Estimation of Pollutant Discharge in the Bohai Sea with Variational Assimilation Method

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Abstract—**Based on the hydrodynamic background field, a Variational Assimilation (VA) Model of pollutant in the Bohai Sea is constructed. The time-varying contamination concentrations (CCs) from the pollution source (PS) are estimated using this model and a new inversion theory is proposed. Some points in the time series are selected as the independent points (IPs), while concentrations of other points are calculated through linear interpolation of these IPs. Through twin numerical experiment, all the given time-varying concentrations are successfully estimated through adjoint method. The cost function decrease greatly, and the ratio of the cost function to its initial value can even reach the magnitude of 10^{-5}, indicating that the adjoint technique is computationally efficient to recover the CCs from the PS**.

Keywords—**VA; Time-varying; IPs; CCs; Pollutant flux**

I. INTRODUCTION

The Bohai Sea is China's only inland sea, which receives large volumes of domestic and industrial discharges and even accidental or intentional spills from moving ships. With limited flushing capacity, the multiple pollutant discharges in the Bohai Sea can deteriorate the water quality significantly [1].

The issue of the PS has been extensively investigated in the past years [2-4], and several authors have proposed models to study the pollutant discharges and transport from the PS [5-7]. However, with limited observations, numerical simulation causes the uncertainty and even deviates from the real world. VA method can optimize the unknown ocean elements using limited observations, and then simulate the whole field accurately. In this study this method is used to inverse the CCs from the PS and computes the pollutant flux.

VA technique has been widely used in the ocean modeling, such as the inversion of the bottom friction coefficient, the open boundary conditions, the hydro-dispersive parameters and the ecological parameters [8-10]. However, the application has not been found in the optimization of the CCs from the PS, which is shown in this study.

II. MODEL

A. Governing Equation

Based on the hydrodynamic background field which is provided by a 3-D Regional Ocean Model System (ROMS), an advection-diffusion model is constructed:

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}(A_H\frac{\partial C}{\partial x})+\frac{\partial}{\partial y}(A_H\frac{\partial C}{\partial y})+\frac{\partial}{\partial z}(K_H\frac{\partial C}{\partial z}) \quad (1)$$

Where C is the contamination concentration, u and v are the horizontal velocities, w is the vertical velocity, A_H and K_H are the horizontal and vertical diffusion coefficient, respectively.

B. Adjoint Equation

The cost function which is usually used to measure the misfit between the observation and the simulation is defined as:

$$J(C)=\frac{1}{2}K_C\int(C-\overline{C})^2 \quad (2)$$

Where K_C is constant. By introducing Lagrange multipliers, the adjoint equation can be constructed:

$$-\frac{\partial C^*}{\partial t}-\frac{\partial}{\partial z}(K_H\frac{\partial C^*}{\partial z})=\frac{\partial}{\partial x}(uC^*)+\frac{\partial}{\partial y}(vC^*)+\frac{\partial}{\partial z}(wC^*)+\frac{\partial}{\partial x}(A_H\frac{\partial C^*}{\partial x})+\frac{\partial}{\partial y}(A_H\frac{\partial C^*}{\partial y})-K_C(C-\overline{C}) \quad (3)$$

Where C^* is the adjoint variable of C.

C. Model setting

The region of interest is the Bohai Sea (37 °N-41 °N, 117.5 °E-122.5 °E). The horizontal resolution of the model is 4′×4′. In the vertical direction the water is divided into 6 layers, and the thickness of each from top to bottom is 10m, 10m, 10m, 20m, 25m and 25m, respectively. The integral time step is one hour. A bathymetry map of the Bohai Sea is shown in Fig. 1.

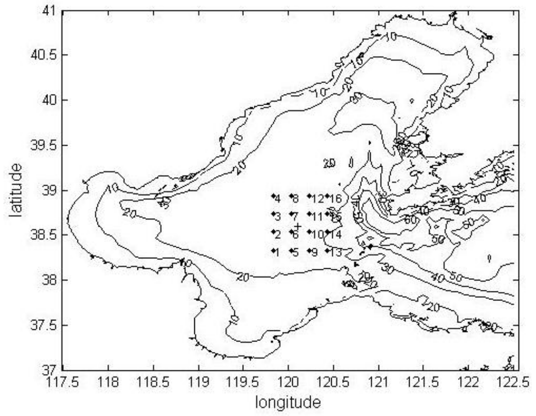


Fig. 1. Topography of the Bohai Sea and distribution of the observation sites. '+'is the location of the PS, and the dots are the observations.

III. TWIN EXPERIMENT (TE)

A. Correction of CCs at IPs

In this study, a new inversion theory is proposed. Suppose $D^{ll}_{i,j,k}$ is the value of the independent points, $C^{l}_{i,j,k}$ is the contamination concentration from the PS after linear interpolation (l denotes calculated point, ll stands for the independent point), then they have relationship as follows:

$$C^{l}_{i,j,k} = \sum_{ll} w_{l,ll} \cdot D^{ll}_{i,j,k} \tag{4}$$

Where $w_{l,ll}$ is the weight coefficient in the Cressman [11] form. After derivation, the gradient of cost function J with respect to $D^{ll}_{i,j,k}$ is

$$\frac{\partial J}{\partial D^{ll}_{i,j,k}} = \sum_{l} w_{l,ll} \cdot \frac{\partial J}{\partial C^{l}_{i,j,k}} \tag{5}$$

Considering the variable adjusted in the inverse direction of the gradient above, the independent contamination concentration from the PS is as follows:

$$K_D(D^{ll}_{i,j,k} - \overline{D^{ll}_{i,j,k}}) + \frac{\partial J}{\partial D^{ll}_{i,j,k}} = 0 \tag{6}$$

Where $\overline{D^{ll}_{i,j,k}}$ is the initial value of independent point, and K_D is the adjustment coefficient.

B. Settings of TE

Considering the real variation of the CCs from the PS, we set the varying types as follows:

$$Type\ 1: C(t) = 100 - 25\frac{(t-169)^2}{167^2},\ t \geq 2 \tag{7}$$

$$Type\ 2: C(t) = 100 - 25\frac{(t-85.5)^2}{83.5^2},\ t \geq 2 \tag{8}$$

$$Type\ 3: C(t) = 75 + 25\sin(\frac{\pi(t-1)}{84}),\ t \geq 2 \tag{9}$$

During the inversion process, eight IP strategies are the following:

Strategy (A): Three evenly distributed grid points are taken as IPs, and the influence radius is the length of 84 grids.

Strategy (B) to Strategy (H): The numbers of IPs are 5, 7, 9, 12, 15, 18 and 22 respectively, which are distributed evenly. Radiuses are the lengths of 84, 42, 28, 21, 15, 12, 10 and 8 grids, respectively.

In type1 and type2, strategies (A)-(E) are used to inverse the CCs, and in type3, strategies (B)-(H) are used.

IV. RESULTS AND DISCUSSION

A. The Inversion Result of Type1

The errors after assimilation for Type 1 are shown in Table 1, which shows that the cost function, the mean absolute errors between the given concentration and the inversed concentrations (ECC), and the mean absolute errors between the given pollutant flux and the inversed pollutant fluxes (EPF) decrease greatly, and the cost function even decreases to the scale of 10^{-5} of its initial value, indicating that the given time-varying distributions are successfully inversed. Results using Strategy (A) are most consistent, whereas those obtained with Strategy (E) are least consistent

TABLE I. RATIO OF ERRORS AFTER ASSIMILATION TO THEIR INITIAL VALUES

TE-strategy	cost function	ECC	EPF
(A)	1.66×10^{-5}	2.08×10^{-2}	6.37×10^{-3}
(B)	2.18×10^{-5}	4.60×10^{-2}	1.42×10^{-2}
(C)	1.24×10^{-5}	5.56×10^{-2}	1.67×10^{-2}
(D)	1.19×10^{-5}	7.19×10^{-2}	2.06×10^{-2}
(E)	1.56×10^{-5}	7.19×10^{-2}	2.04×10^{-2}

The given distributions and the inversion results using strategy (A) are shown in Fig. 2. It is can be seen that the inversed time-varying concentration fluctuates around the given time-varying concentrations, without any larger deviation. The pollutant flux simulated is also well inversed, and the errors at any moment are within 5 tons. It is concluded that the given time-varying concentrations are successfully inversed by using strategy (A).

The ratio of cost function to its initial value versus assimilation step using strategy (A) is shown in Fig. 3 from which the cost function decreases quickly in the beginning, and after 500 iteration steps the cost function can even reach the scale of 10^{-5} of its initial value, indicating that the observations are successfully assimilated.

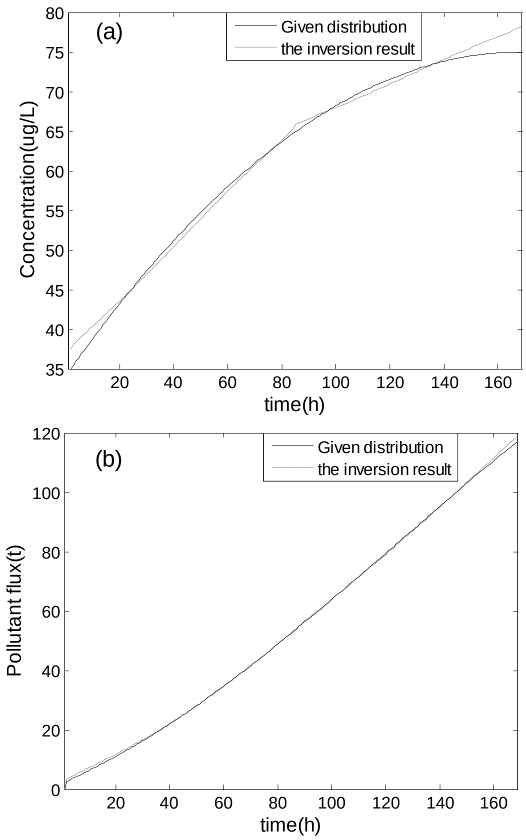


Fig. 2. Given distributions and the inversion results.

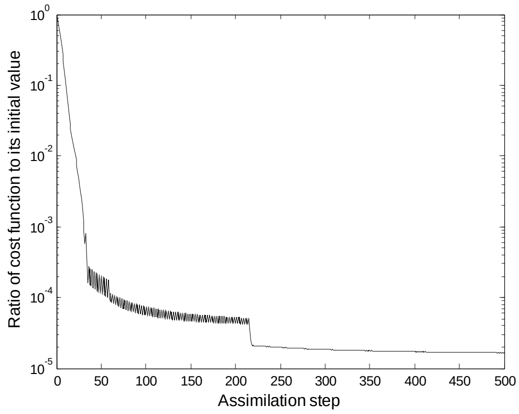


Fig.3. Ratio of cost function to its initial value versus assimilation step.

B. The Inversion Result of Type 2

The given distribution and the inversion results using strategy (C) are shown in Fig. 4, which shows the deviation ranges of concentration in some moments are within 6%, while others are within 3%. The given pollutant flux is also well inversed, and the relative errors are less than 0.1% in the whole time steps. The inversion result is not as good as that of Type 1, which because the variation of that concentration is more complex.

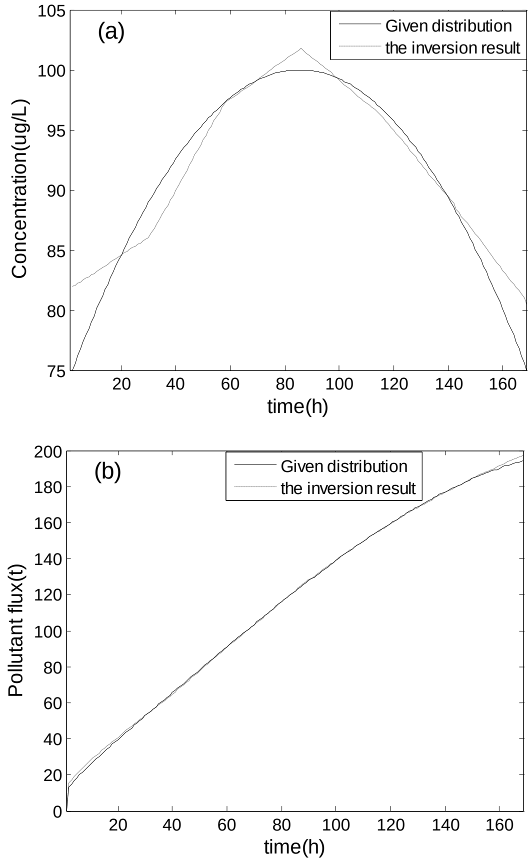
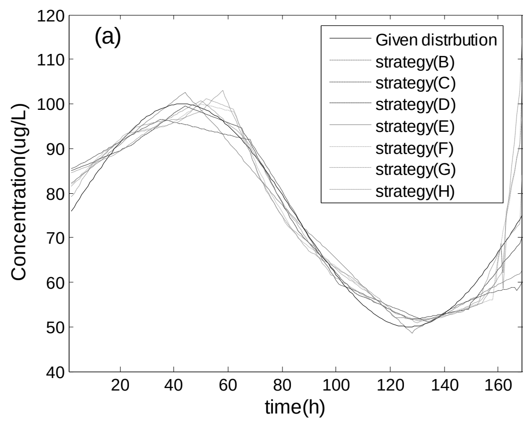


Fig. 4. Given distributions and the inversion results.

C. The Inversion Result of Type 3

The inversion results of the given time-varying concentration and errors between the given time-varying concentrations and the inversion results using strategies (B)-(H) are shown in Fig. 5, which shows a bigger deviation in the last few moments, which may because the observations could not get any feedback on the variation of concentration in those moments. While in other moments the errors are within 5%. It is clearly that the strategy of IPs has significant influence on inversion results, in other words, more IPs can cause the results to deviate from the given distributions greatly.



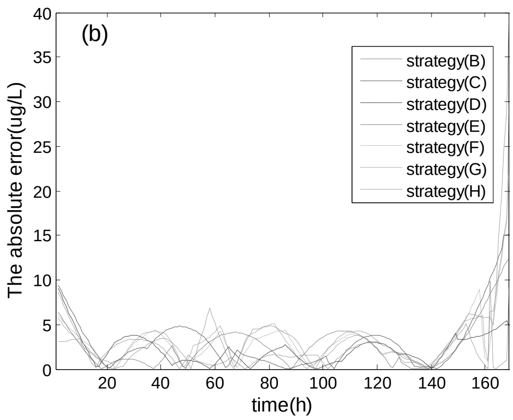


Fig. 5. Inversion results of the given time-varying concentration (a) and the errors between them (b)

The inversion results of the given time-varying pollutant flux and the errors between the given time-varying pollutant flux and the inversion results using strategies (B)-(H) are shown in Fig. 6, which shows the deviation ranges in the last few moments are about 10%, while others are within 3%. It is can be seen that the given time-varying pollutant flux is also successfully inversed.

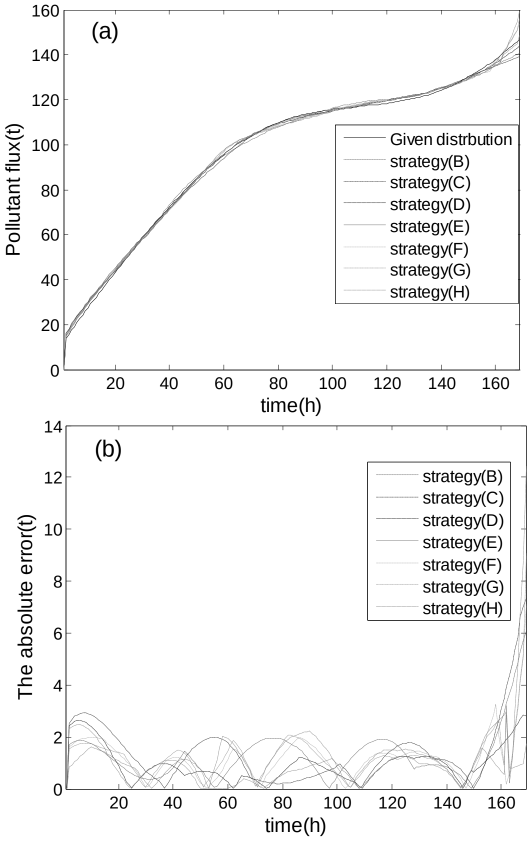


Fig. 6. Inversion results of the given time-varying pollutant flux (a) and the errors between them (b).

V. CONCLUSIONS

Based on the hydrodynamic background field, a VA Model of pollutant in the Bohai Sea is constructed. A new inversion theory is proposed in this study. Some points in the time series are selected as the IPs, while concentrations of other points are calculated through Cressman linear interpolation of these IPs.

All the given time-varying concentrations are successfully estimated by this method. The cost function decrease greatly, and the ratio of the cost function to its initial value can even reach the scale of 10^{-5}. In the inversion process, the strategy of the inversion is significant for the inversion result, and more IPs can cause the inversion results to deviate from the given distributions greatly. More work will be done to meet the actual demand.

ACKNOWLEDGEMENT

Partial support for this research was provided by the National Natural Science Foundation of China through grant 41076006 and 41206001, Natural Science Foundation of Jiangsu Province of China through grant BK2012315, the Fundamental Research Funds for the Central Universities 201261006 and 201262007.

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