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Numerical simulation of hydrodynamic and pollutant diffusion in coastal waters of Qinhuangdao

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ABSTRACT

In this study, a two-dimensional hydrodynamic modeling and pollutant transport model were firstly established. The experiments verify the feasibility of the models. Through the hydrodynamic and the pollutant diffusion model, the numerical simulation of the pollutant diffusion in Bohai Bay is simulated. The diffusion characteristics of pollutant emission were obtained. At the same time, we analyzed the present situation of shallow water quality from chemical oxygen demand, nitrite nitrogen, total phosphorus content, and heavy metal content.

Keywords: Water quality testing; Hydrodynamic; Pollutant diffusion

1. Introduction

Bohai is the largest closed inland sea in China. It is one of the most obvious waters affected by human activities along the coast. Its sea water exchange cycle is long, and its regeneration capability is weak. With the rapid development of economy [1], rapid population growth, and rapid development of coastal aquaculture, the amount of pollutants entered the sea has increased year by year in the Bohai region. The marine environment in the coastal waters of Bohai has been deteriorating, and environmental problems are becoming more and more prominent [2].

Qinhuangdao is located in the south of Bohai, located in the central area of the Bohai area. The coordinates are 39°24′–40°37′ in the north latitude and 118°33′–119°51′ in the east longitude [3]. It is an important foreign trade port in North China, and it is a national class tourist city approved by the State Council. Beidaihe is the jurisdiction of Qinhuangdao [4]. Located in the central part of the north coast of Bohai Bay, northeast of Hebei, the geographical coordinates in the north latitude are 39°47′48″–39°53′17″ and in east are 119°24′08″–119°31′31″ [5,6].

Tidal movement is one of the main hydrodynamic conditions in estuaries and coastal waters, and the transport process of sediment, salt, all kinds of pollutants, and heat is accompanied by the tide. The simulation by describing the motion control equations of tidal current numerical tidal using numerical discrete approximate to simulate the trend of movement. There are two kinds of control equations, two-dimensional model and three-dimensional model [7]. Estuaries and near shore waters are broad shallow waters, the two-dimensional numerical model can basically reflect the horizontal motion law of the flow, and it has received certain effect in some practical problems.

The sewage will be migrated under the action of the seawater movement when it enters the sea. Due to the effect of turbulent diffusion and dilution, the temporal and spatial

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distribution of pollutant concentration prediction in water were used to evaluate sea water pollution, water environmental capacity, and the development of water pollution control planning scheme [8]. It has an important meaning to implement objective management of water environment. Field observation, physical model test, and numerical model methods were used to study the migration and diffusion laws of water pollutants. Due to the limitation of conditions and the difficulty of grasping the natural laws of wave [9], the establishment of mathematical models of water quality is currently the main and commonly used method in water pollution control research [10]. The mathematical model of water quality is mainly composed by the material convection diffusion equation. It can also according to different research objects and different water environment. Different supplementary equations can be added to achieve the purpose of solving the problem. There are two main models of water quality in coastal waters: two-dimensional model and three-dimensional model. The control equation of the water quality model can be solved coupled with the hydrodynamic control equation, and it can be solved separately. The solution method is similar to the numerical simulation method of the tidal current.

2. Experiments

This study was based on the Delft3D model by the Delft Hydraulic Research Institute in Holland.

Delft 3D is composed by the flow model (hydrodynamic module), and other models (such as water environment, water ecology, topography evolution, sediment transport, and so on) are extended and configured on the flow model. The basis of hydrodynamic module is Navier–Stokes equation, and the shallow water is simplified. The governing equations of the coordinate system are discretized by the alternating direction method (ADI). According to the characteristics of Beidaihe and coastal waters, this paper uses Delft 3D to simulate the hydrodynamics and pollutant migration.

2.1. Mathematical model

2.1.1. Hydrodynamic model

The continuity equation in the curvilinear coordinate system is as follows [11,12]:

$$\frac{\partial\zeta}{\partial t}+\frac{1}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\left(\frac{\partial[(d+\zeta)u\sqrt{G_{\eta\eta}}]}{\partial\xi}+\frac{\partial[(d+\zeta)v\sqrt{G_{\xi\xi}}]}{\partial\eta}\right)=0 \quad (1)$$

The equations of motion in the ξ and η directions are as follows:

$$\begin{aligned}&\frac{\partial u}{\partial t}+\frac{u}{\sqrt{G_{\xi\xi}}}\frac{\partial u}{\partial\xi}+\frac{u}{\sqrt{G_{\eta\eta}}}\frac{\partial u}{\partial\eta}\\&+\frac{uv}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\frac{\partial\sqrt{G_{\eta\eta}}}{\partial\eta}-\frac{v^2}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\frac{\partial\sqrt{G_{\eta\eta}}}{\partial\xi}-fv=\\&-\frac{1}{\rho_0\sqrt{G_{\xi\xi}}}P_\xi-\frac{gu\sqrt{u^2+v^2}}{(d+\zeta)C^2}+F_\xi+M_\xi\end{aligned} \quad (2)$$

$$\begin{aligned}&\frac{\partial v}{\partial t}+\frac{u}{\sqrt{G_{\xi\xi}}}\frac{\partial v}{\partial\xi}+\frac{v}{\sqrt{G_{\eta\eta}}}\frac{\partial v}{\partial\eta}+\frac{uv}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\frac{\partial\sqrt{G_{\eta\eta}}}{\partial\xi}\\&-\frac{u^2}{\sqrt{G_{\xi\xi}}\sqrt{G_{\eta\eta}}}\frac{\partial\sqrt{G_{\xi\xi}}}{\partial\eta}+fu=\\&-\frac{1}{\rho_0\sqrt{G_{\eta\eta}}}P_\eta-\frac{gu\sqrt{u^2+v^2}}{(d+\zeta)C^2}+F_\eta+M_\eta\end{aligned} \quad (3)$$

In the above equations, u is the ξ directional velocity component; v is the η directional velocity component; $G_{\xi\xi}$ and $G_{\eta\eta}$ are the coordinate transformation coefficients; P_ξ and P_η are the pressure gradient forces; ρ_0 is the density of water; ζ is the water level above the datum level; d is the water depth below the datum plane; $d + \zeta = H$ is the actual depth; F_ξ and F_η are Reynolds stress terms; M_ξ and M_η are subsidiary loads affecting the secondary flow; and f is Coriolis force.

2.1.2. Pollutant diffusion model

The transport equation of pollutant diffusion is as follows [9]:

$$\begin{aligned}\frac{\partial(\mathrm{HP})}{\partial t}+\frac{\partial(\mathrm{HUP})}{\partial x}+\frac{\partial(\mathrm{HVP})}{\partial y}&=\frac{\partial}{\partial x}\left(HD_x\frac{\partial P}{\partial x}\right)\\&+\frac{\partial}{\partial y}\left(HD_y\frac{\partial P}{\partial y}\right)+HS\end{aligned} \quad (4)$$

where U, V, and P are the propagation velocities and concentration in x,y space; D_x and D_y are dispersion coefficients; and H is the depth of water.

2.2. Computing method

The main calculation method of Flow model is the finite difference method. It uses interlaced grids and alternating direction explicit and implicit hybrid schemes based on the finite difference method. The grid in this format is square or rectangular, and the variables are interlaced on both sides or central position of the grid. The layout of the grid is shown in Fig. 1.

In staggered grids, not all quantities, such as water level, water depth, velocity, or concentration, are defined at the same point of grid, which is a characteristic of staggered grid. Real line indicates numerical grid network. In the definition of flow, "+" indicates the water level, concentration, and salinity; "–" represents horizontal velocity in the horizontal direction; "|" represents the horizontal velocity in the vertical direction; the black point indicates the depth of the average water level; and the gray area represents the content of the point in this area with the same grid index (M.N).

ADI is not a direct solution to a differential equation, but a differential dispersion first. And each time step Δt is divided into two segments. The time in the front $t/2$, the momentum equation and the continuous equation in the X direction, the momentum equation with u and ξ into Y direction, then the V is obtained by explicit solution. In the post $\Delta t/2$, x is replaced by y, and U is obtained by explicit solution.

This study is a two-dimensional hydrodynamic simulation. After the water level is determined, the water depth is simulated as the initial data, the water depth is obtained through the water level minus the bottom elevation.

2.3. Boundary conditions and parameter setting

The coastline near the estuary is used as the closed boundary of the simulated region, and the free-slip condition is adopted at the closed boundary. And the harmonic driving force is used in the simulation.

Flow uses alternating direction explicit and implicit mixed schemes based on finite difference method (ADI). The grid of the format is square or rectangle, and the variables ξ, u, and v are arranged alternately on both sides or center of the grid.

The computational area of the numerical simulation method is 5 km radius of the river estuary. The minimum width of the grid near the outfall is about 20 m, the width of the offshore grid is relatively large, about 500 m. A total of 740 curvilinear grids and 798 nodes are generated in all the computational regions.

In this model, the latitude of the simulated region is N39°40′1-51″, with a precision of 12.96″. The main driving forces are earth gravity, rotation force, river driving force, tide, wave, and so on; gravity acceleration was 9.81 m^2/s; sea water density is 1,024 kg/m^3; the atmospheric density is 1 kg/m^3; the tidal type is irregular semidiurnal tide; the temperature is set according to the climate conditions of the simulated area; turbulence model is k–ε; eddy viscous coefficient are 10 m^2/s and 10^{-6} m^2/s in horizontal and vertical directions; when the water temperature range is 10°C–28°C, the coefficient of degradation is generally between 0.02 and 0.02 d^{-1}; the highest salinity in Beidaihe sea appeared around June, about 32 psu, the minimum peak occurred around August, about 25 psu; the lowest value of dissolved oxygen appeared around July, about 6 mg/L, and the highest value appeared around September, which is 9 mg/L; the sea water temperature begin to rise from May, the highest value appeared around August, the highest value is about 26°C, and the water temperature begin to decline in September, and the water temperature is about 17°C in October.

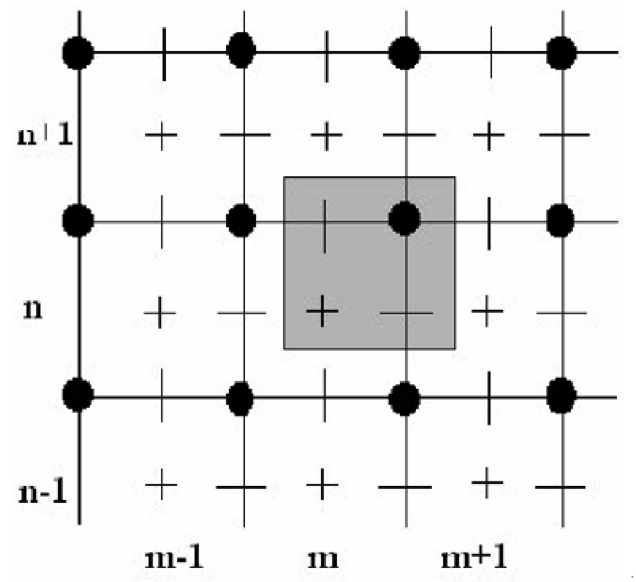

Fig. 1. Schematic diagram of Delft3D-FLOW staggered grid arrangement.

2.4. Model validation

2.4.1. Hydrodynamic model validation

In order to simulate the diffusion law of the emission pollutants in the coastal waters, this project put float tracers in the Yinma River estuary and the Yang River estuary. The trace and influence range of pollutants in the near sea water environment are simulated by the float tracers [13]. The location of the tracer floats is shown in Fig. 2. The trajectories of the tracer are shown in Fig. 3. Due to the influence of flow field and wind speed, it has to go through the trend of parallel movement along the coastline. It is very bad for the diffusion of pollutants to the sea. The float can be obtained by tracer diffusion of pollutants in the Yinma River, near the Yang River. It is helpful to the control of the offshore pollutants and the management of the water environment. Through the simulation of the velocity of the observation point, it can be found that the simulation results coincide with the measured data. This proves the credibility of the hydrodynamic model and the rationality of the selection of the parameters. The chemical oxygen demand (COD_{MN}) equivalent distribution at a typical time is shown in Figs. 4 and 5.

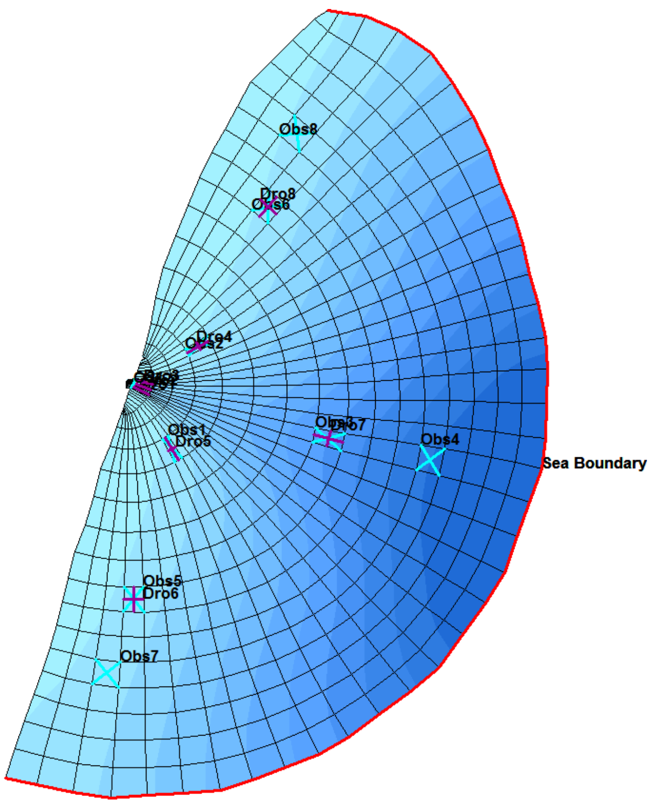

Fig. 2. Yinma River tracer floats position.

2.4.2. Pollutant diffusion model validation

In order to effectively analyze the variation and regional characteristics of the environmental quality in the near sea water, this paper chooses the typical water quality indicators in coastal water quality management: COD, nitrite, total phosphorus, and the concentration of copper, lead, zinc, and chromium ions. We selected 30 actual monitoring points as the monitoring points of the simulated area, coupled simulation of coastal water quality with Flow module and Waq module in Delft3D. And we used the water quality module to simulate the diffusion of pollutants in the computational domain. The characteristics of the diffusion of pollutants were obtained. The results of diffusion characteristics of pollutant emissions are shown in Fig. 5. Simulation results indicate the pollutants in coastal waters move obviously along with the wind direction, and the influence of wind force is an important factor of pollutant dispersion in shallow sea.

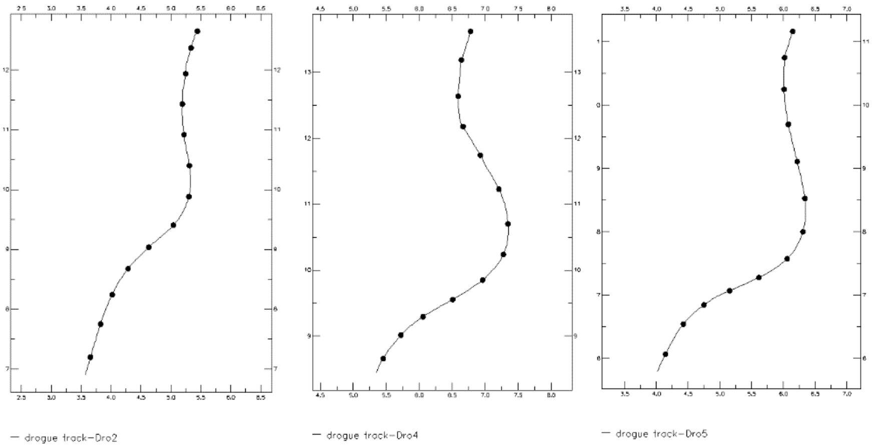

Fig. 3. Yinma River estuary tracer float trajectory simulation results.

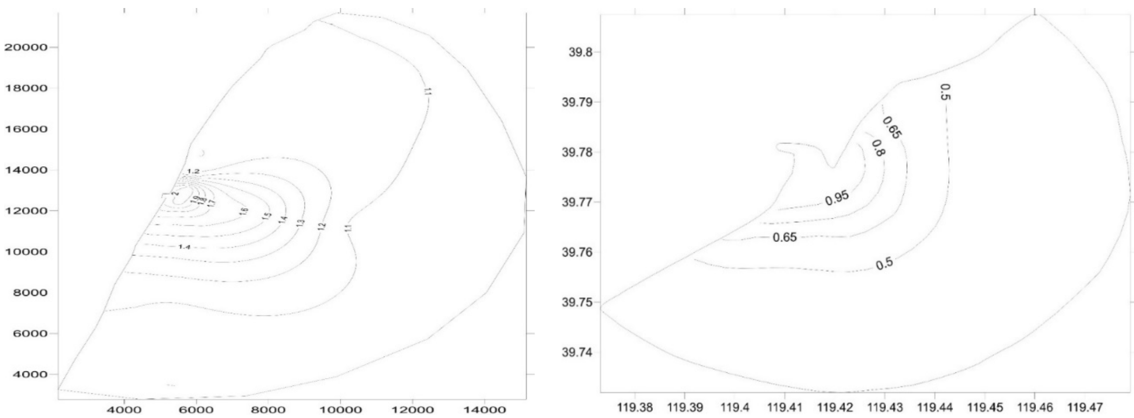

Fig. 4. Equivalent distribution maps of Yinma River COD_{MN}.

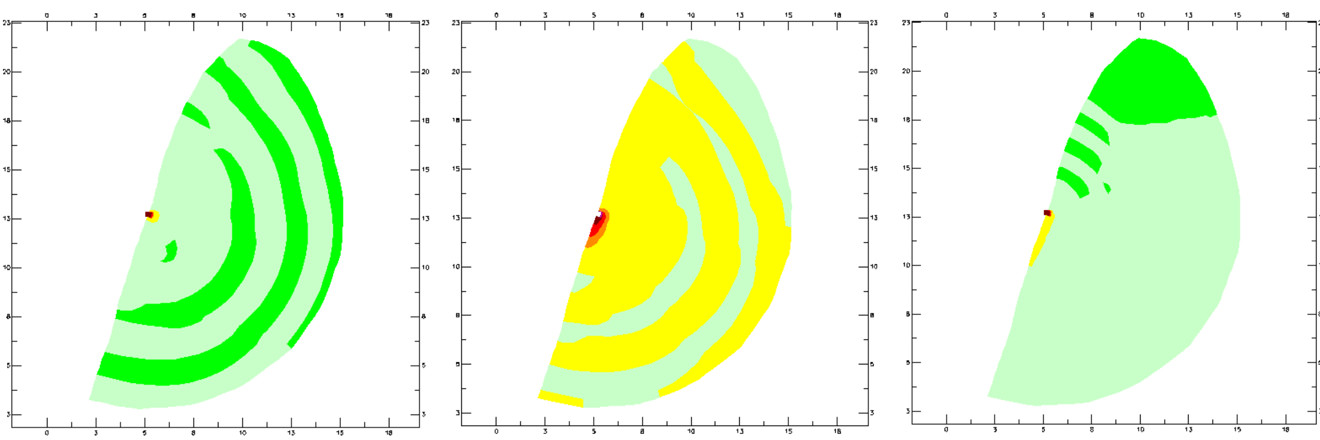

Fig. 5. Yinma River estuary flow diffusion of pollutant effects.

3. Results and discussion

The graphics of the comparison between the results extracted from Delft3D simulation and field measurements for surface elevation are presented. For these comparisons, a time series from the simulation results of surface elevation at the grid point was extracted. So, the time series was compared with the temporal series already shown in the figures. The comparison between the simulation results of main pollutants and the measured values in Yinma River is shown in Figs. 6 and 7. Error rate analysis is shown in Fig. 8. The error rate of COD_{MN} is less than 28%, among which the error rate is less than 20%, accounting for 83% of the total point. The error rate of heavy metal zinc is less than 31%, among which the error rate is less than 30%, accounting for 97% of the total point. The error rate is less than 20% accounting for 63% of the total point. The error rate of heavy metal cadmium is less than 31%, among which the error rate is less than 30%, accounting for 97% of the total point. The error rate is less than 20% accounting for 60% of the total point. The error rate of heavy metal lead is less than 29%, among which the error rate is less than 20%, accounting for 87% of the total point. The error rate of heavy metal copper is less than 31%, among which the error rate is less than 30%, accounting for 97% of

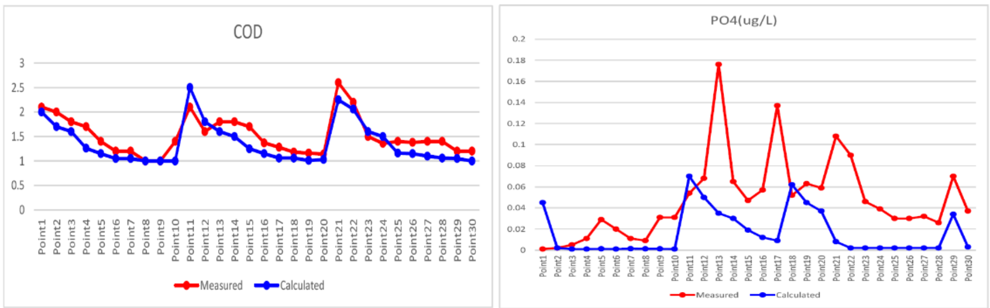

Fig. 6. Changes of COD_{MN} and PO4 concentration of Yinma River.

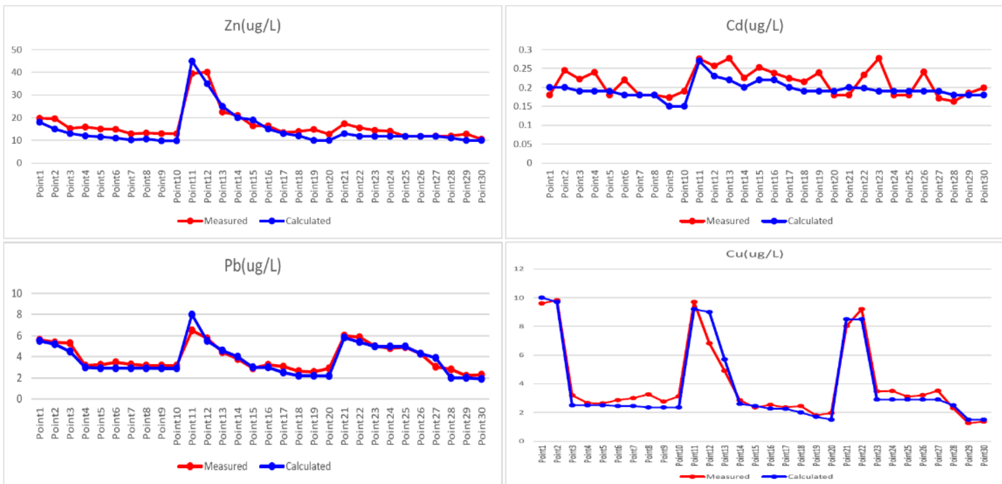

Fig. 7. Changes of heavy metals concentration of Yinma River.

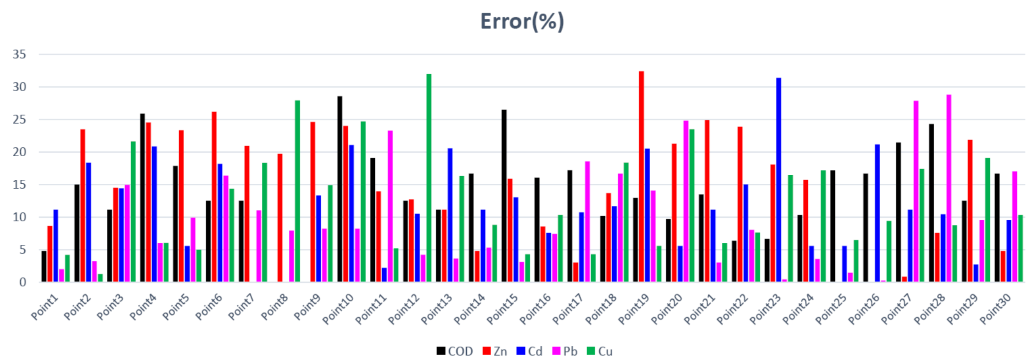

Fig. 8. The Yinma River error rate distribution of pollutants.

the total point and the error rate is less than 20% accounting for 83% of the total point.

From the above simulation results, it can be seen that the direction of the COD_{MN} transport is in line with the direction of Ebb and Flow. The distribution of COD_{MN} concentration decreases from the estuary to the sea, the dilution of channel COD_{MN} is high after discharging into sea area; the gradient of the concentration field is smaller than that of the offshore area. When the tide rises, the high concentration area of COD_{MN} moves toward the river course, the high concentration area of COD_{MN} in offshore is the smallest. When the low tide, the COD_{MN} high concentration zone goes offshore, the high concentration area of COD_{MN} in offshore is the largest.

The time period of the model calculation is mainly based on the test time, and the model is corrected and verified according to the experimental data. The pollutant transport model is verified by the measured concentration of Yinma River. The comparison and analysis of the COD_{MN} concentration calculated from the model and the measured value of the measured COD_{MN} can be obtained. The coastal waters of Yinma River and the relative error that is close to the artificial river estuary waters are relatively large, and the mean deviation is less than 20%. The main reasons of the error are as follows: (1) site detection time is not synchronized, and the calculated value and the true value cannot guarantee the water quality at the same time; (2) the mathematical model only takes account of pollutants entering the sea area. The influence of nearby estuaries is not considered. For example, the total phosphorus and COD_{MN} emissions of man-made estuaries are relatively high, the relative error of the position near the artificial estuary is also larger; (3) the waters near the mouth of Yinma River are two, the two are merged into one entrance to the sea in the process of simulation, so the influence of other estuaries on the space point pollution is ignored.

Through the simulation, it is found that the transport direction of COD_{MN} is in accordance with the trend of the fluctuation tide. As the movement of the rising tide changes periodically, the high-concentration region is mainly concentrated in the coastal waters of the river outlet, which has no obvious effect on the open seas. Cu, Pb, Cd, and Zn characteristics of the four kinds of heavy metals, from inshore to offshore direction decreases, the high-value area appears near the river entrance to the sea and the artificial estuary.

4. Conclusion

The distribution of heavy metals in sea water at each observation point shows that the distributions of copper, zinc, cadmium, and lead are similar, they are all decreased from offshore to high seas, and the heavy metal concentration area is mainly located in the coastal waters near the estuary. The concentration of simulation area near high seas is relatively low. Heavy metals are below the second-class water quality standards and do not cause pollution. At the same time, the simulation of COD_{MN}, total phosphorus, and inorganic nitrogen content also confirmed this conclusion. It shows that the pollution areas caused by land-based pollutants are mainly distributed in the coastal waters of the Qinhuangdao sea area. The COD_{MN} range of the surveyed sea area is between 1 and 3 mg/L. The value of COD_{MN} meets second-class water quality standards in wet period, and most of the COD_{MN} values in dry season and normal water period meet first-class water quality standards.

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