¹ **Machine learning reveals biological activities as the dominant**

² **factor in controlling deoxygenation in the South Yellow Sea**

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Abstract:

 Dissolved oxygen (DO) is a crucial element for both biotic and abiotic processes in marine ecosystems, but has declined globally in recent decades. Therefore, there is an urgent need for solid large-scale and continuous estimation of DO concentration in vital ecosystems, such as coastal areas. A random forest (RF) model for DO in South Yellow Sea (SYS) was developed by integrating satellite data and simulation data during 2011–2019. The root mean squared error (RMSE) for the training and test sets were 0.514 mg/L and 0.732 mg/L, respectively. Spatiotemporal distributions of DO of multiple layers in the study area during 2011–2019 were very well reproduced by the RF model and showed a slight decline trend in most SYS areas, while more intense decline occurred in the deep central SYS. The analysis of the mechanisms of DO decline in the South Yellow Sea cold water mass (SYSCWM), located in the deep central SYS, indicates that the deoxygenation here is largely due to biological activities. This finding may have implications for studies on drivers of deoxygenation in coastal areas. Furthermore, integrating satellite data with machine learning models can offer a powerful approach to capturing the continuous spatiotemporal characteristics of ocean parameters over large spatial scales.

1. Introduction

 Dissolved oxygen (DO) concentration in seawater is a crucial parameter that impacts both biotic and abiotic processes. It influences the growth, reproduction, and feeding of organisms [\(Batziakas et al., 2020;](#page-25-0) [Flint et al., 2015;](#page-26-0) [Fock and Czudaj, 2019\)](#page-26-1),

 while also playing a crucial role in regulating biogeochemical cycles involving carbon, nitrogen, and many other elements [\(Banks et al., 2012;](#page-25-1) [Codispoti et al., 2001;](#page-26-2) [Levin,](#page-27-0) [2018;](#page-27-0) [Lonborg et al., 2020;](#page-28-0) [Mathew et al., 2022\)](#page-28-1). However, global warming has led to the heating of seawater and stronger stratification; in the meantime, rising nutrient loads resulted in increased productivity in the upper water column. All of this caused increased oxygen consumption, leading to "deoxygenation" in the ocean [\(Breitburg et](#page-25-2) [al., 2018;](#page-25-2) [Fennel and Testa, 2019;](#page-26-3) [Keeling and Garcia, 2002\)](#page-27-1). The DO content in the global ocean has declined by over 2% since 1960 [\(Schmidtko et al., 2017\)](#page-29-0), with coastal waters experiencing worse deoxygenation than the open ocean in recent decades [\(Gilbert et al., 2010\)](#page-26-4). This decline in DO at the coastal water poses a potential threat to marine ecosystem health, which could ultimately impact not only the well-being of marine life but also the livelihoods of approximately 10-12% of the global population who rely directly on marine resources for their survival and economic activities [\(Wenning, 2020\)](#page-29-1). Despite growing attention to the issue, there is a strong lack of continuous dataset to help fully understand its underlying mechanisms and quantify its declining rates, especially in the marginal seas.

 Traditionally, DO concentrations have been measured using titration facilitated by cruises [\(Bushinsky et al., 2016;](#page-25-3) [Edwards et al., 2010\)](#page-26-5). However, this approach is labor- intensive and costly, and is also subject to weather conditions. Even with improved accessibility, Argo floats face challenges in achieving large-scale, continuous observations. In this context, numerical simulations can be valuable, especially when a

 significant amount of *in-situ* data have been collected. At present, numerical simulation methods used for DO estimation include process-based (mechanistic) models and data- driven models. Process-based models, such as high-resolution numerical simulation models, can effectively reproduce real-world scenarios through extensive calculations across the entire spatial extent of the study area [\(Scully, 2013;](#page-29-2) [Xu et al., 2011\)](#page-29-3). Even though such models may provide higher accuracy, they demand extensive multidisciplinary knowledge of the specific study area and are not easily adjustable. By contrast, data-driven models have emerged as a promising approach. They demonstrate significant potential for high efficiency in various fields [\(Beyan and Browman, 2020;](#page-25-4) [Chen et al., 2020;](#page-25-5) [Goldstein et al., 2019;](#page-26-6) [Malde et al., 2020;](#page-28-2) [Pahlevan et al., 2022;](#page-28-3) [Rubbens et al., 2023;](#page-28-4) [Xiao et al., 2019\)](#page-29-4). When combined with satellite data at high spatiotemporal resolution, these models have been proven effective in modeling DO concentrations [\(Sadaiappan et al., 2023\)](#page-29-5). For example, [Guo et al. \(2021\)](#page-26-7) used support vector regression (SVR) to predict DO concentration at the surface of lakes. [Li et al.](#page-27-2) [\(2023b\)](#page-27-2) employed multiple machine learning models to reproduce hypoxia events in the bottom of the Gulf of Mexico. All of this shows that machine learning performs well at DO simulation. If machine learning methods can be integrated with some marginal seas where DO is at risk of declining, it may offer enlightening information. The South Yellow Sea (SYS) is a significant marginal sea in the western Pacific 83 Ocean, providing crucial ecological and economic services [\(Barbier et al., 2011;](#page-25-6) Dong,

[2019;](#page-26-8) [Hou et al., 2020;](#page-27-3) [Long et al., 2023;](#page-28-5) [Yu et al., 2022\)](#page-30-0). However, it is experiencing

 local deoxygenation [\(Lin et al., 2005;](#page-27-4) [Wei et al., 2021\)](#page-29-6), and this has a significant impact on the marine ecosystem. The South Yellow Sea Cold Water Mass (SYSCWM) in the SYS plays a vital role in its hydrodynamics and significantly affects its primary 88 production [\(Guo et al., 2020a;](#page-26-9) [Li et al., 2019\)](#page-27-5), maintaining high DO concentration (> 6 mg/L) year around [\(Xin et al., 2013;](#page-29-7) [Zhang et al., 2008\)](#page-30-1). Although recent reports suggest warming in the SYSCWM [\(Yang et al., 2023\)](#page-29-8), the trend in DO concentration remains uncertain. Moreover, it is unknown whether deoxygenation is taking place in the entire SYS and what its driving mechanisms. Existing studies on deoxygenation mechanisms often focus on solubility changes, with less emphasis on the role of biological processes (Oschlies et al., 2018). Thus, we aim to gather large-scale DO data alongside biomass data from satellite observations to explore the mechanisms involved. Using machine learning to generate such DO data is a suitable choice. Therefore, we developed a machine learning model for reproducing DO concentration in the SYS during 2011–2019. We evaluated four models and 15 sets of 99 inputs, identified the optimal model, and applied it to generate a high-resolution $(1/12^{\circ})$ multi-layer map of DO concentration in the SYS. Through analyzing the model outputs, this study aims to determine the spatial and temporal distributions of DO in the SYS, assess whether DO levels are declining, especially in the SYSCWM region, and understand the roles of warming and biological activities in the DO change. This study may have implications for studies on drivers of deoxygenation in the SYS and other

coastal areas.

2. Data and Methodology

2.1 Study area

 The study area includes the SYS and parts of the north East China Sea, specifically 109 ranging from the northern boundary of the SYS (marked by a black dashed line in Fig. $\frac{1}{a}$ to 30°N. The SYS is a semi-enclosed marginal sea bordered by the North Yellow Sea to the north and the East China Sea to the south, constituting a part of the Northwest 112 Pacific Ocean. It has an average depth of 44 m [\(Liu et al., 2009\)](#page-28-6). The coastal areas of Jiangsu and Shandong provinces are of great significance for coastal aquaculture, while most of the SYS shows potential for deep-sea aquaculture [\(Hou et al., 2020;](#page-27-3) [Yu et al.,](#page-30-0) [2022\)](#page-30-0). The prevailing ocean currents in this region follows a counterclockwise pattern. There is the strong northwestward YSWC in the central area and southward YSCC along the western coasts [\(Naimie et al., 2001\)](#page-28-7). This circulation pattern results in relatively high temperature in the central SYS during winter. In the deep central SYS, the SYSCWM undergoes seasonal formation, weakening, and disappearance from summer to winter.

121 **Fig. 1** (a) Geographic location and topography of the study area (NYS: North Yellow Sea; ECS: 122 East China Sea; YSWC: Yellow Sea Warm Current; YSCC: Yellow Sea Coastal Current) and (b) 123 Distribution of *in-situ* DO samples by horizontal location.

124 **2.2 Data**

125 **2.2.1 In-situ data**

 The *in-situ* DO concentration data (3214 data points) used for modeling were compiled from previous studies, including some from the National Earth System Science Data Center (http://www.geodata.cn/index.html). Details about the data source can be found in Table S1. Data samples show a higher frequency in Jun and Aug 130 (usually when DO is low) as shown in Fig. S1a. Spatially, the distribution of samples 131 adequately covers the entire study area $(Fig. 1b)$ and both above and below the mixed 132 layer depth (MLD) (Fig. S1b). The climatological seawater temperature at the vertical profile relating to the DO in Section 4 was obtained from the Regional Climatological Dataset of East Asia (RCDEA; [https://www.ncei.noaa.gov/products/regional-ocean-](https://www.ncei.noaa.gov/products/regional-ocean-climatologies)

[climatologies\)](https://www.ncei.noaa.gov/products/regional-ocean-climatologies).

2.2.2 Satellite data

Table 1 Data sources used in this study.

2.2.3 Simulated data acquisition and processing

 8-day composite MLD data at a resolution of 1/12° were derived from GLBu0.08 from the Hybrid Coordinate Ocean Model (HYCOM; https://www.hycom.org/). The simulated DO concentration data were obtained from the Global Ocean Biogeochemistry Hindcast (GOBH) model, produced by the Copernicus Marine Environment Monitoring Service (CMEMS; [http://marine.copernicus.eu/\)](http://marine.copernicus.eu/) and were used for comparison with our model. Monthly three-dimensional seawater temperature and salinity data were obtained from the Global Ocean Physics Reanalysis (GLORYS) product from the CMEMS and were used to define the SYSCWM region. This region 161 was defined as areas within the 10 \degree C isotherm at the bottom layer for a given month.

2.3 Models

 The model selection and development procedures are illustrated in Fig. 2a, with more detailed steps are shown in Fig. 2b. The model selection included 15*4*50 independent simulations. The number 15 represents the number of input variable sets. Each set consists of SST, water depth, MLD, Chl-*a*, and time (coded by an integer). In every set, only the Chl-*a* varies while the other variables stay unchanged. We focused on the cumulative effect of surface Chl-*a* prior to *in-situ* DO. Subsequently, Chl-*a* from

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$$
R = \frac{\sum_{i=1}^{N} (y_i - \bar{y}_i) * (\hat{y}_i - \bar{\hat{y}}_i)}{\sqrt{\sum_{i=1}^{N} (y_i - \bar{y}_i)^2 * (\hat{y}_i - \bar{\hat{y}}_i)^2}}
$$
(1)

185 Where N represents the number of the match-up pairs, y_i , \bar{y}_i , \hat{y}_i , and $\bar{\hat{y}}_i$ are the 186 *in-situ*, mean *in-situ*, simulated, and mean simulated DO concentrations, respectively.

187 **Fig. 2** Sketch diagrams showing (a) overall procedures of model selection and (b) the detailed

188 procedures of modeling.

3. Results

3.1 Performance of models

 The RF model, which used the mean of 8 weeks'Chl-*a* as one of the input variables, produces the lowest RMSE and highest R values. This indicates its superior performance compared to the other models (Fig. S2). The results predicted by the RF model closely match the *in-situ* DO observations (Fig.S2b), confirming its effectiveness. Hence, we selected the RF model with the 8 weeks mean Chl-*a* concentration as one input variable as our final model. However, when comparing its performance on the test set with training dataset, we observe slight overfitting of the RF model to the 198 training data (Fig. 3). In Fig. 3b, some outliers appear in the low DO segment ($\leq 4mg/L$), indicating that the model overestimates DO in this range. Despite of this defect, the model demonstrates reliable performance in both the training and test sets, with RMSE \leq 0. 8 mg/L, R $>$ 0. 95, and mean absolute error (Eq. S2) \leq 0. 5 mg/L. We also compared the model performances above and below the MLD. Both regions exhibit a similar 203 ability to the overall model (Fig. S3), indicating consistent performance across different

water depths.

Fig. 3 Scatter plots of results of the RF model alongside the *in-situ* data. (a) Training set, (b) Test

set.

3.2 Variation of Monthly DO during 2011–2019

 The monthly climatological DO derived from the model outputs during 2011– 209 2019 reveals that DO generally decreased from the inshore to the center of the SYS and 210 from the upper layer to the deeper layer in most months $(Fig. 4)$. However, above the 211 10 m layer from Jun to Sep, DO increases from the inshore to the center of the SYS. In addition, both the surface and the 10 m layers show prominent bands of high DO inshore in most months, especially from Apr to Jun. Furthermore, from Jun to Aug, an area with DO higher than both the upper and deeper layers is displayed at the 30 m layer in the center of the SYS.

 The DO in the SYS also exhibits significant seasonal variations. Generally, DO exhibits a gradual decline from late winter (Jan, Feb) to midsummer (Aug), followed by a subsequent increase after early autumn (Sep, Oct). The lowest DO levels are observed in August, while the highest levels occur in Mar. However, the recovery of DO does not take place during autumn (Sep, Oct, and Nov) in the center of the SYS (SYSCWM region) at a depth of 60 m.

222 **Fig. 4** Simulated monthly climatological DO concentrations from Jan 2011-Dec 2019. The surface and bottom layers are defined as the layer with a depth of 1 m and

223 the depth of the seabed topography, respectively.

3.3 Long-term patterns of DO during 2011–2019

4. Discussion

4.1 Mechanisms underlying the spatiotemporal patterns of DO

246 We observe close relationship between SST and DO, as evident from Figs. 4 and [S4.](file:///C:/Users/LENOVO/Desktop/论文修改/审稿意见/Supplementary%20material.docx%23figs4) DO shows a gradual decline from late winter (Jan, Feb) to midsummer, followed by an increase after early autumn (Sep, Oct). Meanwhile, SST increases from early spring (Mar) and declines after autumn (Sep). This negative correlation is mainly explained by the lower DO solubility in warmer seawater. In addition, enhanced stratification caused by high seawater temperature at the surface can also limit ventilation into deep water, leading to depletion of DO at the bottom. In Jan and Feb, the dominant current patterns of YSCC and YSWC result in high seawater temperature in the central region and low temperatures inshore. The spatial patterns of DO at surface, 255 10 m and 30 m layers in these months closely match the patterns of SST (Fig. S4), with high DO inshore and low DO in the center of the SYS. This indicates that DO in these months is primarily driven by seawater temperature. This is likely due to the well-mixed water column in winter (Fig. S5), leading to sufficient replenishment of DO, thus

 the 60 m layer in the following months. This can be attributed to the persistence of the 281 stratification until Nov (Fig. S7). In the absence of sufficient ventilation, DO in deep water is depleted by the remineralization of sinking organic particles.

4.2 Mechanisms of DO decline in the SYSCWM

 Even though our results suggest that seasonal DO variations are highly correlated with seasonal seawater temperature changes in Section 4.1, the long-term downward trend in the center of the SYS is not solely caused by rising temperature. Thus, we used a computational method to separate the effect of biological activities and warming on deoxygenation. The details of this method are described in the [supplementary materials.](file:///C:/Users/LENOVO/Desktop/论文修改/审稿意见/Supplementary%20material.docx%23calculationmethod) In the SYSCWM region, either above or below the MLD, the primary factor accounting for decline in DO is the biological activity (Table S2). These could be interpreted as either a decline in oxygen production or an increase in oxygen consumption. Above the MLD in the water column, DO often appears oversaturated as phytoplankton thrives under optimal temperature and light conditions (Wei et al., 2021). This suggests that the decline in DO above the MLD can be attributed to a decrease in oxygen production during photosynthesis. Below the MLD in the water column, the decline in DO may be attributed to the more intense oxygen consumption of sinking organic particles through respiration. To see if phytoplankton biomass is changing as expected, the trends of sea surface Chl-*a* at the annual and monthly scales were plotted respectively (Fig. 6, S8).

After examining the trend of the sea surface Chl-*a*, a declining trend was found

315 the SYSCWM region [\(Chen, 2009;](#page-26-10) [Hickox et al., 2000\)](#page-27-10).

316 **Fig. 6** Long-term monthly variations of Chl-*a* concentration during 2011–2019.

 To investigate whether the biological contribution to the decline in DO in the SYSCWM (i.e., below the MLD in the SYSCWM region) can be attributed to the stronger early spring bloom, we plotted the Chl-*a* in Mar and the DO in Aug in the SYSCWM region (blow the MLD). These months were chosen because they denoted the increase in phytoplankton bloom in early spring and the peak phase of the 322 SYSCWM, respectively. The correlation between them is -0.772 ($P < 0.05$), indicating a plausible link between stronger early spring phytoplankton blooms and reduced DO in the SYSCWM (Fig. S9). We also calculated the correlation between DO in Jun in the 325 SYSCWM and that in Aug ($P < 0.05$). The strong correlation suggests that the low DO

Chl- a (mg/m³ per month)

 in Aug may be due to that in Jun. Similarly, we investigated whether the Chl-*a* in the southern part of the study area in Jun was related to the DO of the SYSCWM. The 328 results showed that there was no significant correlation between them $(p > 0.05)$, suggesting the effect of the seawater temperature fronts as a barriers. Collectively, our hypothesis that the organic particles formed in spring may account for the decline in DO in the SYSCWM remains valid. The proposed mechanism is visually represented in Fig. 7.

 In addition, physical processes also play a role in this process. For instance, the process illustrated in Fig. 7 may be augmented by the mixed layer pump (MLP) observed in many studies. That is, in regions with significant seasonal variation in the MLD, surface organic particles are pushed into deeper waters by intensified wind mixing during the colder seasons [\(Lacour et al., 2019;](#page-27-11) [Xing et al., 2020\)](#page-29-12). Stronger stratification due to warming can reduce nutrient supply to the surface, subsequently decreasing primary production [\(Dave and Lozier, 2013\)](#page-26-11). It can also limit the extent of ventilation from the surface to the deep water. In essence, warming and biological activities can sometimes interact. Aside from directly affecting the DO content entering the ocean (through air-sea exchange), warming can also change DO content by influencing ocean hydrology which then regulates the biological activities.

 Fig.7 Schematic of the mechanisms of deoxygenation explained by biological activities in the SYSCWM. In spring, stronger phytoplankton blooms formed more sinking particles, while the mixing gradually weakened and the water column gradually stratified in the following months. Then these particles continued to sink and gradually consumed more DO below the MLD through respiration. In summer, or the SYSCWM period, lower DO is present and it is difficult to be replenished from the upper layers of the stratified water column.

 In addition to the overall downward trend, there are some details worth our attention in Fig.5, such as DO in the year 2013 is considerably lower than any other years. After plotting the interannual variation of SST in Aug and Chl-*a* in Feb and Mar, we found that 2013 had a higher SST than most years and the highest spring Chl-*a* (Fig. S10) High seawater temperatures and strong stratification, combined with enough sinking particles produced by phytoplankton, contributed to the low DO in summer

2013.

4.3 Advantages and drawbacks of the study

 Based on extensive previous studies, our modelling study provides distribution and trends of DO with higher spatial-temporal resolution, thus highlighting locations of more intense deoxygenation. The spatial patterns of DO exhibited by our model aligns closely with a substantial body of empirical studies [\(Guo et al., 2020b;](#page-26-12) [Guo et](#page-26-13) [al., 2020c;](#page-26-13) [Li et al., 2015;](#page-27-12) [Lu et al., 2017;](#page-28-9) [Luo et al., 2018;](#page-28-10) [Qu et al., 2015;](#page-28-11) [Xiong et](#page-29-13) [al., 2020;](#page-29-13) [Zhu et al., 2017\)](#page-30-4). Besides, the declining DO observed by our model in the SYS is consistent with previous findings [\(Wei et al., 2021\)](#page-29-6), which also show a more significant decline in DO in the deeper layers of the SYS. This further substantiates the reliability of modeling as an approach to comprehensively capture spatiotemporal patterns despite limited *in-situ* data availability. Although global model data with similar functions are available, our model exhibited higher accuracy and higher resolution in comparison to the global model in our study area (Fig. S11). Moreover, the error observed in our study is considered acceptable compared to similar studies, which achieved an RMSE of approximately 1 mg/L [\(Guo et al., 2021;](#page-26-7) [Kim et al., 2020;](#page-27-13)

[Li et al., 2023b;](#page-27-2) [Ross and Stock, 2019\)](#page-28-12).

 This study not only captures the spatial and temporal characteristics of DO, but also demonstrates the feasibility of machine learning combined with satellite data to predict the DO concentration in the SYS. This approach would reduce the cost of instruments and labor. However, narrowing down the error caused by potential

 inaccuracies in satellite data as well as the inherent limitations of the model itself remains a challenging task. Our model may not fully capture the actual variations in extremely low DO conditions (e.g., < 4 mg/L). This can be attributed to the involvement of more intricate processes in DO dynamics in these cases, such as sediment consumption and advection transport. There are also other challenges that remain to be further addressed. For example, the precision of input data and the comprehensiveness of *in-situ* data need improvement. In the future, we anticipate that more *in-situ* data will be collected, satellite data will be accurately calibrated, and additional variables will be incorporated to enhance the precision of the model. Moreover, due to the introduction of the time variable into the model and its significant contribution to the result (Fig. S6), the accuracy of dissolved oxygen simulation beyond the time range cannot be guaranteed. It is expected that the model's time variable will be adjusted or deleted in the future to enhance the usability of the model in forecasting. More discussions on the time variable and the partial correlation curves (Fig. S12) can be found in the supplementary material. Additionally, the potential of the proposed approach for achieving similar performance in other waters remains to be tested.

5. Conclusion

 In this study, an RF model was presented to efficiently and accurately simulate the DO conditions of multiple layers in the SYS during 2011–2019. This provided a comprehensive spatiotemporal distribution of DO within the SYS. The model has achieved good accuracy and effectively captures a declining trend of DO in the SYS,

Declaration of competing interest

The authors declare that they have no competing financial interests or personal

- relationships that could have appeared to influence the work reported in this paper. All
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