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Abstract

A simplified conceptual model based on timescales of gravitational circulation, vertical exchange, and total oxygen consumption rate of the biochemical processes is presented to provide insight into the relationships between estuarine dynamics and bottom water dissolved oxygen (DO). Two dimensionless parameters are introduced to diagnose the relationship between the vertical exchange process and the biochemical DO consumption and the influence of gravitational circulation on replenishment of bottom DO. The relative magnitudes of these timescales provide a linkage between the physical and biochemical processes. The hypoxic and anoxic conditions in deep waters of Chesapeake Bay are successfully interpreted with these three proposed timescales. Because the Bay is a long estuary, the replenishment of the bottom DO due to gravitational circulation diminishes as the bottom water travels farther upstream. The bottom DO is mainly modulated by the vertical exchange process in the middle and upper portions of the Bay. In addition to other physical processes that affect vertical exchange, wind and freshwater are the major predictors of the vertical exchange time. The model is applicable to Chesapeake Bay and other estuaries with persistent gravitational circulation if the dimensionless parameters can be appropriately estimated.

Hypoxia and anoxia occurrences in estuaries appear to be increasing and are most likely accelerated by human activities (Cloern 2001; Diaz 2001). Persistent seasonal hypoxia occurs in many stratified, partially mixed estuaries and shelf regions worldwide (Diaz 2001; Nixon 1995). The formation of chronic (days to months) hypoxic bottom waters in deep estuaries and coastal oceans is a common phenomenon of eutrophication in the aquatic environment and has been widely studied for many years (Diaz 2001; Kemp et al. 1992, 2005). Hypoxia and anoxia develop in Chesapeake Bay from the middle to upper Bay in summer (Kemp et al. 2005). The U.S. Environmental Protection Agency monitoring data (http://www.chesapeakebay.net/data/downloads/) also indicate that the hypoxic condition lessens in the lower Bay and that the bottom dissolved oxygen (DO) concentration at the Bay entrance is near saturation most of the time. Annual summertime occurrences of hypoxia in deep water are driven by seasonal stratification coupled with total respiration. Hypoxia develops when the DO consumption rate of biochemical processes exceeds the oxygen supply for the sub-pycnocline water of an estuary (Officer et al. 1984).

The variation of estuarine dynamics is the key factor controlling the development of hypoxia (Kuo and Neilson 1987; Boicourt 1992; Scully 2010). Kuo and Neilson (1987) analyzed DO budgets in Virginia tributary estuaries of Chesapeake Bay. They pointed out that gravitational circulation plays an important role in modulating DO in these tributaries. High DO water at the estuarine mouth can be transported upstream by the gravitational circulation that replenishes the bottom-water DO. For an estuary with weak gravitational circulation, DO associated with inflow water will be removed by sediment oxygen demand

(SOD) as water parcels move upstream and inflow water replenishment of the bottom-water DO decreases. They concluded that the variations in frequency, duration, and severity of hypoxia in Virginia tributaries are related to the net movement of bottom waters controlled by the strength of the gravitational circulation. In Chesapeake Bay, it has been found that freshwater discharge is a major factor in regulating stratification (Boicourt 1992) and is a predictor of summertime hypoxic volume (Hagy et al. 2004) due to high nutrient input during spring runoff. In addition to the variation of freshwater, wind variations play a critical role in interannual DO variations in estuaries (Malone et al. 1986; Scully 2010). It has been suggested that the lateral exchange of DO between the surface and sub-pycnocline water due to lateral circulation contributes to the variation of hypoxia in Chesapeake Bay (Sanford et al. 1990; Scully 2010). Scully (2010) showed that wind plays a critical role in the modulation of hypoxia in Chesapeake Bay through lateral circulation.

These previous studies show that the development of hypoxia in the bottom layer of estuaries results from the competition between DO consumption and DO supply and is highly correlated to external physical forcings. Kuo and Neilson (1987) proposed a simplified model to examine the contribution of gravitational circulation to the bottom-water hypoxia in Virginia tributaries of Chesapeake Bay, which explains the differences among the hypoxia conditions in these tributaries. Although a strong gravitational circulation develops in the Bay, the strong stratification acts to decrease DO replenishment to the oxygen-depleted waters near the bottom. It appears that vertical stratification dominates over longitudinal advection in the mainstem of the Bay. But the effect of gravitational circulation in determining the oxygen-depletion zone is far from negligible (Boicourt 1992). It will be instructive to have a common relationship linking the competition of the vertical exchange
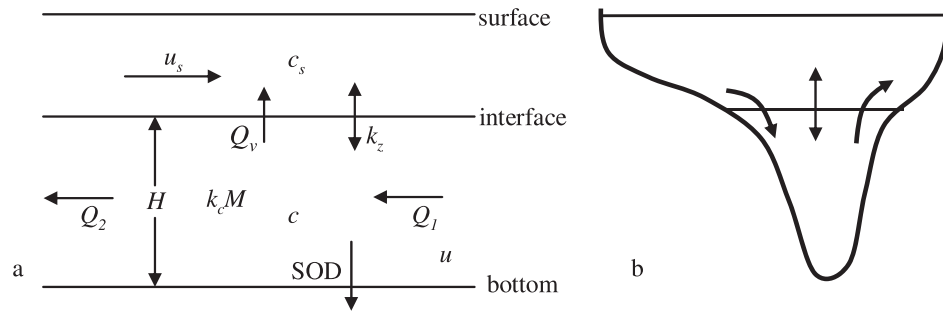

Fig. 1. Diagram of the conceptual DO budget model in a partially mixed estuary. (a) Along mainstem of the estuary; (b) across mainstem of the estuary.

process, gravitational circulation, and biochemical oxygen consumption to depict the occurrence of the hypoxic condition in estuaries. Although complex three-dimensional (3D) eutrophication models have been successfully applied to Chesapeake Bay for water quality management and can be used for the study (Cerco 1995; Shen et al. 2012), it is difficult to discern the separate influences of physical and biochemical processes on DO in a simple and understandable way. For this purpose, we present a simplified conceptual model in this paper that includes parameters accounting for oxygen consumption, vertical exchange, and gravitational circulation in a partially mixed estuary. The model is formulated using a Lagrangian perspective, with both the biochemical DO consumption rate and the physical processes quantified by timescales, which provides a single and comparable currency (Lucas et al. 2009). Using a timescale approach to interpret biochemical and physical processes has been successful for understanding the relationships between phytoplankton biomass and transport time (Lucas et al. 1999*a,b*, 2009), plankton and transport time (Reynolds 2000; Allan and Benke 2005), coupled effects of vertical mixing and benthic grazing and transport time (Koseff et al. 1993), and nutrient export and residence time (Nixon et al. 1996). Despite all of their simplifications and assumptions, they provide frameworks to explain the competition of biochemical and physical processes. In this study, Chesapeake Bay is used to demonstrate that the conceptual model can be used to explain the development of hypoxia in the bottom layer of the Bay and that it is applicable to other estuaries.

Methods

Development of the conceptual model—For a partially mixed estuary, the gravitational circulation can be described by a two-layer model (Pritchard 1952; Kuo and Neilson 1987; MacCready 2004) as shown in Fig. 1. Deepwater DO (the lower layer) in an estuary depends on the vertical exchange, horizontal advection, and biochemical processes, both in the water column and at the water–sediment interface. The mass balance equation of DO in a control volume (ΔV) of bottom waters can be written as

$$\frac{d(\Delta V c)}{dt} = k_z \frac{c_s - c}{d} \Delta A + Q_1 c_1 - Q_2 c \\ - Q_v c - B_{SOD} \Delta A - \alpha k_c M \Delta V \tag{1}$$

where c_s and c are DO concentrations (g O_2 m^{-3}) of the surface and bottom waters, respectively. c_1 is inflow DO concentration (g O_2 m^{-3}). k_z is the vertical exchange rate (m^2 d^{-1}) between the surface and bottom layers, which parameterizes the overall exchanges between two layers and is not restricted to the turbulent mixing. d is the distance between the middle point of the two layers, ΔA is the surface area of the control volume, Q_1 and Q_2 are the horizontal flows transported in and out of the control volume in the bottom layer driven by gravitational circulation, Q_v is the vertical flow due to gravitational circulation, B_{SOD} is the bottom SOD (g O_2 m^{-2} d^{-1}), M is the organic carbon concentration (g m^{-3}), k_c is the carbon decay rate (d^{-1}), and α is the DO to carbon ratio. Because vertical turbulent diffusion is much larger than horizontal diffusion in this vertical–longitudinal two-dimensional model, the longitudinal diffusion is neglected. The flows satisfy the continuity condition (Kuo and Neilson 1987)

$$Q_1 = Q_2 + Q_v \tag{2}$$

Assuming steady state, Eq. 1 can be written as

$$u \frac{dc}{dx} = \frac{k_z}{H} \frac{(c_s - c)}{d} - \frac{B_{SOD}}{H} - \alpha k_c M \tag{3}$$

where x is the axis in the along-estuary direction, and $x = 0$ at the mouth and increases upstream. u is the mean bottom inflow velocity and is assumed to be a constant. This assumption is valid in the central region for a uniform estuary based on the classical two-layer estuarine circulation model (Hansen and Rattray 1965). H is the bottom-layer thickness. Equation 3 is a typical "plug flow" model. The underlying assumptions are uniformity of all the properties along the cross-estuary section, persistence of estuarine circulation, and no longitudinal or horizontal mixing. Letting $D = c_s - c$ as DO deficit, and applying boundary condition $D = D_0$ at $x = 0$, Eq. 3 can be solved as

$$\frac{D}{c_s} = \frac{BHd}{k_z c_s}\left(1 - e^{\frac{-k_z}{Hd}\frac{x}{u}}\right) + \frac{D_0}{c_s} e^{\frac{-k_z}{Hd}\frac{x}{u}} \quad (D \geq 0) \tag{4}$$

where $B = B_{SOD}/H + \alpha k_c M$ is the net oxygen consumption rate (g O_2 m^{-3} d^{-1}). There are three key timescales that can be introduced: two represent physical transport processes (longitudinal and vertical, respectively) and one represents biochemical processes that quantify oxygen consumption.

Let $\tau_e = x/u$ be the longitudinal transport timescale that quantifies the travel time of gravitational circulation and $\tau_v = Hd/k_z$ be the vertical transport timescale that is the time required for the vertical exchange between the surface layer and sub-pycnocline water. If the surface-layer thickness is on the same order as that of the bottom layer, d approaches to H. If the surface-layer thickness is much less than that of the bottom layer, d approaches to $H/2$. $\tau_b = c_s/B$ is the timescale of the biochemical oxygen consumption. Using an approach similar to that of Lucas et al. (2009), we introduce two dimensionless parameters, τ_b^* and τ_e^*, which are scaled by the vertical exchange timescale as

$$\tau_b^* = \frac{\tau_b}{\tau_v} \text{ and } \tau_e^* = \frac{\tau_e}{\tau_v} \qquad (5)$$

Substituting Eq. 5 into Eq. 4 gives

$$\frac{D}{c_s} = \frac{1}{\tau_b^*}\left(1 - e^{-\tau_e^*}\right) + \frac{D_0}{c_s} e^{-\tau_e^*} \qquad (6)$$

The second term on the right-hand side of Eq. 6 accounts for the effect of the boundary condition, which diminishes as x increases. For $D_0 = 0$ at the boundary ($c = c_s$, i.e., the bottom DO concentration equals the surface DO concentration at the estuary entrance), Eq. 6 can be written as

$$\frac{D}{c_s} = \frac{1}{\tau_b^*}\left(1 - e^{-\tau_e^*}\right) \qquad (7)$$

or

$$\frac{c}{c_s} = 1 - \frac{D}{c_s} = 1 - \frac{1}{\tau_b^*}\left(1 - e^{-\tau_e^*}\right) \qquad (8)$$

Equation 8 gives a normalized DO concentration in terms of two dimensionless parameters (τ_b^* and τ_e^*). Here we have transformed Eq. 4, which is a function of distance (x), to an equivalent Eq. 6, which is a function of timescales and gives a Lagrangian perspective of DO balance equation. Dimensionless parameter τ_e^* is a normalized transit time of the gravitational circulation scaled by τ_v. Unlike the traditional point of view that the vertical exchange timescale is to quantify vertical turbulent mixing, τ_v is the vertical exchange timescale, which incorporates both vertical mixing and other processes that induce exchanges between the two layers (Fig. 1b), such as lateral circulation (Malone et al. 1986; Scully 2010). Although the exchange processes differ, the exchange timescale measures the overall exchange rate. τ_b^* is the parameter quantifying the competition of total biochemical oxygen consumption and oxygen replenishment through vertical exchange in the bottom waters. Using these three timescales, we are able to apply this simplified conceptual model to explain the distribution of bottom DO in a complex estuary system.

The normalized DO diagram of Eq. 8 is depicted in Fig. 2a. The contours are the values of $c:c_s$ (the ratio of bottom-layer DO to surface-layer DO). It can be seen that all contour lines become horizontal if transit time is long enough (i.e., if τ_e^* is large enough). Note that, from Eq. 8, DO can be written as
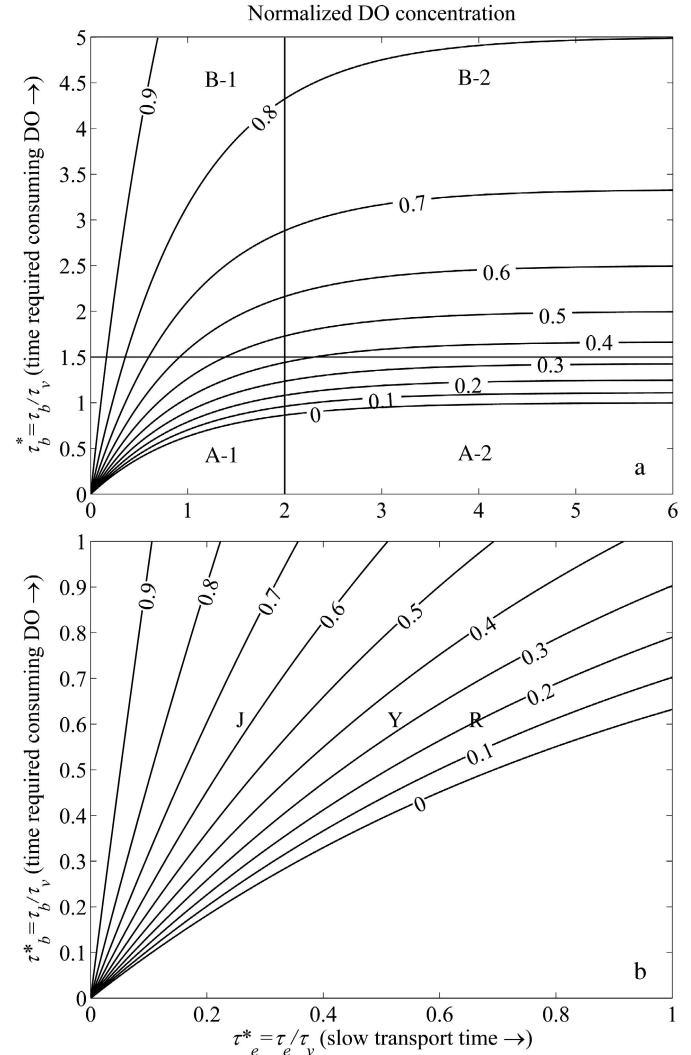
Fig. 2. (a) Normalized DO distribution ($c:c_s$, ratio of the bottom-layer DO to surface-layer DO) with respect to dimensionless timescale parameters. (b) An enlargement of part of (2a).

$$c = c_s - \frac{c_s}{\tau_b^*} + \frac{c_s e^{-\tau_e^*}}{\tau_b^*} \qquad (9)$$

The second term on the right-hand side of Eq. 9 reduces DO due to oxygen consumption, whereas the third term supplies DO through estuarine circulation. The ratio between the third term and the second term, $e^{-\tau_e^*}$, is the relative contribution of estuarine circulation on increasing bottom DO. When $\tau_e^* > 2$, the contribution of estuarine circulation is less than 14%.

As $e^{-\tau_e^*}$ becomes much smaller than 1.0, an equilibrium state is reached. Under this condition, DO consumption by the biochemical processes is balanced by DO replenishment by the vertical exchange processes, and the DO concentration reaches a constant value unless the relative magnitude of either process changes as the bottom water travels farther upstream. When τ_b^* is larger than 1.5, the normalized DO is larger than 0.3 and hypoxia (DO < 2 g m^{-3}) will not likely occur. For the purpose of discussion, Fig. 2a

can be divided into four regions. The figure shows that the biochemical timescale has a strong influence on bottom DO in all regions except for the extreme left side of regions A-1 and B-1, where τ_e is much smaller than τ_v. Hypoxia (e.g., normalized DO concentration less than 0.3) will likely occur in both regions A-1 and A-2, where the biochemical timescale is short. Hypoxia may be avoided in region A-1 if τ_e is much smaller than τ_v or τ_b is larger than τ_v, such as in the geographical region near the mouth (*see* later discussion). In regions A-2 and B-2, where τ_e is much larger than τ_v, the contour lines become horizontal, indicating that DO is mainly controlled by biochemical consumption and vertical exchanges. DO is independent of τ_e and increases with increasing τ_b/τ_v. All three timescales influence the bottom DO concentration in regions A-1 and B-1.

Computing physical timescales—The timescales of physical processes, τ_v and τ_e, can be estimated based on theoretical analysis and field measurements for an estuary with relatively simple geometry. For a complex estuary, the gravitational circulation and the vertical exchange are highly variable. Their timescales are not readily obtainable through theoretical analysis or field observations. However, it is possible to compute these parameters using 3D numerical models. Let us consider a water parcel released from the surface that will be transported to the bottom through physical processes. As the water parcel leaves from the surface, it can travel through different pathways and mix with other water parcels before reaching the bottom. Also, different water parcels released at the surface can reach the same location at the bottom. We want to estimate the mean time required for the parcel to be transported from the surface to the bottom. This mean transport time is a representative mean transport timescale from the surface to any location (Gustafsson and Bendtsen 2007), which can be computed using the concept of the mean water age that references the surface (Deleersnijder et al. 2001). However, the age clock will be reset to zero if the water parcel travels back to the surface before reaching the bottom. This timescale will be referred to as vertical exchange timescale. Similarly, the time required for water parcels to travel from the mouth to a location upstream can be estimated from the water age referenced to the mouth of the estuary. Delhez et al. (1999) provided a way to use a numerical model to compute the water age. Assuming that there is only one tracer released to a system without internal sources and sinks, the transport equations for computing tracer and the age concentrations can be written as (Deleersnijder et al. 2001):

$$\frac{\partial C(t,\vec{x})}{\partial t} + \nabla(\vec{u} C(t,\vec{x}) - K\nabla C(t,\vec{x})) = 0 \tag{10}$$

$$\frac{\partial \alpha(t,\vec{x})}{\partial t} + \nabla(\vec{u}\alpha(t,\vec{x}) - K\nabla\alpha(t,\vec{x})) = C(t,\vec{x}) \tag{11}$$

The mean age can be calculated as follows:

$$a(t,\vec{x}) = \frac{\alpha(t,\vec{x})}{C(t,\vec{x})} \tag{12}$$

where $\nabla = \vec{i}\frac{\partial}{\partial x} + \vec{j}\frac{\partial}{\partial y} + \vec{k}\frac{\partial}{\partial z}$, $C(t,\vec{x})$ is the tracer concentration, $\alpha(t,\vec{x})$ is age concentration, $\vec{u}$ is the velocity field, and K is the diffusivity tensor. Equations 10–12 can be computed by a 3D numerical model with specified initial and boundary conditions.

The Three-Dimensional Hydrodynamic-Eutrophication Model (HEM-3D) using the realistic forcings of observed freshwater discharges, winds, and tides was used to compute these transport timescales for Chesapeake Bay. The model was calibrated for surface elevation, current, and salinity for Chesapeake Bay and is good for hydrodynamic simulations (Hong and Shen 2012). The model was used to study the change of transport time due to sea level rise in the Bay. The model configurations and boundary conditions used for computing age in this study are the same as those used for the Bay.

For computing the timescale of gravitational circulation, tracers with an arbitrary concentration of one unit were continuously released at the open boundary (Hong and Shen 2012). Tracer age was set to zero at the boundary, and the radiation boundary condition was applied to account for the tidal effect (Shen and Haas 2004). For computing the vertical exchange timescale, tracers were continuously released at the surface. Tracer age at the surface boundary was set to zero, and the zero-flux boundary condition was used at the bottom (Gustafsson and Bendtsen 2007). The model simulation of vertical age and age of gravitational circulation started on 01 January 1998 and ran continuously until 2004. The first year's simulation was used for model spin-up.

Parameters applied to the study—The timescale τ_b can be estimated based on temperature, surface DO (c_s), and DO consumption rate. The saturation DO was computed as a function of temperature and salinity (Thomann and Mueller 1987). We used observed surface temperature in each month and interpolated over the entire year to compute the saturation DO. We used an estimated total oxygen consumption rate for this study, which allows us to examine the competition between biochemical and physical processes. The total DO consumption rate was computed as the sum of SOD and net respiration in the water column. Although SOD varies at different locations, we used 1.0 g O_2 m^{-2} d^{-1} for the mainstem of the Bay. This value is slightly higher than the measured high value of 0.86 g O_2 m^{-2} d^{-1} reported by Cowan and Boynton (1996) but is lower than the value reported by Boynton and Kemp (1985). The mean concentration of dissolved organic carbon in the mainstem of the Bay is about 2.7 g m^{-3}, with a minimum value of 2.0 g m^{-3} based on 1995 observation data collected by the Chesapeake Bay Program. A constant organic carbon concentration of 2.0 g m^{-3} was used in the water column. A mean organic carbon decay rate of 0.05 d^{-1} was used (Johnson et al. 1985). For a bottom-layer thickness of 20 m, this oxygen consumption rate is approximately 0.32 g O_2 m^{-3} d^{-1}, or 0.013 g O_2 m^{-3} h^{-1} at 20°C. This value is within the range of measured values for Chesapeake Bay between 0.01 g O_2 m^{-3} h^{-1} and 0.04 g O_2 m^{-3} h^{-1} (Smith and Kemp 1995). Both the decay

rate and the SOD levels change with time as a function of temperature, $1.06^{(T-20)}$, to account for seasonal variation, where T is temperature (°C; Thomann and Mueller 1987). Observations of monthly mean temperatures near the bottom were interpolated over the mainstem and were used to compute the temperature effect. Phytoplankton activities were not considered explicitly because supersaturation DO does not often occur near the surface and the bottom layer is outside of the photic zone. For the Virginia tributaries, measured respiration rates ranged from 0.012 g O_2 m^{-3} h^{-1} to 0.56 g O_2 m^{-3} h^{-1} (Lake 2013). Therefore, a high carbon decay rate and SOD value were used based on previous studies (Kuo and Neilson 1987; Shen and Kuo 1996). The DO consumption rate at 20°C is about 0.73 g O_2 m^{-3} d^{-1} or 0.031 g O_2 m^{-3} h^{-1}. All the parameters are listed in Table 1.

Results

Model bottom DO in tributaries—Low DO often occurs in summer in the deep water of Virginia tributaries. Kuo and Neilson (1987) studied the DO distribution in the Virginia tributaries of Chesapeake Bay—the James, York, and Rappahannock Rivers. They pointed out that DO concentrations near the bottom depend on the bottom-water transit time, which is determined by the gravitational circulation. Hypoxia rarely occurred in the James River, due to its strong gravitational circulation and the resulting short transit time. Because these tributaries have relatively simple geometry, the vertical exchange time can be estimated based on measurements, and the timescale of gravitational flow can be estimated from the horizontal salinity gradient based on classical estuarine theory. We use their estimated horizontal gravitational flow, u, as well as other parameters (Kuo and Neilson 1987; Kuo et al. 1991), for the conceptual model (Table 1). For the calculation, the origin of the longitudinal axis ($x = 0$) is at the mouth of each tributary. Although the bottom DO concentration at the mouth of the tributaries can be lower than the saturation DO in some years, we assume $D = 0$ at the mouth for the purpose of comparison of the three tributaries. The ratio of DO values ($c : c_s$) at a location 40 km upstream from the mouth in summer, where the lowest DO levels often occur, was examined. The results are listed in Table 1 and are marked on Fig. 2b by symbols J, Y, and R for the corresponding values in the James, York, and Rappahannock Rivers, respectively. It can be seen that the James River has the highest bottom DO among the three tributary estuaries because it has the strongest gravitational circulation, resulting in a short timescale of τ_e^*, which is consistent with the results of Kuo and Neilson (1987).

Timescales for mainstem of the Bay—The typical mean-flow year of 2000 and the wet-flow year of 2004 were selected for comparison. The transect and stations used for the following analyses are shown in Fig. 3. Figure 4 shows the 3D model–simulated monthly mean tracer ages at the bottom along the mainstem of the Bay from May to August for years 2000 and 2004, respectively. The ages are

Table 1. Parameters and computed values of timescales for three Virginia tributaries of Chesapeake Bay.

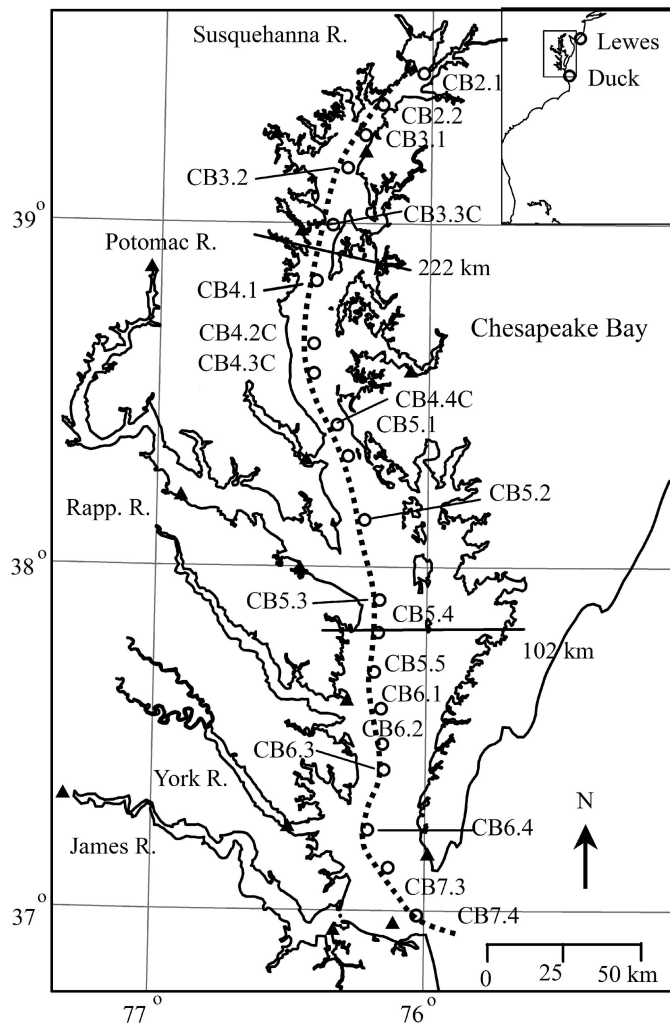| Estuary	Distance (km)	u (m s^{-1})	τ_e (d)	τ_v (d)	τ_b (d)	τ_b^*	τ_e^*	k_c (d^{-1})	SOD (g O$_2$ m^{-2} d^{-1})	k_z (m^2 s^{-1})	M (g m^{-3})	c_s (g O$_2$ m^{-3})	θ	H (m)
James	40	0.16	2.89	11.57	7.63	0.66	0.25							
York	40	0.078	5.94	11.57	7.63	0.66	0.51							
Rappahannock	40	0.062	7.47	11.57	7.63	0.66	0.65							
Tributary								0.1	2	1.0×10^{-4}	2	7	1.06	10
Bay								0.05	1	Varies	2	Varies	1.06	Varies

Fig. 3. Map of Chesapeake Bay. The along-bay transect, the major rivers that input freshwater to the Bay, and the Chesapeake Bay Water Quality Monitoring Program monitoring stations in the mainstem of the Bay are indicated.

representative of the timescale of the gravitational flow (τ_e), which is referenced to the estuary mouth at latitude 37°N, and the timescale of the vertical exchange (τ_v). They are the amount of time required for water parcels to be transported into the estuary through gravitational circulation and through the vertical exchange processes, respectively.

The transport time of the gravitational circulation increased gradually toward locations upstream (Fig. 4a,c). For example, the transport time ranged from 50 d to 120 d for water parcels to travel for a distance of 122 km (latitude 38°N) upstream from the Bay mouth. The transport times were highly variable. Approximately 75 d were required for a water parcel to travel to latitude 38.5°N in July 2004, whereas it required approximately 125 d in 2000. Overall, the transport times were shorter in 2004 than in 2000. The change of transport time depends on the strength of the gravitational circulation. Because the estuary was more stratified in year 2004 than in 2000 (Hong and Shen 2012), the stronger gravitational circulation resulted in a shorter longitudinal transport time.

The transport time of the vertical exchange process at the bottom is shown in Fig. 4b,d for years 2000 and 2004, respectively. The exchange time ranges from 5 d to 15 d in the lower Bay. It increases in the middle portions of the Bay. The maximum exchange time near the bottom is 20 d to 45 d between latitudes 38°N and 39°N, where stratification is much stronger and hypoxia frequently occurs during summer. In a coastal plain estuary, the water column in the mid-estuary is typically more stratified than that in the lower estuary. Therefore, the vertical mixing is more rapid in the lower estuary than in the mid-estuary. In the case of Chesapeake Bay, the lower Bay is wider and shallower, so that the wind-induced mixing is more pronounced there. The gravitational circulation will carry a tracer released at the surface of the mid-Bay downstream before it is mixed downward. The particle will be mixed downward as it travels toward the lower Bay and then is carried upstream by the gravitational circulation. Therefore, the downstream bottom waters have a shorter age than do upstream waters. The exchange time decreases as water depth decreases further in the upper Bay, as vertical mixing increases. The change of vertical exchange time depends highly on the freshwater discharge, wind, and estuarine stratification, which will be noted in the Discussion section.

Model bottom DO in the mainstem Chesapeake Bay— Using the computed timescales for gravitational circulation and vertical exchange, the bottom-water DO of the Bay can be evaluated using Eq. 8. For Chesapeake Bay, the position of the pycnocline is stable horizontally, but the vertical location varies between 5 m and 10 m below the surface, depending on external forcing (Sanford et al. 1990; Smith and Kemp 1995). DO above the pycnocline is often well mixed, with a sharp decrease downward across the pycnocline (Sanford et al. 1990). Mean DO in the surface layer is about 85% of saturation DO along the mainstem of the Bay. The mean vertical exchange time around the pycnocline is ca. 5–10 d. Both upper and lower layers are often well mixed, with a similar vertical pattern as that of salinity (Hong and Shen 2012). We used Sta. CB4.4 as a reference station to determine the location of the pycnocline in the mainstem of the Bay. The estimated pycnocline depth was applied to the mainstem. The timescale at the pycnocline at each model grid was subtracted from the bottom timescale, except in the very shallow regions, where the total depths are less than the upper-layer thickness in deep water. The timescale τ_b was computed using parameter values listed in Table 1.

Calculated monthly mean results of each variable in 2000 along the mainstem of the Bay are shown in Fig. 5. The surface DO shown in Fig. 5 is 85% of saturation DO, and the vertical exchange time shown in Fig. 5 is the bottom timescale less the timescale at the pycnocline. It can be seen that the net oxygen consumption rate varies from 0.4 g O_2 m^{-3} d^{-2} to 0.5 g O_2 m^{-3} d^{-2} in summer. The vertical exchange time varies from 5 d to 35 d, with the maximum exchange time occurring in summer in the middle Bay. The influence of the gravitational circulation is only limited to the 30 km near the mouth ($\tau_e^* < 4$). DO
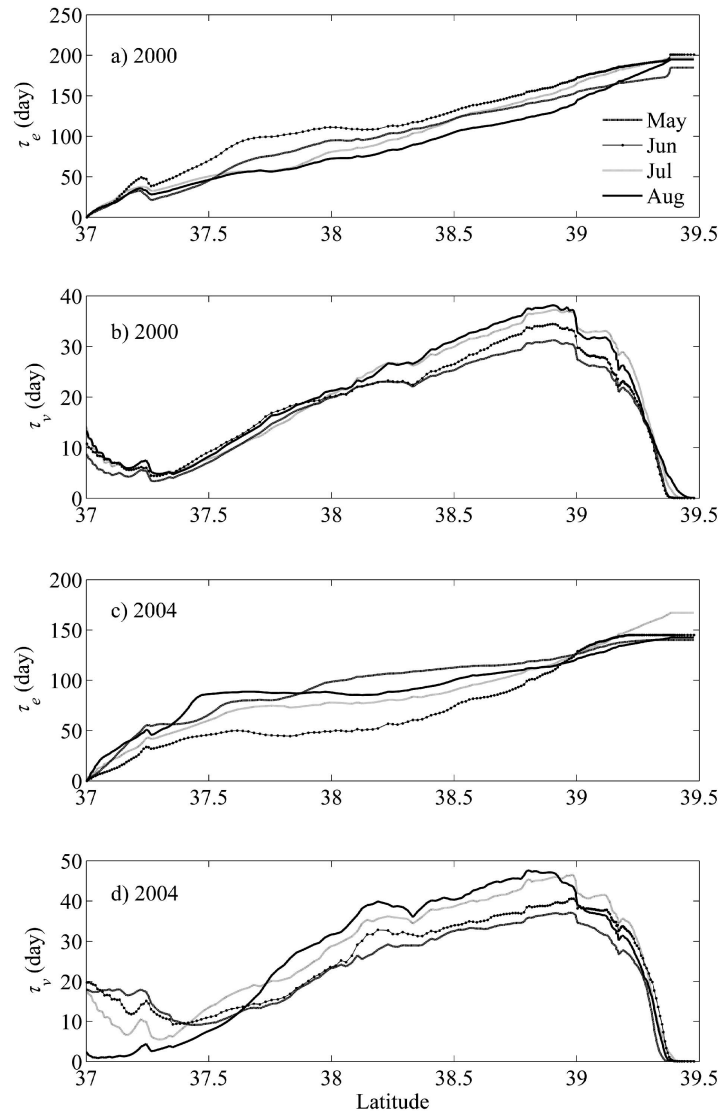
Fig. 4. (a,c) Monthly mean timescales of gravitational flow and (b,d) timescales of vertical exchange in 2000 and 2004, respectively.

distribution was mainly controlled by the balance between the DO consumption and the vertical replenishment.

Comparisons of the conceptual model results and observations of bottom DO along the mainstem of the Bay (*see* Fig. 3) from May to August are shown in Fig. 6, for years 2000 and 2004. Observation data were obtained from the U.S. Environmental Protection Agency's Chesapeake Bay Program (http://www.chesapeakebay.net/data/downloads). Because only one or two measurements were taken in each month and the dates were not the same for each station, we plot all available bottom DO data for each month from May to August. Daily DO was computed; and modeled maximum, minimum, and mean values over a period of 20 d that covered the observations in each month were plotted for comparison.

It can be seen that the DO distribution estimated by the conceptual model matches the observations in general. Because constant DO consumption rates were used, deviations of model results from observations can be expected.

Overall, the model results agree with observations in the same range and show the same temporal and spatial variations as do the observations. Figure 7 compared the model results and observations at selected Sta. CB4.4 and CB3.3C in 2000. It can be seen that the seasonal variation of the bottom-water DO can be modeled by these two dimensionless parameters, indicating that the simplified conceptual model can be used to diagnose the bottom DO conditions based on the variations of dimensionless timescales.

Discussion

Influence of DO consumption—We use the total oxygen consumption rate (B in Eq. 4) to quantify the complex biochemical processes. The purpose is to discern the influences of physical and biochemical processes on bottom DO. With the use of a constant rate corrected by temperature variation, the seasonal variations of the bottom DO concentrations can be estimated. Figure 5
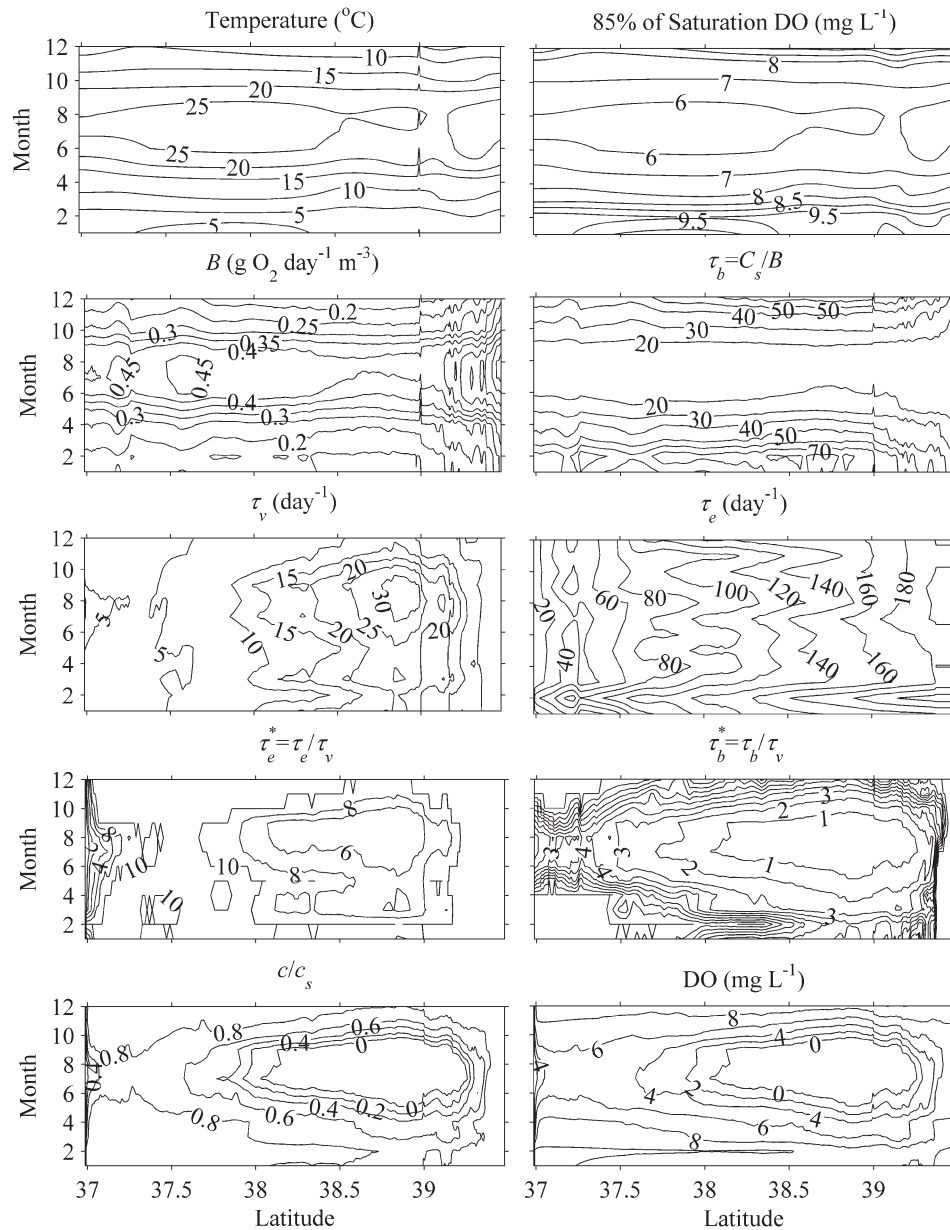
Fig. 5. Distribution of monthly mean key model parameters, computed timescales, and DO along the mainstem of the Bay.

shows that the timescale of DO consumption has the same order as the vertical exchange timescale in summer, but the timescale of DO consumption is about twice as large as the vertical exchange time during spring and winter. Therefore, no hypoxia occurs in spring and winter. On the other hand, from the mouth to approximately latitude 37.7°N, the vertical exchange timescale is shorter than the DO consumption timescale in summer; this results in a good DO condition, even though the DO consumption rate in the lower Bay is the same as that in the upper Bay. Because oxygen consumption rates vary both spatially and temporally, deviations of the model results from the observations can be observed (Fig. 7). The biochemical rates can be obtained from the observations. Boynton and Kemp (1985)

conducted measurements of SOD at selected stations in Chesapeake Bay. By adding the measured water column respiration, total oxygen consumption rates at different stations in May and August ranged from $3.2 \text{ g O}_2 \text{ m}^{-2} \text{ d}^{-1}$ to $19.1 \text{ g O}_2 \text{ m}^{-2} \text{ d}^{-1}$, with a mean value of $7.52 \text{ g O}_2 \text{ m}^{-2} \text{ d}^{-1}$. High rates were observed in the upper and middle portions of the Bay. Assuming the thickness of the lower layer to be 20 m in the middle Bay, the total oxygen consumption rates ranged from $0.16 \text{ g O}_2 \text{ m}^{-3} \text{ d}^{-1}$ to $0.96 \text{ g O}_2 \text{ m}^{-3} \text{ d}^{-1}$, with a mean rate of $0.38 \text{ g O}_2 \text{ m}^{-3} \text{ d}^{-1}$. Our rate is within the same range (Fig. 5), but the model will not capture the DO variations due to biochemical processes that deviate from the mean. It can be seen that biochemical processes have a large influence on DO.
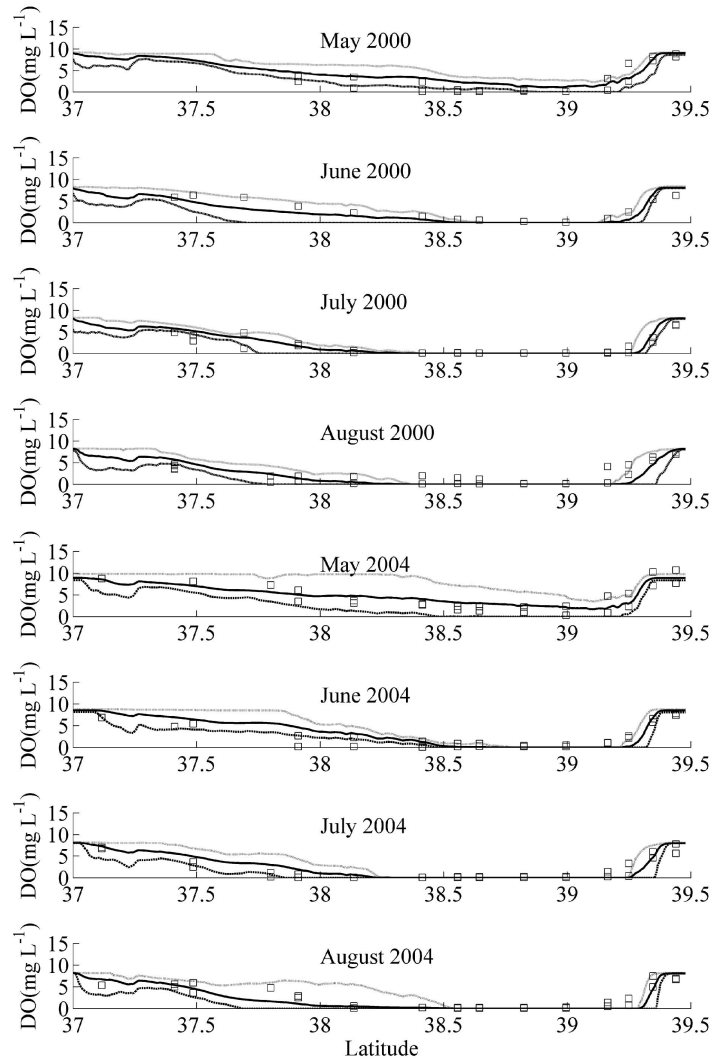
Fig. 6. Comparisons of conceptual model results and observations of the bottom DO from May to August in 2000 and 2004 (lines are model results of monthly mean, minimum, and maximum DO concentrations in each month; squares are available observations in each month).

The conceptual model can also be used for estimating the total oxygen consumption rate if dynamic timescales are known. Based on Eqs. 5 and 7, the total oxygen consumption rate can be expressed as:

$$B = \frac{c_s - c}{\tau_v} \left(1 - e^{-\tau_e^*}\right)^{-1} \qquad (13)$$

For example, surface DO was ca. 7.0 g m^{-3} in May 2000 at Sta. CB4.4 (latitude 38.4°N, Fig. 5b). Measured bottom DO was 0.1 g m^{-3} on day 145 (Fig. 7). τ_e and τ_v in May were ca. 120 d and 15 d, respectively. The computed total DO consumption rate using Eq. 13 was 0.46 g O$_2$ m^{-3} d^{-1}. The estimated total DO consumption rate used in our model application was 0.30 g O$_2$ m^{-3}d^{-1}, which was lower than the calculated value. Therefore, our model result on day 145 was higher than the observation (Fig. 7). In August, our estimated total DO consumption rate was higher than that calculated using Eq. 13. Because the entire bottom DO was consumed in August, the high DO consumption rate used in the model does not make any difference for the DO prediction.

Influence of gravitational circulation—Gravitational circulation is more important in tributaries because it is comparable to vertical transport processes. If bottom DO at the mouth of an estuary is not close to the saturation DO, Eq. 6 should be used to account for the boundary condition. The gravitational circulation has influence near the mouth and has less influence from the middle to the upper Bay. For example, if τ_e^* is larger than 6 in August 2000 at Sta. CB4.4 (Fig. 5), the relative contribution of gravitational circulation to bottom DO, $e^{-\tau_e^*}$ as shown in Eq. 9, is less than 1%. Because all DO is consumed, the effect of gravitational circulation on replenishing bottom DO diminishes toward the middle and upper portions of the Bay. Thus, the bottom DO in the middle to upper Chesapeake Bay is located in the A-2 and B-2 regions shown in Fig. 2a, which are mainly controlled by the
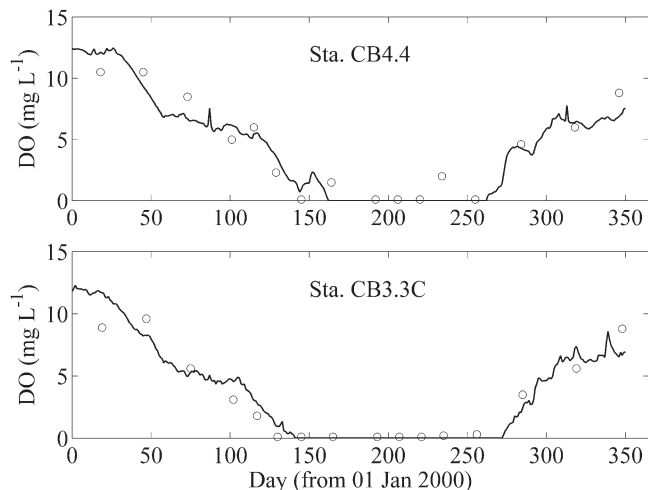
Fig. 7. Comparisons of conceptual model results and observations at Sta. CB4.4 and CB3.3C, respectively, in 2000 (lines are model results, circles are observations).

competition between biochemical processes and vertical exchange processes.

The gravitational flow can be evaluated based on observations of residual current. For a relatively uniform estuary, the gravitational flow can also be estimated based on Hansen and Rattray's (1965) analytical solution, which was derived from the balance between the horizontal density gradient and the vertical turbulent diffusivity. For an estuary with complex geometry, the gravitational flow is not a constant along the estuary, and it is not readily obtainable, due to tide and the geometry effect (Jay and Smith 1990). Therefore, using a 3D numerical model to compute the gravitational flow is an appropriate approach that provides more accurate results. When using the 3D model–computed dynamic timescales, one essentially integrates the conceptual model with varying cross-sections and changes of dynamic fields.

Influence of vertical exchange process—It is interesting to see that hypoxia and anoxia in Chesapeake Bay mainly result from the competition between vertical DO replenishment and biochemical DO consumption. Figure 5 shows that biochemical processes have a pattern of high DO consumption in summer, with little longitudinal variation; whereas vertical transport time increases in summer in the middle Bay. Neither distribution has the pattern of low DO. When plotting τ_b^*, which measures the competition between biochemical and physical processes, the pattern of low DO appears. It can be seen that low DO is due to high DO consumption but is modulated by vertical exchange processes. Because we used a simple approach to determine the pycnocline and used bottom exchange time referenced to the pycnocline to estimate the DO, a discrepancy between model and observations can be expected. However, the results are reasonably good because the bottom exchange time has little vertical variation in the lower layer of the Bay and the horizontal pycnocline is relatively stable.

The vertical exchange time computed by the 3D model is different from the timescale estimated using a constant k_z
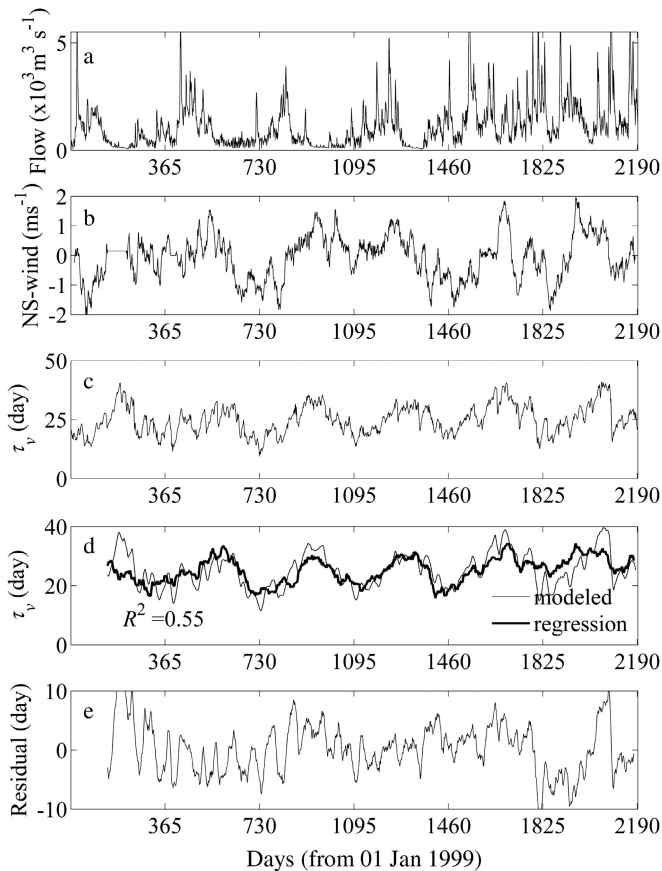

Fig. 8. (a) Daily Susquehanna River discharge, (b) 30 d low-pass-filtered north–south (NS) wind, (c) 3D numerical model calculated vertical exchange timescale at Sta. CB4.4, (d) regression (using Susquehanna River discharge and wind) results of vertical exchange timescale at Sta. CB4.4, superimposed by the 15 d low-pass-filtered vertical exchange timescale shown in (c). The river discharge data used in the regression has a 120 d shift and was moving averaged in 70 d intervals, (e) errors in the regression results. All the data and results (a–e) are presented from 1999 to 2004.

value measured or computed using the turbulent closure models, which is on the order of 1.0×10^{-5} m² s⁻¹ to 1.0×10^{-4} m² s⁻¹. For a depth of 20 m, the timescales for turbulent mixing are on the order of 46 d to 460 d. Significant portions of the estuarine cross-section have Richardson numbers greater than 0.25, an expected threshold value for which direct turbulent flux through the pycnocline is effectively reduced to zero (Scully 2010). Our vertical exchange time is short and changes with external forcings, and it accounts for mixing and lateral circulation–induced exchanges between the surface and bottom layers, which play a critical role in deep-water ventilation processes in the Bay (Scully 2010).

Vertical exchange processes are highly variable depending on the external forcing. The short vertical exchange time in the lower Bay is mainly due to changes of estuarine stratification and wind. The greater width and large shallow areas make the lower Bay more susceptible to wind-induced mixing. On the other hand, the upper middle Bay is narrower and has a higher stratification. Figure 8a,b,c shows,

respectively, the dominant discharge of the Susquehanna River, the north–south monthly wind component at Solomons Island, and the model-calculated vertical exchange timescale at Sta. CB4.4 from 1999 to 2004. These figure parts clearly show annual variations of external forcings. It is found that freshwater discharge is a major factor in regulating stratification (Boicourt 1992) and is a predictor of the summertime hypoxic volume. High discharge increases stratification and nutrient supply, which enhances primary production (Hagy et al. 2004; Murphy et al. 2011). The observations showed that the time required for salinity in the upper Bay at latitude 38.4°N to respond to Susquehanna River discharge is about 1 month (Boicourt 1992). The salinity response can require 2–3 months in the middle to lower portions of the Bay because the estuary–ocean exchange is on the order of 80–120 d (Austin 2002; Shen and Wang 2007). A regression of nontidal vertical exchange timescales at Sta. CB4.4 was conducted with respect to the Susquehanna River discharge and 30 d moving-averaged north–south wind components at Solomons Island. Considering the cumulative effect of freshwater discharge, a 70 d moving-averaged discharge was used for regression. Regressions with different windows of moving-averaged flow and delay time were also tested. The highest correlation ($R^2 = 0.55$, $p < 0.0001$) was attained with the moving average of 70 d and a delay of 120 d. Figure 8d shows the comparison of modeled and regression results of vertical exchange timescales. The large exchange timescale occurred in summer, corresponding to the high flow in spring and change of wind direction. Note that we only fit the low-frequency variation of the vertical exchange timescale because the averaged flows and daily wind are used for the regression. A large deviation can be observed, and the deviation can be up to 10 d (Fig. 8e), which is caused by other high-frequency forcings such as wind- and tide-induced vertical mixing and lateral circulation. Because both wind and freshwater have annual cycles, the contribution of freshwater and wind on vertical exchange cannot be separated based on the current regression approach. Scully (2010) shows that wind is the dominate forcing to modulate the bottom DO in the Bay. Wind and freshwater effect on vertical exchange timescale warrant further study.

This conceptual model quantifies the physical processes with two timescales and the biochemical processes with one single timescale. The single biochemical timescale represents all the oxygen consumption processes as a sink term. As long as the oxygen consumption rate can be determined, and timescales can be appropriately computed, it should be applicable to any estuary with persistent gravitational circulation. The two physical timescales represent two distinctive sources of oxygen replenishment: surface water oxygen and the high-oxygen water at the estuary mouth. The model assumes that both the surface water and the bottom water at the estuary mouth are at or near saturation. The first assumption may be true for most estuaries that have no significant point source of wastewater discharge. However, the second assumption may be violated for an estuary with a short residence time, in which

significant oxygen consumption materials have not been oxidized before being exported out of the estuary. If either of the assumptions is violated, the model is not applicable. Further efforts are needed to modify the model; perhaps an additional parameter quantifying the boundary conditions of oxygen sources will do. The model uses vertical exchange as the pathway for surface-water oxygen to reach the bottom water; it should be applied for the entire water body. However, it relies on the upstream transport of gravitational circulation to carry high-oxygen water from the estuary mouth. The model should not be used in a case in which a persistent gravitational circulation does not exist. For an estuary that violates the underlying assumptions, which would preclude quantitative use of the conceptual model, the model would still be informative in diagnosing the bottom DO condition.

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