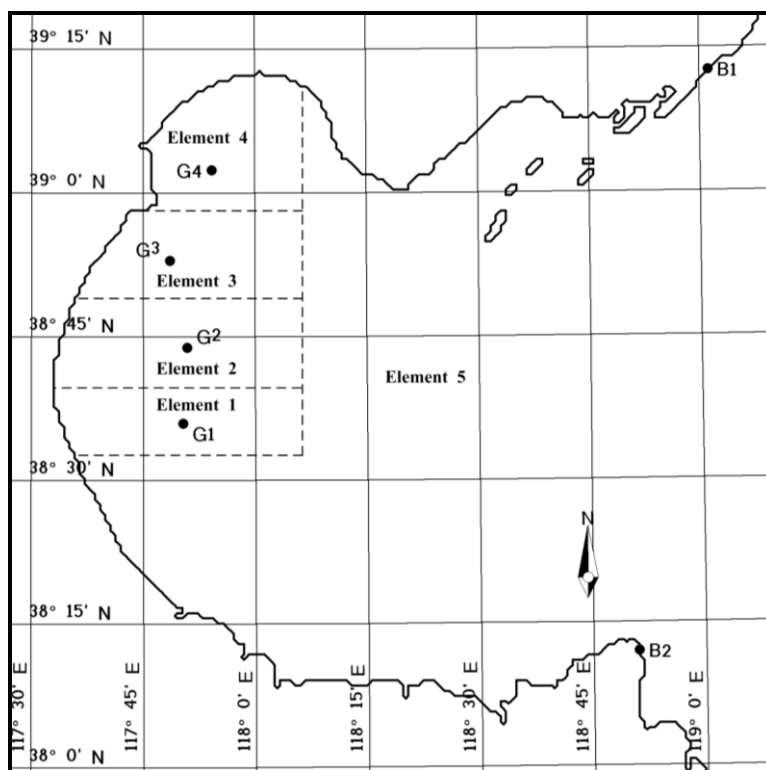
Fig. 5—Diagram of research region and element division

Table 1. State variable and sensitive parameters

State variable	Sensitive parameters	Unit
	Growth rate of phytoplankton（VMMAX）	1/d
DIN	Growth temperature of phytoplankton（TEMPS）	°C
	Decomposed rate of DIN（DRDN）	1/d

In Table 1, DIN has three sensitive parameters. The corresponding ranges of the control variables are set among the initial guess values in Table 2.

Table 2. Values for sensitive parameters

State variable	Sensitive parameters	Values		
	VMMAX	1.44	2.5	3.36
DIN	TEMPS	15	26	35
	VKDN	0.012	0.018	0.026

In Table 2, the values of the control variables are listed. For each control variable, 3 values are taken in its range, and 27 designed cases are obtained.

Bohai Bay is divided into four major elements according to the gauge stations distribution, whereas the rest of the sea area is categorized under element 5 and is not used in the inversion research. There is one state variable and three

sensitive parameters, so the network of multi-parameter matching inversion using data-driven model is determined.

A total of 27 cases of pollution concentration data of 144 hours are acquired 27 times by the MIEWQM computation. After inputting the 27 DIN data of 144 hours and the relative sensitive parameters data in Table 2 into the data-driven model, the relationships between the gauge

stations and the model parameters are generalized.

The parameters (VMMAX=2.4, TEMPS=25.0, DRDN=0.02) are utilized as real values and are inputted into MIEWQM for the pollution concentration data as pseudo-field data. The initial values of multi-parameter are inversed by inputting the pseudo-field data into the abovementioned relationships.

In the precise inversion phase, a new range is obtained from the initial values of multi-parameter matching. It is taken as the constraining conditions for the value-taking range of population in GAs. The maximum generation is 50, the crossover rate was 0.5, and the mutation rate is 0.1. $r = 20$, namely, the amount of chromosome is 20, so the scale of population is 3×20.

Into the generation circulation, MIEWQM is used to perform numerical calculation for each chromosome (20 times in total). The pollutant concentration result of the four gauge stations is output and stored. After 20 repetitions of MIEWQM calculations, the Eqs. (4) is used to calculate the fitness for each chromosome. "RMSE=0.005" is set to be the allowable error and "maximum generation is 50" is considered

as the constraining condition for judging the program end.

If the allowable error and the maximum generations are not satisfied for current population, the genetic calculation module with evolution, crossover and mutation are performed to obtain new values for filial generation and new population. The chromosomes in new population are input into MIEWQM for loop computing until the allowable error or maximum generation conditions are satisfied.

Meanwhile, the data-driven model and GAs method are directly adopted in this paper for multi-parameter inversion. The multi-parameter results of the three inversion methods are input into MIEWQM to calculate for calibration and comparison (Figure 6). The data-driven model method refers to obtain the initial values of multi-parameter matching from step 1 to step 3, whereas the GAs method refers to obtain the multi-parameter values from step 4 to step 7. However, these inversion processes are different from the stepwise coupling inversion method. The maximum and minimum parameter values in table 1 are adopted as the value-taking range of population in this GAs method.
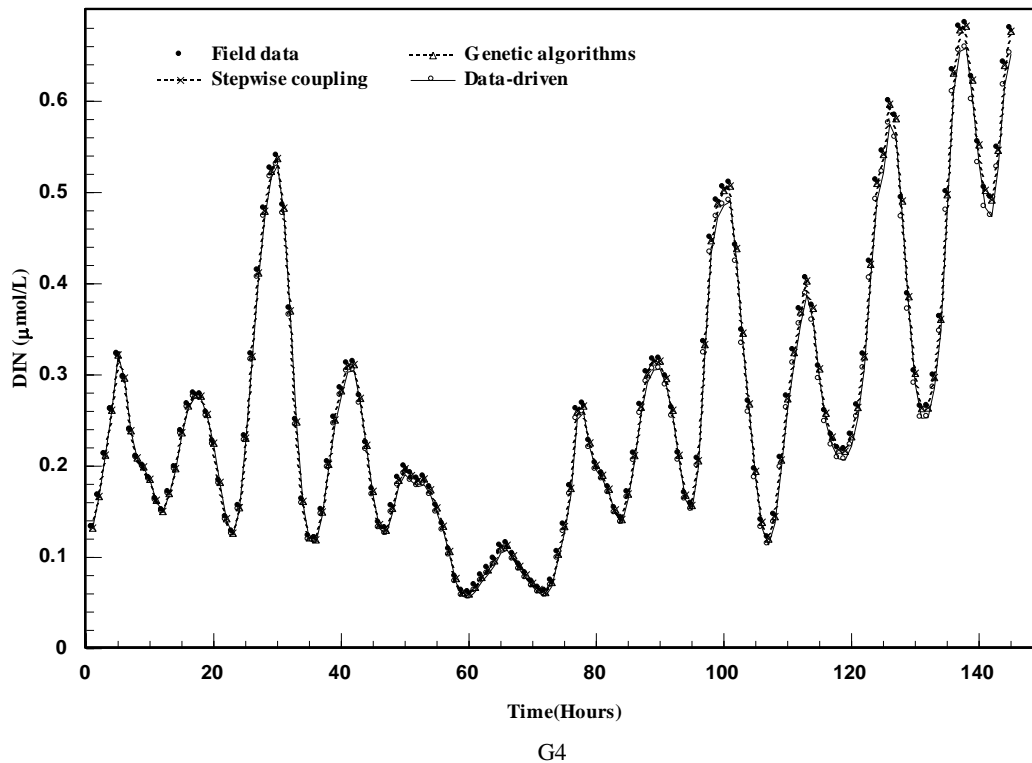
G2

G3

G4
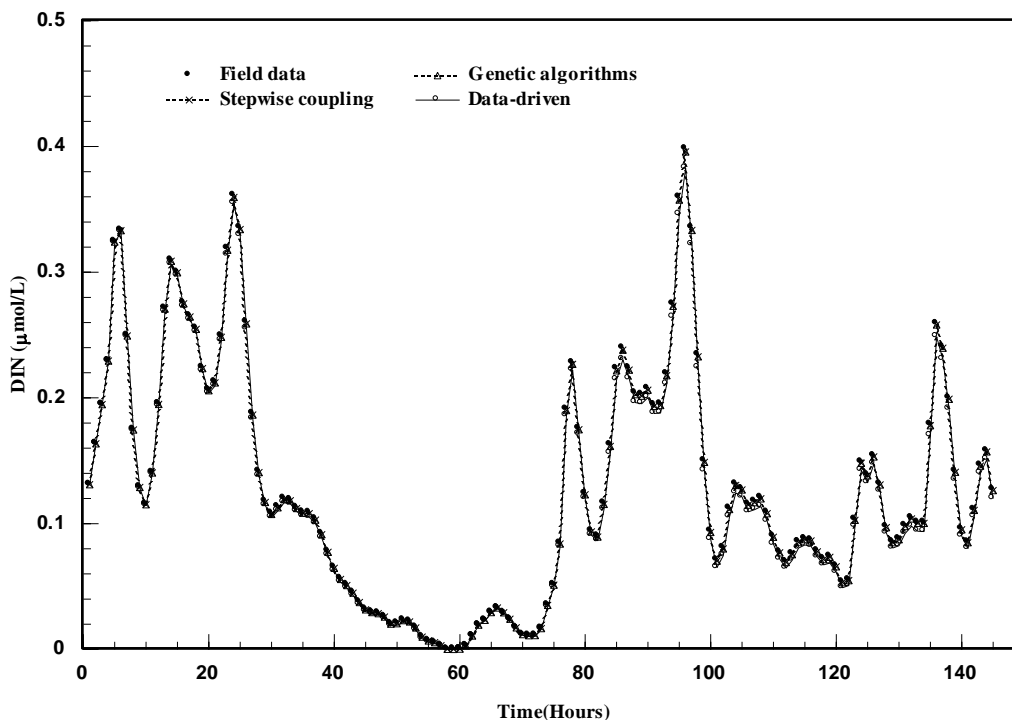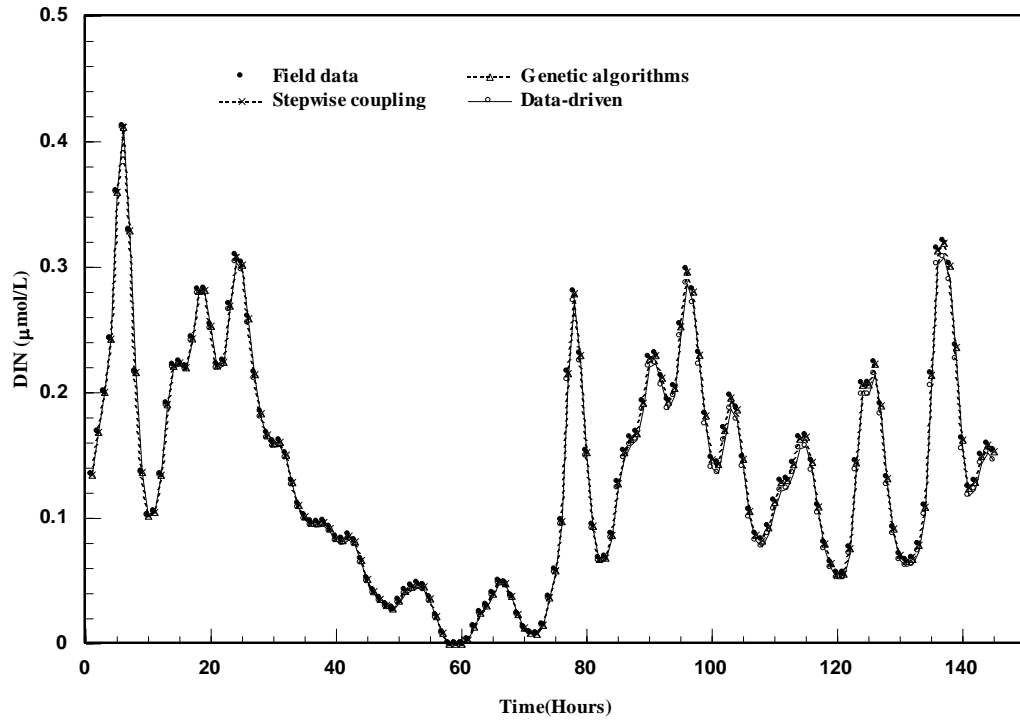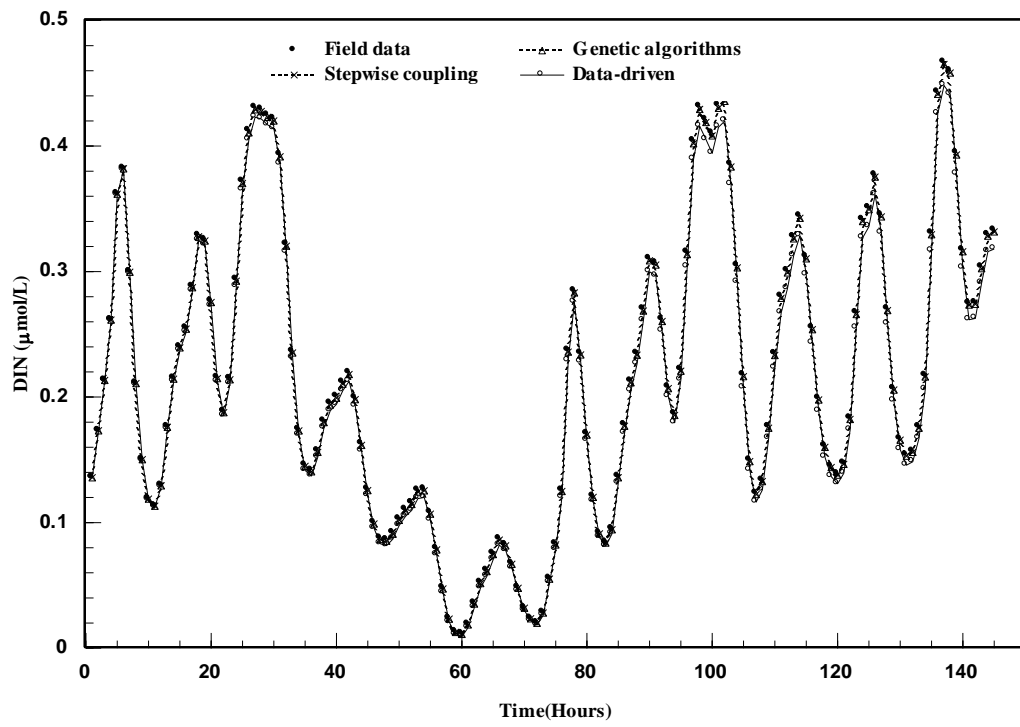
Fig. 6—Comparison of calibration results by three inversion methods

Figure 6 shows that the comparison of calibration results by three inversion methods in the four gauge stations. Compared with the field data, the correlation coefficients of three inversion methods are all exceed 0.99. The high precision cause is the adoption of the "identical twin experiment" method. However, the precisions of stepwise coupling and GAs methods are notably higher than that of the data-driven model method, particularly in terms of peak scope, because the global optimization means is adopted in the stepwise coupling and GAs inversion methods. Meanwhile, the data-driven model method merely presents the initial values of multi-parameter matching according to the nonlinear relationship between the state variables and the control variables, the error is not considered as the model operating constraining condition. The precisions of the stepwise coupling and GAs methods are the same. However, in the stepwise coupling inversion method, the population range is obtained from the initial values of multi-parameter matching by the data-driven model. The data-driven model method in the preliminary inversion steps reduces the range of global optimization in GAs, which is the advantage of stepwise coupling method to save the time consumption. The stepwise coupling inversion method's multi-parameter global optimization range is superior to that of the GAs, so the former's efficiency is much higher than the latter's.

Method calibration by field data

Field data of DIN in August 2004 and the stepwise coupling inversion method are applied to calibrate the MIEWQM of Bohai Bay in this section. Except for the allowable error RMSE=0.05, the other parameters are the same as those in Section 4.2. The multi-parameter optimal solution obtained from the stepwise coupling inversion method is input into the MIEWQM to calculate and verify the feasibility of this method.
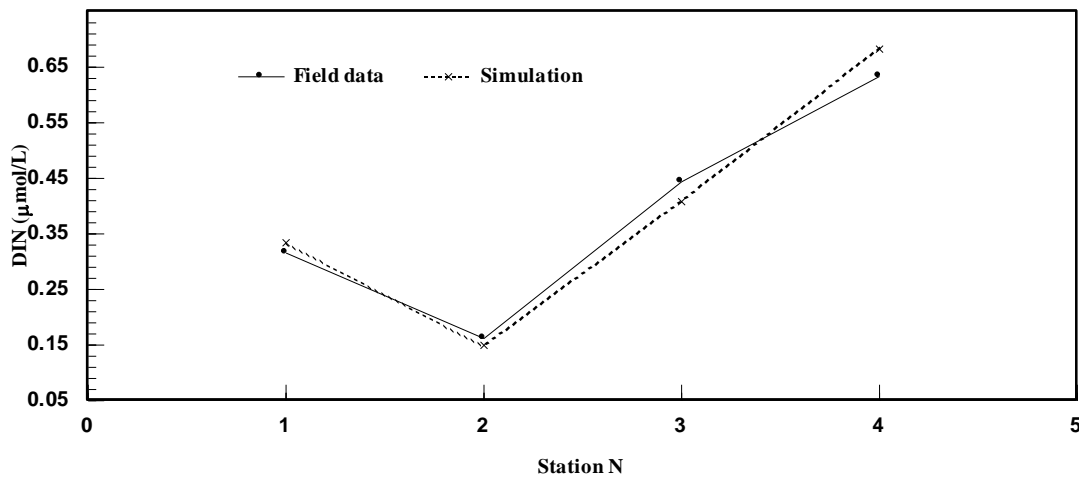
Fig. 7—Comparison of calibration results with field data by stepwise coupling method

Figure 7 is the comparison of calibration results with field data by the stepwise coupling inversion method. The simulation values and field data on the four gauge stations are essentially the same, with a correlation coefficient of 0.97. This finding demonstrates that the independent evaluation of parameters in different elements[29] has advantage of improving the precision of water quality simulation. However, the calibration for the field data still contains certain errors, and the errors in station 3 and 4 are higher than those in station 1 and 2. The errors mainly exist because the complicated nonlinear relationship included in the marine water quality and ecological system is not fully represented in the MIEWQM. Meanwhile, the initial concentration field of DIN and the pollution sources in the MIEWQM are obtained from rough estimation according to the limited data. Station 3 and 4 are in offshore positions, which are more easily controlled by sources, compared with station 1 and 2.

Conclusion

Calibration results indicate that the stepwise coupling inversion method has the advantage of high precision and high efficiency, because global optimization means is applied and its optimization space in the precise inversion phase is shortened by data-driven model in the preliminary inversion. Spatial independent evaluation means in water quality model is found to have superiority in improving the simulated precision. Compared with the adjoint method, the stepwise coupling inversion method does not require complicated deduction and modeling processes, it is simple, flexible and less time consuming. The present stepwise coupling inversion method is found to be suitable for the inverse problem of multi-parameter.

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