



1 Hydrodynamic and Biochemical Impacts on the Development of 2 Hypoxia in the Louisiana–Texas Shelf Part II: Statistical Modeling 3 and Hypoxia Prediction

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10 **Abstract.** In this study, a novel ensemble regression model was developed for hypoxic area (HA) forecast in the Louisiana–
11 Texas (LaTex) Shelf. The ensemble model combines a zero-inflated Poisson generalized linear model (GLM) and a quasi-
12 Poisson generalized additive model (GAM) and considers predictors with hydrodynamic and biochemical features. Both
13 models were trained and calibrated using the daily hindcast (2007–2020) by a three-dimensional coupled hydrodynamic–
14 biogeochemical model embedded in the Regional Ocean Modeling System (ROMS). A promising HA forecast is provided by
15 the ensemble model with a low RMSE (3,204 km²), a high R² (0.8005), and a precise performance in capturing hypoxic area
16 peaks in the summers. To test its robustness, the model was further applied to a global forecast model and produces HA
17 prediction from 2019 to 2020 with the adjusted predictors from the HYbrid Coordinate Ocean Model (HYCOM). Predicted
18 HA shows a high agreement with the ROMS hindcast time series (RMSE=4,571 km², R²=0.8178). Our model can also predict
19 the magnitude and onsets of summer HA peaks in both 2019 and 2020 with high accuracy. To the best of our knowledge, this
20 ensemble model is by far the first one providing fast and accurate daily HA predictions for the LaTex Shelf while considering
21 both hydrodynamic and biochemical effects. This study demonstrates that it is feasible to perform regional ocean HA prediction
22 using global ocean forecast.

23 1 Introduction

24 The Louisiana–Texas (LaTex) Shelf has become a center of hypoxia (bottom dissolved oxygen, DO<2 mg L⁻¹) study since
25 the 1980s (Rabalais et al., 2002; Rabalais et al., 2007a; Justić and Wang, 2014). Regular mid-summer Shelfwide cruises
26 documented that the area and volume of hypoxic bottom water could reach up to 23,000 km² and 140 km³, respectively
27 (Rabalais and Turner, 2019; Rabalais and Baustian, 2020). The aquatic environments, fisheries, and coastal economies are
28 under threat of recurring hypoxia in summer (Chesney and Baltz, 2001; Craig and Bosman, 2013; De Mutsert et al., 2016;
29 LaBone et al., 2020; Rabalais and Turner, 2019; Rabotyagov et al., 2014; Smith et al., 2014). Water column stratification and
30 sediment oxygen consumption (SOC) are two main factors regulating the formation, evolution, and deconstruction of bottom



31 hypoxia from mid-May through mid-September (Bianchi et al., 2010; Conley et al., 2009; Fennel et al., 2011, 2013, 2016;
32 Feng et al., 2014; Hetland and DiMarco, 2008; Justić and Wang, 2014; Laurent et al., 2018; McCarthy et al., 2013; Murrell
33 and Lehrter, 2011; Rabalais et al., 2007b; Wang and Justić, 2009; Yu et al., 2015). However, prevailing prediction models for
34 the hypoxic area (HA) rely most on nutrient-induced mechanisms rather than the hydrodynamic features. Turner et al. (2006)
35 built a multiple linear regression model for summer HA prediction using the annual and May nitrogen flux (nitrate+nitrite) of
36 the Mississippi River as the predictors. The model provides a robust annual prediction when no strong wind was present but
37 underestimates the HA in windy years. Obenour et al. (2015) modeled HA using the empirical relationship between HA and
38 bottom DO concentration derived by a Bayesian biophysical model. Their model accounted for primary biophysical processes
39 solved for steady-state conditions, water transport, May total nitrogen loads by rivers, and parameterized water reaeration.
40 Katin et al. (2021) further adjusted the Bayesian model by taking into account river flows, riverine bioavailable nitrogen
41 loadings, and wind velocity in both summer (June–September) and non-summer (November–May) months. Summer riverine
42 inputs are projected using non-summer riverine variables, river basin precipitation, and river basin temperature, while,
43 however, summer wind velocity is resampled from historical records from 1985 to 2016. Therefore, the model is known as a
44 pseudo-forecast model since predictors in future stages only include riverine inputs. The pseudo-forecast model explains 71
45 % and 41 %–48 % of the variability in hindcast (Del Giudice et al., 2020) and geostatistically estimated HA (Matli et al.,
46 2018), respectively. Another Bayesian model was proposed for summer bottom DO concentration prediction taking account
47 of May total nitrogen loads, distance from the Mississippi River mouth, and downstream velocity (Scavia et al., 2013). The
48 summer HA is determined by hypoxic length ($HA=57.8$ hypoxic length) derived from summer bottom DO concentration. The
49 model explains 69 % of the variability in observed HA by the mid-summer Shelfwide cruises. Different from linear regression
50 and Bayesian analysis, Laurent and Fennel (2019) developed a weighted mean forecast method calibrated on the May nitrate
51 loads and three-dimensional hindcast simulations (1985–2018). Once calibrated, the model requires the May nitrate loads for
52 the forecast year as the only input to produce the seasonal forecast. The model can explain up to 76 % of the year-to-year
53 variability of the HA observation. However, the model is not favorable for years with strong wind events during summer.

54
55 These above-mentioned models share some similar shortages: (1) The effects of water column stratification are not included
56 or only partially considered even though stratification is documented as a crucial factor in regulating HA variability. (2) The
57 information of future conditions is limited although some models are built upon multiple predictors, thus these forecast models
58 are indeed “pseudo-forecast” ones. (3) Most models only capture year-to-year HA variability and fail whenever winds are
59 strong in summers. According to the hindcast results by our three-dimensional coupled hydrodynamic–biogeochemical model
60 described in the accompanying paper (Part I), monthly and daily variabilities of HA cannot be neglected before and after strong
61 wind events. In this study, we aimed to provide a new technique in HA prediction considering both stratification and
62 biochemical effects and executing daily forecasts based on the forecasts of selected predictors. An important assumption is
63 that the future conditions of predictors are accessible. Indeed, it can be fulfilled by using global forecast products such as the
64 HYbrid Coordinate Ocean Model (HYCOM), which provides operational hydrodynamics forecasts for up to one week (eight



65 days). In the accompanying paper (Part I), we demonstrated that the hypoxic volume and the bottom HA over the LaTex Shelf
66 are highly correlated. The former can be reproduced by the latter alone with a quadratic relationship. Thus, in this study, we
67 focused on bottom HA predictions. The rest of the paper is organized as follows: a detailed description of methods and data is
68 given in section 2. The employment of generalized linear models (GLMs) and generalized additive models (GAMs) is given
69 in section 3. The ensemble HA prediction and its application using the global HYCOM is discussed in section 4.

70 2 Methods

71 2.1 Data descriptions

72 We adapted a three-dimensional coupled hydrodynamic–biogeochemical model embedded in the framework of the Regional
73 Ocean Modeling System (ROMS) on the platform of Coupled Ocean–Atmosphere–Wave–Sediment Transport modeling
74 system (COAWST, Warner et al., 2010) to the GoM (Gulf–COAWST, for detailed descriptions, validations, and results of the
75 numerical model see Part I). Numerical hindcasts (hereafter denoted as ROMS hindcasts or ROMS simulations) are output
76 daily from 1 January 2007 to 26 August 2020 and spatially averaged over the LaTex Shelf. In this study, we aim to produce a
77 fast and accurate daily forecast of the shelf HA using models trained from the ROMS outputs.

78 2.1.1 Hydrodynamic-related predictors

79 Both water stratification and bottom biochemical processes modulate the variability of bottom DO concentration in the LaTex
80 Shelf. Potential energy anomaly (PEA, in J m^{-3}) is introduced as an estimate of water column stratification according to:

81

$$82 \text{ PEA} = \frac{1}{H} \int_{-h}^{\eta} (\bar{\rho} - \rho) g z dz, \quad (1)$$

83

84 where ρ is water density profile (estimated by water temperature and salinity profiles) over water column of depth $H = h + \eta$,
85 h is the location of the bed, η is water surface elevation, g is the gravitational acceleration (9.8 m s^{-2}), z is the vertical axis, $\bar{\rho}$
86 is the depth-integrated water density given by $\bar{\rho} = \frac{1}{H} \int_{-h}^{\eta} \rho dz$ (Simpson and Hunter, 1974; Simpson et al., 1978; Simpson,
87 1981; Simpson and Bowers, 1981). The PEA represents the amount of energy per volume to homogenize the entire water
88 column (Simpson and Hunter, 1974). Thus, a greater PEA value represents a more stratified water column. As a river-
89 dominated area, water stratification in the LaTex Shelf is highly affected by freshwater-induced buoyancy from the Mississippi
90 and Atchafalaya Rivers. Sea surface salinity (SSS) is a good proxy in representing the distribution and variability of river
91 freshwater across the shelf. Indeed, the correlation of regionally averaged PEA and SSS is significantly high up to -0.88
92 ($p < 0.001$; Figure 1a) which emphasizes the importance of freshwater-induced stratification. Therefore, we considered SSS as
93 another candidate predictor besides PEA.

94



95 In the meantime, surface heating and wind mixing are other two factors influencing water stratification (Simpson and Hunter,
96 1974; Simpson et al., 1978) and can be quantified as follows:

$$98 \frac{d(PEA)}{dt} = \frac{\alpha gh}{2c} Q - \delta k_a \rho_a W^3, \quad (2)$$

99
100 where Q is the rate of surface heat input, α is the volume expansion coefficient, c is water specific heat capacity, δ is
101 coefficient of wind mixing, k_a is drag coefficient, ρ_a is humid air density near the sea surface, and W is the wind speed near
102 sea surface. The first term on the right-hand side of Eq. (2) represents the rate of change of water stratification due to surface
103 heating, while the second term is the rate of working by wind stress contributing negatively to water stratification. Therefore,
104 the heat-induced change of PEA is proportional to the product of heat input and water depth, which is,

$$106 d(PEA)_{heat} \propto Qh, \quad (3)$$

107
108 The total net heat flux, a sum of net shortwave and net longwave radiation flux, is derived from the National Centers for
109 Environmental Prediction Climate Forecast System (NCEP) Reanalysis (CFSR) 6-hourly products (Saha et al., 2010; 2011) in
110 this study. The term (Qh) is added to the candidate list of predictors and is denoted as PEA_{heat} (heat-induced PEA changes)
111 for simplification.

112
113 Daily variability of term ($\delta k_a \rho_a W^3$) is dominated by that of W^3 , since the ρ_a fluctuates much less than the W^3 in a daily
114 scale (Figure A1). We obtained the ρ_a according to (Picard et al., 2008) :

$$116 \rho_a = \frac{pM_d}{ZRT} \left[1 - x_v \left(1 - \frac{M_v}{M_d} \right) \right], \quad (4)$$

117
118 where p represents the absolute air pressure, M_d ($=28.96546 \text{ g mol}^{-1}$) is the molar mass of dry air, M_v ($=18.01528 \text{ g mol}^{-1}$) is
119 the molar mass of water vapor, Z indicates compressibility, R ($=8.314472 \text{ J mol}^{-1} \text{ K}^{-1}$) is the molar gas constant, T is
120 thermodynamic temperature, x_v is the mole fraction of water vapor. We assumed that air parcels at the sea surface are ideal
121 gases ($Z = 1$) and are always saturated with water vapor. Thus, x_v is a function of absolute air pressure (p) and saturation
122 vapor pressure of water (p_{sat}) and can be calculated as follows:

$$124 x_v = \frac{p_{sat}}{p}, \quad (5)$$

125
126 According to the Tetens equation (Monteith and Unsworth, 2014), p_{sat} (in Pa) can be estimated for the following:



127

128
$$p_{sat} = 610.78e^{\frac{17.27(T-237.3)}{T}},$$
 (6)

129

130 Substitute Eqs. (5)–(6) to Eq. (4) with the assumption of $Z = 1$, we obtained air density as a function of both air pressure and
131 air temperature in the following:

132

133
$$\rho_a = \rho_a(T, p) = \frac{pM_d}{ZRT} \left[1 - \frac{1}{p} \left(1 - \frac{M_v}{M_d} \right) e^{\frac{17.27(T-237.3)}{T}} \right],$$
 (7)

134

135 The ρ_a is then estimated using sea surface air pressure and air temperature 2 meters above the sea surface provided by NCEP
136 CFSR 6-hourly products. Correlation of daily $\rho_a W^3$ and W^3 (provided by NCEP CFSR 6-hourly products) is significantly
137 high as 0.9989 ($p < 0.001$, Figure A1) emphasizing the importance of term W^3 in controlling the daily variability of wind-
138 induced PEA changes over the shelf. We, thus, approximated the relationship as:

139

140
$$d(PEA)_{wind} \propto W^3,$$
 (8)

141

142 The term W^3 is introduced as another candidate predictor and is denoted as PEA_{wind} (wind-induced PEA changes) for
143 simplification.

144 2.1.2 Biochemical-related predictors

145 Sedimentary biochemical processes directly influence the bottom DO consumption rate. However, by far, global forecast
146 model systems like HYCOM does not include biochemical fields. Therefore, the biochemical-related term SOC needs to be
147 replaced by an alternative term (denoted as SOCalt) that does not rely on biochemical simulations. According to the SOC
148 scheme stated in Eq. (8) and Eq. (10) in Part I, the biochemical features are attributed to the sedimentary particulate organic
149 nitrogen (PONsed, derived from ROMS hindcasts) concentration. The total nitrate and nitrite load by the Mississippi River are
150 used to represent the PONsed variability, because inorganic nitrogen is the primary nutrient resource for plankton bloom. Daily
151 updates of measured riverine nitrate+nitrite loads are accessible from U.S. Geological Survey (USGS) National Water
152 Information System (NWIS). Due to lateral transports and vertical settling of particulate organic matter, a leading period should
153 be introduced to the time series of riverine nutrient loads. The optimal length of leading days is obtained by examining the
154 highest linear correlation of regionally averaged ROMS-hindcast SOC and SOCalt following Eq. (9) and is calculated as 19
155 days (Figure A2a). The exponential term in Eq. (9) estimates the temperature-dependent decomposition rate of organic matter.
156 A significant correlation coefficient between daily SOCalt and ROMS-hindcast SOC is found as 0.8157 ($p < 0.001$, Figure A2).

157

158
$$SOCalt = \text{Mississippi River inorganic nitrogen loads (led by 19 days)} \cdot e^{0.0693T_b},$$
 (9)



159

160 where T_b indicates bottom water temperature (in °C). Along with SOCalt, the temperature-dependent decomposition rate
 161 $e^{0.0693 \cdot T_b}$ is also considered as a candidate predictor in statistical models and is denoted as DCP_{Temp} for simplification.

162 2.1.3 HA estimation

163 As listed in Table 1, there are six candidate predictors considered in the statistical models including four stratification-related
 164 variables (PEA, SSS, (Qh), and W^3) and two bottom biochemical variables (SOCalt and $e^{0.0693 \cdot T_b}$). For simplification, we
 165 denoted this variable as (Qh), W^3 , and $e^{0.0693 \cdot T_b}$ as PEA_{heat}, PEA_{wind}, and DCP_{Temp}, respectively. Correlation coefficients
 166 matrix (Figure 1a) indicates that multicollinearity may become a problem in regression models since linear correlations among
 167 some predictors are significantly high, e.g., 0.76 ($p < 0.001$) between PEA and SOCalt, and -0.88 ($p < 0.001$) between PEA and
 168 SSS. The frequency distribution of HA (Figure 1b) illustrates that the response variable is highly right-skewed with ~51 % of
 169 samples (2,506 out of 4,968) being exactly zero. The HA is estimated by the number of hypoxia cells times a constant value
 170 (area of the computational cell). Thus, the HA can be estimated by the number of grid cells when the Poisson and negative
 171 binomial regression models are applied. However, the great portion of zero samples leads to overdispersion (magnitude of
 172 variance \gg magnitude of mean, i.e., 52,161,613 \gg 4,378) and zero-inflated problems (Lambert, 1992). The overdispersion
 173 issue violates the mean-variance equality assumption employed in regular Poisson regression models, while zero-inflated
 174 problems can weaken the model performances.

175 **Table 1. Description of daily response variable and candidate predictors. The data cover a time range from 1 January 2007 to 26**
 176 **August 2020. Prescribed min and max are used for min–max normalization.**

Variables [units]	Description	Min	Median	Mean	Max	Prescribed (Min:Max)
HA [km ²]	Area of extremely low dissolved oxygen concentration (< 2 mg L ⁻¹)	0	0	4,378	40,561	Non-normalized
PEA [J m ⁻³]	Potential energy anomaly measuring the water stratification	3.1	36.9	49.2	190.4	(0:200)
SSS [non-dim]	Sea surface salinity	20.7	31.8	31.4	34.4	(0:40)
PEA _{heat} [W m ⁻³]	=Qh, an approximation of surface heat-induced water stratification	-1,472.9	3,986.3	3,717.2	6,829.7	(-2,000:7,000)



PEA _{wind} [m ³ s ⁻³]	=W ³ , an approximation of water stratification changes due to wind mixing	0.8	175.1	305.4	6,415.8	(0:6,500)
SOC _{alt} [mmol m ⁻³ s ⁻¹]	An alternative term for sediment oxygen consumption.	874,870	10,103,864	12,604,970	41,530,153	(800,000:42,000,000)
DCP _{Temp} [non-dim]	= e ^{0.0693·T_b} , temperature-dependent decomposition rate of organic matter	2.6	5.1	5.2	8.0	(0:10)

177

178 2.2 Data pre-processes

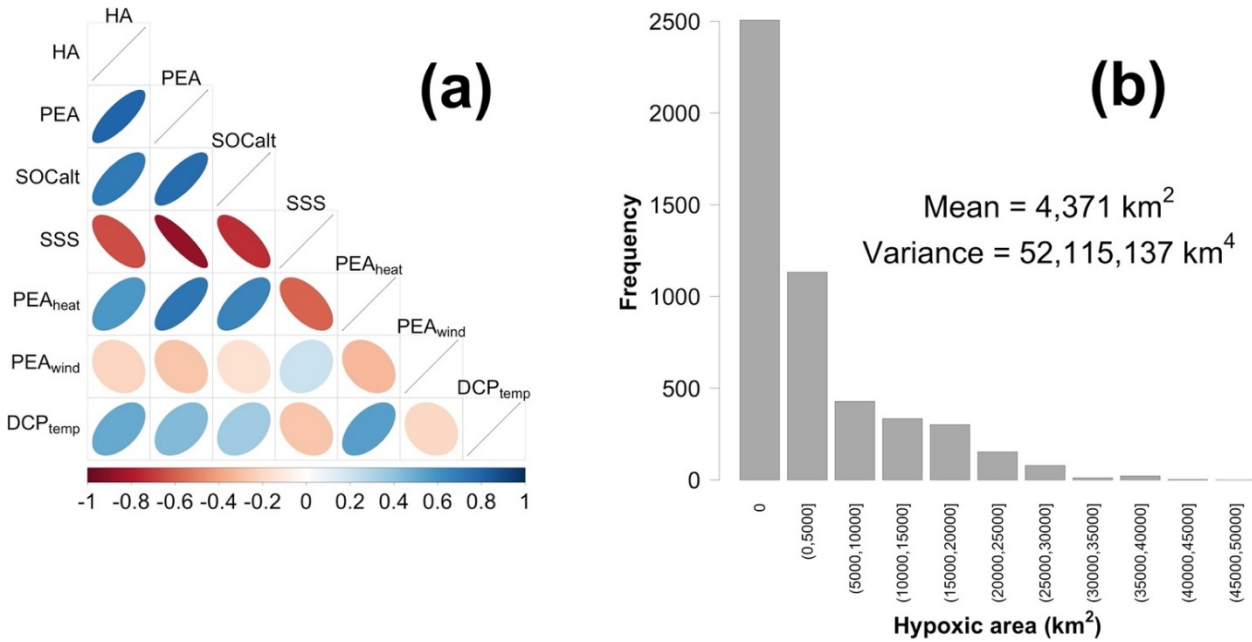
179 We applied the spatially averaged daily ROMS-derived predictors over the LaTex Shelf, then applied the min–max
 180 normalization (Eq. (10)) to the one-dimensional time series. Predictive models can be beneficial from the min–max
 181 normalization when applying to a new dataset since the method guarantees that the normalized predictors from different
 182 datasets range from 0 to 1 as the minimum and maximum values are prescribed. Note that the response is not normalized.

183

$$184 X_{nor} = \frac{X_{org} - Min_{prescribed}}{(Max_{prescribed} - Min_{prescribed})}, \quad (10)$$

185

186 where X_{nor} , X_{org} , $Min_{prescribed}$, and $Max_{prescribed}$ represent normalized value, original value, prescribed minimum, and
 187 prescribed maximum, respectively. The daily samples are then split into a training set (for model construction) accounting for
 188 80 % of the total samples and a test set (for assessment of model performances) accounting for the rest 20 %. To maintain the
 189 HA distribution in both sets, a random resampling method is applied in different HA intervals individually. For example, 80
 190 % of samples with HA=0 is chosen randomly for the training set out of all daily samples with HA=0, while the rest of samples
 191 with HA=0 is grouped into the test set. The HA=0 is the first interval to which the resampling process is applied, while the rest
 192 of samples are split every 5,000 km². However, the distribution of HA from each year is similar with a right-skewed structure
 193 and numerous zero values. Thus, even though through random processes, both the training and test sets contain samples from
 194 each year including samples with non-peak and peak HA. Samples shown in Figure 4 are listed sequentially in the time
 195 dimension from 2007 to 2020 but are not equally distributed along time, which means that the listed samples should not be
 196 regarded as time series. This splitting method increases the model applicability and provides a comprehensive assessment of
 197 prediction performances on both non-peak and peak HA.



198

199 **Figure 1. (a) Correlation coefficient matrix of the response variable and candidate predictors, and (b) frequency distribution of HA.**

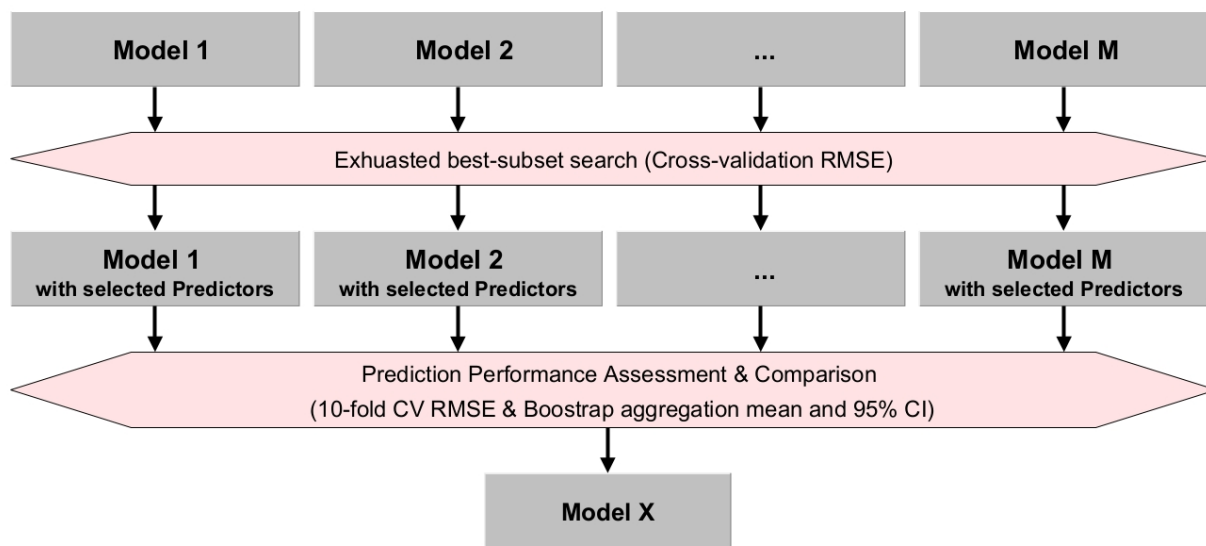
200 3 Model construction

201 3.1 Model built-up process

202 Several regression models are explored using the statistical programming language R. To find the “best” model balancing both
 203 model interpretability and prediction performance, a procedure is conducted for model selection (Figure 2) and is summarized
 204 below. (1) Choose a regression model. (2) Apply an exhaustive best-subset searching approach to the chosen model. Models
 205 with possible combinations of candidate predictors from the ROMS training set are built. A 10-fold cross-validation (CV)
 206 method is applied to each model yielding 10 root-mean-square errors (RMSEs) and 1 corresponding mean. The candidate
 207 predictors of PEA and SOCal are forced into each subset. Thus, the number of fitted models with a subset size of k is
 208 $C(6 - 2, k - 2) = \frac{4!}{(6-k)!(k-2)!}$, $2 \leq k \leq 6$ (the total number of candidate predictors is 6). The optimal subset of this size is
 209 found as the one with the lowest mean CV RMSE among these models. The best subset is then obtained by comparing mean
 210 CV RMSEs of the optimal subsets of different sizes. (3) Steps (1)–(2) are repeated for the selected M candidate regression
 211 models. (4) Prediction performances of different models with the corresponding best subsets are assessed by the 10-fold CV
 212 RMSEs and Bootstrap (1,000 iterations) aggregating (i.e., Bagging) ensemble algorithms. The Bagging method builds the
 213 given model N ($=1,000$) times during each of which the given model is trained using different samples chosen randomly and
 214 repeatedly from the ROMS training set and is executed for HA prediction using samples in the ROMS test set. The ensemble
 215 means and ensemble 95 % prediction intervals (PIs) of forecast HA are given according to the prediction results in the 1,000



216 iterations. The best model (Model X in Figure 2) is chosen according to the comparisons of the 10-fold CV RMSEs and the
217 Bagging results.



218
219 **Figure 2. A flow chart of building up regression models.**

220

221 **3.2 Generalized linear models (GLMs)**

222 **3.2.1 Regular GLMs and zero-inflated GLMs**

223 The response variable can be treated as count data. Regular Poisson (function `glm` in R package “stats” version 3.6.2), quasi-
224 Poisson (function `glm` in R package “stats” version 3.6.2), and negative binomial (function `glm.nb` in R package “MASS”
225 version 7.3-54; Venables and Ripley, 2002) GLMs are explored in this section. The latter two GLMs are known for solving
226 overdispersion problems by relaxing the mean-variance equality assumption. These GLMs make use of a natural log link
227 function. Thus, a natural logarithm of the area of a single ROMS cell ($\sim 25.56 \text{ km}^2$) is added to the models as an offset term
228 (an additional intercept term).

229

230 In addition, the overdispersion issue can result from the great percentage ($\sim 51 \%$) of zero values in the response variable
231 (Figure 1b). Zero-inflated GLMs (using function `zeroinfl` in R package “pscl” version 1.5.5; Jackman, 2020; Zeileis et al.,
232 2008) are developed for dealing with response variables of this kind. Rather than resetting dispersion parameters, a zero-
233 inflated count model is a two-component mixture model blending a count model and a zero-excess model. The count model is
234 usually a Poisson or negative binomial GLM (with log link), while the zero-excess model is a binomial GLM (with logit link
235 in this study) estimating the probability of zero inflation. An offset term of $\log(25.56)$ is also introduced into the count model.
236 Instead of applying the best-subset searching to the count and zero-excess models simultaneously, in this study, the searching



237 is conducted respectively for these two models to reduce demands of computational resources. The best subset of the zero-
238 excess model (binomial GLM) is given first. The best subset of the count model (Poisson or negative binomial GLMs) is then
239 provided blending the zero-excess model with the corresponding selected best subset fixed.

240

241 However, it is hard to determine whether a given zero value of HA is excessive, instead, it is relatively easy to model hypoxia
242 occurrence assuming that all the zero values are excessive. A new binary response, hypoxia, stated in Eq. (11) is introduced
243 for modeled hypoxia occurrence using regular binomial GLMs (function `glm` in R package “stats” version 3.6.2). The hypoxia
244 is equal to 0 when HA is 0 (no hypoxia), otherwise, is equal to 1. The optimal model selected three predictors: PEA, SOCalt,
245 and DCP_{Temp} (Figure 3b).

246

$$247 \text{ hypoxia} = \begin{cases} 0, & \text{no hypoxia} \\ 1, & \text{hypoxia occurs} \end{cases}, \quad (11)$$

248

249 3.2.2 Performance of GLMs

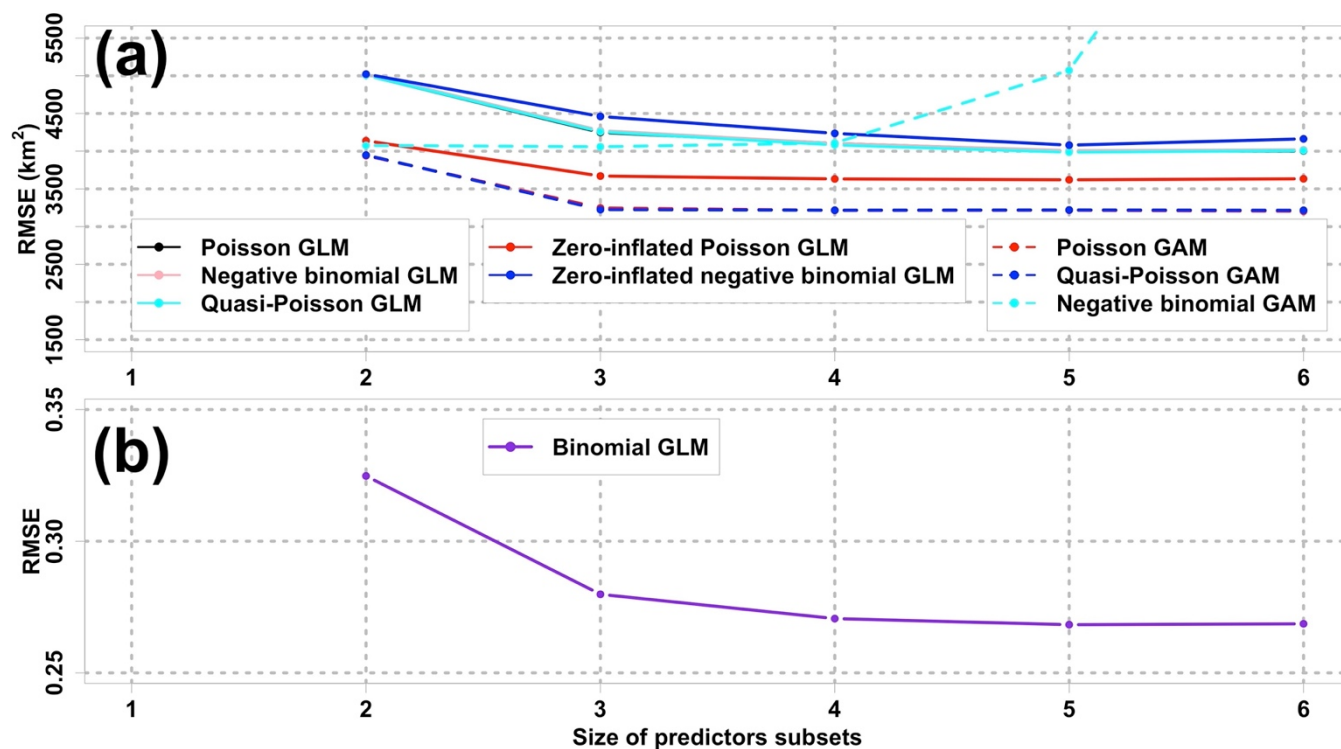
250 The zero-inflated Poisson GLM serves as the best GLM in terms of prediction performances since it has the lowest mean CV
251 RMSE (Figure 3a) among the five candidate GLMs. The relaxation of the mean-variance equality assumption by the negative
252 binomial GLM and the quasi-Poisson GLM does not guarantee salient improvement of performances when comparing their
253 CV RMSEs to those of regular Poisson GLM. The zero-inflated negative binomial GLM yields poorest performance with the
254 largest mean CV RMSE. The mean CV RMSEs of zero-inflated Poisson GLM hit the trough (3,621 km²) at the size of five.
255 However, the greatest drop of RMSEs (3,671 km²) occurs at the size of three beyond which the RMSEs remain stable. It is
256 worth considering a model with fewer predictors satisfying model interpretability. Thus, the best zero-inflated Poisson GLM
257 accounts for three predictors (PEA, SOCalt, and DCP_{Temp}) in the count model and three predictors (PEA, SOCalt, and DCP_{Temp})
258 in the zero-excess model. As indicated in the correlation matrix (Figure 1a), the robustness of a model can be impaired by
259 multicollinearity which can be estimated by variance inflation factors (VIFs). VIFs among the selected predictors are 2.60,
260 2.43, and 1.23 for PEA, SOCalt, and DCP_{Temp}, respectively. The VIFs are all less than 5 suggesting that predictors subsets
261 involved in both the count and the zero-excess models are merely violated by multicollinearity. For simplicity, the best zero-
262 inflated Poisson GLM is symbolized as GLMzip3.

263

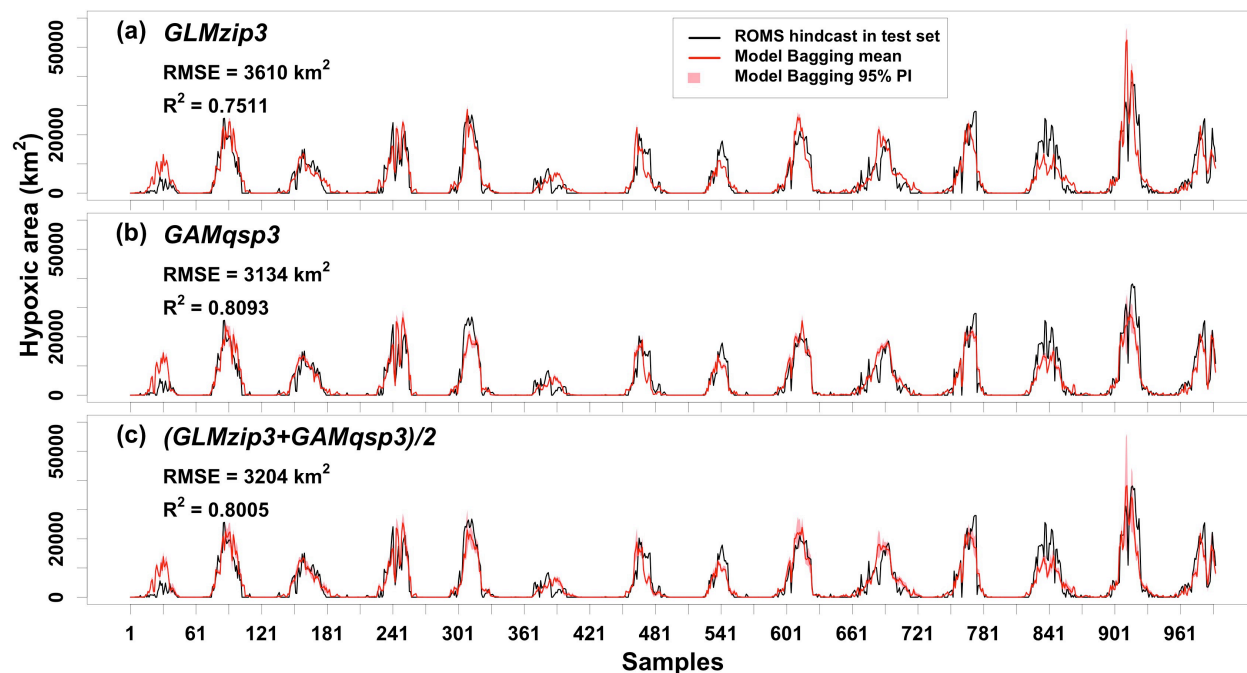
264 The Bagging ensemble method is implemented to estimate the prediction performance of GLMzip3 (Figure 4a). The Bagging
265 means of predicted HA provides an RMSE of 3,610 km² and an R² of 0.7511 against the ROMS hindcasts. The Bagging 95 %
266 PIs of the predicted values are restricted within a narrow range with a slight increase at the predicted peaks. We want to address
267 that the comparisons are not between the time series. The training set and test set are resampled according to different HA
268 intervals, while the distributions of HA in each year are similar. Thus, HA in both the training set and test set contains



269 observations of peak and non-peak values in each year. The results suggest that GLMzip3 is capable of providing not only
 270 accurate but also stable HA forecasts. Nevertheless, we noted salient overestimations (e.g., around the 30th and 920th samples)
 271 and underestimations (e.g., around the 540th and 830th samples) at some peaks. Instead of the prediction performance at non-
 272 peak HA, here we are more focused on forecasts at HA peaks which impose more threatens to the shelf ecosystem. In section
 273 3.3, GAMs are investigated with an expectation of further improvements in peak predictions by considering non-parametric
 274 or non-linear effects of the predictors.



275
 276 **Figure 3.** Comparisons of mean 10-fold CV RMSEs among different regression models with various sizes of predictors subsets. The
 277 response variable in (b) binomial GLM and (a) other models is hypoxia occurrence (hypoxia) and hypoxic area (HA), respectively.
 278 Note that the CV RMSE of negative binomial GAM with the size of six is out of the range shown. CV RMSE curves of the Poisson
 279 GLM, negative binomial GLM, and quasi-Poisson GLM overlap, while those of Poisson GAM and quasi-Poisson GAM overlap. The
 280 minimum size of predictor subsets is two since PEA and SOCalt are forced into every subset.



281
 282 **Figure 4. Comparisons of model predicted HA and ROMS-hindcast HA in the test set. RMSEs and R²s are derived between model**
 283 **Bagging mean and ROMS-hindcast HA.**

284 3.2.3 Model interpretation for GLMzip3

285 We applied the complete ROMS training set to the model construction of GLMzip3 and found the coefficients for PEA,
 286 SOC_{alt}, and DCP_{Temp} (Table 2) are all significantly positive ($p < 0.001$) in the count model, while coefficients for these
 287 predictors are significantly negative ($p < 0.001$) in the zero-excess model. The count model simulates the HA while the zero-
 288 excess model estimates the probability of HA being zero. Higher PEA is consistent with stronger water stratification, while
 289 higher SOC_{alt} and DCP_{Temp} are both corresponding to higher sediment oxygen consumption. Therefore, there is no surprise
 290 that higher PEA, SOC_{alt}, and DCO_{Temp} are related to greater HA and higher hypoxia occurrence or lower probability of HA
 291 being zero. Results indicate that the GLMzip3 essentially builds up reasonable relationships between the response and
 292 predictor variables with a high agreement with physical and biochemical mechanisms.

293 **Table 2. Regression coefficients of GLMzip3.**

Count model coefficients (Poisson with log link):					Zero-excess model coefficients (binomial with logit link):				
	Estimate	Std. Error	z value	Pr (> z)		Estimate	Std. Error	z value	Pr (> z)
Intercept	1.9897	0.0021	948.2	<2E-16***	Intercept	9.1993	0.3181	28.9	<2E-16***
PEA	2.6763	0.0016	1681.4	<2E-16***	PEA	-10.0945	0.5986	-16.9	<2E-16***
SOC _{alt}	0.9228	0.0014	663.6	<2E-16***	SOC _{alt}	-8.7784	0.5508	-15.9	<2E-16***
DCP _{Temp}	3.5940	0.0031	1168.2	<2E-16***	DCP _{Temp}	-9.4939	0.4346	-21.9	<2E-16***



Significance codes: 0 (***) 0.001 (**) 0.01 (*)

Log-likelihood: -2.4E6 on 8 degrees of freedom

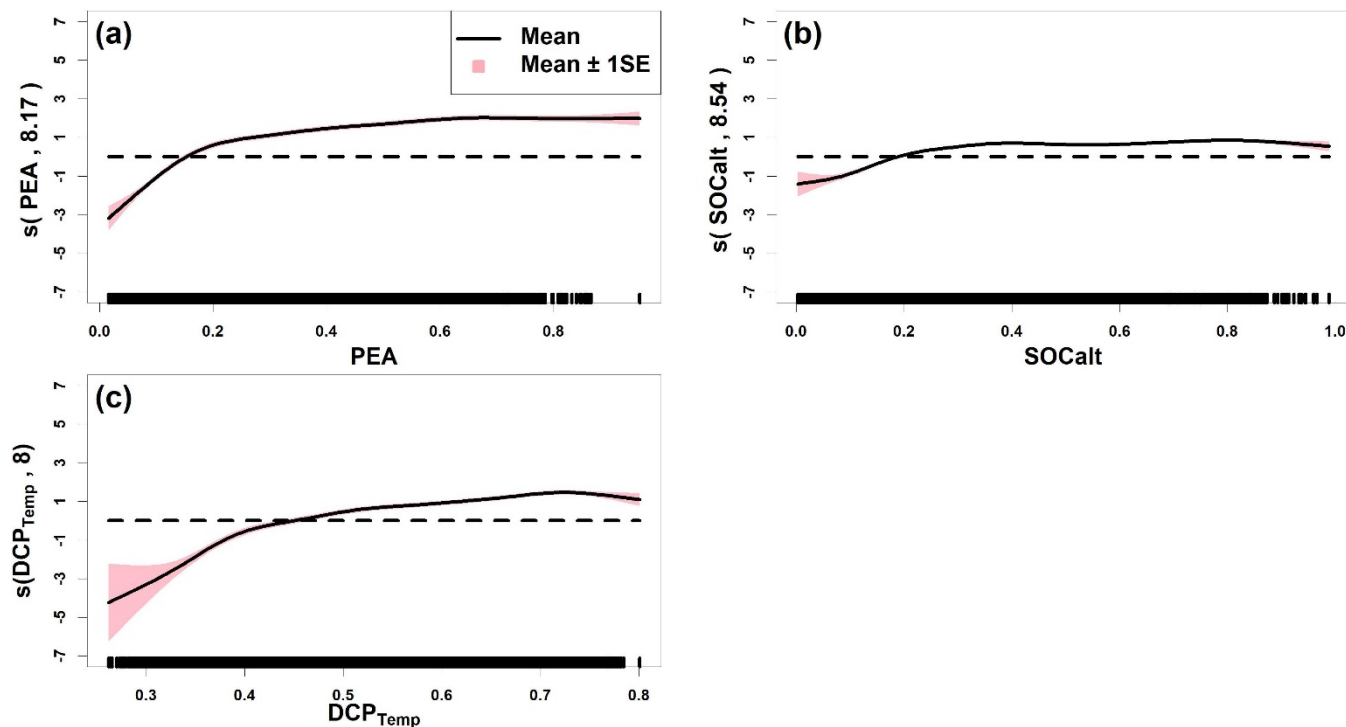
294

295 3.3 Generalized additive models (GAMs)

296 GAMs are explored with an expectation of improving prediction performance in HA peaks by introducing non-parametric
297 effects of predictors. Using function "gam" in R package "mgcv" (version 1.8-36; Wood, 2011) with smooth functions as pure
298 thin plate regression splines (degree of freedom=9; Wood, 2003), three GAMs are studied and compared, i.e., Poisson GAM,
299 quasi-Poisson GAM, and negative binomial GAM. Following the same procedure in GLM exploration, the best subset
300 searching approach is applied to the GAMs first. The mean 10-fold CV RMSEs for the Poisson and quasi-Poisson GAMs
301 (Figure 3a) exhibit insignificant differences and are the lowest among those for all GLMs and GAMs studied. Although the
302 mean CV RMSEs for these two types of GAMs both reach the lowest at the size of five, the best size is considered as three
303 (considering PEA, SOC_{alt}, and DCP_{Temp}) at which CV RMSEs exhibits most saline decline, and beyond which mean CV
304 RMSEs stabilize around 3,200 km². The negative binomial GAM has the greatest mean CV RMSEs among the GAMs studied
305 and has an extremely high mean CV RMSE at the size of six. It is, therefore, dropped out of the list of candidate models. The
306 quasi-Poisson GAM with three predictors involved (symbolized as GAM_{qsp3}) is chosen as the best GAM since it relaxes the
307 mean-variance equality assumption which should not be applied to the HA dataset due to the overdispersion issue.

308

309 Component plots of model GAM_{qsp3} (Figure 5) imply that HA generally increases as the chosen predictors increase. The
310 smooth functions of PEA and DCP_{Temp} are considerably greater than the smooth function of SOC_{alt} indicating that the
311 contributions of the former two predictors are greater than the effect of SOC_{alt} on the daily variability of HA. Note that the
312 fitted HA equals the summation of all smooth function terms. Such results agree with those found by model GLM_{zip3}.
313 However, the component plots provide more detailed information about the rate of changes of HA. The effective degrees of
314 freedom range from 8 to 8.54 indicating strong non-linear effects of the predictors on the changes of HA. The HA is more
315 sensitive to the predictors in the low-value ranges but becomes nearly stable in the medium- and high-value ranges of
316 predictors. It implies that bottom hypoxia develops rapidly in early summer when water stratification and sediment oxygen
317 demand start to increase. The bottom hypoxic water further extends with a much lower expansion speed as the stratification
318 and SOC further intensify. Nevertheless, the smooth function of PEA is slightly greater also with a more acute slope than those
319 found for SOC_{alt} and DCP_{Temp} in the medium- and high-value regimes of the predictors. It indicates that the HA variability is
320 more related to the hydrodynamic changes in the shelf than the biochemical effects. The result is consistent with the findings
321 by previous studies of the shelf hypoxia (Yu et al., 2015; Mattern et al., 2013) emphasizing that the physical impacts are
322 stronger than the biological impacts on HA estimates. A short conclusion is made that the GAM_{qsp3} model provides reasonable
323 interpretations on the hypoxic area mechanisms.



324

325 **Figure 5. Component plots of model GAMqsp3. Solid black lines represent the mean of the smooth function, while the pink area**
326 **denotes the range of mean \pm 1SE. Numbers in brackets represent effective degrees of freedom for the corresponding smooth terms.**
327 **Black bars at the x axis indicate the density of corresponding predictors. Dashed black lines are straight lines of zero along the**
328 **predictor domains. Note that the predictors shown have been normalized.**

329 The prediction performance of GAMqsp3 is estimated using the Bagging ensemble method (Figure 4b). The RMSE and R^2
330 between the Bagging mean and ROMS-hindcast HA is 3,134 km² and 0.8093, respectively. They are 13 % lower and 8 %
331 higher than the corresponding statistics found for the GLMzip3, respectively, suggesting that GAMqsp3 outcompetes
332 GLMzip3 in terms of overall performance. However, GAMqsp3 tends to produce underestimated predictions at HA peaks
333 (like peaks around the 310th and 920th samples) some of which are overestimated by the GLMzip3. Therefore, instead of
334 determining the best model out of the two, ensemble HA predictions blending efforts of both GLMzip3 and GAMqsp3 are
335 carried out with an expectation to improve model performance in the peak forecast. We assumed that the contributions of
336 GLMzip3 and GAMqsp3 are equally weighted since there is no clue showing the apparent superiority of either model in HA
337 peak predictions. We thus averaged the predicted HA by GLMzip3 and GAMqsp3 and calculated the 95 % PIs given the
338 Bagging results of these models (Figure 4c). As expected, the overall performance of the ensemble forecast is somewhere
339 between the performance of GLMzip3 and GAMqsp3 with an RMSE of 3,204 km² and an R^2 of 0.8005. However, some HA
340 peak events (like peaks around the 310th and 920th samples) which are overestimated by GLMzip3 but are underestimated by
341 GAMqsp3 are accurately predicted by the ensemble approach. The ensemble model provides higher accuracy in peak forecast
342 given minor sacrifices in overall performance.



343 4 Discussion

344 A promising HA forecast is provided by the ensemble model with a low RMSE (3,204 km²), a high R² (0.8005), and a precise
345 performance in capturing hypoxic area peaks in the summers. The power of the prediction model relies on the availability of
346 the forecast of predictors. In this section, we discuss the model's transferability using an independent global ocean product.

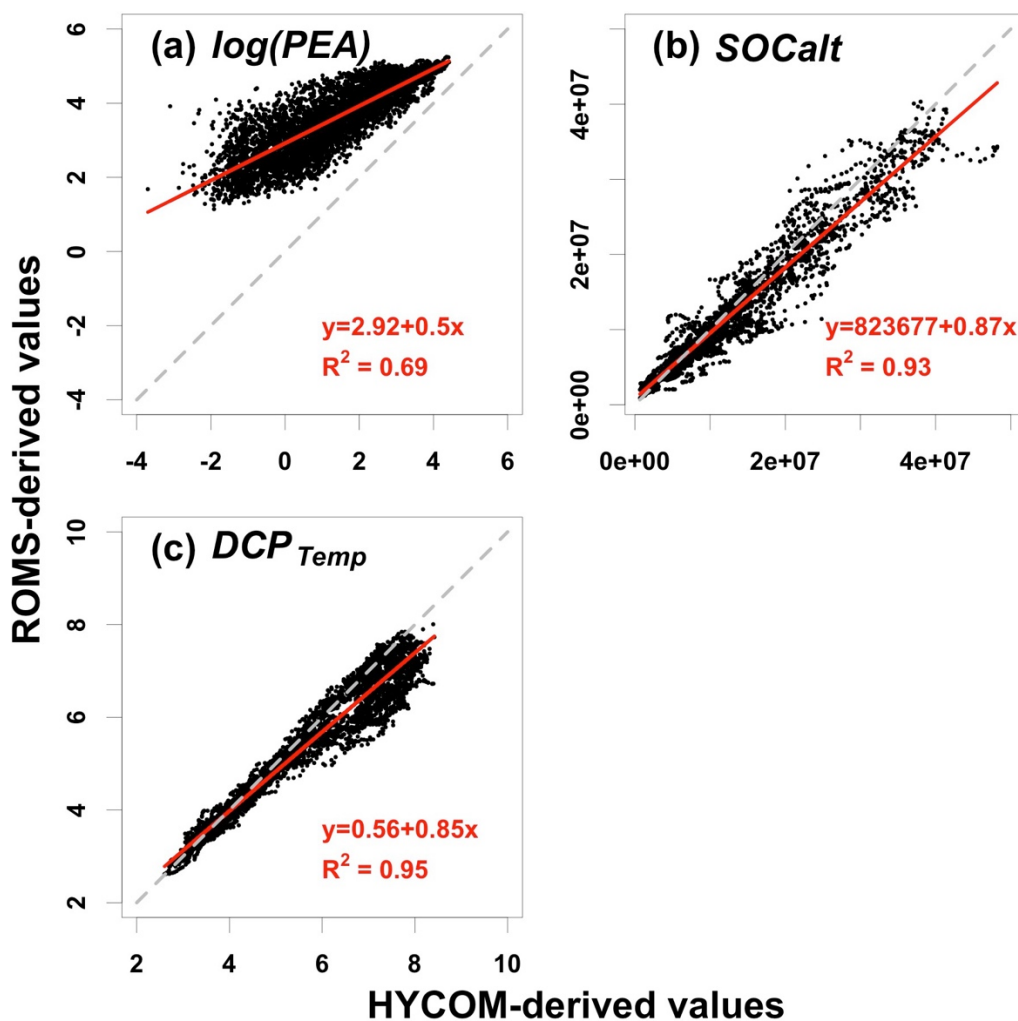
347
348 The Global Ocean Forecasting System (GOFS) 3.1 provides global daily analysis products and an eight-day forecast in a daily
349 interval with a horizontal resolution of 1/12 °. The products (hereafter referred to HYCOM-derived products) are derived by a
350 41-layer HYCOM global model with data assimilated via the Navy Coupled Ocean Data Assimilation (NCODA) system
351 (Cummings, 2005; Cummings and Smedstad, 2013). Daily data from 1 January 2007 to 26 August 2020 are retrieved and
352 studied. Predictors of PEA, SOCalt, and DCP_{Temp} are reconstructed using HYCOM-derived variables and Mississippi River
353 daily total nitrate and nitrite loadings downloaded from the USGS NWIS. Relationships of ROMS-derived and HYCOM-
354 derived predictors are examined in Figure 6. The magnitudes of HYCOM-derived SOCalt and DCP_{Temp} match up with the
355 corresponding ROMS-derived predictors, respectively, although HYCOM-derived predictors are found slightly greater.
356 Simple linear regression for these predictors illustrates that the linear relationships between the ROMS and HYCOM products
357 are significant with the R² ranging from 0.93 to 0.95. The intercept terms are at least one-order smaller than the magnitudes of
358 corresponding predictors. Therefore, the HYCOM global products are deemed to agree with the ROMS hindcasts for SOCalt
359 and DCP_{Temp}. Nevertheless, the magnitude of HYCOM-derived PEA is found much lower than the ROMS-derived PEA
360 (Figure 6a). Simple linear regression indicates a significant linear relationship between the natural log transformation of PEA
361 from the two datasets (R²=0.69).

362
363 At land-sea interfaces, the HYCOM global model is forced by monthly riverine discharges, which weakens the model
364 performance in coastal regions. The hydrodynamics in the LaTex Shelf is highly affected by the freshwater and momentum
365 from the Mississippi and the Atchafalaya Rivers. Monthly river forcings in HYCOM are essentially weaker than daily forcings
366 used in our ROMS set up and can result in a less stratified water column (i.e., lower PEA). Therefore, it is necessary to scale
367 the magnitude of HYCOM-derived PEA to that of the ROMS hindcast. It can be achieved by using the natural log
368 transformation and simple linear regression as discussed. We then adjusted HYCOM-derived PEA but kept the HYCOM-
369 derived SOCalt and DCP_{Temp} unchanged before the application of the ensemble model.

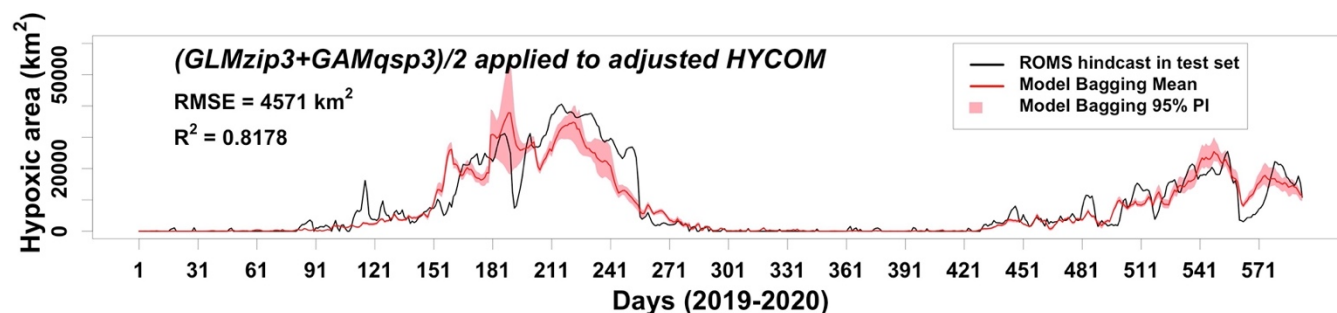
370
371 The Bagging approach is implemented again to assess the performances of the ensemble model. During each iteration
372 (N=1,000), the GLMzip3 and GAMqsp3 are trained using the ROMS training set and then applied to the adjusted HYCOM-
373 derived predictors for HA prediction from 1 January 2019 to 26 August 2020. The ensemble method provides averages and 95
374 % PIs of predicted HA blending Bagging results by GLMzip3 and GAMqsp3. Compared to the ROMS-hindcast HA, the
375 ensemble model performs an overall accurate HA forecast with an RMSE and an R² of 4,571 km² and 0.8178, respectively



376 (Figure 7). The HA peaks in both 2019 and 2020 summers are well captured by the model with slight underestimates at the
377 first peak and slight overestimates at the second. The width of 95 % PI is larger during high HA periods suggesting less stability
378 in the HA peak forecast. Discharges measurements for the Mississippi and the Atchafalaya Rivers are provided and updated
379 daily by USGS NWIS, assuring a possible improvement of HYCOM model performance in the LaTex Shelf. Once the
380 performance of hydrodynamics predictions in the LaTex Shelf is guaranteed, predictions performance of the ensemble model
381 on HA would be further improved.



382
383 Figure 6. Scatter plots of (a) $\log(PEA)$ (unit: $\log(\text{J m}^{-3})$), (b) $SOCal_t$ (unit: $\text{mmol m}^{-3} \text{s}^{-1}$), and (c) DCP_{Temp} (unit: 1) between
384 ROMS and HYCOM simulations. Note that the solid red lines represent linear regression lines, while the dashed grey lines are
385 diagonals with a slope of 1 and an intercept of 0. Daily data compared are from 2007 to 2020.



386

387 **Figure 7. Daily time series of predicted HA by ensemble model ((GLMzip3+GAMqsp3)/2) when applied to adjusted HYCOM**
388 **products and ROMS-hindcast HA from 2019 to 2020.**

389 5 Conclusion

390 In this study, an ensemble HA forecast model for the LaTex Shelf is developed using the state-of-the-art statistic programming
391 language R. The model is trained using numeric simulations from 1 January 2007 to 26 August 2020 generated by a coupled
392 hydrodynamic–biogeochemical model. Before splitting data into a training set and a test set, we applied regional average over
393 the LaTex Shelf and min-max normalization to the hindcast data.

394

395 Multiple GLMs (regular Poisson GLMs, quasi-Poisson GLMs, negative binomial GLMs, zero-inflated Poisson GLMs, and
396 zero-inflated negative binomial GLMs) and GAMs (regular Poisson GAMs, quasi-Poisson GAMs, and regular negative
397 binomial GAMs) are assessed for HA prediction. Comparisons of model prediction performance illustrate that an ensemble
398 model combing the prediction efforts of a zero-inflated Poisson GLM and a quasi-Poisson GAM provides the most accurate
399 HA forecast with a variability explanation high up to 80 %, a low overall RMSE of 3,204 km², and a high precision in
400 forecasting peak HA when compared to the hindcasts by the coupled model. Predictors PEA, SOCal_t, and DCP_{Temp} are involved
401 in the GLM and GAM. Statistically significant coefficients for the predictors (for the GLMzip3) and component plots (for the
402 GAMqsp3) agree well with the physical and biochemical mechanisms.

403

404 The ensemble model is then migrated to the GOFS 3.1 products based on HYCOM,s which provides eight-day forecast of
405 global hydrodynamics. The ensemble model is trained using the ROMS training set and then is used for the HA prediction
406 covering the period from January 1st, 2019 to August 26th, 2020. The prediction is robust when compared to the ROMS
407 simulations (2019–2020), with a low overall RMSE (4,571 km²) and a high R² (0.8178). The model can also accurately predict
408 the magnitude and onset of summer HA peaks in 2019 and 2020, respectively. To our best knowledge, this ensemble model is
409 the first model providing efficient yet accurate daily HA forecast for the LaTex Shelf while considering both hydrodynamic
410 and biochemical effects. This model is also the first model successfully applying global hydrodynamic forecast in regional HA
411 predictions.

412



413 **Author contribution:** Bin Li and Z. George Xue designed the experiments and Yanda Ou carried them out. Yanda Ou
414 developed the model code and performed the simulations. Yanda Ou, Bin Li, and Z. George Xue prepared the manuscript.

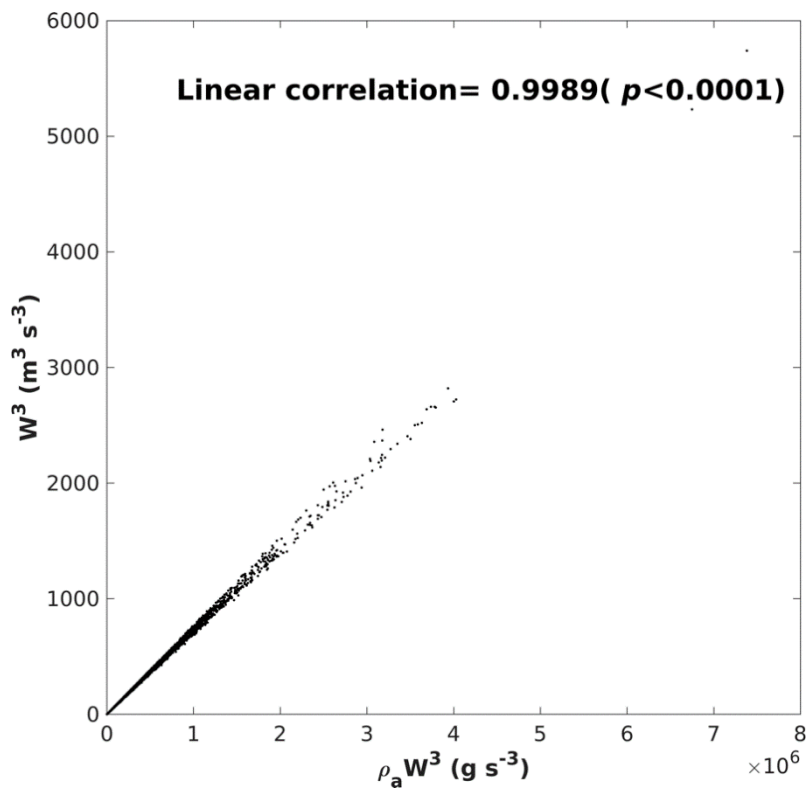
415
416 **Competing interests:** The authors declare that they have no conflict of interest.

417
418 **Acknowledgment:** Research support was provided through the Bureau of Ocean Energy Management (M17AC00019,
419 M20AC10001). We thank Dr. Jerome Fiechter at UC Santa Cruz for sharing his NEMURO model codes. Computational
420 support was provided by the High-Performance Computing Facility (clusters SuperMIC and QueenBee3) at Louisiana State
421 University.

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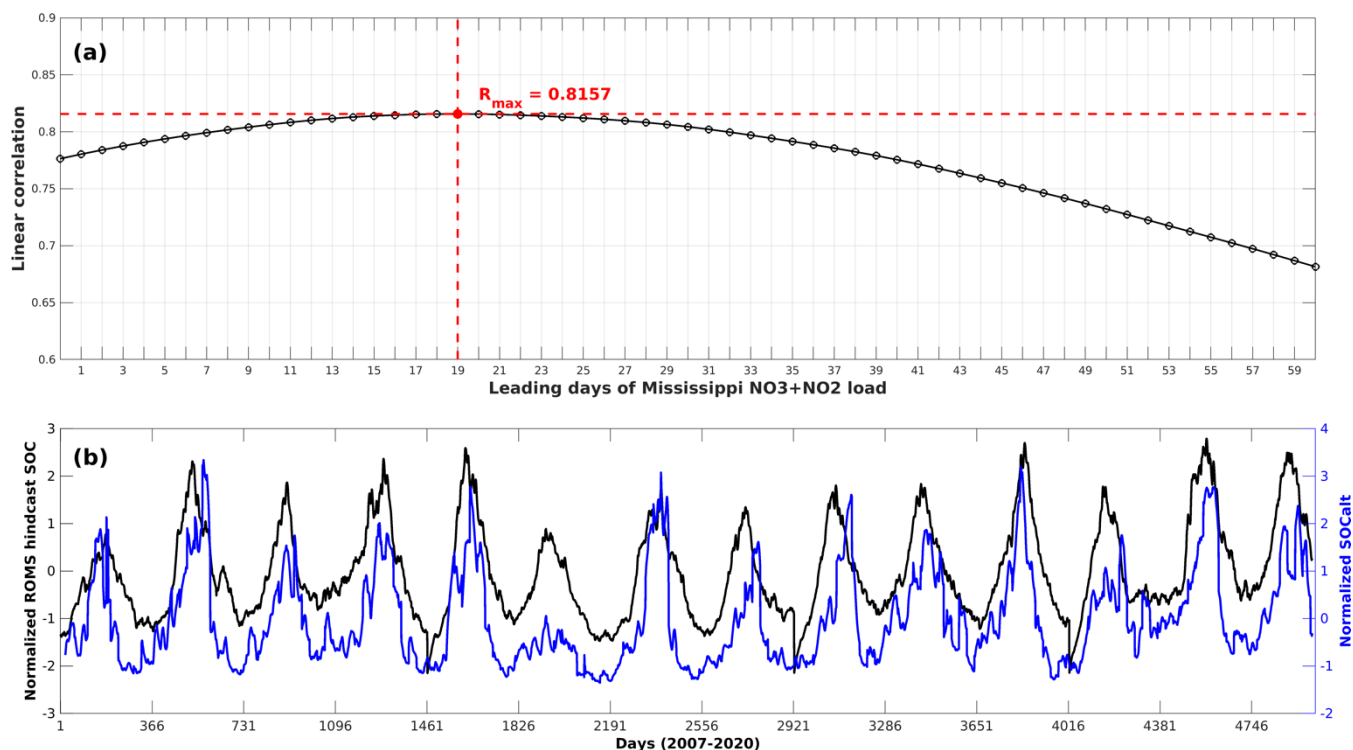


424 **Appendix A:**



425

426 **Figure A1. A scatter plot of $\rho_a W^3$ and W^3 and their linear correlation.**



427

428 **Figure A2. (a) Lead/lag correlation coefficients between ROMS hindcast daily SOC and SOCalt (=**
429 **Mississippi River inorganic nitrogen loads $\cdot e^{0.0693T_b}$) with the Mississippi nitrogen loads led by different days; (b) daily time**
430 **series of ROMS hindcast SOC and SOCalt when the Mississippi nitrogen loads led by 19 days. Time series of compared is averaged**
431 **over the LaTex Shelf and is normalized.**

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