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## A coastal three-dimensional water quality model of nitrogen in Jiaozhou Bay linking field experiments with modelling

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## ABSTRACT

With anthropogenic changes, the structure and quantity of nitrogen nutrients have changed in coastal ocean, which has dramatically influenced the water quality. Water quality modeling can contribute to the necessary scientific grounding of coastal management. In this paper, some of the dynamic functions and parameters of nitrogen were calibrated based on coastal field experiments covering the dynamic nitrogen processes in Jiaozhou Bay (JZB), including phytoplankton growth, respiration, and mortality; particulate nitrogen degradation; and dissolved organic nitrogen remineralization. The results of the field experiments and box model simulations showed good agreement ( $RSD = 20\% \pm 2\%$  and  $SI = 0.77 \pm 0.04$ ). A three-dimensional water quality model of nitrogen (3DWQMN) in JZB was improved and the dynamic parameters were updated according to field experiments. The 3DWQMN was validated based on observed data from 2012 to 2013, with good agreement ( $RSD = 27 \pm 4\%$ ,  $SI = 0.68 \pm 0.06$ , and  $K = 0.48 \pm 0.04$ ), which testifies to the model's credibility.

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### 1. Introduction

Land-based pollution is the primary cause of environmental issues in Jiaozhou Bay (JZB) (Wang et al., 2006; Zhang, 2007; Liu et al., 2010). With the rapid development of industrial and agricultural activities and urbanization in the JZB Rim Region, anthropogenic wastewater, mainly through rivers and wastewater treatment plants, has been discharged into JZB (Sun et al., 2007; Han et al., 2011). Green tide (*Enteromorpha*), the depletion of fish biodiversity and ecosystem degradation in JZB (Rabalais, 2002; Dai et al., 2007; Borja et al., 2008), are the result of eutrophication subjected to the high concentration of dissolved inorganic nitrogen (DIN) (Shen, 2001; Liu et al., 2005; Meng et al., 2013). Previous survey data showed that not only the load of land-based total dissolved nitrogen (TDN) into JZB increased year by year, but the components of TDN have also changed, with the contribution of dissolved organic nitrogen (DON) particularly increasing gradually in recent years (Liu et al., 2005; Yang, 2014; Lu et al., 2016). Generally, various biogeochemistry processes of TDN in the coastal area lead to DON being transformed into DIN, which affects the water quality of JZB. However, the transport and transformation processes of different nitrogen forms are complicated and difficult to explain. These processes should be analyzed, and their effects on the corresponding water quality should be assessed. A coastal three-dimensional water quality model can describe the transformation processes of different nitrogen forms,

help predict changes in water quality, and contribute strongly to the necessary scientific grounding of coastal management (Srinivasan and Arnold, 1994; Krysanova et al., 1998; Drago et al., 2001; Howarth et al., 2002).

Water quality modeling is an instrumental methodology for studying different nitrogen forms and dynamics in coastal areas because the model results not only confirm existing knowledge derived from field work but also provide insight into the functioning mechanisms of ecosystems, which are difficult to understand only by observations (Liu et al., 2007). Crise et al. attempted to use a seasonal 3D model to study the nitrogen cycle in part of the Mediterranean Sea. They found that the circulation directly or indirectly determines the distribution of the dissolved inorganic nitrogen (Crise et al., 1998). Han et al. (2011) and Li et al. (2015) studied the environmental capacity of nitrogen pollution in JZB based on a 3D water quality model (Han et al., 2011; Li et al., 2015). Previous studies have shown that the stability and veracity of a 3D water quality model depend not only on the hydrodynamic force but also on the functions and parameters of the dynamic processes of an ecosystem (Fasham et al., 1995; Walters et al., 1997; Mann and Lazier, 2006; Ayata et al., 2013). Therefore, the biogeochemical processes of different nitrogen forms might change with changes in the land-based TDN composition in JZB. Thus, it is necessary to correct the dynamic equations and parameters of the water quality model through field culture experiments (Vavilin et al., 2014). Based on a single season/form/process culture experiment, the biogeochemical processes and parameters of the multiple nitrogen forms were mostly systematic and unsuitable for the water quality model (Jørgensen et al., 1981, 1986; Morton and Frith, 1995; Suzuki et al., 2000; Fennel et al., 2001).

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Therefore, we must comprehensively and systematically understand the transformation processes of the multiple nitrogen forms in JZB, which include phytoplankton uptake, death, and respiration; particulate nitrogen (PN) degradation, and DON remineralization processes, through a field culture experiment in JZB.

Although the method of system field culture research can be completed as a multistep process, with different nitrogen sources and a complete period for the transformation processes of multiple nitrogen forms in JZB, the objective of this research is to build and calibrate the structure and dynamic parameters of the water quality model and improve the simulation accuracy. The results of this study can be further applied to evaluate plans for water quality management and lay a foundation for effectively improving water quality in JZB.

## 2. Material and methods

### 2.1. Study area

The JZB is located in the southern coastal area of the Shandong peninsula in China, surrounded by the city of Qingdao (Fig. 1). It is a typical semi-enclosed bay with a channel 2.5 km in width connected with the Yellow Sea. The bay has a surface area of 360 km<sup>2</sup> and an average depth of 7–8 m (Liu et al., 2005). The bay is increasingly affected by anthropogenic activities. A large amount of land-based pollutants enter JZB mainly through the six rivers of the Dagu, Licun, Yanghe, Loushan, Lianwan, Moshui and five wastewater treatment plants of Haibohe,

Licunhe, Loushanhe, Lianwanhe and Tuandao, leading to water quality degradation in JZB.

### 2.2. Field culture experiments

Nitrogen-enrichment culture experiments were performed at the Zhongyuan dock (N36°6'10", E120°14'48") and the deck of the ship "Dongfanghong II" of Ocean University of China, with anchorage located in the bay mouth (N36°2'6", E120°18'15") (Fig. 1). Four batches of experiments were performed to examine the transport and transformation, the dynamic processes of nitrogen in autumn (5–30 September in 2014), winter (18 January–10 February in 2015), spring (18–26 May in 2015) and summer (16 July–12 August in 2015). The whole culture experiment was designed in 4 stages based on time segments. The first stage from 0 d to 7 d was the phytoplankton growth period, the second stage from 8 d to 12 d was the phytoplankton mortality period, the third stage from 13 d to 18 d was the degradation of PN period, and the last stage was the period of DON remineralization into DIN. The experimental conditions were kept as similar as possible to the actual condition. Surface seawater was filtered through a 0.2 mm Nitex screen after sampling at the central part of JZB (N36°6'10", E120°14'48") to remove large particles or zooplankton. The filtrated seawater (15 L) was poured into a low-density polyethylene barrel (20 L) for culture experiments. DON (from the Licunhe wastewater treatment plant), NH<sub>4</sub>-N (NH<sub>4</sub>Cl AR) and NO<sub>3</sub>-N (NaNO<sub>3</sub> AR) were enriched with multi phytoplankton, light and bacteria-controlled conditions (Table 2). Phytoplankton and bacteria in seawater were removed with 1.22- $\mu$ m and 0.22- $\mu$ m filters (cellulose acetate membrane, Diqing, Shanghai), respectively. DON addition was conducted by concentrating water using tangential flow fractionation filtration with a Millipore Pellican-2 system with a 1000D pore diameter membrane (Ou et al., 2014), which retains particles larger than 1000D, improves the DON concentration, and removes inorganic nitrogen and small-molecule DON interference. Nitrogen treatments were conducted by adding DON, NH<sub>4</sub>-N and NO<sub>3</sub>-N to the culture buckets. The field culture experimental design and conditions are shown in Tables 1 and 2.

### 2.3. Field survey

Land-based pollution (rivers and wastewater treatment plants) was investigated at 11 sites and seawater samples were collected from 23 stations in July (summer) and November (autumn) 2012 and in March (winter) and May (spring) 2013 (Lu et al., 2016). DIN, DON and Chl-*a* are used to validate the simulated results of the water quality model in JZB. The investigated sites are shown in Fig. 1.

### 2.4. Sample collection and analysis

Four hundred-milliliter seawater samples were collected from culture buckets during the culture experiments at 9:00 am every day during the first week and every two days from the second week on. Two hundred-milliliter and 150-mL samples were filtered immediately

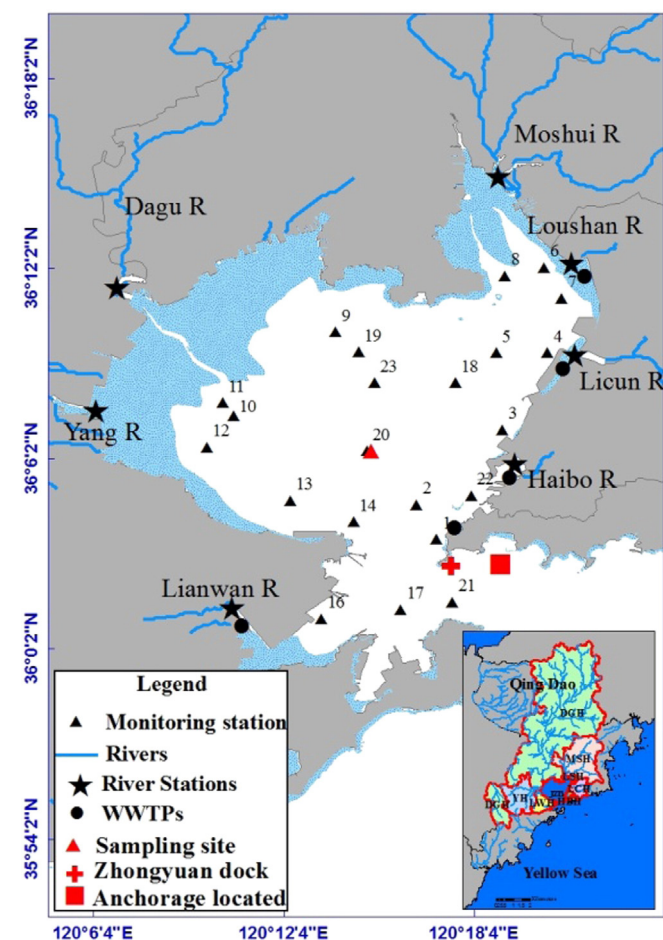


Fig. 1. Schematic of survey stations in Jiaozhou Bay. WWTPs represent wastewater treatment plants, and  $\Delta$ , + and  $\blacksquare$  represent the raw seawater collection point, the field culture experiment site and the ship anchorage location, respectively. The inset shows the location of the study area on a larger map.

Table 1  
Field culture experimental conditions.

Parameters	Spring	Summer	Autumn	Winter
Concentration (N-add $\mu\text{mol L}^{-1}$ )	50	30	30	30
Experimental location	Ship	Ship	Dock	Dock
Light ( $\text{W/m}^2$ )	225–630	750–1120	620–950	123–520
Temperature ( $^{\circ}\text{C}$ )	7–8	23–24	22–23	4–5
Salinity (‰)	30	29	29	31
Initial Chl- <i>a</i> ( $\mu\text{g L}^{-1}$ )	0.64	1.43	0.28	0.75
Dominant species	<i>Skeletonema costatum</i>	<i>Skeletonema costatum</i>	<i>Nitzschia</i>	<i>Skeletonema costatum</i>

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