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Numerical simulation of water quality in Yangtze Estuary

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Abstract: In order to monitor water quality in the Yangtze Estuary, water samples were collected and field observation of current and velocity stratification was carried out using a shipboard acoustic Doppler current profiler (ADCP). Results of two representative variables, the temporal and spatial variation of new point source sewage discharge as manifested by chemical oxygen demand (COD) and the initial water quality distribution as manifested by dissolved oxygen (DO), were obtained by application of the Environmental Fluid Dynamics Code (EFDC) with solutions for hydrodynamics during tides. The numerical results were compared with field data, and the field data provided verification of numerical application: this numerical model is an effective tool for water quality simulation. For point source discharge, COD concentration was simulated with an initial value in the river of zero. The simulated increments and distribution of COD in the water show acceptable agreement with field data. The concentration of DO is much higher in the North Branch than in the South Branch due to consumption of oxygen in the South Branch resulting from discharge of sewage from Shanghai. The DO concentration is greater in the surface layer than in the bottom layer. The DO concentration is low in areas with a depth of less than 20 m, and high in areas between the 20-m and 30-m isobaths. It is concluded that the numerical model is valuable in simulation of water quality in the case of specific point source pollutant discharge. The EFDC model is also of satisfactory accuracy in water quality simulation of the Yangtze Estuary.

Key words: *water quality; chemical oxygen demand; dissolved oxygen; Yangtze Estuary; EFDC model*

1 Introduction

The water quality of the Yangtze River is for the most part controlled by river discharge, ocean dynamics, and human activities. It is always of concern for Shanghai, a metropolis located on the South Branch of the Yangtze River. As shown in Fig. 1, from Xuliujing to the sea there are three points of bifurcation and four river discharges, one of which, the Yangtze Estuary, is divided into a South Branch and a North Branch. The region relevant to the present study stretches from the Yangtze Estuary to Hangzhou Bay. The hydrodynamic factors in this area are tides and river discharge. The annual river discharge is 9.21×10^{11} m^3 with significant

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seasonal variation. The tidal system in the estuary is driven by East China Sea tides and Yellow Sea tides, and is strongly influenced by topographical variation. Early geochemical research on the Yangtze Estuary was carried out by the Institute of Oceanology of the Chinese Academy of Sciences in the 1960s (Gu 1966). The issue of qualitative simulation of water quality has drawn wide attention since the 1980s because of deterioration of the living environment. A considerable amount of field data has been collected for water engineering projects, including large projects such as the Three Gorges Dam and the South-to-North Water Transfer. In order to investigate the water quality, field observation of current and velocity stratification has been conducted using the shipboard acoustic Doppler current profiler (ADCP), with simultaneous collection of water samples (Zhu et al. 2003; Chen and Chen 2002; Shen et al. 2003; Deng et al. 2003; Tu and Wang 2004; Li and Shi 2005; Shi et al. 2006; Zhang 2007; Yan et al. 2007; Wang and Li 2007; Li and Wang 2008). However, there have been few real-time simulations of water quality.

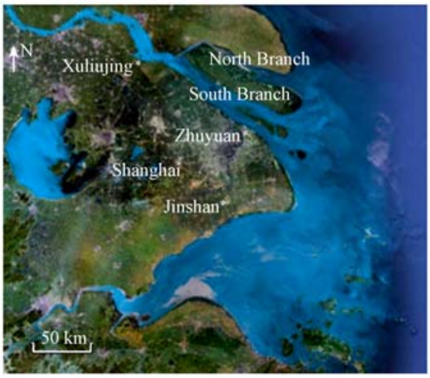


Fig. 1 Yangtze Estuary study domain (Google Earth 2009)

This study sought to develop a method based on the Environmental Fluid Dynamics Code (EFDC) (Hamrick 1992) for the simulation of water quality of the Yangtze Estuary. In the EFDC, dynamic variables such as depth, velocity, and mixing coefficients are directly coupled with the water quality modules. There have been some good case studies from the United States (Kuo et al. 1996; Shen and Kuo 1999; Shen et al. 1999; Shen and Haas 2004; Shen and Lin 2006; Jin et al. 2000, 2007). Standard water quality variables produced by the EFDC model can be divided into two sets: those with an initial value of zero (new additives) and those with non-zero initial values (existing substances). Two representative water quality variables were selected for detailed study: chemical oxygen demand (COD) and dissolved oxygen (DO), with COD representing new additives to the water quality model and DO representing existing substances in the Yangtze Estuary.

2 Numerical model setup

In the study domain, shown in Fig. 1, two point sources of sewage were selected: Zhuyuan and Jinshan. Zhunyuan has been the main sewage and pollutant outlet of the

Huangpu River in Shanghai since 1993, and Jinshan is a perpetual heavy industrial zone of Shanghai. Considering the complexity of pollutant outlets and limitations of field data, these two point sources constitute a simplified conceptualization of sewage discharge in the Yangtze Estuary.

The EFDC water quality model estimates three-dimensional distribution of hydrodynamic environmental variables including salinity and organic pollutants through consideration of river discharge, tides, sewage outlets, and exchange between the ocean and air. Fig. 2 is a simplified sketch of model variables, where the total suspended solids are provided by the hydrodynamics model. In the Yangtze Estuary model setup, 21 state variables are initialized: cyanobacteria, diatoms, green algae, refractory particulate organic carbon, labile particulate organic carbon, dissolved organic carbon (DOC), refractory particulate organic phosphorus, labile particulate organic phosphorus, dissolved organic phosphorus, total phosphate, refractory particulate organic nitrogen, labile particulate organic nitrogen, dissolved organic nitrogen, ammonium nitrogen, nitrate nitrogen, particulate biogenic silica, available silica, chemical oxygen demand, dissolved oxygen, total active metal, and fecal coliform bacteria. The units are g/m^3 for all variables except total active metal, which is in mol/m^3, and fecal coliform bacteria, which is in MPN (most probable number) per 100 m. All 21 variables were classified in two sets: new additives and existing substances. In consideration of the available field data, COD (new additives) and DO (existing substances) were selected for detailed analysis as representative variables. The quantitative description of DO is related to the initial value of DO and consumption of DO in this area; thus, only spatial distribution is extracted for illustration in the following discussion. The variation of COD is directly related to the point source discharge from sewage outlets; thus, temporal and spatial variations of COD are of interest.

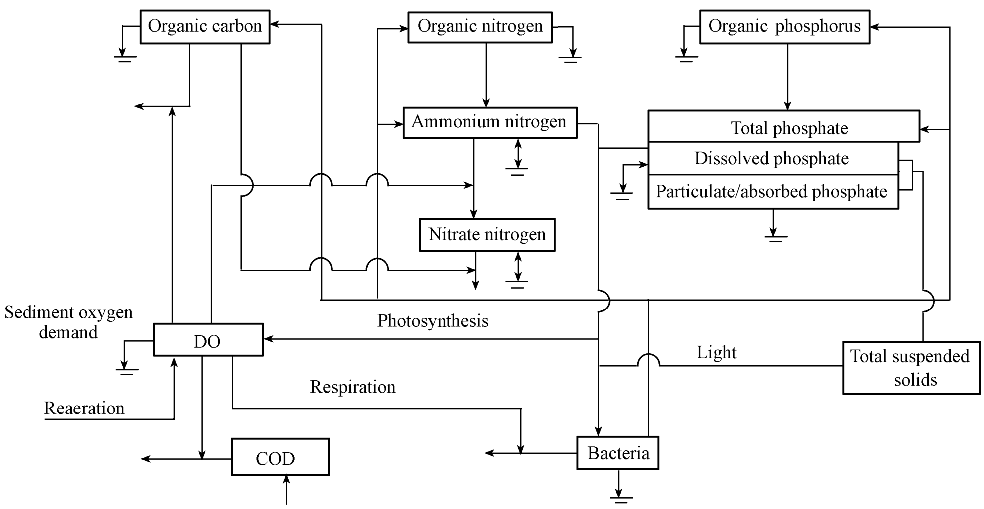


Fig. 2 Simplified water quality model in EFDC

3 Governing equations of EFDC water quality model

The governing continuity equation of water quality variables is as follows (Mellor and Yamada 1982; Mellor and Blumberg 1985; Hamrick 1986; Rosati and Miyakoda 1988; Mellor 1991; Hamrick 1992; Hamrick and Wu 1997; Ji et al. 2001):

$$\frac{\partial C}{\partial t}+\frac{\partial(uC)}{\partial x}+\frac{\partial(vC)}{\partial y}+\frac{\partial(wC)}{\partial z}=\frac{\partial}{\partial x}\left(K_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(K_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial x}\left(K_z\frac{\partial C}{\partial z}\right)+S_{\mathrm{c}} \tag{1}$$

The hydrodynamics equation is

$$\frac{\partial C}{\partial t}=S_{\mathrm{c}} \tag{2}$$

which can also be expressed as

$$\frac{\partial C}{\partial t}=KC+R \tag{3}$$

where the continuity equation consists of physical transport, convection, and hydrodynamics; C is the water quality variable concentration; u, v, and w are velocity in Cartesian coordinate directions x, y, and z, respectively; K_x, K_y, and K_z are the diffusion coefficients in the x, y, and z directions, respectively; S_{c} is the source/sink term per volume; K is the kinetic rate; and R is a source/sink term.

3.1 Governing equation of DO

The source/sink term for DO in the model corresponds to the following processes: (1) photosynthesis and respiration of algae, (2) denitrification, (3) heterotrophic respiration of dissolved organic carbon, (4) aeration of COD, (5) surface reaeration, (6) oxygen demand of bottom sediment, and (7) external loads. The equation describing the DO hydrodynamic process is as follows (Cline and Richards 1969; Di Toro 1980):

$$\begin{aligned}\frac{\partial\rho(\mathrm{DO})}{\partial t}=&\sum_{x=\mathrm{c,d,g}}\left[\left(1.3-0.3P_{\mathrm{N}_x}\right)P_x-\left(1-F_{\mathrm{CD}_x}\right)\frac{\rho(\mathrm{DO})}{K_{\mathrm{HR}_x}+\rho(\mathrm{DO})}B_{\mathrm{M}_x}\right]A_{\mathrm{OCR}}B_x\\&-A_{\mathrm{ONT}}N_{\mathrm{it}}N_{\mathrm{H_4}}-A_{\mathrm{OCR}}K_{\mathrm{HR}}\rho(\mathrm{DOC})+K_{\mathrm{r}}\left[\rho(\mathrm{DO_S})-\rho(\mathrm{DO})\right]\\&-\frac{\rho(\mathrm{DO})}{K_{\mathrm{H_{COD}}}+\rho(\mathrm{DO})}K_{\mathrm{COD}}\rho(\mathrm{COD})+\frac{S_{\mathrm{OD}}}{\Delta z}+\frac{W_{\mathrm{DO}}}{V}\end{aligned} \tag{4}$$

where the subscript x is used to denote three algal groups: c for cyanobacteria, d for diatoms, and g for green algae; P_{N_x} is the preference for ammonium uptaken by algal group x ($0\le P_{\mathrm{N}_x}\le 1$); P_x is the production rate of algal group x (d^{-1}); F_{CD_x} is the fraction of the basal metabolism exuded as dissolved organic carbon with an infinite DO concentration for algal group x; K_{HR_x} is the half-saturation constant of DO for algal dissolved organic carbon excretion for group x ($\mathrm{g/m^3}$); B_{M_x} is the basal metabolism rate of algal group x (d^{-1}); B_x is the algal biomass of algal group x (g/m^3); N_{it} is the nitrification rate (d^{-1}); $N_{\mathrm{H_4}}$ is ammonium nitrogen concentration (g/m^3); $K_{\mathrm{H_{COD}}}$ is the half-saturation constant of dissolved oxygen required for oxidation of chemical oxygen demand (g/m^3); K_{COD} is the oxidation rate of chemical oxygen demand (d^{-1}); Δz is layer thickness (m); V is cell volume (m^3); A_{ONT} is the DO demand per unit mass for ammonia nitrogen nitration (A_{ONT} = 4.33); A_{OCR} is the DO-to-carbon ratio in respiration (A_{OCR} = 2.67); W_{DO} is externally loaded DO (g/d); K_{r} is the re-aeration coefficient (d^{-1}) (re-aeration only applies to the surface layer); $\rho\left(\mathrm{DO_S}\right)$ is DO saturation concentration (g/m^3); and S_{OD} is the DO demand of sediment (g/(m^2·d)), which only applies to the bottom layer.

3.1.1 Algae

Algae consumes oxygen during photosynthesis. This production of oxygen is related to nitrogen consumption during growth, and is expressed as (Morel and Hering 1983)

$$\begin{aligned}&106\mathrm{CO_2}+16\mathrm{NO_3^-}+\mathrm{H_2PO_4^-}+122\mathrm{H_2O}+17\mathrm{H^+}\longrightarrow \mathrm{protoplasm}+138\,\mathrm{O_2}\\&106\mathrm{CO_2}+16\mathrm{NH_4^+}+\mathrm{H_2PO_4^-}+106\mathrm{H_2O}\longrightarrow \mathrm{protoplasm}+106\mathrm{O_2}+15\mathrm{H^+}\end{aligned}\tag{5}$$

In Eq. (4), $(1.3-0.3P_{\mathrm{N}_x})$ is the rate of photosynthesis. Consumption of oxygen during respiration is

$$\mathrm{CH_2O}+\mathrm{O_2}=\mathrm{CO_2}+\mathrm{H_2O}\tag{6}$$

It can be concluded from the chemical reaction formula that $A_{\mathrm{OCR}}=$ 2.67.

3.1.2 Denitrification

The process of denitrification is nitrifying bacteria oxidizing ammonia nitrogen to create nitrite and oxidizing nitrite to create nitrogen, as described by the following chemical reaction formula (Wezernak and Gannon 1968):

$$\mathrm{NH_4^+}+2\mathrm{O_2}\longrightarrow\mathrm{NO_3^-}+\mathrm{H_2O}+2\mathrm{H^+}$$

Since nitrifying bacteria may obtain oxygen by fixing CO_2, consumption of 1 mol of ammonia requires less than 2 mol of oxygen, which means that $A_{\mathrm{ONT}}=4.33$.

3.1.3 Reaeration

Assuming that the oxygen is saturated in the air, the DO reaeration rate is proportional to the oxygen gradient $\left[\rho\left(\mathrm{DO_S}\right)-\rho\left(\mathrm{DO}\right)\right]$ across the air-sea interface. The DO saturation concentration decreases with the increase of temperature and salinity. This is expressed as (Hamrick 1992)

$$\begin{aligned}\rho\left(\mathrm{DO_S}\right)=&\,14.553\,2-0.382\,17T+5.425\,8\times10^{-3}T^2-\\&C_{\mathrm{L}}(1.655\times10^{-4}-5.866\times10^{-6}+9.796\times10^{-8}T^2)\end{aligned}\tag{7}$$

where S is salinity, T is temperature, and C_{L} is the chloride concentration, equal to $S/1.806\,55$.

The reaeration coefficient, which includes the effects of turbulence through bottom friction and surface wind force, is the following (Banks and Herrera 1977; O'Connor and Dobbins 1958; Hamrick 1992):

$$K_{\mathrm{r}} = \left(K_{\mathrm{ro}} \sqrt{\frac{u_{\mathrm{eq}}}{h_{\mathrm{eq}}}} + W_{\mathrm{rea}} \right) \frac{1}{\Delta z} K_{T_{\mathrm{r}}}^{T-20} \tag{8}$$

where K_{ro} is a proportional constant equal to 3.933 (in meter-kilogram-second unit system); u_{eq} is the weighted average velocity at a cross section (m/s), $u_{\mathrm{eq}} = \sum (u_k V_k) / \sum V_k$, where V_k is the weight factor; h_{eq} is the weighted average depth at a cross section (m); W_{rea} is reaeration induced by wind (m/d). $W_{\mathrm{rea}} = 0.728 U_{\mathrm{w}}^{0.5} - 0.317 U_{\mathrm{w}} + 0.037\,2 U_{\mathrm{w}}^{2}$, U_{w} is the wind velocity at a height of 10 m; and $K_{\mathrm{T_r}}$ is the constant of the DO reaeration rate adjusted by temperature.

3.2 Governing equation of COD

In the model, the equation to describe COD with consideration of external loads is the following (Hamrick 1992):

$$\frac{\partial \rho(\mathrm{COD})}{\partial t} = -\frac{\rho(\mathrm{DO})}{K_{\mathrm{H_{COD}}} + \rho(\mathrm{DO})} K_{\mathrm{COD}} \rho(\mathrm{COD}) + \frac{B_{\mathrm{FCOD}}}{\Delta z} + \frac{W_{\mathrm{COD}}}{V} \tag{9}$$

where K_{COD} is the reaeration rate of COD (d^{-1}), $K_{\mathrm{H_{COD}}}$ is the half-saturation constant of DO required by COD reaeration ($\mathrm{g/m^3}$), B_{FCOD} is the sediment flux of COD applied to the bottom layer only ($\mathrm{g/(m^3 \cdot d)}$), and W_{COD} is the out-loading of COD (g/d).

The reaeration rate K_{COD} is related to the temperature, and may be expressed through an exponential function:

$$K_{\mathrm{COD}} = K_{\mathrm{CD}} \exp\left[K_{T_{\mathrm{COD}}} \left(T - T_{\mathrm{R_{COD}}} \right) \right] \tag{10}$$

where $T_{\mathrm{R_{COD}}}$ is the reference temperature of COD (℃), K_{CD} is the reaeration rate of COD at the reference temperature $T_{\mathrm{R_{COD}}}$ (d^{-1}), and $K_{T_{\mathrm{COD}}}$ is the reaeration rate of COD induced by the temperature ($℃^{-1}$).

4 Numerical simulation results

4.1 Hydrodynamic results and verification

The calculation domain is shown in Fig. 3. Velocity fields were calculated with the EFDC hydrodynamics module and verified with field data (Yu 2005), and the water quality factors were coupled with the hydrodynamics module in the model. Fig. 4 shows depth-averaged three-dimensional calculation results in a sigma-coordinate system. Fig. 5 shows vertical velocity distributions as examples for six layers of depth *h*: 0*h*, 0.2*h*, 0.4*h*, 0.6*h*, 0.8*h*, and 1.0*h*. Basically, the field data and numerical results agree.

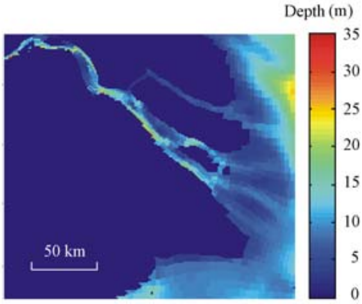


Fig. 3 Bathymetry of calculation domain

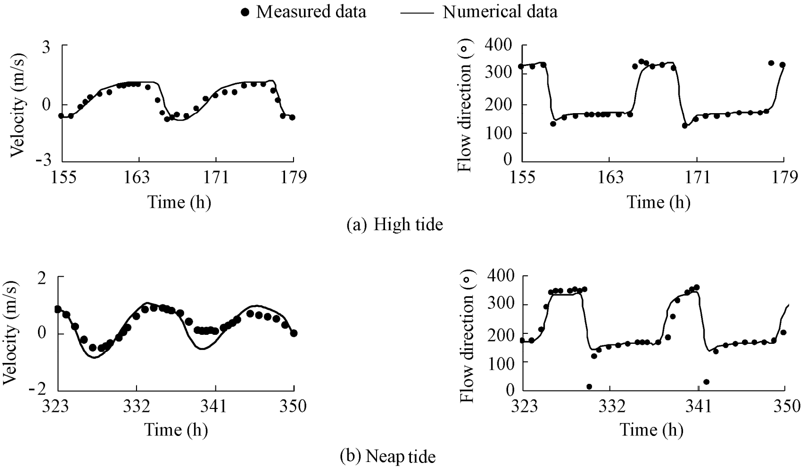


Fig. 4 Verification of depth-averaged velocity with field data for Zhuyuan

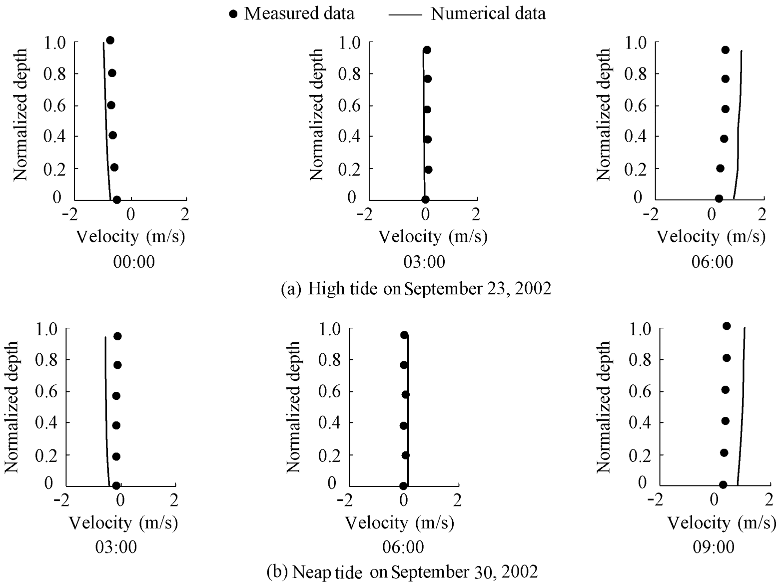


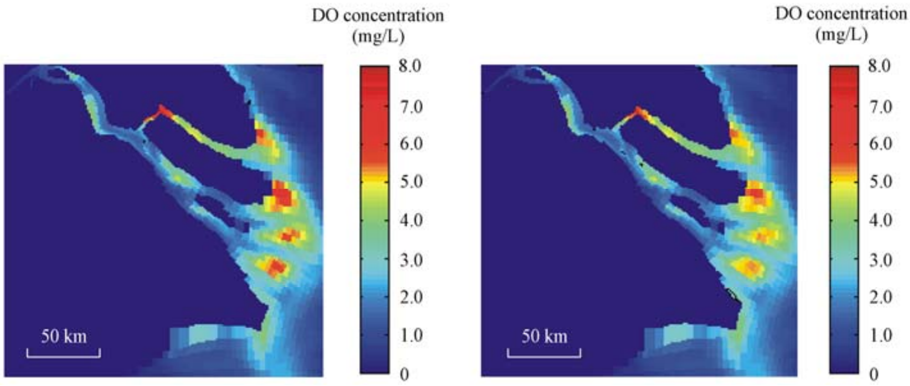
Fig. 5 Verification of vertical velocity with field data for Zhuyuan

4.2 Spatial distribution of DO

The DO distribution in the Yangtze Estuary has the following characteristics: DO concentration is higher in the surface layer and decreases toward the bottom; as shown in Fig. 6 and Fig. 7, DO concentration is higher in the North Branch than in the South Branch; the regions around the 20-m isobaths show a low DO concentration, as DO has been consumed by organic pollutants in the upper river discharge; between the 20-m isobath and the 30-m isobath is a high DO concentration region, which includes the maximum gradient of DO. The DO concentration is influenced by biological, chemical, and physical processes. When the phytoplankton density and the concentration of chlorophyll a are high, photosynthesis is strong, leading to high levels of DO. When phytoplankton dies off, the oxidization is stronger than photosynthesis, DO concentration decreases sharply, and the sea is oxygen-deficient. Similarly, when the temperature is low, DO concentration increases, and when the temperature is high, DO concentration decreases. DO is also related to physical processes such as tide-induced mixing. The high-DO concentration regions are located at the surface and near banks, and are mainly influenced by low temperatures, low salinity, high levels of nutrients in river discharge, and air-sea exchange, which provides a supplement to DO in the water. Basically, the DO concentration in the surface layer is higher than in the middle of the bottom layer, approximately at saturation. It is higher near the coast than out at sea. The results of this analysis are similar to those of previous research (Shi et al. 2006).

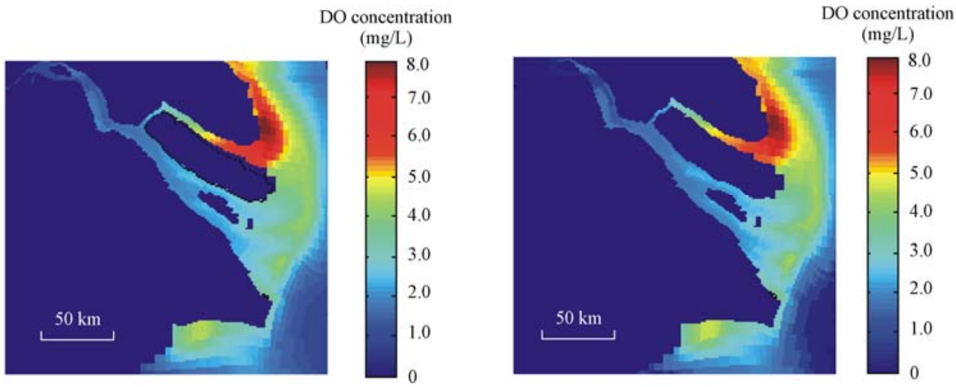
4.3 Temporal and spatial distribution of COD

The numerical model was used to monitor pollutant transport in the Yangtze Estuary. Important point sources are located along the banks in Shanghai. It was necessary to consider the chemical reaction of organic substances in simulating specific parameters of water quality. As a common water quality parameter, COD at two point sources of sewage, Zhuyuan (domestic sewage) and Jingshan (industrial waste), was simulated in order to monitor the transportation of pollutants. The initial value in the domain was zero. Shown in Figs. 8(a)-(d) are the temporal and spatial distributions of COD. The initial release of COD from the Zhuyuan point source was 150 mg/L with the background value throughout the model set to zero. The COD was significantly diluted immediately after release, as shown in Fig. 8(a). After nine days, the mixing area was approximately stable, fluctuating slightly with the influence of tides. The collected field data (Meng et al. 2004) show that the COD concentration at the intake point for drinking water 8 km above the release point was 2.8 mg/L near the bank, which is slightly smaller than the numerical result of 3.0 mg/L neglecting the background value. It is concluded that the numerical results agree with field data, and the model provides a method of simulating transportation of pollutants.



(a) Surface layer (b) Bottom layer

Fig. 6 Distribution of DO during neap tide

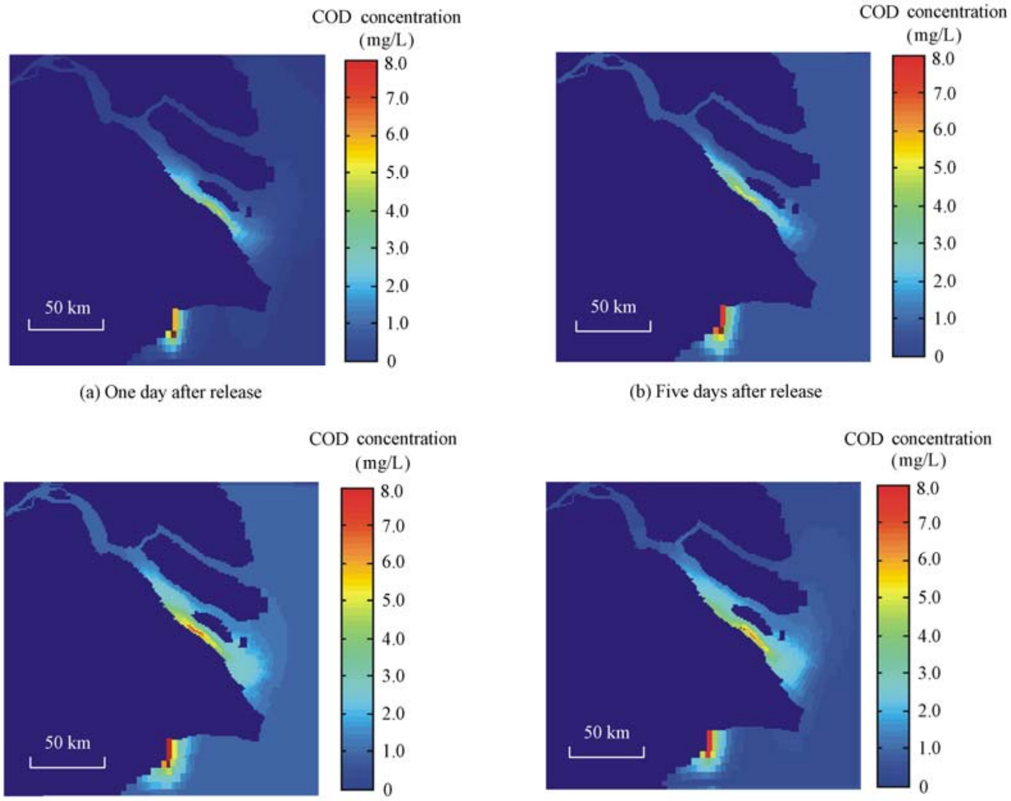


(a) Surface layer (b) Bottom layer

Fig. 7 Distribution of DO during high tide

5 Conclusions and discussion

The Yangtze River is a sediment-loaded river, and saline water mixes with fresh water in the estuary, which leads to complex mixing and difficulty in accurately quantifying the diffusion coefficient. In a numerical model, calibration of numerical data with field observation is always important. The numerical results of this model were compared with field data, and the field data provided verification of numerical application: this model is an effective water quality simulation tool. For point sources, the COD concentration was simulated with an initial value of zero in the river. The simulated increment and distribution of COD in the water body had a trend in agreement with field observation, and the concentration of DO in the North Branch was much higher than in the South Branch due to consumption of oxygen in the South Branch by sewage discharged from Shanghai. It is concluded that the numerical model is valuable in water quality simulations that include specific point source pollutant discharge, and also that the EFDC model is of satisfactory accuracy in simulation of the water quality of the Yangtze Estuary. More study on the influence of ocean circulation and mixing processes on water quality is expected in the future through both field and numerical methods.



(a) One day after release
(b) Five days after release
(c) Nine days after release
(d) Thirteen days after release

Fig. 8 Temporal and spatial simulation of COD variation after release of point source discharges

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