Numerical simulation of three-dimensional hydrodynamic characteristics and pollutant diffusion behavior by ROMS model

Jing Ren, Chazhong Ge, Chunxu Hao, Rui Hu, Kefu Cui, Chen Peng, Quan Zhou, Aiyu Yu, He Xu, Shiqing Liu and Feng Li

ABSTRACT

Based on the ROMS (Regional Ocean Modeling System) model, a three-dimensional hydrodynamic model and a convection diffusion model are built in this paper. The three-dimensional tidal current model is intended to reflect the distribution characteristics of the tidal level and the flow field of water with different depths of the Bohai Bay. On this basis, a water exchange correlation matrix is adopted to analyze the water exchange characteristics of the offshore area of Binzhou City in the offshore planning functional area of Bohai Bay. Considering the functional planning of the offshore area of Binzhou city, the paper simulates how COD and NH_4^+-N in the water discharged from the sewage outfall of the city migrate and disperse under tidal current. In this way, the paper concludes the concentration distribution patterns of pollutants at different times. The results serve as basis and reference to delimitation of environmental management and control unit demarcation in Binzhou nearshore.

Key words | pollutant diffusion, ROMS, three-dimensional numerical simulation, water exchange characteristics

HIGHLIGHTS

- Establish 3D hydrodynamic model of Bohai Bay.
- Establish water exchange correlation matrix to analyze nearshore water transport characteristics.
- Quantify the contribution of water exchange.
- Effects of river pollution load on nearshore water quality were simulated by our hydrodynamic model.
- Results serve as basis in delimitation of environmental management and control zone demarcation.

Jing Ren
School of Environment,
Liaoning University,
No.66, Chongshan Middle Road, Huanggu District, Shenyang,
China, 110036

Jing Ren
Chazhong Ge
Chunxu Hao (corresponding author)
Rui Hu
Chen Peng
Quan Zhou
Aiyu Yu
Chinese Academy of Environmental Planning of the Ministry of Ecology and Environment,
Beike Chuangye Building, No. 10, Dayangfang, Beiyuan Road, Chaoyang District, Beijing,
China, 100012
E-mail: *haocx@caep.org.cn*

Jing Ren
He Xu
School of Environment,
College of Environmental Science and Engineering, Nankai University,
No.38, Tongyan Road, Haihe Education Park, Jinnan District, Tianjin,
China, 300350

Kefu Cui
Central Research Institute of SIASUN Co., Ltd,
Xinsong Intelligent Industrial Park, No. 33, Quanyun Road, Hunnan New District, Shenyang,
China, 110168

Shiqing Liu
Binzhou Ecology and Environment Service Center,
No. 669, Bohai 18th Road, Binzhou,
China, 256600

Feng Li
Binzhou Ecology and Environment Monitoring Center,
No. 669, Bohai 18th Road, Binzhou,
China, 256600

INTRODUCTION

As China's coastal economy and marine industry gain traction in these years, the offshore area has been exposed to aggravating pollution due to rapid expansion of production

doi: 10.2166/ws.2020.380

activities, such as building ports, shipping transportation, building breakwaters, reclaiming land from the sea, protecting beaches, discharging pollutants into the sea, and harnessing estuaries and aquaculture. Pollutants can mix with surrounding waters through dilution, diffusion, convection and transportation after they go with the surface runoff into the ocean, which quickly brings down the concentration. Driven by the dual pressure from environmental protection and economic growth, research on the power system in the offshore area and the pollutant migration and diffusion pattern can make a great difference. Policies including Eco-functional Regionalization and Guidelines for Demarcation of Red Lines for Ecological Protection released by the Ministry of Ecology and Environment (hereinafter referred to as MEE) aim to guide localities through the principal function regionalization process, bringing a step closer the intensified protection of the ecological environment and natural resources in important regions and an optimized spatial development pattern (Li *et al.* 2019). After the 18th National Congress of the Communist Party of China, China has set out on a new mission of spatial management and control of sea areas to make progress in marine ecological red line and marine main function zoning across the board (Gao *et al.* 2018). What makes marine space management and control stand out lies in it being available to determine the structure and function of the ecosystem based on the physical, chemical and bio-ecological characteristics of the ecosystem in different locations, identify the important bio-ecological areas, and thus manage them in a differentiated way (Fock 2008). However, problems still exist such as relying on the original environmental function division and insufficient estimation of marine hydrodynamic diffusion conditions (Wang 2018) when delivering the work, especially for marine environmental control units division.

Three-dimensional hydrodynamic models become the mainstream of hydrodynamic numerical simulation as a better way to simulate what is really happening. Regarding water transport engineering and water environment application, the DHI Mike3 model, the Estuarine Coastal Ocean Model and the Princeton Ocean Model are all three-dimensional mathematical models based on static pressure assumption. In recent years, considering the realities of short wave driven flow, strong density gradient stratified flow and flow with large topographic changes, some achievements (Song *et al.* 1999; Koçyigi *et al.* 2002) have been made in the research into three-dimensional hydrodynamic mathematical models based on the non-hydrostatic assumption. Among them, ROMS (Regional Ocean Modeling System), as an open-source three-dimensional regional ocean model (Haidvogel *et al.* 2000), has been widely used in flow field simulation at different scales. It has obvious advantages in water level and flow field simulation caused by meteorological factors or astronomical tides, small-scale water physical movement simulation such as coastal ports, river channels, etc. (Budgell 2005).

Bohai Bay is a typical semi-closed bay. Its main hydrodynamic factors, wave and current (including tidal current, runoff, circulation, wave-generated nearshore current, etc.), interact with each other to shape a complex dynamic system. Its poor exchange capacity between the sea water and the outside world takes a toll on water quality of the offshore area as polluted water cannot spread rapidly. This paper takes the offshore area of Binzhou City in Shandong Province as the research object to analyze the dynamic factors in the ocean, adopting a hydrodynamic model based on the ROMS platform to simulate the water exchange characteristics of each area of the Bohai Bay and the migration and diffusion pattern of pollutants in the water. This can serve as a basis and reference for Binzhou city to demarcate environmental management and control units in offshore areas combined with how the marine environmental function zone and the marine ecological red line are identified.

METHODS

Construction of 3D hydrodynamic model

ROMS is an approximate solution to the N-S equation of Reynolds average under the Boussinesq assumption and the vertical static pressure assumption. Boussinesq assumes that differences in density within a body of water can be ignored unless the difference is caused by gravity. The vertical static pressure assumption holds that the depth scale in the coastal waters is much smaller than the horizontal scale, so the vertical equation of motion can be approximated by static equilibrium; that is, the vertical pressure gradient force and gravity balance. Cartesian coordinates are used horizontally and Sigma coordinates are used vertically.

The research takes the entire Bohai Sea area as the computational domain. To build an accurate three-dimensional hydrodynamic model of ocean scale, the open boundary of the calculation domain need to be accurate and stable. Besides, its continuous water level and velocity information should be easy to obtain. Thus, the open boundary of the tide on the east side is set between the National Marine Data Information Center at Tiger Beach (121°41′E,38°52′N) and Yantai Port (121°23′E,37°33′N). The data of moon phase, tidal hour and height of tide are obtained from the National Marine Data Information Center.

As Bohai Bay includes many ports in several provinces, data on human activities are difficult to estimate without reliable investigation; the effects of pollution caused by human were not quantified in this model.

The research adopts an orthogonal grid generated by the seagrid toolkit of Matlab. The total number of grid is 140 × 150, and the areas with large grid scales concentrate on the northern coastal area of Liaodong Bay, which has a relatively small driving effect on the tidal currents of Bohai Bay. This will not generate great effects on numerical simulation accuracy. Computational domain and computational grid are shown in Figure 1. Considering the overall shape characteristics of the Bohai Sea, the eastern open boundary extends from southwest to northeast; setting the grid along the open boundary is conducive to calculating the driving force. Besides, there are sparse grids in the northern part and a dense grid in the southern area, which can concentrate the calculation resources in the areas of our primary concern. At the beginning of calculation, water level and velocity of the model will adopt a zero initial condition. The water level of the opening boundary will adopt the harmonic constant interpolation of eight tidal constituents from Tiger Beach to Yantai, including M2,S2,K1,O1,N2,P1,K2 and Q1. Based on the wind rose chart of Binzhou, the model simulates the characteristics of the monsoon, continuously changes the wind direction, then calculates the average wind speed of each specific direction as a wind speed of 10 m above the sea surface, to estimate the influence of wind on water flow. After verification, it shows that the error of harmonic water level is very small. Hence, we can use the harmonic water level to replace the tidal table water level as the tidal boundary of the hydrodynamic model. The major parameters of the model are set as follows:

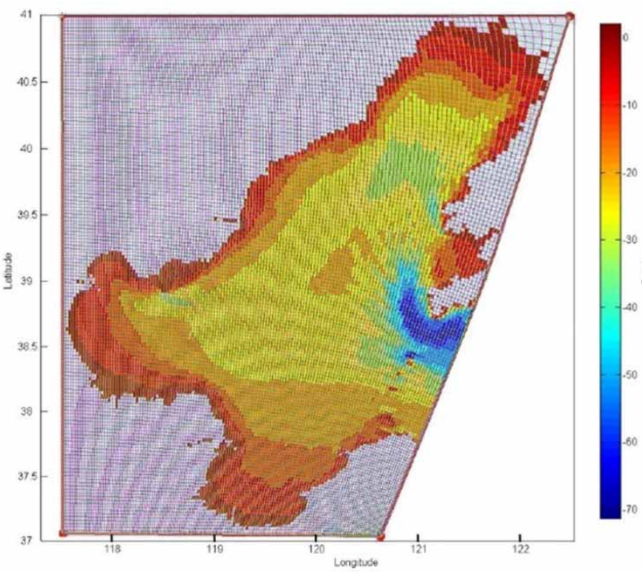

Figure 1 | Water depth distribution of research area and orthogonal grid setup.

(1) Time step. Limited by CFL conditions, the time step of the internal model of the tide numerical model is 300s, and the time step of the external model is 15s. The water level information of the east side opening boundary will be read every time step.
(2) Bottom calculation parameter. Since the sediments of Bohai Bay are mainly silt and clay, the granularity is relatively small, the roughness length is 0.005 m, and the drag coefficient of bottom friction is 0.0008.
(3) Set up appropriate vertical calculation parameters, which mainly include a vertical mixing coefficient, momentum vertical mixing coefficient, surface tensile parameter and bottom tensile parameter.

RESULTS AND DISCUSSION

The status quo of environmental quality in Binzhou offshore areas

The northern coast of Binzhou City, Shandong Province, is located in the South Bank of Bohai Bay, with gentle slope and a shallow water, wide span of intertidal zone. Southwest wind is the predominant wind direction, featuring continental climate. Many rivers, such as Dakou River, Majia River and Taoer River, cross into the sea. The tidal current in the Binzhou waters are the regular semidiurnal tides. The rising tide flows to the southwest and the falling tide flows to the northeast. The reversing current is the typical tidal movement (Liu 2020). The Binzhou sea area is open to the east and north, with large waves, mainly wind and waves, supplemented by swell. Binzhou is home to a vast sea area, rich coastline resources, broad continental shelf and endowed natural environment.

At present, the Binzhou nearshore area is mainly developed for the sake of mariculture, raw salt production, port shipping, shipping industry, electric power industry, oil and gas exploitation, urban construction, road and bridge and coastal protection (Tian 2018). The water quality of Binzhou nearshore in 2017 and 2018 is shown in Table 1, dominated by the heavily and moderately polluted sea areas respectively. The results of the seawater quality monitoring data in the past five years show that inorganic nitrogen, total nitrogen, total phosphorus and other nutrient pollutants exceed the limits, and the eutrophication phenomenon is most visible around March every year in offshore areas of Binzhou.

Flow field feature analysis of Bohai Bay

It can be seen from different levels of velocity that in jet stream waters, the vertical differences of velocity are relatively evident. However, in areas with relatively small velocity, the velocities of surface, middle and bottom have almost no differences (see Figure 2). Besides, the simulation flow result shows the influences of nearshore engineering and natural structures on the direction of current motion (Zhou & Yang 2019; Li *et al.* 2020). In general, the flow field of Bohai Bay is characterized by a regular east-west reciprocating flow. In the northern part, due to the blocking of the coast line of Caofeidian, Tangshan (Point A), the tidal currents wind along the coast line. The northwestern area takes Nanjiang Port (Point B) of Tianjin as its boundary. When the tide rises, the flow direction of waters in northern Nanjiang Port is north by northwest, while the flow direction of waters in southern Nanjiang Port is mainly west, and the flow direction of some areas is slightly south. When the tide falls, the flow direction is the opposite.

By comparing flow directions of different depths at the same time, we can see that the flow directions of the surface, middle and bottom of Bohai Bay are basically the same. From the velocity at high tide, the velocity of northern Bohai Bay is greater than that of the southern area. On the east side of Caofeidian, the flow velocity of the surface, middle and bottom level is decreasing, while on the west side of Caofeidian, where streaming is generated, the velocity of tidal currents increases dramatically. The tidal currents then flow to the inshore region of Tianjin Binhai New Area, with a decreasing velocity. There is little difference in velocity in most of central area of Bohai Bay; at the inshore region of east Huangye Port (Point C) of Cangzhou, the velocity of tidal currents gradually decreases. At low tide, the velocity in most areas of Bohai Bay is similar to that of high tide. However, the velocity feature of streaming near Caofeidian is opposite to that of high tide, and the greatest velocity appears at the east side of Caofeidian.

Table 1 | Areas of sea water with different levels of quality in Binzhou (2017–2018)

	Sea area (km^2)				
Sea water quality	**I**	**II**	**III**	**IV**	**Inferior to IV**
2017 average	130.22	458.53	465.19	318.77	627.29
2018 average	390.86	285.89	616.51	275.07	431.66

Water exchange feature of Bohai Bay

In general, the water exchange capacity of Bohai Bay is rather poor. The southeast region has the largest semi-exchange period. The water exchange capacity of the northwest and north beach area is relatively poor, which is adverse to pollutant discharge. In the wave breaking region, pollutant transport and diffusion is characterized by parallel shoreline diffusion, so the pollutants cannot diffuse to open seas along with tidal currents. The pollutants emitted outside the wave-breaking region may generate influences on the offshore area in the south part of the emission point.

Based on water exchange relational matrix analysis (Sun 2007) and the coastline of Bohai Bay, combined with characteristics of nearshore human activities, we divided Bohai Bay into six subdomains (Figure 3). District I represents the southwest part of Bohai Bay, including the offshore sea of Binzhou. District II is the southeast part of the computational domain, namely the east part of Binzhou. District III and IV represent

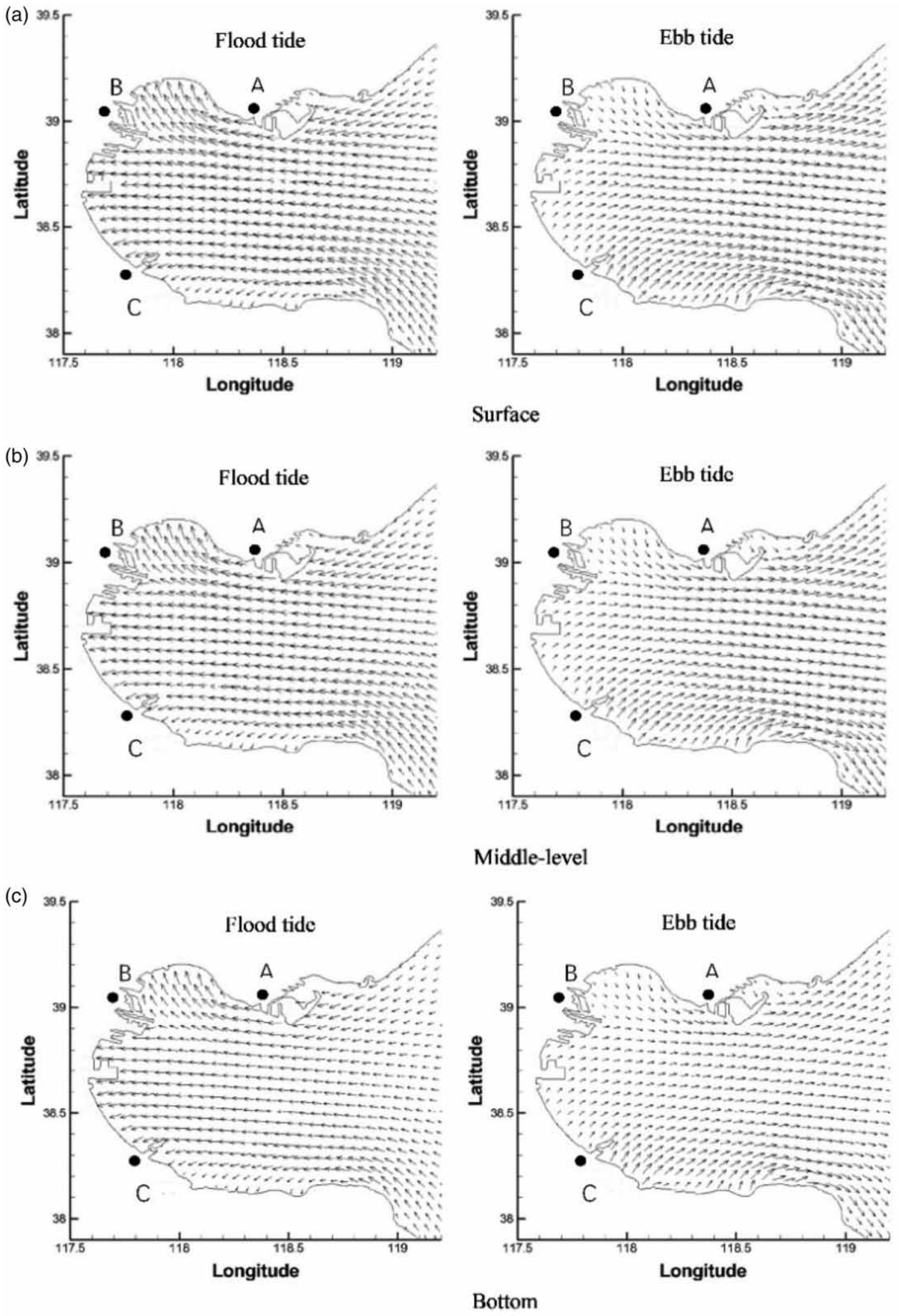

Figure 2 | Vector diagram of velocity at high tide and low tide in Bohai Bay. *Note*: Point A is Caofeidian of Tangshan, Point B is Nanjiang Port of Tianjin, Point C is Huangye Port of Cangzhou.

the middle west and middle east part of the computational domain respectively. District V and VI are the northwest and northeast part of the computational domain respectively. We simulated the water-exchange features of six subdomains, and the simulation period is a month. The simulation result is shown in Figure 4.

Figure 4(a) indicates that the original water of District I continuously flows out via water exchange to other

Figure 3 | Bohai Bay subdomain division plan.

subdomains. Six days after the simulation, the water exchange rate of this region exceeds 50% for the first time. On the 30th day, the original water of this region only accounts for 13.7% of the current water. During flow field movement, the original water of this region mainly flows to District III and IV, namely the middle west and middle east part of the computational domain; the water in this region contributes little to the output to District II, V and VI during water exchange. Only less than 1% of the water in District I flows to District VI. Therefore, during the simulation period, the sea water quality of Binzhou offshore sea has little influence on the offshore sea of Dongying, Shandong Province (District II), and the offshore sea of Tianjin (District V). And it has almost no influence on the offshore sea of Tangshan (District VI).

Figure 4(b)–4(e) show the proportion of the water exported to District I after water exchange in District II ~ VI to the original water in each district. It can reflect the influences of sea water quality of each region on the water quality of Binzhou offshore sea. According to the simulation result, the original water of the offshore sea of Dongying, Shandong Province, flows out to Binzhou at a relatively large amount; the sea water quality of Tianjin offshore sea and Tangshan offshore sea has little effect on the water quality of Binzhou. The offshore sea of Tangshan, Hebei Province almost has no influence on the water quality of Binzhou waters. It is worth noting that the results of the water exchange feature can explain the offshore seawater exchange pattern between Binzhou and surrounding cities. The water exchange feature should not be completely equivalent to the impact of pollution caused by surrounding cities.

Simulation of pollutant diffusion in offshore sea of Binzhou

The offshore sea of Binzhou includes Wuli County and Zhanhua District. Wuli County has three seagoing rivers, which are Dehuixin River, Majia River, and Zhangweixin River. The coordinates of the sea access monitoring section are E117.6871°/N37.9914°, E117.5987°/N37.9731° and E117.5641°/N38.0502° respectively; there are two sea access drain outlets in Zhanhua District, the coordinates of which are E 118.2353°/N 37.8044° and E 118.2163°/N 37.9970°.

Based on the above grid, we established a simulation environment of Binzhou offshore sea, wind velocity was set up according to the average wind direction and speed provided by Binzhou Meteorological Bureau. Based on the background values of COD and the NH_4^+-N indicator of Binzhou offshore sea from 2017 to 2018 (Ecological Environment Department of Shandong Province 2019), we simulated the influences of pollution discharge from the offshore sea access drain outlet and upstream rivers on the water quality of Binzhou offshore sea within 30 days, so as to investigate the potential for improving the marine environment. Since there is no reliable data to support and train the model, the transport/absorption/decomposition of pollutants by marine animals and plants are not taken into account in this paper. The model uses inert tracer particles to simulate pollutants, which can simulate the migration and diffusion of pollutants under physical conditions.

The result shows that the diffusivity of pollutants along the coastline is poor. This is mainly because the sea is making a reciprocating motion with the tide, leading to accumulated pollutants along the coast line (Figure 5). According to the marine environment function planning of Binzhou, this region is close to the harbor approach. Therefore, production activities have great effects on the water quality in this region. Besides, this region is close to the

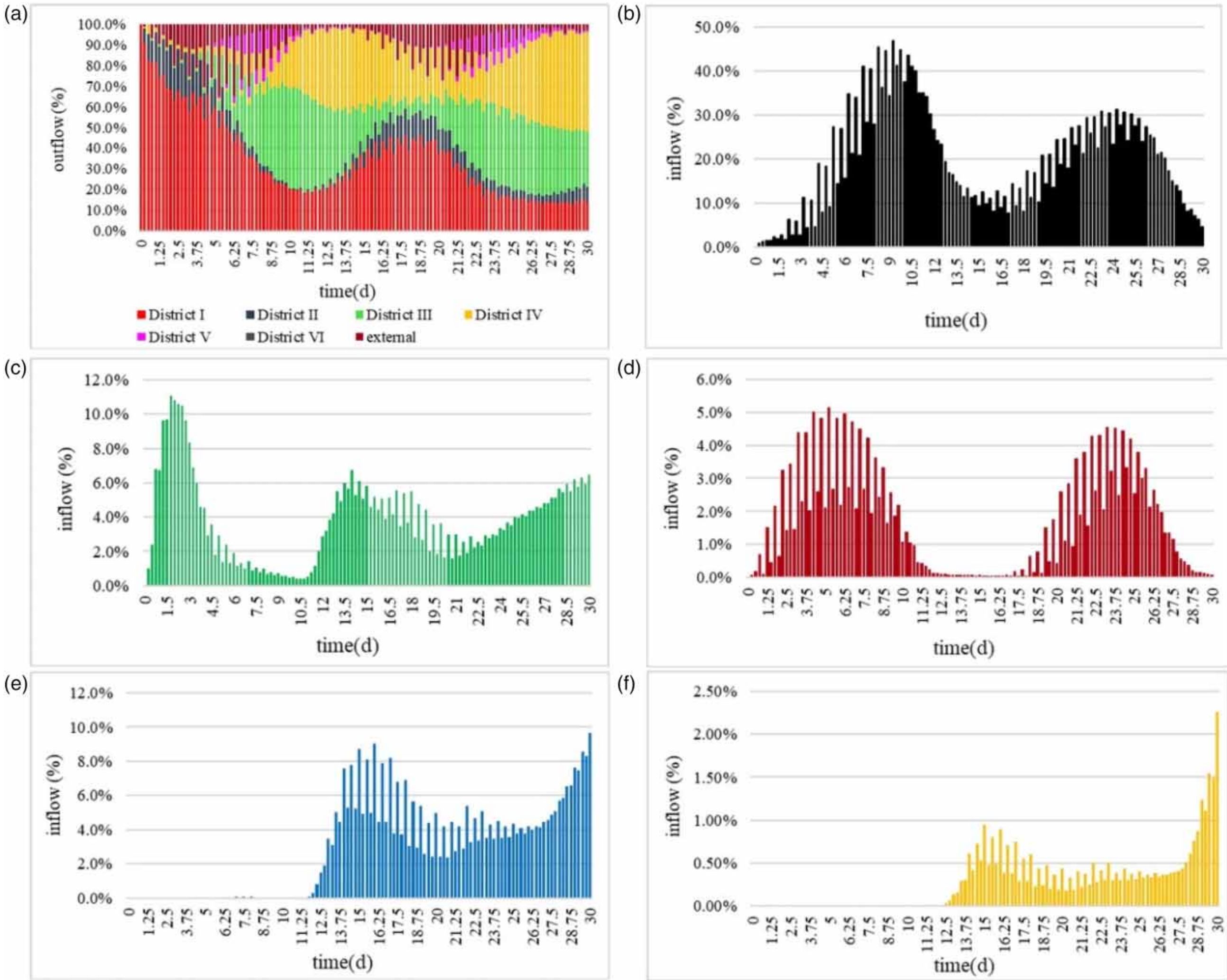

Figure 4 | Water exchange simulation result of District I and other subdomains. *Note*: (a) represents water exchange outflow result of District I; (b), (c), (d), (e) and (f) represent water exchange inflow results from District II, III, IV, V and VI to District I.

offshore sea, so at the entrance drain outlet, the emission concentration of COD in discharged water (from Wuli County, Zhanhua District Industry Park and factories) has a significant effect on the pollutant concentration of the offshore sea. If no water is discharged from the entrance drain outlet of Binzhou, then within 30 days of simulation, the COD concentration in the offshore sea can decrease by 19.11% (Figure 6). As for the NH_4^+-N, the potential reduction excent is 10.85%. According to the water quality monitoring results of Binzhou offshore sea in 2017 and 2018, the simulated pollutant concentration accumulation area agrees well with the water quality monitoring results of Binzhou offshore sea.

CONCLUSIONS

(1) *Publish technical guidelines of offshore Marine Control Unit division*

This research used ROMS to construct the hydrodynamic model, to simulate the water exchange features of Bohai Bay. In the simulation, we considered the influences of wind speed, tide level and other factors, preliminarily determined the area with poor diffusivity in Binzhou offshore sea, and used it as the basis for the Binzhou marine control unit division. In China, the division of Environmental Control Areas is in progress; meanwhile, no unified division method for

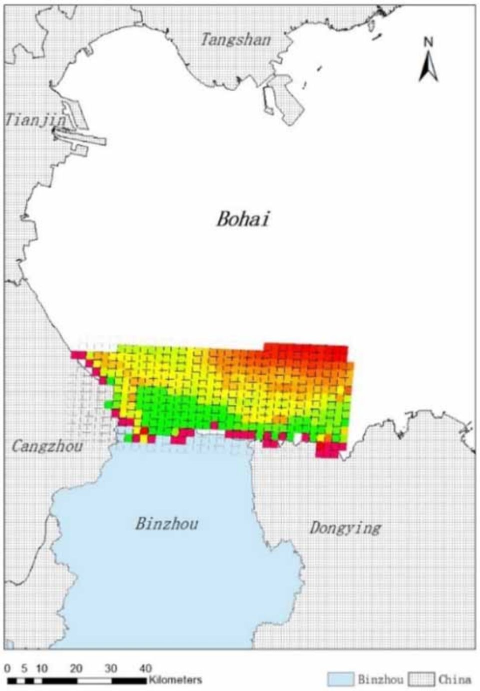

Figure 5 | Simulation of pollutant diffusion in Binzhou offshore sea.

Marine Control Areas has been published yet. In the demarcation of Key Marine Control Areas, it is necessary to identify weak dispersion regions in the nearshore. It has been verified by our study that ROMS has considerable advantages in this respect. We shall carry out in-depth research on pollutant diffusion behavior patterns (Chen *et al.* 2017.), combined with ocean vertical exchange analysis, and establish a better offshore sea diffusion model, so as to provide a theoretical basis for marine control unit division.

(2) *Accelerate the implementation of sea space control division results, improve supporting control system*

Binzhou should accelerate the ratification of marine control unit and marine ecology red line division results, implement marine ecology red line control requirements, accelerate the construction of a supporting control system (Huang *et al.* 2016), improve water quality monitoring capacity for the offshore sea, improve the marine control unit performance appraisal system, carry out research on an ecological compensation system for the red line region, so as to guarantee major progress in ecological environmental protection and resources conservation in the offshore sea.

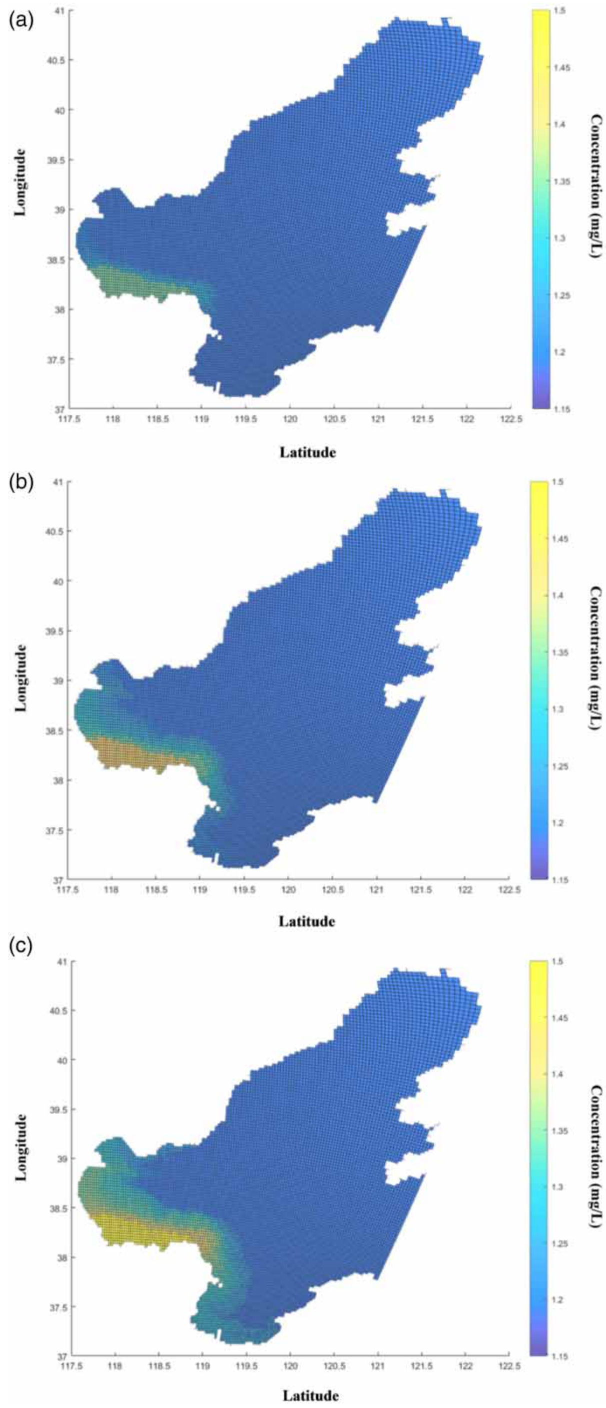

Figure 6 | Simulation of pollutant reduction potential in Binzhou offshore sea. *Note*: (a)-(c) represent COD concentration in the offshore sea in 5 days, 15 days and 30 days, respectively.

(3) *Strengthen coast line management, strictly control land reclamation projects*

The simulation results of water exchange features shows that the water exchange capacity of Bohai Bay is poor in general, especially the southeast area, which has the largest semi-exchange period and is not conducive to pollutant discharge. Ocean development processes such as getting soil from the coast, hydraulic reclamation and burying will generate negative influences on hydrodynamic conditions of the offshore sea, increasing the risks of typhoons, storm tides and other marine disasters (Sun *et al.* 2020). We should accelerate top level design of offshore sea development control, strictly control land reclamation and introduce marine emerging industry projects, to scientifically and rationally promote the sustainable development of the offshore sea economy.

ACKNOWLEDGEMENTS

The authors would like to thank Binzhou Ecology and Environment Service Bureau for help on management recommendations. The work was supported by funding from the National Financial Program 'the Red Line of ecological protection, the bottom line of environmental quality, the upper line of resource utilization and the negative list of environmental admittance' Pilot Construction and Implementation of Ecological and Environmental Protection Project (2110107).

DATA AVAILABILITY STATEMENT

All relevant data are included in the paper or its Supplementary Information.

REFERENCES

Budgell, W. P. 2005 Numerical simulation of ice-ocean variability in the Barents Sea region. *Ocean Dynamics* **55** (3), 370–387.
Chen, G., Hu, W., Chen, B., Ma, Z. & Liao, J. 2017 Marine spatial planning using in marine ecological red line zoning – a case study of Dongshan County. *Journal of Applied Oceanography* **36** (01), 6–15.
Ecological Environment Department of Shandong Province 2019 *Environmental Status Bulletin of Shandong Province.* Available from: http://zlc.sdein.gov.cn/zkgb/ (accessed 5 June 2019)
Fock, H. O. 2008 Fisheries in the context of marine spatial planning: defining principal areas for fisheries in the German EEZ. *Marine Policy* **32** (4), 728–739.
Gao, Y., Zeng, J., Huang, W., Chen, Q., Shou, L. & Xu, X. 2018 The relationship between marine functional zoning and marine ecological red line. *Ocean Development and Management* **35** (01), 33–39.
Haidvogel, D. B., Arango, H. G., Hedstrom, K., Beckmann, A., Malanotte-Rizzoli, P. & Shchepetkin, A. F. 2000 Model evaluation experiments in the North Atlantic Basin: simulations in nonlinear terrain-following coordinates. *Dynamics of Atmospheres and Oceans* **32** (3), 239–281.
Huang, W., Zeng, J., Chen, Q., Du, P., Tang, Y. & Yang, H. 2016 Preliminary research on the zoning method of the marine ecological red line: a case study of Hainan Province. *Acta Ecologica Sinica* **36** (01), 268–276.
Koçyigi, M. B., Falconer, R. A. & Lin, B. 2002 Three-dimensional numerical modelling of free surface flows with non-hydrostatic pressure. *International Journal for Numerical Methods in Fluids* **40** (9), 1145–1162.
Li, Q., Wang, Z., Liu, Y., Li, W., Zeng, S., Xiang, W. & Xu, K. 2019 Research on Beijing-Tianjin-Hebei region environment control division and different access. *Environmental Impact Assessment* **41** (01), 28–33.
Li, Z., Liu, A. & Mo, X. 2020 A numerical method for solving 3D marine dynamics model based on surface state parameter. *Journal of Tropical Oceanography* **39** (01), 12–19.
Liu, S. 2020 Spatial distribution characteristics of heavy metals in soil and bottom sediments in Binzhou Coast Zone. *Shandong Land and Resources* **36** (01), 7–12.
Song, Z., Xue, H., Yan, Y., Mao, L. & Xu, F. 1999 Quasi-3D numerical simulation of tidal hydrodynamic field. *China Ocean Engineering:English Version* **3**, 265–276.
Sun, J. 2007 *The Relation Matrix Method and Its Application of Water Exchange Study for Sea Bay and Coastal Water.* Tianjin Univesity, Tianjin, China.
Sun, Y., Qiao, Y., Liu, C., Yu, H. & Wang, W. 2020 Marine ecological pressure and countermeasure in Tianjin. *Ocean Development and Management* **37** (02), 58–62.
Tian, G. 2018 Research on marine ecological environment quality anaysis and comprehensive management – Binzhou. In *Ecological Economy and Healthy China-China Ecological Economics Society 2018 Academic Annual Conference*, Xi'an, Shanxi, China.
Wang, S. 2018 Optimization of evaluation method of marine resources and environmental carrying capacity based on scientific management and control. *Marine Environmental Science* **37** (04), 608–612.
Zhou, Z. & Yang, N. 2019 Study on dynamic simulation of river water quality based on three-dimensional numerical model. *Environmental Protection Science* **45** (06), 108–113.

First received 18 August 2020; accepted in revised form 15 December 2020. Available online 30 December 2020