

A simple surface water biogeochemical model

2. Simulation of selected lacustrine and marine settings

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Abstract. A linear, three-component (nitrate, phytoplankton, and zooplankton) biogeochemical model coupled to a one-dimensional turbulence closure fluid dynamic model successfully reproduces most of the thermal and biogeochemical features of three marine settings (Bermuda Station “S” in the oligotrophic portion of the North Atlantic subtropical gyre, Ocean Weather Station “India” in the North Atlantic subpolar gyre, and the 60-m isobath of the New York Bight) and one freshwater lake (South Bluehill Pond in Newfoundland). Model reproduction of temperature in all four settings is good. Model temperature gradients in the thermocline are somewhat steeper than those observed in the data of the three marine settings due to the inability of the one-dimensional fluid flow model to reproduce internal waves which can be a significant source of vertical mixing in large water bodies. Nitrate and chlorophyll are predicted reasonably well by the model at Bermuda Station “S” and the New York Bight. Underprediction of surface nitrate at Station “India” is probably due to the lack of an ammonium component in the model. Model reproduction of the spring bloom productivity in the marine settings is good, although post-bloom model productivity is generally too low. Biogeochemical simulations of South Bluehill Pond are strongly dependent on the value of the light attenuation coefficient used in the model. A relatively high attenuation coefficient (most likely representing high inorganic sediment concentrations) is necessary to accurately reproduce nitrate and chlorophyll concentrations. These results illustrate the necessity of accurately characterizing the light regime prior to using the model in lacustrine settings.

Introduction

Numerical models have emerged as a fundamental tool for studying a wide variety of geochemical processes. Modeling nutrient and oxygen cycles in surface water is particularly important for understanding both modern and ancient aquatic environments. Examples include lakes and reservoirs [*Gachter and Imboden*, 1985; *Jewell*, 1992], estuaries [*Kremer and Nixon*, 1978; *Cero and Cole*, 1992], marine continental shelves [*Walsh*, 1975; *Walsh et al.*, 1988; *Hofmann*, 1988], ocean basins [*Wroblewski et al.*, 1988; *Sarmiento et al.*, 1993], the modern world ocean [*Najjar et al.*, 1992], and the world ocean in the geologic past [*Shaffer*, 1989].

Two difficulties are inherent in the design and application of these models. One is the necessary complexity of a model which attempts to simulate the myriad biogeochemical processes and components observed in nature. Developers of even the most complex models acknowledge that they fall short of capturing the multitudinous processes of an aquatic ecosystem [e.g., *Fasham et al.*, 1990]. A second feature of existing biogeochemical surface water models is the relatively restricted scope of their applications. For instance, models of open ocean ecosystems are rarely applied to estuaries, while those developed for lakes have not been tested against data from the marine mixed layer.

This paper is the second in a series aimed at developing simple biogeochemical surface water models which are applicable in a wide variety of surface water aquatic settings. The

biogeochemical model, sensitivity analyses, and idealized simulations are described by *Jewell* [this issue]. In this paper the model is applied to four marine and lacustrine settings with very extensive databases and diverse physical and biogeochemical characteristics.

Model Description

The majority of previously developed biogeochemical models employ seven or more components coupled by rate constants and a variety of parameters which must be determined empirically from field or laboratory studies [e.g., *Hofmann and Ambler*, 1988; *Fasham et al.*, 1990, 1993; *Ambrose et al.*, 1993]. However, the basic dynamics of photosynthesis and respiration in surface water settings can be reproduced with a three-component biogeochemical model (a generic limiting nutrient, phytoplankton, and zooplankton/detritus) which is coupled to a one-dimensional (vertical) turbulence closure fluid dynamic model [*Jewell*, this issue]. Zooplankton/detritus is transferred from the euphotic zone to depth by an empirical biogenic flux-depth equation. The model reproduces standard features observed in temperate-latitude surface waters including a spring phytoplankton bloom following convective overturn of the water column as well as depletion of surface water nutrients, and deep water nutrient enrichment following the spring bloom. The model also produces features such as a late-season, deep chlorophyll maximum which have been described in the literature, but whose origins are poorly understood [e.g., *Steele*, 1964; *Kiefer et al.*, 1972; *Fee*, 1976; *Fasham et al.*, 1993].

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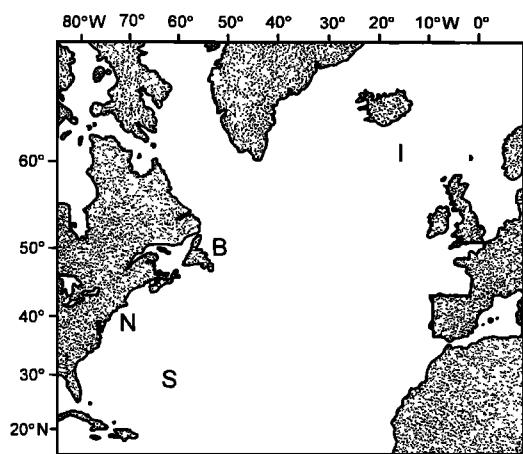


Figure 1. Location of field localities described in the text. S denotes Bermuda Station "S" in the Atlantic. I denotes Weather Station "India" in the northern Atlantic. N denotes New York Bight off the coast of the eastern United States. B denotes South Bluehill Pond, Newfoundland.

Model Applications

Several criteria were used to select sites for model application. Locations were sought which had excellent biogeochemical databases and which had been published in widely circulated journals or books. Within this general framework a diversity of physical and chemical characteristics was considered desirable. The four sites (two open ocean, one coastal ocean, and one lacustrine) selected for model validation lie between 30° and 60° latitude (Figure 1). All show convective overturn in the spring followed by a bloom of biological productivity and subsequent vertical segregation of biogeochemical components.

The two open ocean settings (Bermuda Station "S" and Ocean Weather Station "India") were chosen for model validation on the basis of their excellent biogeochemical databases and extensive exposition in a previous, ocean general circulation-ecosystem model study [Fasham *et al.*, 1993; Sarmiento *et al.*, 1993]. Both the Bermuda and the India stations are in the open ocean over water deeper than that considered appropriate for this model (<1000 m) [Jewell, this issue]. For these simulations the model domain only encompassed the maximum depth of the seasonal thermocline [Levitus, 1982] (Table 1). In this way, the physics of the biologically active portion of the water column, the seasonal character of the spring bloom, and the subsequent biogeochemical evolution of the mixed layer could be examined without the necessity of modeling the entire water column.

Coastal marine settings represent a potentially complicated setting for model validation. Freshwater input from rivers can cause density stratification which is difficult to reproduce with a one-dimensional model. Furthermore, the temperature and biogeochemistry of coastal settings can be strongly influenced by exchange with the open ocean. The New York Bight was chosen for model validation on the basis of its excellent databases collected over a number of years [Walsh, 1981, 1988]. Density stratification due to salinity (approximately 1.5‰ from the top to the bottom of the water column) is not as important as stratification brought about by temperature in this setting. The uncertainties involved in advective transport

of heat and chemical components from the open ocean to the New York Bight are discussed below.

Small lakes are relatively amenable to one-dimensional models since horizontal gradients of heat and chemical components are minor relative to vertical gradients [e.g., Gachter and Imboden, 1985]. Lakes can present additional complications, however. They are often shallow and have a tendency to freeze during the winter at temperature latitudes. Inorganic sediment in the water column can attenuate light in a manner which is often difficult to model without knowledge of the optical features of a particular lake. South Bluehill Pond in Newfoundland was selected for model validation on the basis of the extensive temperature, geochemical, and light attenuation data described by Kerekes [1974].

The model used in this study is constructed so that either nitrate or phosphate can be used as a limiting nutrient [Jewell, this issue]. Nitrate is modeled in each of the four settings of this study. For all model applications the initial nitrate and temperature conditions were close to those of the vertically homogeneous water column observed during the spring overturn (Table 1). A fixed surface temperature boundary condition consisting of measured temperatures was used in all simulations. The bottom temperature boundary condition was set at 60 mW/m², an average value for continental heat flow. Zero-flux boundary conditions were specified for all biogeochemical components at both the bottom and the surface [Jewell, this issue].

Wind was modeled as a diurnally varying sine wave. Maximum wind strength was varied until the depth of the thermocline in the model simulations was close to the observed thermocline depth. Alternating the direction of the wind over a period of 1 day provides time-varying kinetic energy input to the aquatic domain in a fashion similar to that of natural settings, although the diurnal frequency is obviously not the same as wind variations in natural settings. While determining wind strength and variability in this fashion is very idealized, it should be emphasized that the purpose of this study was to study the biogeochemistry rather than the physics of these four domains.

The physical model used in this study is based on the second-

Table 1. Summary of Variables Used in Applications of the Biogeochemical Model

Variable	Bermuda Station "S"	Station India	New York Bight	South Bluehill Pond
Depth, m	150 ^a	400 ^a	60	23
Latitude, degrees	30	60	40	48
Initial temperature, °C	20 ^b	9 ^b	9 ^c	4 ^d
Initial nutrient concentration, mmol/m ³ NO ₃ ⁻	0.7 ^b	10. ^b	6.0 ^c	3.0 ^d
Maximum wind strength, m/s	14	14	12.7	9
Cloudiness, %	0.4 ^e	0.8 ^e	0.6 ^e	0.7 ^e
Water attenuation coefficient, m ⁻¹	0.04 ^f	0.04 ^f	0.04 ^f	0.04, 0.35 ^{d,f}

^aMaximum depth of the seasonal thermocline [Levitus, 1982].

^bFasham *et al.* [1993].

^cWalsh [1981].

^dKerekes [1974].

^ePeixoto and Oort [1992].

^fJerlov [1976].

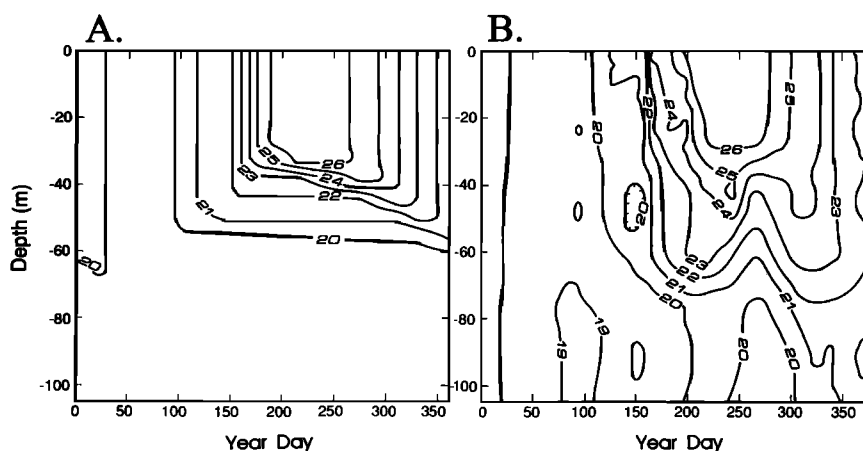


Figure 2. Time-depth temperature at Bermuda Station "S": (a) model computations; (b) data [from *Fasham et al.*, 1993].

order turbulence closure scheme described by *Mellor and Yamada* [1974, 1982]. One-dimensional versions of the Mellor-Yamada model have a track record of accurately reproducing the thermal structure of marine and lacustrine domains [*Mellor and Durbin*, 1975; *Klein and Coste*, 1984; *Jewell*, 1992]. Even though only idealized wind forcing was used in this study, realistic formulation of vertical eddy diffusivity through the water column was possible with the Mellor-Yamada turbulence closure scheme. Realistic vertical mixing is a very important control of the vertical transfer of biogeochemical components.

The time step for the model simulations was 30 min. Forty vertical grid points with logarithmic spacing for the top three grid points were used in all of the model runs. For all four settings the model was run for 3 years with output from the final year being saved for analysis. Differences between model results of the second and third year were minimal.

Bermuda Station "S"

Bermuda Station "S" is located in the middle of the subtropical gyre of the Atlantic Ocean (Figure 1). Previous studies of the biogeochemistry of Bermuda Station "S" include *Menzel and Ryther* [1960], *Be et al.* [1971], *Deevey* [1971], and *Altabet* [1989]. Results of these studies have been summarized by *Fasham et al.* [1990, 1993]. Although the model depth for Bermuda Station "S" was 150 m (Table 1), only the upper 110 m is shown in Figures 2–5. In this manner, the model results can be more directly compared with the data summaries and model results given by *Fasham et al.* [1993].

The general thermal structure of Bermuda Station "S" is reproduced reasonably well by the model (Figure 2). The numerical model produces a thermocline which is much sharper than that seen in the data. As discussed by *Jewell* [1992], this is probably due to the fact that while the one-dimensional fluid dynamic model accounts for both shear and buoyant turbulent energy production, it cannot reproduce horizontal features such as internal waves, which tend to increase the amount of vertical mixing in stratified waters. Incursions of water with variable temperature between 40–100 m depth observed in the data (Figure 2b) are probably the result of horizontal advection, which also obviously cannot be reproduced by the one-dimensional model. More realistic formulation of the surface

wind boundary condition might also have improved model simulations of temperature.

The general features of the seasonal nitrate structure are also reproduced by the model, although some discrepancies can be noted (Figure 3). The model shows complete vertical mixing of nitrate around year day 70, whereas the nitrate data retain some vertical stratification during this period of time. In contrast to simulations of temperature, the model produces late-season vertical nitrate gradients which are much more diffuse than those in the data. The depth of the greatest vertical nutrient gradient (the nutricline) is greater in the data than it is in the model. This discrepancy was also noted in the ocean general circulation–ecosystem model simulations of Bermuda Station "S" described by *Fasham et al.* [1993], who attributed it to the relatively shallow mixed layer produced by their general circulation model. Note, however, that the thermocline and the nutricline in the model results presented here are at the same depth (approximately 40–50 m) (Figures 2a and 3a), whereas the data show a thermocline and nutricline at distinctly different depths (Figures 2b and 3b). Like the temperature data, irregularities in the deep nitrate data are most likely the result of horizontal nutrient advection.

It is important to reemphasize that the model depth at Bermuda Station "S" (150 m) (Table 1) is greater than the depths shown in Figures 2–5 (110 m). This means that relatively high concentrations of nutrients are present between 110 and 150 m during periods of thermal stratification in the model. These nutrients reenter the photic zone when the stratification breaks down. As stated previously, this procedure was undertaken as an alternative to modeling complete, deep ocean settings.

The general structure of the chlorophyll data produced by the model (Figure 4) is not as good as that for temperature and nitrate. In both data and model, the maximum chlorophyll concentration during the spring bloom is about 0.5 mg/m^3 , although the most intense portion of the spring bloom occurs approximately 1 month later in the model than in the data. A deep chlorophyll maximum (DCM) of approximately 0.5 mg/m^3 appears in both the model and the data, although like nutrients, the DCM shallower in the model than it is in the data. A similar, shallow DCM is reported in the simulations of *Fasham et al.* [1993], who attribute it to the phytoplankton

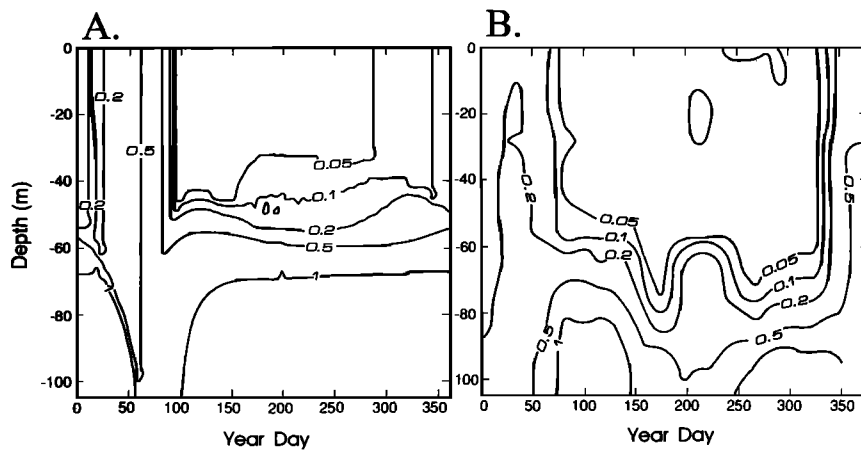


Figure 3. Time-depth nitrate concentrations (millimoles per cubic meter) at Bermuda Station "S": (a) model computations; (b) data [from *Fasham et al.*, 1993].

mortality rate of their model being too high. Decreasing phytoplankton mortality in this model still produced a DCM and in fact had very little influence on the overall pattern of biological productivity. As pointed out in a discussion of generalized simulations using this model [*Jewell*, this issue], the model DCM appears to be a result of sharply increased vertical eddy diffusivity (and hence increased nutrient flux) immediately below the thermocline. The DCM is a noteworthy feature of a variety of marine settings [e.g., *Parsons et al.*, 1984; *Walsh*, 1988; *Fasham et al.*, 1990, 1993], and determining its precise cause must await further, careful field and modeling studies.

Biological productivity simulations as a function of depth closely follow those of chlorophyll (Figure 5a). Surface productivity in both the simulations and the data from Bermuda Station "S" reach a maximum value of approximately $10 \text{ mg C m}^{-3} \text{ d}^{-1}$, although maximum productivity in the data is approximately 20 days earlier than it is in the model. Surface productivity drops off sharply in both the model and the data after year day 100. A late-season deep productivity maximum of approximately $2 \text{ mg C m}^{-3} \text{ d}^{-1}$ produced by the model is only weakly seen in the data between year days 200 and 300.

Vertically integrated productivity generally parallels published data (Figure 6). The spring bloom is reproduced quite

well, although the measured productivity data are generally higher than the model in the later part of the year.

Ocean Weather Station "India"

Data from Ocean Weather Station "India" are given by *Williams and Robinson* [1973] and *Williams* [1988] and are also summarized in the ecosystem model study of *Fasham et al.* [1993]. Like Bermuda Station "S," Ocean Weather Station "India" is exceptional in its seasonal data coverage of many biogeochemical components including surface productivity. The modeled depth of Station "India" (i.e., maximum seasonal mixed layer depth) is significantly greater than Bermuda Station "S" (350 versus 150 m). Station "India" makes an interesting contrast to Bermuda Station "S" because (1) its relatively high latitude (60°N) means that surface productivity is light limited for much of the year and (2) nutrient concentrations at this location are much higher than those of Bermuda Station "S."

Like Bermuda Station "S" the modeled thermocline at Station "India" is steeper than that observed in the data (Figure 7). The observed temperature profile is also much more irregular than that produced by the model. Again, horizontal ad-

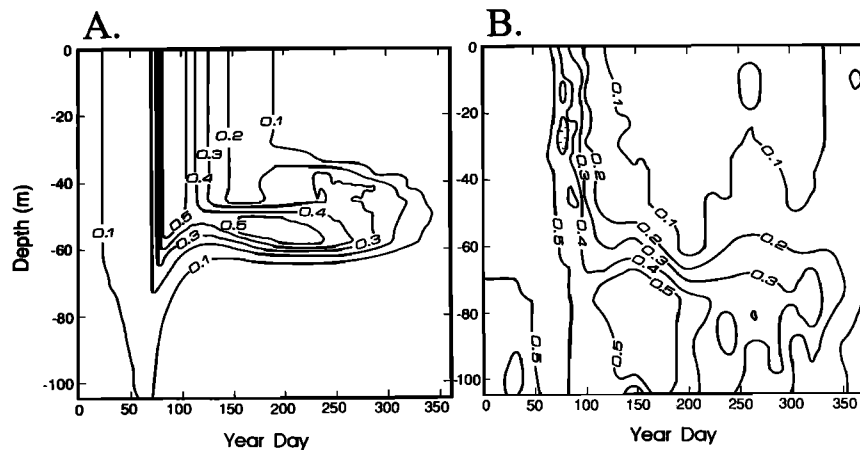


Figure 4. Time-depth chlorophyll *a* concentrations (milligrams per cubic meter) at Bermuda Station "S": (a) model computations; (b) data [from *Fasham et al.*, 1993].

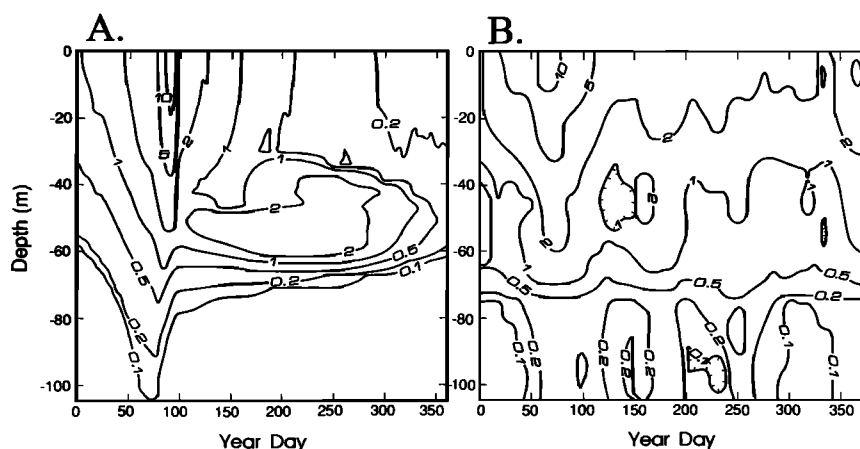


Figure 5. Time-depth productivity ($\text{mg C m}^{-3} \text{d}^{-1}$) at Bermuda Station "S": (a) model computations; (b) data [from *Fasham et al.*, 1993].

vection of thermally variable water is the most likely cause of these irregularities.

Nitrate data for Station "India" are also irregular and somewhat discontinuous due to incomplete sampling (Figure 8). Nitrate in the shallow depths during seasonal stratification of the model is much lower than that observed in the data. The relatively high surface nutrients observed in the North Atlantic [*Williams and Robinson*, 1973; *Williams*, 1988] were also reproduced by the ocean general circulation–ecosystem model of *Fasham et al.* [1993] and *Sarmiento et al.* [1993]. These authors attribute the high-latitude surface nutrients to (1) high nutrient concentrations at depth which cause high diffusive fluxes across the nutricline and into the surface layer and (2) preferential uptake of ammonium relative to nitrate by phytoplankton. The large ammonium concentrations produced in the models of *Fasham et al.* [1993] and *Sarmiento et al.* [1993] are the result of excretion from large amounts of zooplankton produced by the spring bloom. Ammonium is not included in the three-component model of this study, and this may be the reason modeled nitrate concentrations in surface waters are much lower (Figure 8a).

The initial spring bloom seen in the data (occurring around year day 150) is well reproduced by the model (Figure 9). Maximum chlorophyll concentrations are greater than 2 mg/m^3 in both the data and the model. Two smaller phytoplankton blooms observed in the data in midsummer and early fall (maximum chlorophyll concentration of approximately 1 mg/

m^3) are not reproduced by the model. These secondary blooms were, however, reproduced by the model of *Fasham et al.* [1993] and *Sarmiento et al.* [1993], who attribute them to high summertime ammonium concentrations. If so, this would explain the lack of secondary blooms in this model. Note, however, that the modeled productivity does show three progressively smaller surface blooms (maximum productivity values of 5, 1, and $0.5 \text{ mgC m}^3/\text{d}$) throughout the summer and fall (Figure 10a). These relatively small blooms are not reflected in modeled surface chlorophyll between year days 170 and 270 (Figure 9a).

Interestingly, neither the data nor the model results show a deep chlorophyll maximum similar to that observed and modeled at Bermuda Station "S" (Figure 4). The lack of a deep chlorophyll maximum in the model appears to be the result of generally low productivity after year day 200 (Figures 10 and 11).

Vertically integrated productivity calculated by the model agrees quite well with that shown by the data (approximately $1.5 \text{ g C m}^{-2} \text{ yr}^{-1}$) (Figure 11). Model productivity drops off sharply following the spring bloom, while measured values remain as high as $0.7 \text{ g C m}^{-2} \text{ yr}^{-1}$ between year days 200 and 300 (approximately mid-July to late October).

New York Bight

The hydrography, biology, and geochemistry of the New York Bight have been studied extensively [*Walsh et al.*, 1978, 1987; *Conway and Whitedge*, 1979; *Falkowski et al.*, 1980, 1983; *Harrison et al.*, 1983]. These field studies have also been incorporated into a numerical study of productivity and phytoplankton of the New York Bight [*Walsh et al.*, 1988].

The New York Bight was the most computationally challenging of the four domains used for model validation. Continental shelf hydrography and geochemistry are often influenced by advection of water from both continental runoff and the open ocean. In the New York Bight, river runoff produces some salinity stratification. Vertical salinity differences as high as 1.5‰ and temperature differences as high as 9°C have been documented at the 60-m isobath [*Walsh et al.*, 1978]. Density stratification due to salinity (approximately 1 kg/m^3) is therefore not as great as density stratification due to temperature (approximately 3 kg/m^3) [e.g., *Pond and Pickard*, 1983, Figure 2.1]. Vertical homogenization of both temperature and nutri-

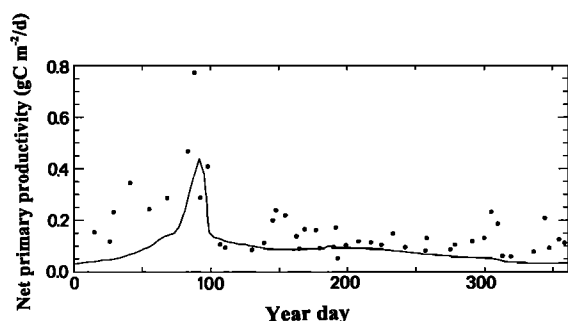


Figure 6. Vertically integrated surface productivity at Bermuda Station "S" as computed by the model (solid line) and as measured in the field (solid circles) [from *Fasham et al.*, 1993].

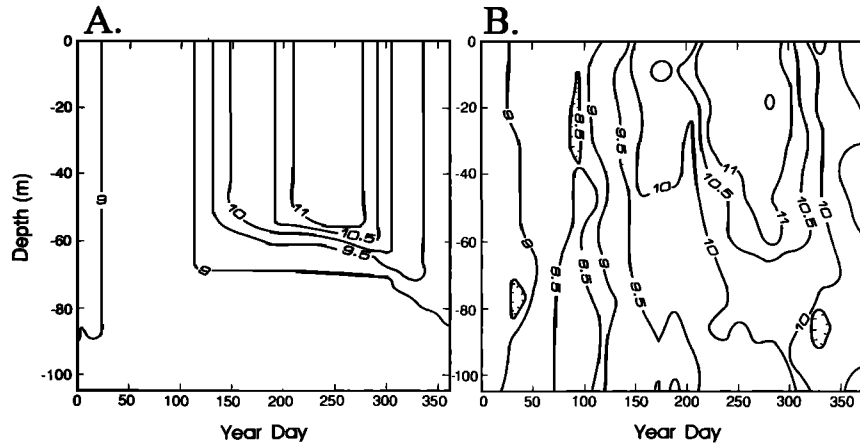


Figure 7. Time-depth temperature at Weather Station "India": (a) model computations; (b) data [from Fasham *et al.*, 1993].

ents is observed during spring and fall in the composite data of Walsh [1981] and Walsh *et al.* [1987] (Figures 12 and 13), suggesting that salinity does not dominate the density structure of this portion of the New York Bight.

For the New York Bight simulations both observed surface and bottom water temperatures were used as fixed-value boundary conditions, rather than assuming a bottom heat flux boundary condition as was done for the other simulations. This was done in order to more accurately model the effects of the incursion of water with varying thermal characteristics over the New York Bight. Again, it should be emphasized that the purpose of this study was simulation of biogeochemical rather than physical features of these settings. Model results of temperature using this method of boundary condition formulation appear to be reasonable (Figure 12). As with the two open ocean simulations, modeled temperature gradients in the thermocline are steeper than those observed in the data.

Initial nutrient concentrations in the simulations were set equal to an averaged homogeneous value of the spring overturn ($6 \text{ mmol NO}_3^-/\text{m}^3$) (Table 1). Variations in observed, vertically homogeneous nutrient concentrations ($5\text{--}7 \text{ mmol NO}_3^-/\text{m}^3$) during spring overturn (Figure 13b) suggest horizon-

tal advection of water with variable nutrient concentrations into waters at the 60-m isobath. This is also suggested by irregular, high ($>10 \text{ mg/m}^3$) chlorophyll concentrations between 30 and 50 m depth during the spring (Figure 14).

Numerical simulations of nitrate following convective overturn show good correspondence with the data (Figure 13). Surface nitrate concentrations are drawn down to $<1 \text{ mmol/m}^3$ during the height of seasonal stratification, while bottom water nitrate concentrations as high as 9 mmol/m^3 are seen in both model simulations and the data. The late-season nutricline is observed between 30 and 50 m depth in both the simulations and the data. Phytoplankton concentrations are somewhat less well predicted by the model (Figure 14). The model shows a high of 2 mg/m^3 chlorophyll associated with the spring bloom at approximately year day 130. Maximum spring chlorophyll occurs earlier (year day 80–90) and in deeper water (30–50 m), although as mentioned previously, this may be due to horizontal advection of water with different biogeochemical characteristics. The late-season deep chlorophyll maximum at approximately 30 m depth can be seen in both model and data, although the feature is much more diffuse in the data.

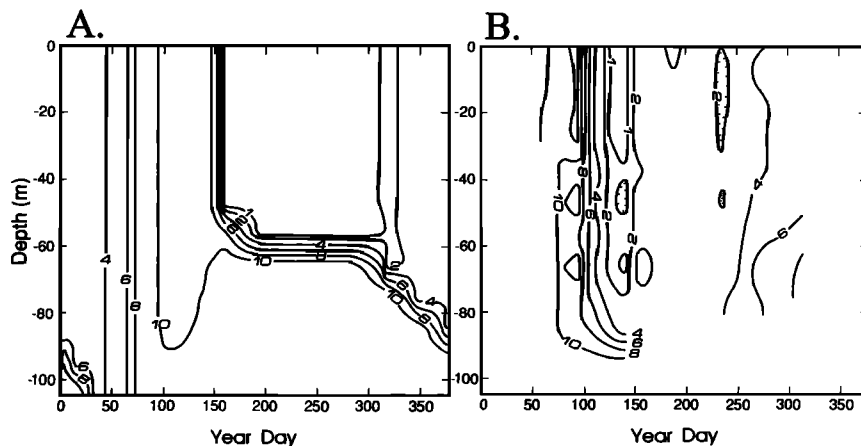


Figure 8. Time-depth nitrate concentrations (millimoles per cubic meter) at Weather Station "India": (a) model computations; (b) data [from Fasham *et al.*, 1993].

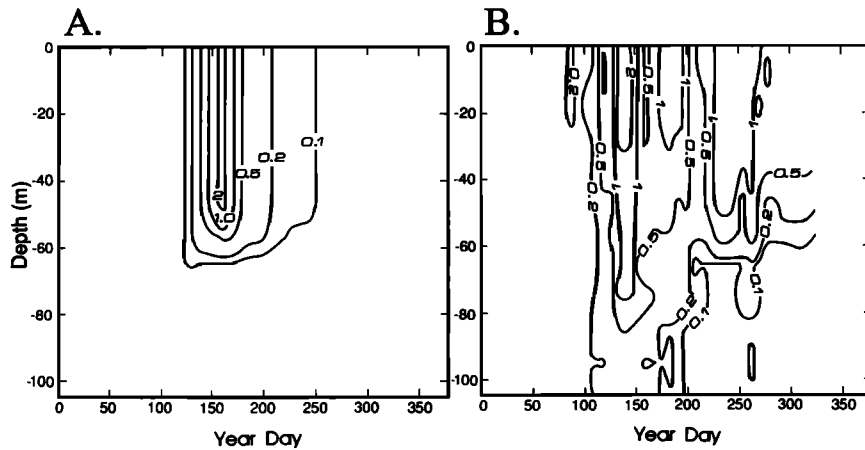


Figure 9. Time-depth chlorophyll *a* concentrations (milligrams per cubic meter) at Weather Station “India”: (a) model computations; (b) data [from *Fasham et al.*, 1993].

South Bluehill Pond, Newfoundland

South Bluehill Pond is the deepest of five oligotrophic lakes in eastern Newfoundland studied in detail by *Kerekes* [1974]. All of the lakes lie within Terra Nova National Park, have mean depths between 1.6 and 9.2 m, and are within 3 km of the ocean. South Bluehill Pond is the deepest of the five lakes (maximum depth of 23 m).

Two aspects of modeling South Bluehill Pond differed from modeling the three marine domains. Ice formed on the surface of the lake from December through April during the period of reported observations (1969–1970). Although ice formation and dissolution are not a specific part of this model, the effects of ice were accounted for by (1) setting wind velocity to zero and (2) changing the surface water attenuation coefficient during the period of observed ice cover on the lake. The degree of light attenuation change depends on the character of the ice (surface roughness, amount of bubbles, presence of snow, and so forth). *Wetzel* [1975, Table 5-4] reports that the percentage of surface light transmission for a variety of snow and ice settings varies between 8% and 72%, but averages about 50%. The water attenuation coefficient in this portion of the model study was therefore doubled in order to account for the effects of ice.

A second change in the South Bluehill Pond model was formulation of the light attenuation coefficient in the water column during ice-free periods. Terrestrial sediment can alter the optical characteristics of water, and yet suspended sediment concentrations are not predicted by most biogeochemical models, including the one employed here. (One notable exception is the model of *Peterson and Festa* [1984]). In order to account for this feature, a wide range of light attenuation constants were tested in the model using the equation

$$I(z) = I_0 \exp \left(-k_w z - \int_z^0 (0.054 \text{Chl-}a^{2/3} + 0.0088 \text{Chl-}a) dz \right)$$

$I(z)$ is depth-dependent light intensity (watts per square meter), I_0 is surface light intensity, k_w is water light attenuation, z is depth, and Chl-*a* is chlorophyll in units of milligrams per cubic meter. Chlorophyll is predicted by the geochemical model, while k_w is dependent on the intrinsic characteristics of the water and concentrations of sediment [*Jerlov*, 1976].

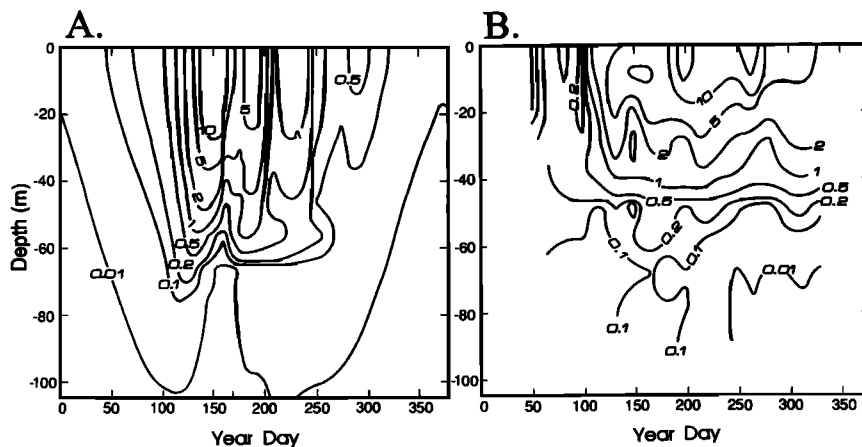


Figure 10. Time-depth productivity ($\text{mg C m}^{-3} \text{d}^{-1}$) at Weather Station “India”: (a) model computations; (b) data [from *Fasham et al.*, 1993].

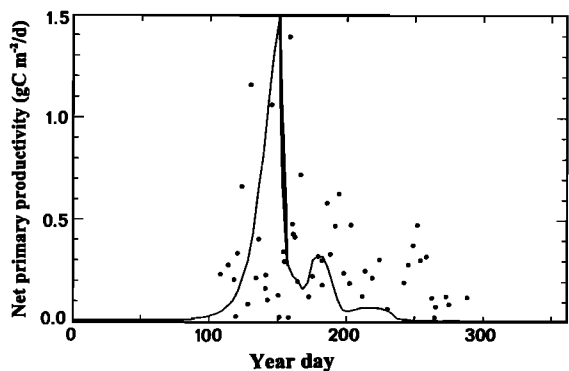


Figure 11. Vertically integrated surface productivity at Weather Station “India” as computed by the model (solid line) and as measured in the field (solid circles) [from *Fasham et al.*, 1993].

Depth versus percent light values for South Bluehill Pond have been reported by *Kerekes* [1974]. Using a light attenuation coefficient of 0.35 in the model produces geochemical gradients which are reasonably close to the published data (Figure 15). Initial model runs employing a variety of values for k_w showed that the commonly reported value for pure water (0.04) [*Jerlov*, 1976] is clearly too low. These two values ($k_w = 0.04$ and 0.35) were therefore used as end-members for the biogeochemical simulations described below.

Modeled temperature profiles for South Bluehill Pond are in reasonable agreement with temperature data for the ice-free period (Figure 16). Unlike the three marine settings, temperature gradients in the thermocline are comparable to those of the data. This is probably due to the relatively small lake area (111 ha), which would result in relatively low energy internal waves. For the ice-covered period the data show a greater

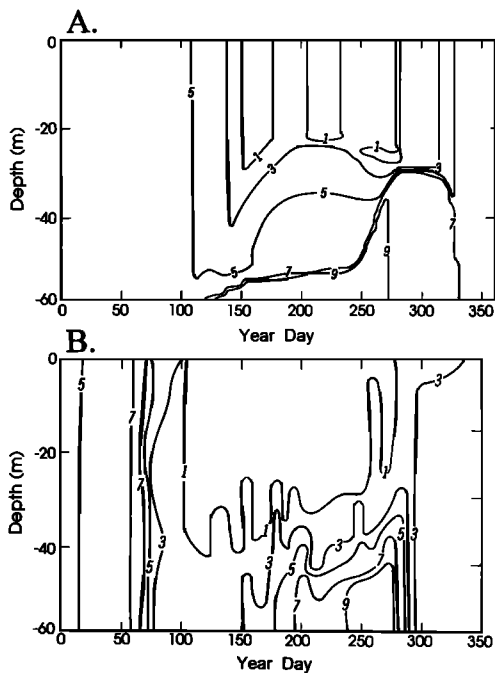


Figure 13. Time-depth nitrate (millimoles per cubic meter) at 60-m isobath of the New York Bight: (a) model computations; (b) data [from *Walsh et al.*, 1987].

degree of thermal stratification than does the model, although for any point in the domain the difference between calculated and observed temperature is only about 1°C (Figure 16).

Modeled nitrate profiles produced using the high-light attenuation coefficient ($k_w = 0.35$) show modest surface depletions in the euphotic zone (i.e., the epilimnion) and concurrent

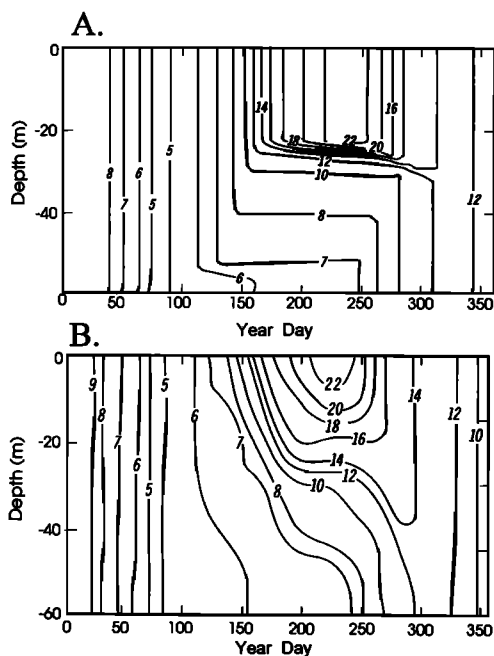


Figure 12. Time-depth temperature at 60-m isobath of the New York Bight: (a) model computations; (b) data [from *Walsh*, 1981].

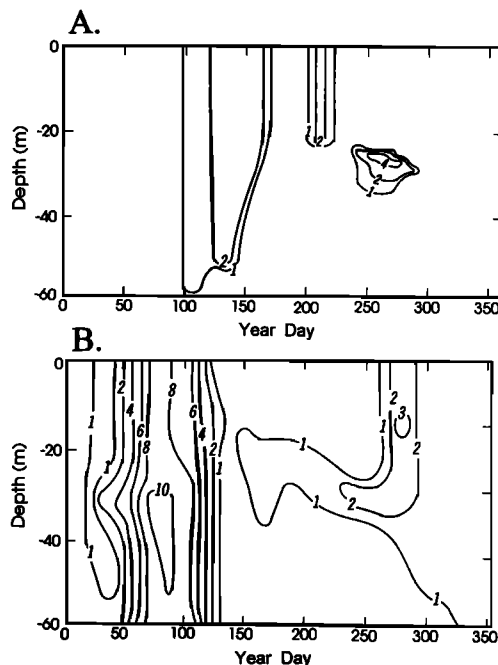


Figure 14. Time-depth chlorophyll *a* (milligrams per cubic meter) at 60-m isobath of the New York Bight: (a) model computations; (b) data [from *Walsh*, 1981].

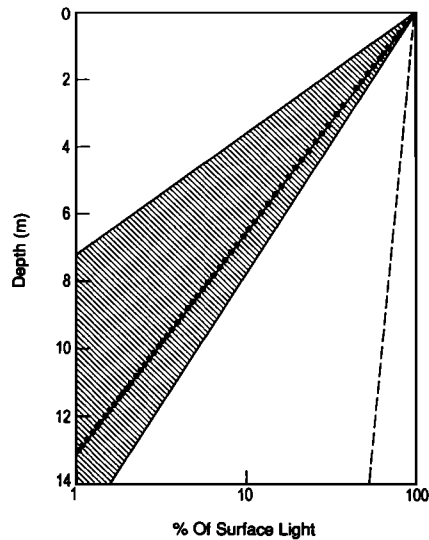


Figure 15. Depth versus percent light attenuation for South Bluehill Pond, Newfoundland. Hatched area represents range of values reported by Kerekes [1974]. Solid circles represent values calculated by the model using a k_w of 0.35 and dashes represent a k_w of 0.04.

nutrient buildup in the subeuphotic zone (i.e., the hypolimnion) (Figure 17a). Similar depletion and enrichment of nutrients can be observed in the data (Figure 17b), although the period of maximum surface nutrient depletion precedes that produced in the model by approximately 1 month. During the ice-covered period the model predicts vertical segregation of nutrients (Figure 17a) which is not observed in the data. Although it is difficult to determine the exact cause of this feature, it might be the result of underrepresentation of light attenuation by ice, which would result in significant wintertime, subice biological productivity in the model.

Nutrient model results produced with the low-light attenu-

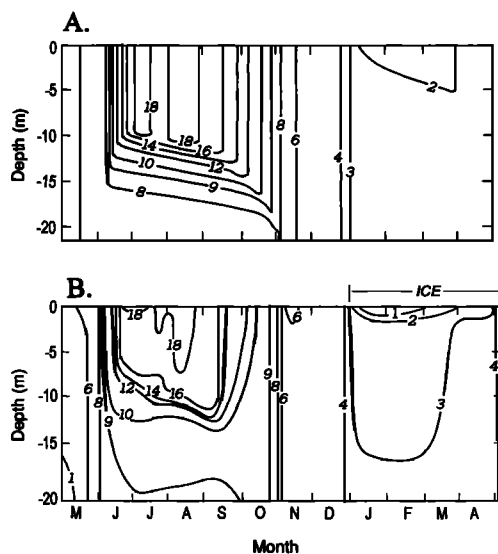


Figure 16. Time-depth temperature of South Bluehill Pond: (a) model computations; (b) data from Kerekes [1974]. The period of ice formation extends from late December through late April.

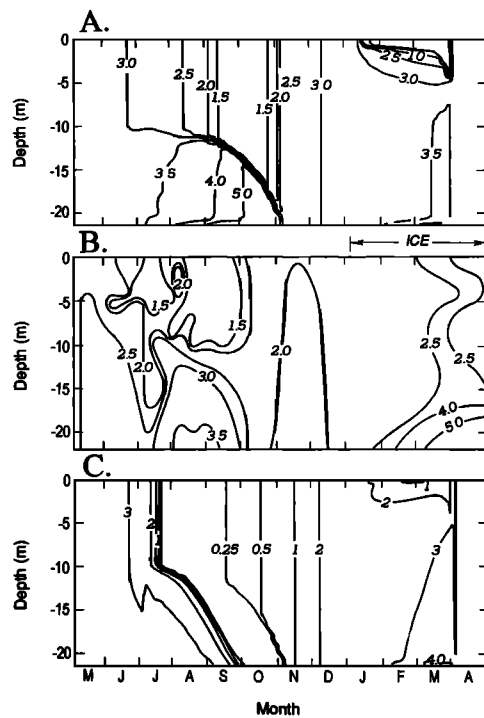


Figure 17. Time-depth nitrate (millimoles per cubic meter) of South Bluehill Pond: (a) model computations using $k_w = 0.35$; (b) data [from Kerekes, 1974]; (c) model computations using $k_w = 0.04$.

ation coefficient ($k_w = 0.04$) (Figure 17c) are at clear variance with the data (Figure 17b). The much smaller vertical nutrient gradients during the ice-free period are a direct result of significant light penetration to the bottom of the relatively shallow (23 m) lake (Figure 15). Vertical nutrient gradients during the ice-covered period of time are not as extreme as those produced by the high-attenuation model (Figure 17a), although they are greater than those observed in the data (Figure 17b).

Phytoplankton simulated by both the high- and low-attenuation models is at variance with published phytoplankton data (Figure 18). The high-light attenuation model produces phytoplankton concentrations which are consistently lower than data values, although stratification is evident in both the high-light attenuation model and the data (Figures 18a and 18b). The low-light attenuation model produces somewhat more realistic phytoplankton concentrations, although, as with nutrients, vertical gradients are considerably lower in this version of the model (Figure 18c) than in the high-light attenuation version of the model (Figure 18a).

Discussion

Integrated Surface Productivity

The numerical models of open ocean, coastal ocean, and lacustrine settings described above can be roughly compared by examining vertically integrated biological productivity averaged over long time periods. Reported productivity from Bermuda Station "S" is significantly higher than that produced by the model (Table 2). This discrepancy appears to be a result of underpredicted model productivity very early and late in the year (Figure 6). On the other hand, the predicted productivity

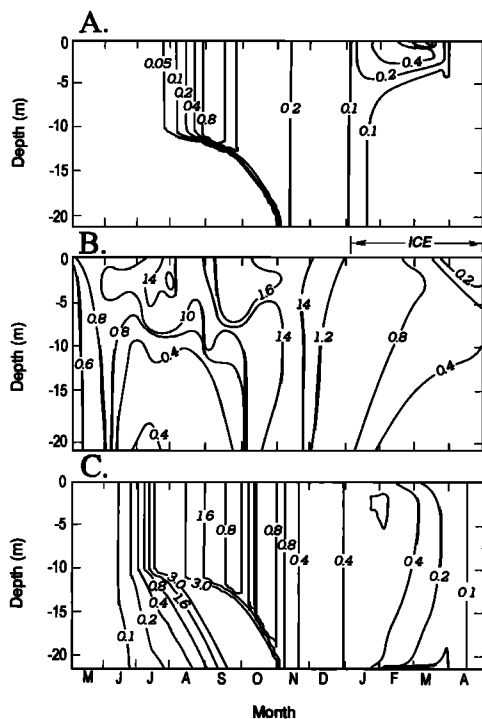


Figure 18. Time-depth chlorophyll *a* (milligrams per cubic meter) of South Bluehill Pond: (a) model computations using $k_w = 0.35$; (b) data [from Kerekes, 1974]; (c) model computations using $k_w = 0.04$.

at Ocean Weather Station "India" in the northern Atlantic is within the range reported by field studies (Table 2). However, this may be in part fortuitous, since there are relatively few field measurements during the late season at this locality, and it is during this period that the model predicts surface productivity to be almost nonexistent (Figure 11).

Calculated and measured integrated productivities for the New York Bight and South Bluehill Pond are in reasonable agreement (Table 2). Unfortunately, time series productivity data for both of these localities have not been published, and so it is difficult to discuss details of the data and model output.

Model Strengths and Deficiencies

Simulation of the four settings described above reveals a number of model strengths and deficiencies which can be discussed within the context of other biogeochemical models as well as future, three-dimensional simulations with this model.

1. Reproduction of the seasonal thermal features of all domains is reasonably good (Figures 2, 7, 12, and 16). Most of the discrepancies between model output and the data are artifacts of three-dimensional features (e.g., internal waves, horizontal advection) found in nature, but which cannot be reproduced with the present, one-dimensional formulation of the model. Future three-dimensional mesoscale models with sufficient grid resolution and real-time wind data will significantly improve model reproduction of temperature.

2. The lack of an ammonium component appears to produce poor model simulation of surface nutrient concentrations in the most productive of the four settings tested (Ocean Weather Station "India"). In nature, ammonium is preferentially taken up relative to nitrate by phytoplankton, leaving relatively high nitrate concentrations in the most productive

portions of a water column. This model deficiency might be less apparent if phosphorus were used as the limiting nutrient in the simulations.

3. The model is quite successful in reproducing vertically integrated surface productivity during the spring bloom. Late-season, integrated surface productivity is underpredicted by the model (Figures 6 and 11). In the case of Ocean Weather Station "India" this may be due to the lack of an ammonium component (see paragraph 2 above), although data for this period of time are sparse.

4. The model produces a late-season, deep chlorophyll maximum (DCM) in the two settings where it is observed (Bermuda Station "S" and the New York Bight). A DCM is not produced by the model in the two settings where it is not seen in the data (Ocean Weather Station "India" and South Bluehill Pond).

5. The correspondence between biogeochemical data and model output for the lacustrine setting is poorer than that of the three marine settings. There are two possible reasons for the discrepancy. As pointed out above, the light regime in terrestrial settings can be very complex, and time-invariant representation of light attenuation in this model may not be adequate. As discussed by Jewell [this issue], the three empirical constants in the model which deal with light (light attenuation coefficient, initial slope of the light-productivity curve, and photosynthetically active radiation) show the greatest sensitivity to integrated productivity calculated by the model. Clearly, determining the light regime for a specific lacustrine setting is one of the most critical aspects of any further application of biogeochemical models such as the one described here, and it should be a primary concern prior to modeling specific lacustrine domains.

6. Perhaps the greatest strength of the three-component model is that realistic simulations of a variety of biogeochemical features can be attained with minimal computing resources. Individual, 3-year simulations reported above took only 7 min of CPU time on a Sun Sparc 4/330 workstation. Three-dimensional simulations would, of course, be much more computationally intensive. Nevertheless, the simple biogeochemical model employed in this study holds considerable promise for conducting real-time, three-dimensional water quality simulations in a desktop environment.

The simple, three-component biogeochemical model described above is currently being integrated with the three-

Table 2. Summary of Integrated Productivity As Calculated by the Model and Reported in the Literature

Productivity	Bermuda Station "S"	Station India	New York Bight	South Bluehill Pond
Measured	60–125 ^a	24–66 ^b	200–300 ^c	29 ^d
Calculated	14	42	177	26 ^e

All units are $\text{g C m}^{-2}/\text{yr}$ except for South Bluehill Pond, which has units of $\text{mg C m}^{-2}/\text{day}$ for the periods indicated in the respective footnotes.

^aDring and Jewson [1982], Lohrenz et al. [1992], Menzel and Ryther [1960].

^bWilliams and Robinson [1973], Fasham et al. [1993].

^cWalsh [1981].

^dAverage of measured values from May to October 1969 and May to August 1970 [Kerekes, 1974].

^eCalculated for the period of May 15 to September 15.

dimensional turbulence closure fluid flow model described by *Blumberg and Mellor* [1987]. Oxygen is being added to the biogeochemical code in a manner similar to *Jewell* [1992]. The resulting model will be capable of explaining spatial and temporal responses of anoxia to nutrient loading and physical forcings (e.g., wind shear stress and solar heating) in a variety of surface water settings. Specific modeling projects include understanding the physical and chemical controls of anoxia in lakes [*Jewell*, 1992, 1993] and the effect of Ekman transport and bathymetry on oxygen and nutrient concentrations in coastal upwelling zones from a variety of geologic time periods [*Jewell*, 1994a, b].

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References

- Altabet, M. A., Particulate new nitrogen fluxes in the Sargasso Sea, *J. Geophys. Res.*, *94*, 12,771–12,779, 1989.
- Ambrose, R. B., T. A. Wool, and J. L. Martin, The water quality analysis simulation program, WASP5, report, 203 pp., Environ. Res. Lab., Environ. Prot. Agency, Athens, Ga., 1993.
- Be, A. W. H., J. M. Forns, and O. A. Roels, Plankton abundance in the North Atlantic Ocean, in *Fertility of the Sea*, vol. 1, edited by J. D. Costlow, pp. 17–50, Gordon and Breach, New York, 1971.
- Blumberg, A. F., and G. L. Mellor, A description of a three-dimensional coastal ocean circulation model, in *Three-Dimensional Coastal Circulation Ocean Models*, *Coastal Estuarine Sci. Ser.*, vol. 4, edited by N. S. Heaps, pp. 1–16, AGU, Washington, D. C., 1987.
- Cero, C. F., and T. M. Cole, Thirty year simulation of Chesapeake Bay eutrophication, in *Estuarine and Coastal Modeling, Proceedings of the 2nd International Conference*, edited by M. L. Spaulding, K. Bedford, A. Blumberg, R. Cheng, and C. Swanson, pp. 116–126, Am. Soc. of Civ. Eng., New York, 1992.
- Conway, H. L., and T. E. Whitledge, Distribution, fluxes, and biogeochemical utilization of inorganic nitrogen during a spring bloom in the New York Bight, *J. Mar. Res.*, *37*, 657–668, 1979.
- Deevey, G. B., The annual cycle in quantity and composition of the zooplankton of the Sargasso Sea off Bermuda, I, The upper 500 m, *Limnol. Oceanogr.*, *16*, 219–240, 1971.
- Dring, M. J., and D. H. Jewson, What does ^{14}C uptake by phytoplankton really measure? A theoretical modelling approach, *Proc. R. Soc. London B.*, *214*, 351–368, 1982.
- Falkowski, P. G., T. S. Hopkins, and J. J. Walsh, An analysis of factors affecting oxygen depletion in the New York Bight, *J. Mar. Res.*, *38*, 479–506, 1980.
- Falkowski, P. G., J. Vidal, T. S. Hopkins, G. T. Rowe, T. E. Whitledge, and W. G. Harrison, Summer nutrient dynamics of the Middle Atlantic Bight: Primary productivity and utilization of phytoplankton carbon, *J. Plankton Res.*, *5*, 515–537, 1983.
- Fasham, M. J. R., H. W. Ducklow, and S. M. McKelvie, A nitrogen-based model of plankton dynamics in the oceanic mixed layer, *J. Mar. Res.*, *48*, 591–639, 1990.
- Fasham, M. J. R., J. L. Sarmiento, R. D. Slater, H. W. Ducklow, and R. Williams, Ecosystem behavior at Bermuda “S” and Ocean Weather Station “India”: A general circulation model and observational analysis, *Global Biogeochem. Cycles*, *7*, 379–415, 1993.
- Fee, E. J., The vertical and seasonal distribution of chlorophyll in lakes of the Experimental Lakes Area, northwestern Ontario: Implications for primary production estimates, *Limnol. Oceanogr.*, *21*, 767–783, 1976.
- Gachter, R., and D. M. Imboden, Lake restoration, in *Chemical Processes in Lakes*, edited by W. Stumm, pp. 363–388, John Wiley, New York, 1985.
- Harrison, W. G., D. Douglas, P. G. Falkowski, G. T. Rowe, and J. Vidal, Summer nutrient dynamics of the Middle Atlantic Bight: Nitrogen uptake and regeneration, *J. Plankton Res.*, *5*, 539–556, 1983.
- Hofmann, E. E., Plankton dynamics on the outer southeastern U.S. continental shelf, III, A coupled physical-biological model, *J. Mar. Res.*, *46*, 919–946, 1988.
- Hofmann, E. E., and J. W. Ambler, Plankton dynamics on the outer southeastern U.S. continental shelf, II, A time dependent biological model, *J. Mar. Res.*, *46*, 883–917, 1988.
- Jerlov, N. G., *Marine Optics*, 231 pp., Elsevier, New York, 1976.
- Jewell, P. W., Hydrodynamic controls of anoxia in shallow lakes, in *Productivity, Accumulation, and Preservation of Organic Matter: Recent and Ancient Sediments*, edited by J. Whelan and J. Farmington, pp. 201–228, Columbia Univ. Press, New York, 1992.
- Jewell, P. W., A prognostic numerical model of nutrient loading and eutrophication in temperate latitude lakes, *Geol. Soc. Am. Abstr. Programs*, *25*, 432–433, 1993.
- Jewell, P. W., Deep water nutrient and oxygen gradients in a modern coastal upwelling zone and their paleoceanographic implications, *J. Geophys. Res.*, *99*, 7845–7850, 1994a.
- Jewell, P. W., Mass balance models of Ekman transport and nutrient fluxes in coastal upwelling zones, *Global Biogeochem. Cycles*, *8*, 165–177, 1994b.
- Jewell, P. W., A simple surface water biogeochemical model, 1, Description, sensitivity analyses, and idealized simulations, *Water Resour. Res.*, this issue.
- Kerekes, J. J., Limnological conditions in five small oligotrophic lakes in Terra Nova National Park, Newfoundland, *J. Fish. Res. Board Can.*, *31*, 555–583, 1974.
- Kiefer, D. A., O. Holm-Hansen, C. R. Goldman, R. Richards, and T. Berman, Phytoplankton in Lake Tahoe: Deep-living populations, *Limnol. Oceanogr.*, *17*, 418–422, 1972.
- Klein, P., and B. Coste, Effects of wind stress variability on nutrient transport into the mixed layer, *Deep Sea Res.*, *31*, 21–37, 1984.
- Kremer, J. N., and S. W. Nixon, *A Coastal Marine Ecosystem*, 217 pp., Springer-Verlag, New York, 1978.
- Levitus, S., Climatological atlas of the world ocean, *NOAA Prof. Pap.* *13*, 173 pp., Natl. Oceanic and Atmos. Admin., Silver Spring, Md., 1982.
- Lohrenz, S. E., G. A. Knauer, V. L. Asper, M. Tuel, A. F. Michaels, and A. H. Knap, Seasonal variability in primary production and particle flux in the northwestern Sargasso Sea: US JGOFS Bermuda Atlantic Time-Series Study, *Deep Sea Res.*, *39*, 1373–1391, 1992.
- Mellor, G. L., and P. A. Durbin, The structure and dynamics of the ocean surface mixed layer, *J. Phys. Oceanogr.*, *5*, 718–728, 1975.
- Mellor, G. L., and T. Yamada, A hierarchy of turbulence closure models for planetary boundary layers, *J. Atmos. Sci.*, *31*, 1791–1806, 1974.
- Mellor, G. L., and T. Yamada, Development of a turbulence closure model for geophysical fluid problems, *Rev. Geophys.*, *20*, 851–875, 1982.
- Menzel, D. W., and J. H. Ryther, The annual cycle of primary productivity in the Sargasso Sea off Bermuda, *Deep Sea Res.*, *6*, 351–367, 1960.
- Najjar, R. G., J. L. Sarmiento, and J. R. Toggweiler, Downward transport and fate of organic matter in the ocean: Simulations with a general circulation model, *Global Biogeochem. Cycles*, *6*, 45–76, 1992.
- Parsons, T. R., M. Takahashi, and B. Hargrave, *Biological Oceanographic Processes*, 330 pp., Pergamon, New York, 1984.
- Peixoto, J. P., and A. H. Oort, *Physics of Climate*, 520 pp., American Institute of Physics, New York, 1992.
- Peterson, D. H., and J. F. Festa, Numerical simulation of phytoplankton productivity in partially mixed estuaries, *Estuarine Coastal Shelf Sci.*, *19*, 563–589, 1984.
- Pond, S., and G. L. Pickard, *Introductory Dynamical Oceanography*, 329 pp., Pergamon, New York, 1983.
- Sarmiento, J. L., R. D. Slater, M. J. R. Fasham, H. W. Ducklow, J. R. Toggweiler, and G. T. Evans, A seasonal three-dimensional ecosystem model of nitrogen cycling in the North Atlantic euphotic zone, *Global Biogeochem. Cycles*, *7*, 417–450, 1993.
- Shaffer, G., A model of biogeochemical cycling of phosphorus, nitrogen, oxygen, and sulfur in the ocean: One step toward a global climate model, *J. Geophys. Res.*, *94*, 1979–2004, 1989.
- Steele, J. H., A study of production in Gulf of Mexico, *J. Mar. Res.*, *22*, 211–222, 1964.
- Walsh, J. J., A spatial simulation of the Peruvian upwelling ecosystem, *Deep Sea Res.*, *22*, 201–236, 1975.
- Walsh, J. J., Shelf-sea ecosystems, in *Analysis of Marine Ecosystems*,

- edited by A. R. Longhurst, pp. 158–196, Academic, San Diego, Calif., 1981.
- Walsh, J. J., *On the Nature of Continental Shelves*, 520 pp., Academic, San Diego, Calif., 1988.
- Walsh, J. J., T. E. Whittedge, F. W. Barvenik, C. D. Wirick, S. O. Howe, W. E. Esaias, and J. T. Scott, Wind events and food chain dynamics with the New York Bight, *Limnol. Oceanogr.*, 23, 659–683, 1978.
- Walsh, J. J., T. E. Whittedge, J. E. O'Reilly, W. C. Phoel, and A. F. Draxler, Nitrogen cycling on Georges Bank and the New York shelf, in *Georges Bank*, edited by R. H. Backus, pp. 234–246, MIT Press, Cambridge, Mass., 1987.
- Walsh, J. J., D. A. Dieterle, and M. B. Meyers, A simulation analysis of the fate of phytoplankton within the Mid-Atlantic Bight, *Cont. Shelf Res.*, 8, 757–787, 1988.
- Wetzel, R. G., *Limnology*, 743 pp., W. B. Saunders, Philadelphia, Pa., 1975.
- Williams, R., Spatial heterogeneity and niche differentiation on oceanic zooplankton, *Hydrobiologia*, 167/168, 151–159, 1988.
- Williams, R., and G. A. Robinson, Primary production at Ocean Weather Station India (59°00'N, 19°00'W) in the North Atlantic, *Bull. Mar. Ecol.*, 8, 115–121, 1973.
- Wroblewski, J. S., J. L. Sarmiento, and G. R. Flierl, An ocean basin scale model of plankton dynamics in the North Atlantic, 1, Solutions for the climatological oceanographic conditions in May, *Global Biogeochem. Cycles*, 2, 199–218, 1988.
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