RESEARCH ARTICLE

Predicting dissolved oxygen in the Chesapeake Bay: applications and implications

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Abstract Eutrophic depletion of dissolved oxygen (DO) and its consequences for ecosystem dynamics have been a central theme of research, assessment and management policies for several decades in the Chesapeake Bay. Ongoing forecast efforts predict the extent of the summer hypoxic/anoxic area due to nutrient loads from the watershed. However, these models neither predict DO levels nor address the intricate interactions among various ecological processes. The prediction of spatially explicit DO levels in the Chesapeake Bay can eventually lead to a reliable depiction of the comprehensive ecological structure and functioning, and can also allow the quantification of the role of nutrient reduction strategies in water quality management. In this paper, we describe a three dimensional empirical model to predict DO levels in the Chesapeake Bay as a function of water temperature, salinity and dissolved nutrient concentrations (TDN and TDP). The residual analysis shows that predicted DO values compare well with observations. Nash–Sutcliffe efficiency (NSE) and root mean square error-observations standard deviation ratio (RSR) are used to evaluate the performance of the empirical model; the scores demonstrate the usability of model predictions (NSE, surface layer = 0.82–0.86; middle layer = 0.65–0.82; bottom layer = 0.70–0.82; RSR surface layer = 0.37–0.44; middle layer = 0.43–0.58 and bottom layer = 0.43–0.54). The predicted DO values and other physical outputs from downscaling of regional weather and climate predictions, or forecasts from hydrodynamic models, can be used to forecast various ecological components. Such forecasts would be useful for both recreational and commercial users of the Chesapeake Bay.

Keywords Dissolved oxygen · Dissolved nutrients · Multi-regression equation · Long-term variability · Chesapeake Bay

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Introduction

Depletion of dissolved oxygen (DO) in coastal and marine waters is a widespread phenomenon that appears to be growing globally and impacts the physiology and energetics of coastal ecosystems (Montagna and Froeschke 2009; Rabalais and Gilbert 2009). Nutrient pollution in estuarine and coastal ecosystems adversely affects DO levels by reducing them to critical levels where the structure and function of the biological communities suffer due to falling growth rate and fecundity (Wu et al. 2003; Chai et al. 2006; Bishop et al. 2006; Ripley and Foran 2007; Steyaert et al. 2007; Costantini et al. 2008; Ludsin et al. 2009). In addition to harmful effects on organisms and ecosystems, changes in frequency and intensity of low-oxygen events could also have broader implications for global biogeochemical cycling of nutrients (Henrichs 1992).

The Chesapeake Bay with an area of 64,000 squares miles is the largest, most productive and biologically

diverse estuary in North America (Fig. 1). Episodes of oxygen depletion in the Chesapeake Bay were first reported in the 1930s (Newcombe and Horn 1938) and is primarily due to anthropogenic nutrient discharge from agriculture and urban development within the watershed (Breitburg et al. 2001; Kemp et al. 2005; Kaushal et al. 2008). Since then, the temporal and spatial extent of these events has increased progressively and has become a major environmental concern (Officer et al. 1984). Physical and biological factors contribute to the seasonal reduction in the bottom water DO (e.g. Kemp et al. 1992; Boynton and Kemp 2000). During spring, DO levels are depleted because large volumes of nutrient rich freshwater advection stimulates phytoplankton production, which subsequently sinks from the surface to deeper waters and sustains oxygen-consuming metabolism (e.g. Tuttle et al. 1987; Malone et al. 1988). The depletion of oxygen due to bacterial degradation is further exacerbated due to its co-occurrence with the onset of increased stratification (Batiuk et al. 2009).

The timing and extent of hypoxic/anoxic conditions in Chesapeake Bay vary year to year and prediction is challenging. Seasonal oxygen depletion is persistent in the mesohaline main-stem of the Bay that typically occur from spring to fall (Hagy et al. 2004; Zhang et al. 2006). The large volume of hypoxic water creates unsuitable habitat for pelagic communities (mainly fishes) by affecting the

behavioral response of developing fish embryo, especially those species that live in subpycnocline water for forage, growth and reproduction (Rombough and Randall 1988). Keister et al. (2000) asserted that overall fish and larvae abundance is low when hypoxic volume is high; i.e. low oxygen water is not physiologically favorable for fish metabolism. Furthermore, fishes living in hypoxic waters are highly susceptible to bacterial infections as is evidenced by outbreaks of mycobacteriosis in the Chesapeake Bay striped bass (*Morone saxatilis*) and papillomatosis in North Sea dab (*Limanda limanda*) that may also be related to low DO levels (Mellergaard and Nielsen 1997; Vogelbein et al. 1999). Therefore, ecological prediction of DO is imperative for ecosystem management, especially to understand climate change and anthropogenic impacts on ecosystem metabolism of Chesapeake Bay.

Generally, ecological models have been used by ecosystem managers, scientists and policy makers to investigate interactions among various ecosystem components (e.g. nutrients, dissolved oxygen, salinity, temperature and biological structure) both qualitatively and quantitatively (Cerco and Cole 1993; Cerco 1995; Hagy et al. 2004; Scavia et al. 2006; Stow and Scavia 2009). All these water quality models have been used to guide policy makers to estimate the pollution load targets that are needed to achieve desired improvements in ecosystem quality. The complexity of these models has ranged from statistical models (Hagy et al. 2004; Scavia et al. 2006) to mechanistic ecological simulations (Cerco and Cole 1993; Cerco 1995; Xu and Hood 2006). A wide range of ecological models used in Chesapeake Bay reveals an ongoing discussion among water quality modelers and ecosystem managers regarding the relative efficacy of simple versus complex models; both have their limitations (Borsuk et al. 2001).

The Chesapeake Bay Forecast System (CBFS) is a flexible, end-to-end prediction tool for decision makers to provide customizable, user-specified forecasts from days to seasons and projections for decades into the future (Murtugudde 2009). As a part of CBFS, long-term data of ecological parameters of Chesapeake Bay have been assembled to develop prototype ecological and biogeochemical models for the sustainable management of the Bay (Anderson et al. 2010; Constantin de Magny et al. 2010; Meng et al. 2010; Prasad et al. 2010). Because the Susquehanna River supplies substantial loads of nutrients to Chesapeake Bay, current water quality models being used to study dissolved oxygen dynamics in Chesapeake Bay are primarily based on Susquehanna nutrient loads (Hagy et al. 2004; Scavia et al. 2006). However, other tributaries within the watershed also supply considerable nutrient loads to the Bay that influence phytoplankton dynamics and oxygen variability (Boesch et al. 2007; Prasad et al. 2010). Furthermore, Susquehanna nutrient loads are mainly confined
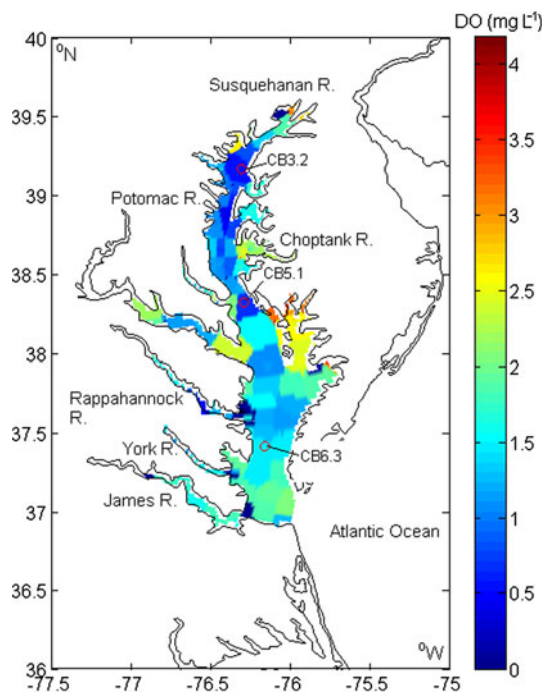
Fig. 1 Bottom water dissolved oxygen concentrations for 2006 summer (average June–September) in Chesapeake Bay. The *red circles* denote stations (CB3.2, CB5.1 and CB6.3) were used for model validations (color figure online)

to within the upper to mid Bay region due to the high residence time, thus they may have little influence over nutrient and phytoplankton dynamics in the lower Bay (Schubel and Pritchard 1986). The present study includes the use of a multi-regression statistical approach to develop a three dimensional oxygen model for prediction of spatially explicit DO levels in Chesapeake Bay by accounting for long-term variability of nutrient concentrations (TDN and TDP), water temperature and salinity across the Bay. Thus, we represent the role of nutrient biogeochemical dynamics and their causative factors on oxygen variability in different zones of Chesapeake Bay. Water temperatures regulate water column nutrient dynamics and sedimentary diagenetic processes that affect biological production (Gudasz et al. 2010). In coastal waters, freshwater discharge from tributaries regulates salinity and stratification, hence salinity is considered as an indirect proxy for freshwater discharge (Buzzelli et al. 2002). This model is thus an intermediate model with a process-based statistical approach; i.e. integration of physical controls on nutrient processes and biological responses to predict DO levels in Chesapeake Bay. With this rather simple model formulation, we can limit the number of parameters to the most critical ones and create functions based on statistical relationship between the expected variable (DO) and control variables (nutrients, temperature and salinity), and apply statistical methods to validate model performance.

Materials and methods

Data collection and analysis

Long-term data (1990–2006) of water temperature, salinity, and dissolved nutrients of Chesapeake Bay were extracted from the US Environmental Protection Agency Chesapeake Bay Program (US EPA–CBP) database from 101 stations across the Bay. Each station was sampled once each month during the colder-late fall and winter months and twice each month in the warmer months. At each station, a hydrographic profile was made and water samples for chemical analysis were collected from the surface, bottom, and (for deeper stations) at two additional mid-water depths, depending on the existence and location of the pycnocline. The collected water samples were analyzed for nutrients using standard analytical protocols.

The collected nutrient parameters are interpolated over the Chesapeake Bay Regional Modeling System (ChesROMS) grid, which is a curvilinear grid system of size 150×100, by the equal weight average method (Anderson et al. 2010; Constantin de Magny et al. 2010; Prasad et al. 2010). We used the gridded data to build the empirical model to predict DO in Chesapeake Bay.

Inter-annual variability and secular trends of DO, water temperature, salinity and nutrient concentrations were analyzed by removing the seasonal climatology computed for the observational period by subtracting the mean for each month from each month in the time-series. The monthly anomaly was then divided by the monthly standard deviation to get the standardized monthly anomaly (Cullen et al. 2007; Li and Harrison 2008). An average of all 12 month anomalies in a year constitutes the annual standardized anomaly.

Statistical DO model

In general, oxygen concentrations in aquatic systems are primarily regulated by physical factors such as water temperature, salinity (Mee 1988; Nezlin et al. 2009) and dissolved nutrients, primarily nitrogen and phosphorus (Alexander et al. 2000; Krug and Marrifield 2007; Nezlin et al. 2009). A correlation analysis was employed to assess the statistical associations between DO and measured controlling factors (temperature, salinity, nitrogen, phosphorus). In Chesapeake Bay, DO has a significant relationship with total dissolved nitrogen ($TDN = NO_3 + NO_2 + NH_4 + DON$), total dissolved phosphorus ($TDP = Ortho\text{-}PO_4 + DOP$), water temperature and salinity (Table 1). Therefore, our model is robustly based on TDN, TDP, water temperature and salinity as a multi-regression model for prediction of DO in Chesapeake Bay. In the present study, data from 1990 to 2004 were used to construct the model and the 2005 to 2006 data were used to evaluate model performance by predicting DO levels with the known inputs.

Based on correlation analysis, a step-wise regression approach was used to select a starting point for the multiple regression models relating DO concentrations to monthly water temperature, water salinity, TDN and TDP levels. The step-wise regression was performed term by term with the addition of an independent variable until the Akaike information criterion was minimized. Multi-regression models can be assessed using a coefficient of determination (R^2) that provides a measure of how well results are likely

Table 1 Correlation coefficient matrix of DO, water temperature, salinity and dissolved nutrients in Chesapeake Bay ($n = 204$; $p < 0.05$)

	DO	Temp	SAL	TDN	TDP
DO	1.000				
Temp	−0.861	1.000			
SAL	−0.124	−0.022	1.000		
TDN	0.654	−0.605	−0.566	1.000	
TDP	−0.343	0.097	0.019	0.133	1.000

to be predicted by the statistical model (Draper and Smith 1998). In addition, the F value is also computed to test statistical variability between the observed and predicted DO values by the step-wise multi-regression method. The multi-regression model is as follows:

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \beta_4 X_4 \qquad (1)$$

where y is the dependent variable (DO), X_{1-4} are independent variables, water temperature, TDN, TDP and salinity, respectively, and β_{0-4} are the model coefficients. A regression model between the response and explanatory variable is generally site-specific and may change over time if changes occur in the sources of the constituent or an improved sensor or modified nutrient analytical scheme becomes available. This is because of simplifying assumptions implicitly built into the regression analysis. For example, oxygen levels in the water column are presumed to be regulated by nutrient levels, water temperature, salinity (Stanley and Nixon 1992; Buzzelli et al. 2002; Hagy et al. 2004; Batiuk et al. 2009). All of these complexities are simplified and aggregated into the values of coefficients (β) computed by the regression analysis. It is very unlikely that any two locations within the system would simultaneously have identical temperature, salinity and nutrient levels. Therefore, we computed regression coefficients at each grid-point and at each vertical level for the spatially explicit prediction of DO in Chesapeake Bay.

Model validation

Multiple regression models are generally evaluated by examining the distribution of residuals and other diagnostics. In addition to residual analysis, we tested the performance of the DO model by two statistical methods, the Nash–Sutcliffe efficiency (NSE) and root mean square error (RMSE)-observations standard deviation ratio which have been widely used in water quality assessment and modeling studies (e.g. Moriasi et al. 2007) as described below.

(1) *Nash–Sutcliffe efficiency*. NSE is a normalized statistical measure that explains the model efficiency as a fraction of the observed value variance that is reproduced by the model (Nash and Sutcliffe 1970). NSE describes the graphical distribution of observed and predicted values along the 1:1 line. NSE is computed as shown in Eq. 2:

$$NSE = 1 - \frac{\sum_i^n (o_i - p_i)^2}{\sum_i^n (o_i - o_{avg})^2} \qquad (2)$$

where o_i is observed (measured) value, p_i is predicted value and o_{avg} is the mean of observed data. NSE ranges between $-\infty$ and 1.0. Values between 0.0 and 1.0 are normally considered as acceptable levels of the model performance (Moriasi et al. 2007), whereas NSE 0.75 is considered to be

an excellent estimate, and NSE between 0.75 and 0.36 is regarded to be satisfactory (Motovilov et al. 1999).

(2) *Root mean square error-observations standard deviation ratio* (*RSR*). RSR standardizes the RMSE which accounts for the bias due to variability in the data set (Singh et al. 2004). RSR varies from the optimal value of 0, which indicates zero RMSE or residual variance and therefore perfect model prediction, to a large positive value. RSR is computed as the ratio of the RMSE and standard deviation of observed data, as shown in Eq. 3:

$$RSR = \frac{RMSE}{Std\ Dev_{obs}} = \frac{\sqrt{\sum_i^n (o_i - p_i)^2}}{\sqrt{\sum_i^n (o_i - o_{avg})^2}} \qquad (3)$$

Where o_i is observed (measured) value, p_i is predicted value and o_{avg} is the mean of observed data. A RMSE value closer to zero indicates a better fit to observed values. The denominator in the RSR minimizes the influence of a few observations that have very large or small values (outliners) relative to the observations as a whole. The lower RSR, the lower the RMSE, indicating better model prediction capability (Moriasi et al. 2007).

Results

Trends in DO, water temperature, salinity and nutrient concentrations

Variability of DO, water temperature, salinity, TDN and TDP in Chesapeake Bay for a 17-year period (1990–2006) are shown in Fig. 2 and long-term means of these environmental variables at three different levels; i.e. surface, middle and bottom are depicted in Fig. 3. The long-term average of surface DO concentrations in Chesapeake Bay demonstrated a clear annual cycle and range between 6.58 to 13.46 mg L^{-1} (mean $\pm$ SD $=$ 9.58 mg L^{-1} $\pm$ 1.94) (Fig. 2a). Standardized anomalies of DO represent interannual variability in DO levels and appear to decrease from 1996 to 2002, and then rise till 2006 (Fig. 2b). The interannual variability in DO levels were primarily regulated by water temperature and dissolved nutrients. Over the ecosystem scale, low values of bottom layer DO ($\leq$2 mg L^{-1}) in Chesapeake Bay were largely isolated towards the mid-Bay region and its associated tidal tributaries (Fig. 3a). High DO levels ($\geq$5 mg L^{-1}) were observed at the river-front zones primarily because of the freshwater influence (Fig. 3a).

Seasonality in water temperature (mean $\pm$ SD $=$ 14.68°C $\pm$ 8.54) showed a minimum of 4–6°C in December/January and a maximum of 27–28°C in July/August (Fig. 2c). Interannual variability in water temperature was
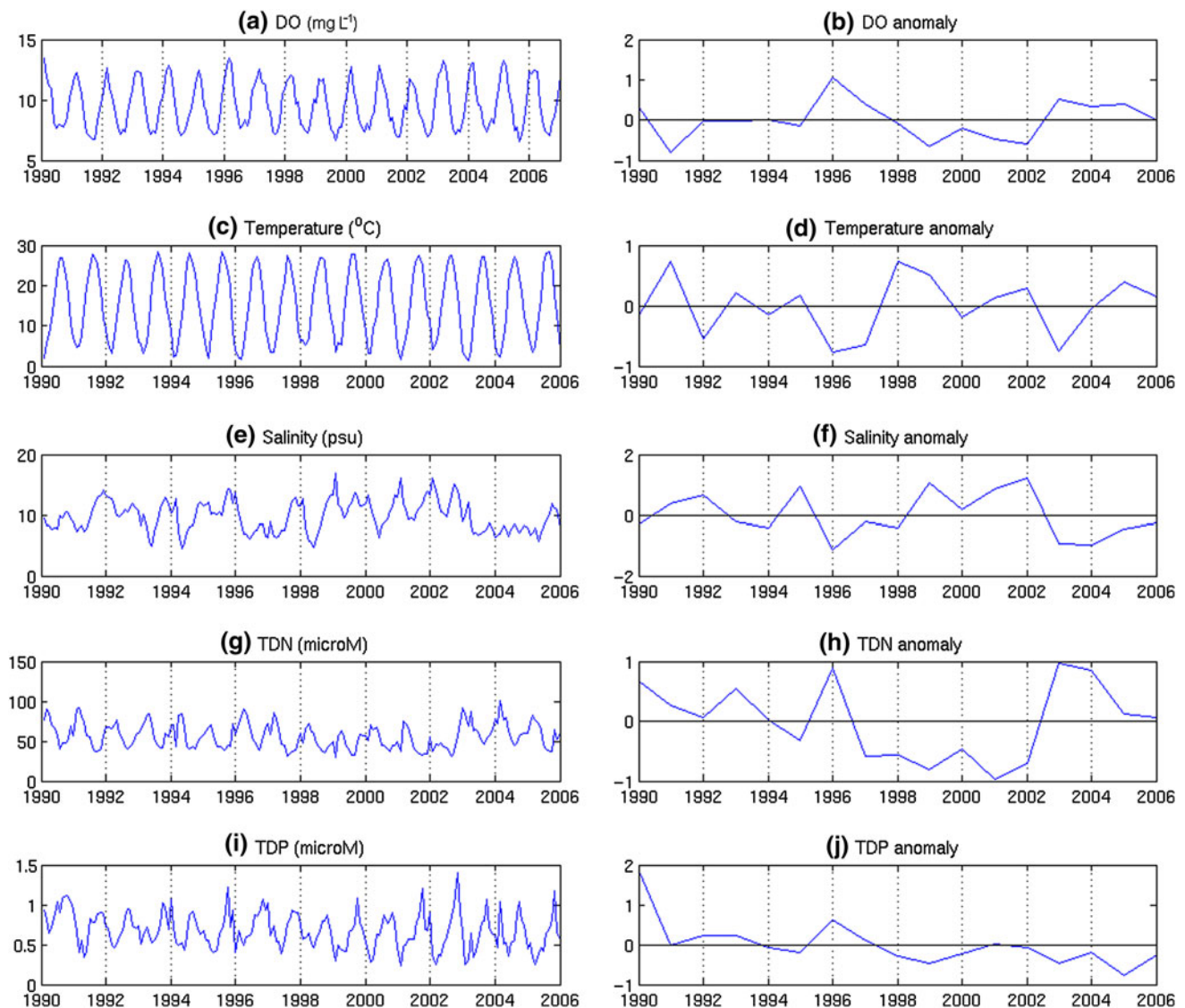
Fig. 2 Long-term distributions (1990–2006) and annual standardized anomalies of the surface average values of dissolved oxygen, water temperature, salinity, total dissolved nitrogen (TDN) and total dissolved phosphorus (TDP) in Chesapeake Bay

observed with relatively high temperatures recorded in 1998–1999 (Fig. 2d). The lower Bay water was significantly warmer than the upper Bay water because of high residence time of the water in the lower Bay (Fig. 3b). Salinity (mean ± SD = 11.03 psu ± 2.48) also exhibited a seasonal pattern and ranged from 4 psu (in winter) to 17 psu (in summer) with the highest mean salinity (12 psu) being recorded in 1999 (Fig. 2e). Spatial distribution and variability of salinity clearly demonstrates that the upper Bay is oligohaline and lower Bay is polyhaline (Figs. 3c, 4b).

The long-term distribution of TDN displayed an interannual variability with a range from 28 to 76 μM (mean ± SD = 37.26 μM ± 11.79) (Fig. 2g). Standardized annual anomalies of TDN were characterized by secular trends

with a decrease between 1996 and 2002 and an increase over 2002–2006 (Fig. 2h). Surface TDP concentrations ranged from 0.17 to 1.16 μM (mean ± SD = 0.52 μM ± 0.20) and decreased from 1999 with a multi-year fluctuation (Fig. 2i). Higher levels of TDN and TDP were observed in the upper Bay and the river fronts than the lower Bay for all three vertical layers (Fig. 3d, e), which is mainly because of river inputs of nutrients from the watershed to the Bay. However, comparatively high TDP levels in the bottom layer are driven by autochthonous sources (Fig. 3e). The spatially explicit variability in TDN and TDP distributions demonstrates that high variability in the upper Bay is mainly due to allochthonous nutrients from the watershed (Fig. 4d, e).

Fig. 3 Long-term averages (1990–2006) of dissolved oxygen, water temperature, salinity, total dissolved nitrogen (TDN) and total dissolved phosphorus (TDP) for surface, middle and bottom layers
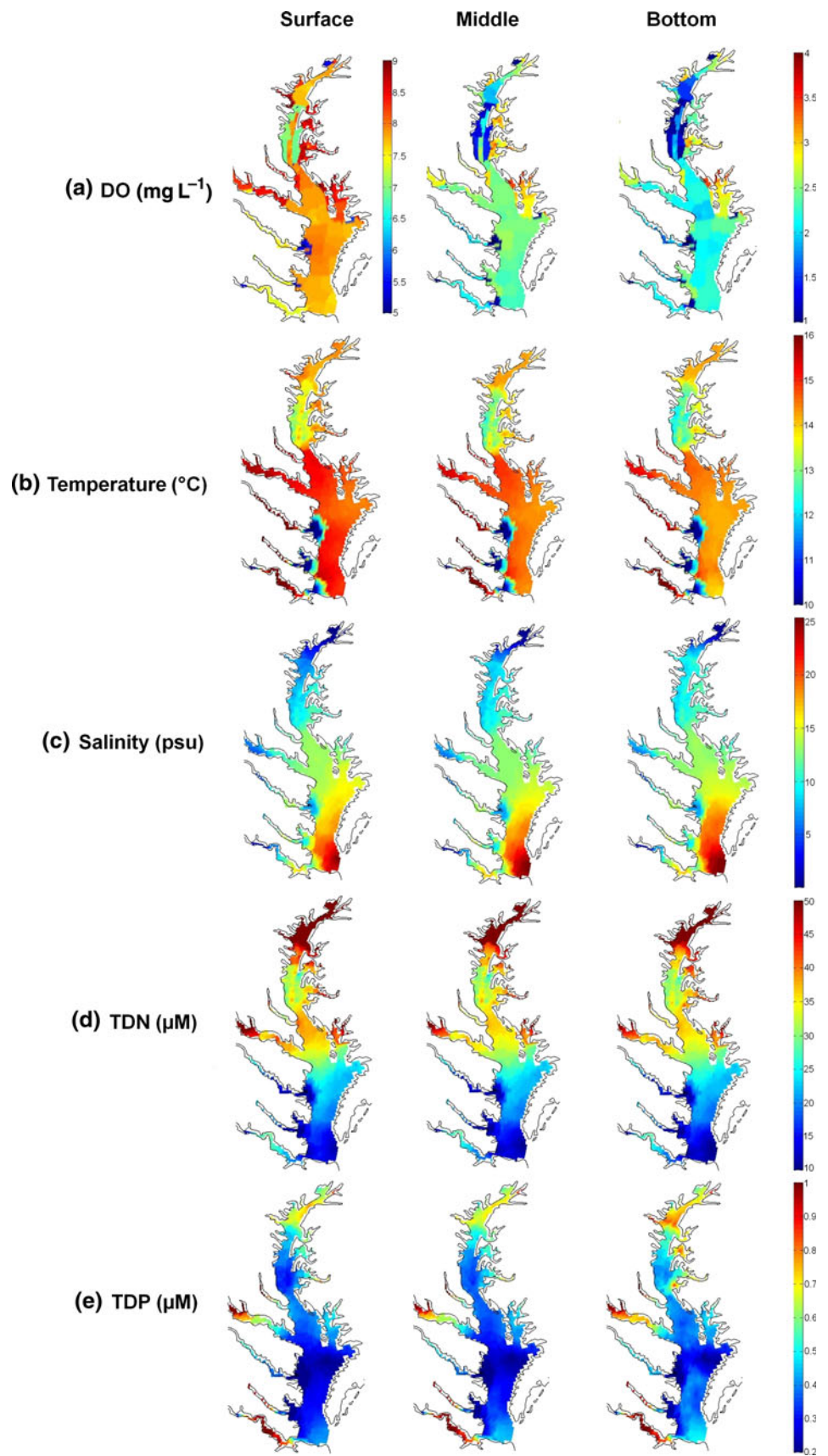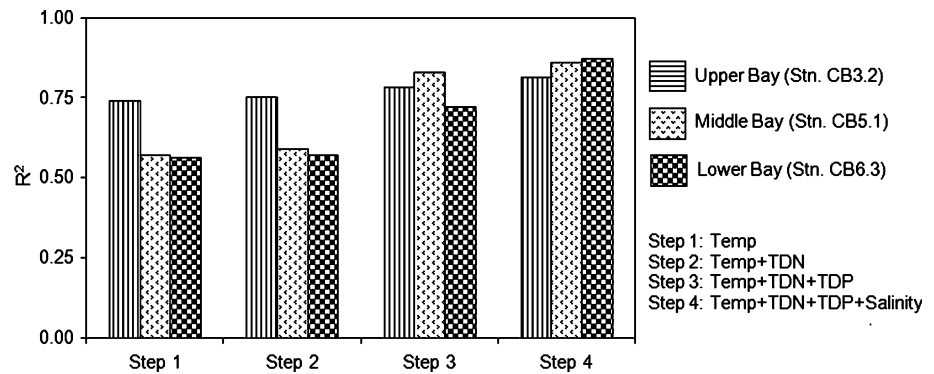
Fig. 4 Standard deviations of dissolved oxygen, water temperature, salinity, total dissolved nitrogen (TDN) and total dissolved phosphorus (TDP) for surface, middle and bottom layers
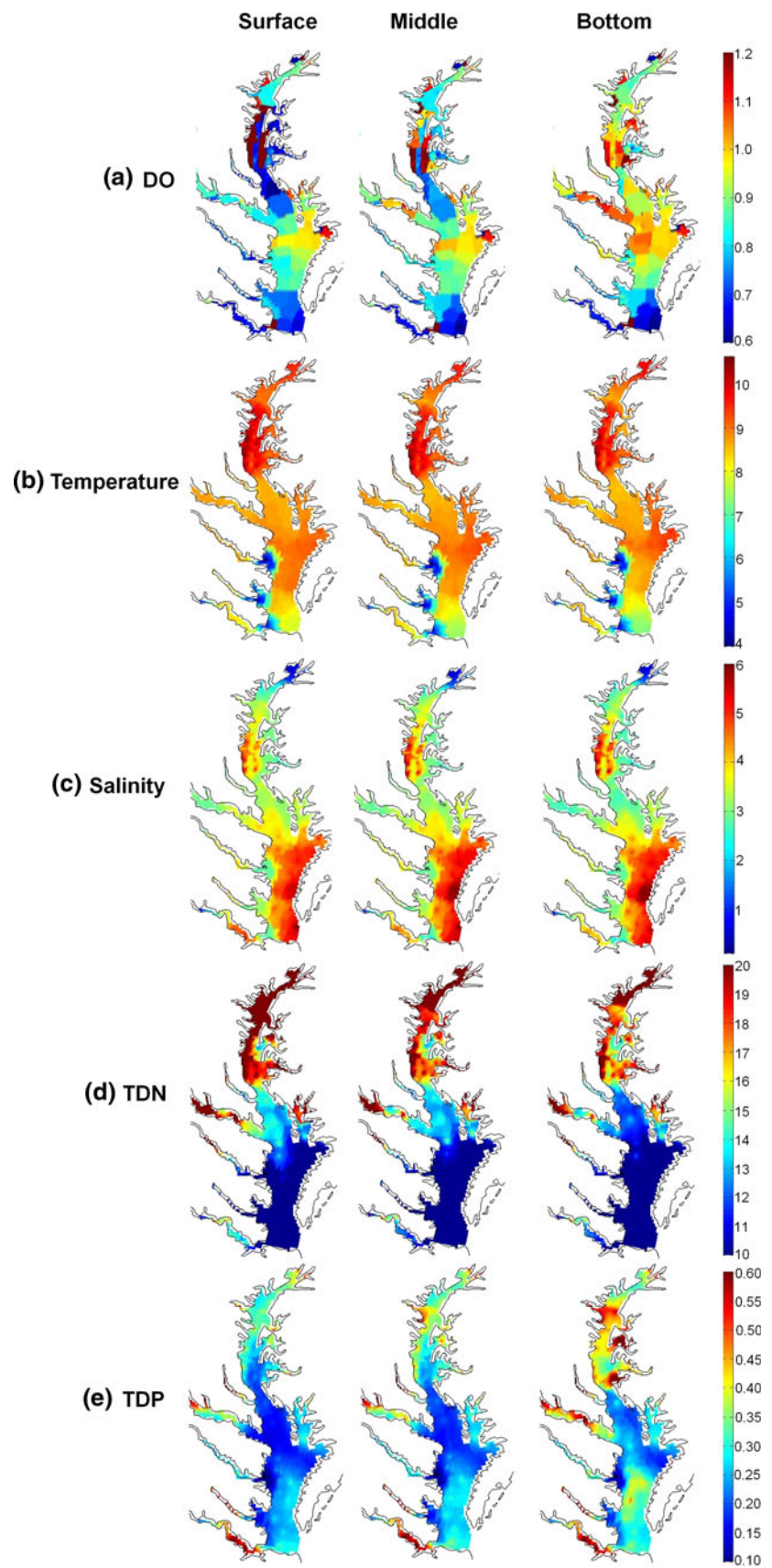
Fig. 5 Coefficient of determination (R^2) of the four different multi-regression approaches to predict DO concentrations

DO empirical model

In general, oxygen dynamics in coastal ecosystems are largely influenced by nutrient concentrations (mainly N and P) and water temperature (e.g. Kemp et al. 2009). In addition, salinity is an important parameter because it is largely regulated by freshwater discharge. The correlation analysis of the response variable (DO) and the driving environmental variables, indicated a strong relationship between DO and water temperature ($r = –0.86$; $p < 0.05$), TDN ($r = 0.65$; $p < 0.05$) and TDP ($r = –0.34$; $p < 0.05$). Statistically significant, albeit weak, correlation between DO and salinity ($r = -0.12$) was observed (Table 1). Besides this, salinity is also an important parameter that regulates nutrient biogeochemistry and vertical stratification in estuarine ecosystems. Moreover, vertical salinity stratification inhibits the exchange of surface-oxygenated water with deep water that depletes the bottom layer oxygen levels to critical value (i.e. 2 mg L^{-1}), which is detrimental for biological communities (Stanley and Nixon 1992).

We demonstrated model performance by choosing three stations from the upper (CB3.2), the middle (CB5.1) and the lower (CB6.3) Bay. The step-wise regression approach was used to identify the best fit model for prediction of oxygen by adding the model variables, and the coefficient of determination (R^2) was used to measure how best the predicted values from the statistical models match with observations. The highest R^2 of the 4th step model with all four variables can be expected to be the most likely to predict DO in Chesapeake Bay (Fig. 5). The F-statistic analyses ($p = 0.05$) further reinforce that oxygen prediction by the 4th step regression model is comparable with observations; i.e. the calculated F value (F_{cal}) is greater than the critical F value (F_{cri}) (Table 2). The model equations (4th step) for the three stations (CB3.2, CB5.1 and CB6.3) for three levels along the main stem are given in Table 3 and the spatial distribution of coefficients are also given in Fig. 6.

Table 2 Statistical analyses (F value, $p = 0.05$) of step-wise regression to select the appropriate model equation for the oxygen prediction

|	F_{cal}	F_{cri}	df
CB3.2			
Step 1	1.66	1.57	33
Step 2	1.67	1.57	33
Step 3	1.56	1.57	33
Step 4	1.59	1.57	33
CB5.1			
Step 1	2.28	1.57	33
Step 2	2.08	1.57	33
Step 3	2.39	1.57	33
Step 4	2.01	1.57	33
CB6.3			
Step 1	1.88	1.65	27
Step 2	1.84	1.65	27
Step 3	1.45	1.65	27
Step 4	1.72	1.65	27

Model validation

In order to use the predicted DO values in practical operations, it is imperative to evaluate the performance of the model. Cross-validation and residual analysis describe the degree of collinearity between predicted values and the observed data (Figs. 7, 8). A variance of 81, 92 and 87% for the surface layer; 66, 81 and 82% for the middle layer, and 77, 78 and 82% for the deep layer in the measured data was explained by the model for stations CB3.2, CB5.1 and CB6.3, respectively (Fig. 7). In addition, the statistical scores (NSE and RSR) demonstrated the predictive ability of model (Table 4). NSE score was consistently above 0.70 for the three stations, which indicates acceptable performance of the model. In addition, RSR score for the three stations ranged between 0.37 and 0.59, which was used as an indication of reliable DO predictions by the model.

Table 3 Multi-regression model parameter estimates for the three stations along the central axis of Chesapeake Bay

| Predictor	Surface layer			Middle layer			Bottom layer		
	CB3.2	CB5.1	CB6.3	CB3.2	CB5.1	CB6.3	CB3.2	CB5.1	CB6.3
Intercept	21.41	16.41	15.49	18.31	18.01	15.86	14.49	16.49	16.69
Temperature	−0.42	−0.36	−0.32	−0.35	−0.36	−0.27	−0.22	−0.22	−0.18
TDN	−7.24	−5.14	−2.86	−4.16	−4.69	−1.88	−0.74	−1.61	−1.81
TDP	28.39	−5.55	0.24	22.74	−1.93	−4.13	−17.58	2.88	−20.19
Salinity	−0.30	−0.034	−0.057	−0.099	0.0093	−0.036	−0.22	−0.21	−0.19
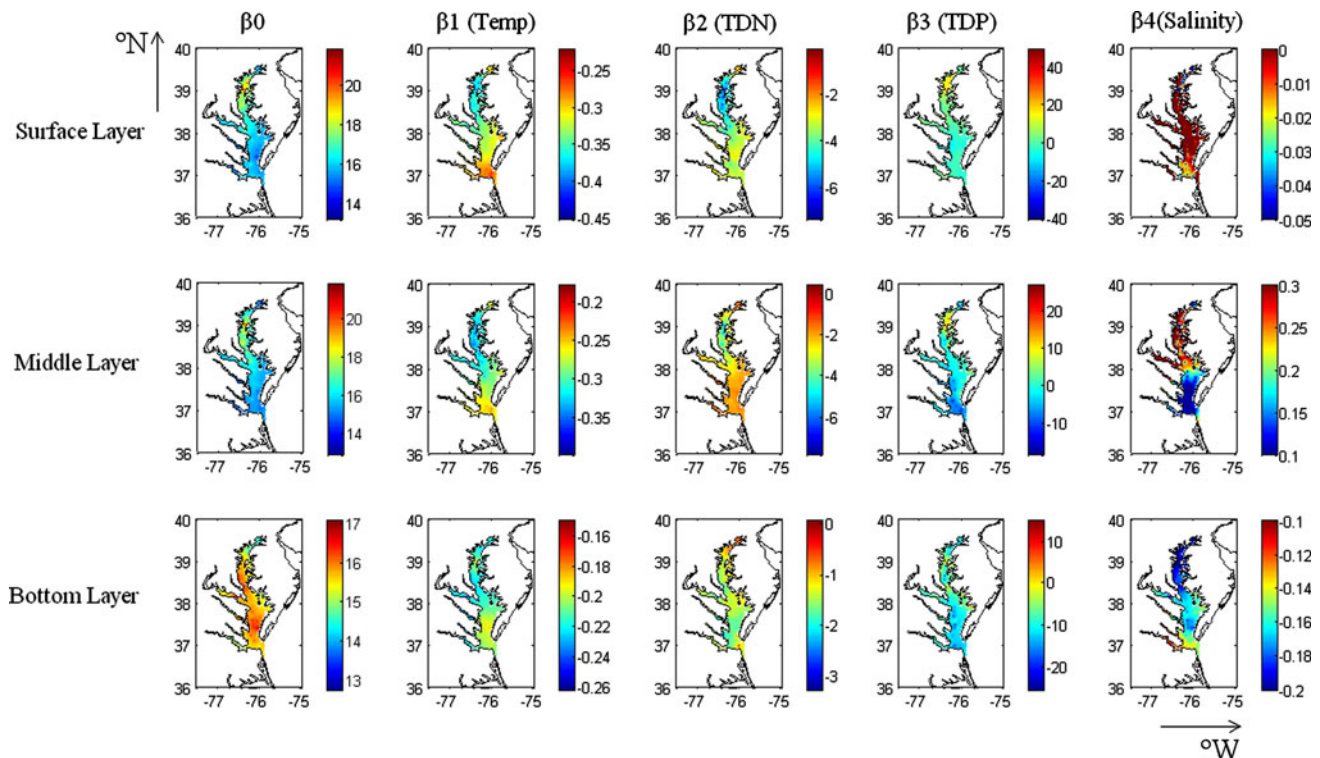
Fig. 6 Multiple regression coefficients used in the empirical prediction of DO for surface, middle and bottom layers. These coefficients are computed from the spatially and vertically interpolated data sets of DO, water temperature, salinity, TDN and TDP

Discussion

Controls on DO dynamics

Depletion of the coastal dissolved oxygen to below the critical level (<2 mg L^{-1}) has spread worldwide since the 1960s (Diaz and Rosenberg 2008) and has received significant scientific and policy attention (e.g. Boesch et al. 2007) as well as escalating documentation of its negative consequences on ecosystem dynamics (e.g. Vanquer-Sunyer and Duarte 2008; Ludsin et al. 2009; Kemp et al. 2009). Rapid changes in land-use/land-management practices within the Chesapeake Bay watershed have increased the delivery of nutrient loads that increase the biological production, which is shown to be responsible for the depletion of DO (Zimmerman and Canuel 2000). Moreover, the decadal variability in low oxygen conditions may be closely linked with climatological factors influencing fluvial loads from the watershed (Karlsen et al. 2000). High DO levels in river-mouth zones (Fig. 3a) are due to ventilation from rapid mixing of Bay water with freshwater from tributaries. High DO in surface waters may be due to supersaturation conditions caused by photosynthesis, which reinforces phytoplankton as a critical factor that regulates oxygen dynamics in Chesapeake Bay (Kemp et al. 1990, 2005). The vertical gradient in DO levels is mainly due to photosynthetic activity, which is further accelerated by increased nutrient concentrations associated with anthropogenically driven eutrophication (Hagy et al. 2004; Breitburg et al. 2009). Sedimentary oxygen demand and suspended
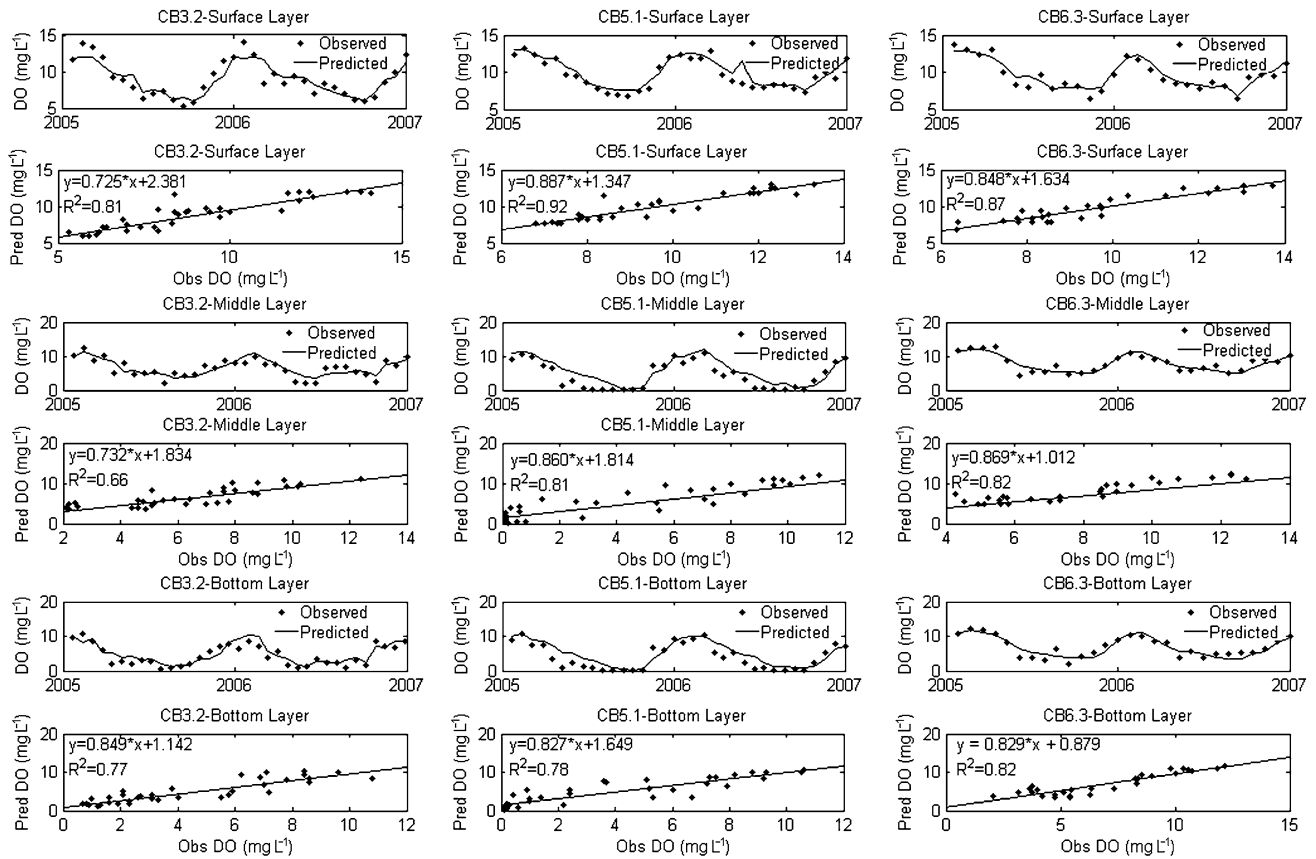
Fig. 7 Comparisons between observed and predicted DO values for the three stations, upper Bay (CB3.2), mid Bay (CB5.1) and lower Bay (CB6.3). Data point in red color is not considered for the analysis
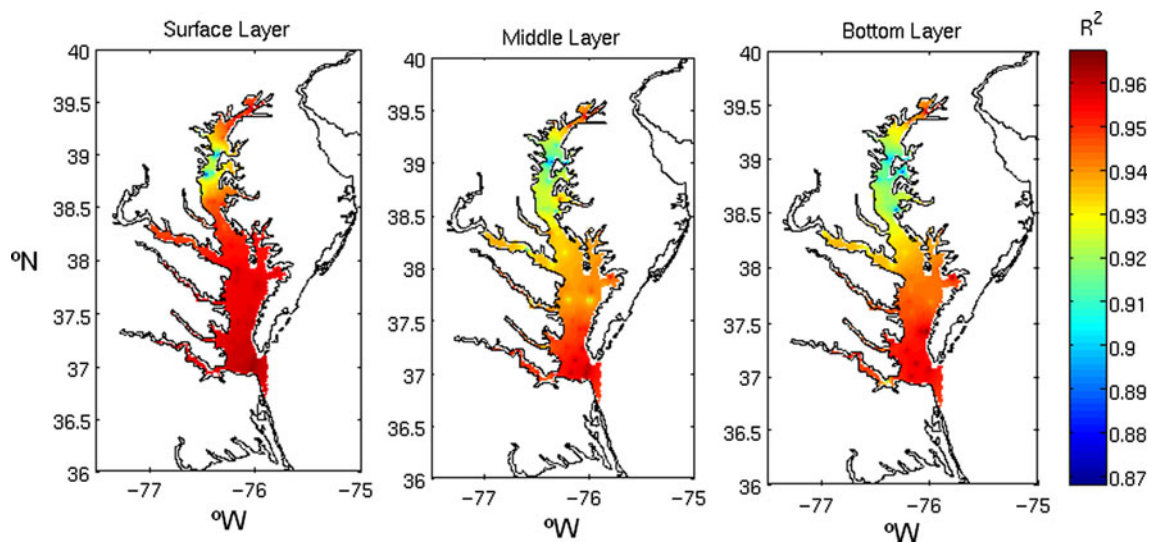
Fig. 8 Correlations (R^2) between observed and predicted DO concentrations for both surface, middle and bottom layers

microbial oxygen demand might have caused a significant variability in DO distribution in the water column (Cowan and Boynton 1996) (Fig. 4a).

High nitrogen levels in coastal waters enhance phytoplankton blooms, which in turn increase DO values in the surface layer due to photosynthesis (D'Avanzo and Kremer

1994). However, low DO values in the bottom layer are a result of respiration and biodegradation of organic matter produced by macro-algae (Valiela et al. 1992). Under low DO conditions, a larger fraction of the total nitrogen load is recycled from sediments as NH_4^+ due to the coupled nitrification–denitrification and is mixed vertically into the euphotic zone where it can fuel further algal growth that subsequently reduces oxygen levels (Kemp et al. 1990, 1992). Furthermore, sulfur-reducing bacteria in sediments consume oxygen at a rate of ~ 9 mg L^{-1} d^{-1} for 1 mol of sulfate in this ecosystem, further causing an oxygen deficit in deep layers (Jonas 1997). Geochemical leaching of phosphate (PO_4^{3-}) from anoxic sediments in polyhaline zones by metal reducers could accelerate phytoplankton growth and respiration in the water column and affect DO dynamics (Froelich et al. 1982; Caraco et al. 1989).

In coastal waters, salinity plays an important role in ecological processes because it represents vertical stratification and is highly influenced by freshwater discharge and wind forcing (Buzzelli et al. 2002). An increase in freshwater discharge from tributaries reduces salinity and elevates nutrient levels, and has a profound influence on phytoplankton growth that subsequently leads to drawdown of DO in coastal waters following the spring freshet of river flow (Seliger and Boggs 1988). Generally, the vertical salinity gradient contributes to the majority (>90%) of density stratification in this estuary (e.g. Goodrich et al. 1987) and the vertical density stratification inhibits mixing of oxygenated surface waters into bottom layers independent of season and temperature. Vertical stratification is also temperature dependent; hence an increase in temperature due to global warming enhances stratification in estuaries, which in turn seriously impacts oxygen dynamics and distribution in the estuarine water column (Buzzelli et al. 2002; Kemp et al. 2009). Recent modeling analysis demonstrates that sea level rise increases salt flux and bottom layer salinity in Chesapeake Bay, thus favoring increased stratification (Hilton et al. 2008). Once vertical stratification is established and vernal warming begins, bottom water DO concentrations decline steadily through spring (Kemp et al. 1992). Allochthonous nutrients in spring waters, mainly nitrogen species, and autochthonous nutrients in summer from the bacterial mineralization, elevate water column productivity (Malone et al. 1988; Cowan and Boynton 1996). Organic matter derived from spring and summer phytoplankton production provides a substrate for planktonic and benthic respiratory processes (Malone et al. 1988), which tend to increase with warming waters. Thus, the combined effects of vernal increases in both biological (respiration) and physical (stratification) processes regulate estuarine DO dynamics in summer.

Performance of the DO model

Prediction of DO is difficult because of its remarkable variability over short time scales due to variability in consumption and production rates of oxygen, which in turn depend on different environmental and anthropogenic factors (Scavia et al. 2006; Greene et al. 2009). Nonetheless, prediction of DO is a key step in the sustainable management of aquatic ecosystems, and while prognostic and mechanistic models are a superior pathway to skillful DO forecasts, many of the biological mechanisms remain to be fully understood, and thus statistical-empirical models remain extremely valuable and instructive. Furthermore, statistical models are entrenched in empirical observations, which can be optimized by improving the parameterizations over time and appropriate selection of independent variables to characterize system response. However, the increasing demand for predictive information on ecological health issues necessitates the implementation of minimum pragmatic, empirical models that take advantage of available data to assemble mechanisms and prognostic understanding as well as build models to understand oxygen dynamics in coastal ecosystems (Greene et al. 2009). Moreover, they can also guide observational needs to enhance process and mechanistic understanding (Murtugudde 2010).

Model results depicted here for the prediction of DO in Chesapeake Bay join the growing efforts to develop and validate ecological models for various biogeochemical and environmental variables such as sea nettles, harmful algal blooms, pathogens, and nutrient and sediment loadings (e.g. Xu and Hood 2006; Decker et al. 2007; Blauw et al. 2006; Anderson et al. 2010; Constantin de Magny et al. 2010; Meng et al. 2010). In contrast to existing water quality models that are based on the Susquehanna river nutrient loads and are aimed at predicting the annual extent of hypoxic area in Chesapeake Bay (Hagy et al. 2004; Scavia et al. 2006), our model accounted for important variables (TDN, TDP, water temperature and salinity) from the whole Chesapeake Bay grid domain influenced by climatic factors and watershed activities. The challenge is to predict DO without the sedimentary diagenetic and microbial rates, and vertical stratification to support the mechanistic modeling. But, the temperature and salinity fields partially represent these processes in the model. Therefore, we categorize our empirical model is an intermediate range with a process-based empirical approach for the spatially explicit prediction of DO in Chesapeake Bay.

Evaluation of model performance is a crucial step in model applicability in environmental management studies. Hitherto, no commonly accepted guidelines have been established to evaluate ecological models, but specific statistical scores and performance ratings have been

Table 4 NSE and RSR statistical scores for the three stations, CB3.2, CB5.1 and CB6.3

Station	NSE			RSR		
	Surface layer	Middle layer	Bottom layer	Surface layer	Middle layer	Bottom layer
Upper Bay (CB3.2)	0.82	0.65	0.74	0.44	0.58	0.51
Middle Bay (CB5.1)	0.83	0.71	0.70	0.42	0.54	0.54
Lower Bay (CB6.3)	0.86	0.82	0.82	0.37	0.43	0.43

developed (see Moriasi et al. 2007). Grid point residual analysis demonstrates that ≥80% variance in measured data is predicted by the model (Fig. 8). Furthermore, the predicted DO values faithfully reproduce observed DO levels for stations from the upper Bay (CB3.2), middle Bay (CB5.1) and lower Bay (CB6.3) (Fig. 7). In addition, NSE and RSR scores were used to demonstrate DO predictability of the statistical model for ecological and management perspectives (Table 4). These statistical scores further attest the fact that the model presented here has demonstrable skill in predicting observed DO values and the model can be applied in practical ecological management and restoration practices.

Dissolved oxygen forecasts and interdisciplinary applications

The spatially explicit prediction of DO is critical in understanding the ecological management and economic implications of oxygen depletion and its associated ecological consequences. To achieve this, DO predictions in Chesapeake Bay require integration of environmental data from different predictive models into the DO empirical model as input. This can be achieved by coupling the DO model with the ChesROMS ocean model to forecast DO levels in Chesapeake Bay. The ChesROMS ocean model forecast is generated using a six to eight member ensemble forced with the global ensemble system (GENS) every 3 days and can deliver skillful estimates of water temperature and salinity. A seasonal outlook is issued every 10 days by downscaling seasonal climate prediction (see http://cbfs.umd.edu). The ChesROMS model is also being coupled with the Nitrogen-Phytoplankton-Zooplankton-Detritus (NPZD) ecosystem model for nutrient concentrations (Fennel et al. 2006). The outputs from the ChesROMS and NPZD models will be inputs to force the prognostic DO model to forecast DO levels in the Bay, which will subsequently be used to develop ecologically linked products to describe ecosystem structure and function.

The spatially explicit empirical DO model can serve wider applications than the presently available models for DO in Chesapeake Bay (Hagy et al. 2004; Scavia et al. 2006; Stow and Scavia 2009), because the existing water

quality models are parameterized for estimation of the volume of hypoxic water and subpycnocline DO levels, so they do not provide a spatially explicit prediction of oxygen. In addition to the prediction of DO values, the model presented can be used to estimate the extent of summer hypoxia/anoxia (not attempted here). Hence, this model can be coupled with other ecological models to evaluate ecosystem structure and function. For example, improved understanding and forecasting of commercially and recreationally important striped bass (*Morone saxatilis*) habitat suitability (Costantini et al. 2008), and the interactions of striped bass and its prey, are important from both scientific and resource management perspectives. Our predicted DO values can be used as a forcing function along with water temperature and salinity from the hydrodynamic ChesROMS model to force striped bass habitat suitability models that can be used to evaluate and forecast how hydro-climate variability drives variability in habitat quality and quantity. Particular emphasis is placed on summer conditions, when the striped bass population is vulnerable to stress from warm temperatures and low oxygen (Brandt et al. 2009). Our ultimate objective is to provide managers with decision support tools for planning ecosystem-based fisheries management.

Implications: dissolved oxygen and climate change and variability

The Intergovernmental Panel on Climate Change (IPCC) has concluded, based on the synthesis of observations, that the earth's surface temperature has increased by approximately 0.57°–0.92°C over the past century, which is primarily attributed to anthropogenic greenhouse gas emissions (IPCC 2007). For the Chesapeake Bay region, various climate models predict that temperature will rise by 3°–6°C over 2070–2099 with wide-spread impacts on every aspect of the Bay's circulation and functioning (Najjar et al. 2010). Several studies have demonstrated a positive correlation between the Bay water temperature and atmospheric temperature (Cronin et al. 2003; Preston 2004; Kaushal et al. 2010). Therefore, the regional temperature predictions indeed imply a direct effect on Bay water temperature and impacts on nutrient biogeochemistry and oxygen dynamics. High temperature affects the solubility

of oxygen in water and the sensitivity of oxygen saturation levels to sub-pycnocline waters (~ 20°C) in the Chesapeake Bay is estimated to be -0.16 mg L^{-1}°C^{-1} (Najjar et al. 2010). Therefore, a temperature increase by ~ 5°C could tip the severely hypoxic waters into the anoxic range.

Najjar et al. (2000) projected that Susquehanna River discharge in spring could change by $+12$ to -4% by 2030 and $+4$ to -25% by 2095. Based on these projections, Howarth et al. (2006) estimated that the nitrogen flux from the Susquehanna River to the Bay could increase by 3–17% by 2030 and 16–65% by 2095, as high loads of anthropogenic nitrogen are transported by increased rainfall and surface runoff. Increased loads of terrestrial anthropogenic nitrogen affects ecological processes by changing intricate interactions between nutrients and biological systems (Barile 2004; Lotze et al. 2006; Pellerin et al. 2006), which subsequently affects the oxygen distribution in coastal waters (Baird 2009). The functional relationship between the Susquehanna flow and the Bay anoxic/hypoxic volume indicates that a 10% discharge increase will drive an increase in anoxic water volume (DO < 0.2 mg L^{-1}) by 10%, severely hypoxic water volume (DO < 1.0 mg L^{-1}) by 6% and mildly hypoxic volume (DO < 2.0 mg L^{-1}) by 3% in the 21st century (Hagy et al. 2004). From these estimations, it is projected that the volume of anoxic water will grow by 3–17% by 2030 and 16–65% by 2095; hypoxic water by 1.8–10.2% by 2030 and 9.6–39% by 2095; and mildly hypoxic water 0.9–5.1% by 2030 and 4.8–19.5% by 2095. Such estimates are quite uncertain, but they provide a context for evaluating the impacts of nitrogen pollution on oxygen dynamics. In addition, impacts of climate change and land-use/land-management practices will increase nutrient loads from both the watershed and the air-shed, which indeed have a profound impact on oxygen levels in Chesapeake Bay (Howarth et al. 1996; Boesch and Brinsfield 2000).

Conclusion

Anthropogenic induced climate change alters nutrient biogeochemical processes and phytoplankton dynamics in the estuarine environment by delivering substantial nutrients from the watershed (Justić et al. 2005). In response to increasing nutrient pollution from the watershed, oxygen dynamics in Chesapeake Bay have been adversely affected and depleted to below the critical level (<2 mg L^{-1}) mainly in spring and summer, which has several negative impacts on the structure and function of the ecosystem. Therefore, prediction of ecological parameters including oxygen is an important step in the sustainable management of aquatic ecosystems. To achieve this, a multi-regression modeling approach was adopted for prediction of spatially explicit DO levels in Chesapeake Bay as a function of water temperature, salinity, TDN and TDP. Residual analysis shows that the predicted DO values compare well with observations ($R^2 > 0.80$; $p < 0.05$). NSE and RSR are also used to evaluate the performance of the statistical model and demonstrate the acceptability of the model prediction. Coupling the DO model with the physical outputs of a regional climate model or hydrodynamic model can be used to develop a regional earth system model to forecast a range of ecological components that describe the structure and function of the ecosystem. Impacts of climate change and nutrient pollution could increase the extent of hypoxic/anoxic area in Chesapeake Bay that would worsen ecological conditions and economic deliverables. Therefore, effective nutrient reduction strategies are required for the sustainable management of the Bay from cultural eutrophication.

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