A three-dimensional model of Lake Superior with ice and biogeochemistry

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Abstract

The formation of winter ice on Lake Superior has been shown to be important in determining the annual thermal cycle of the lake and long-term trends of surface water temperature increase. However, modeling studies of Lake Superior to date have not included dynamic and thermodynamic ice cover. These physical characteristics of the lake in turn can have significant impacts on biogeochemical cycling within the lake. We present a new three-dimensional model of Lake Superior that includes a dynamic and thermodynamic ice model and a biogeochemical model. Results from the model forced by observed meteorological conditions for the period 1985 to 2008 are discussed and compared with available observations. Modeled long-term interannual trends in increasing water temperature and decreasing ice cover are compared with observed rates. In the model, total annual gross primary productivity is found to correlate positively with mean annual temperature and negatively with mean winter ice-cover magnitude.

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Introduction

Lake Superior is a minimally disturbed, large aquatic system. It is the world’s largest lake by surface area and contains approximately 10% of the Earth’s surface freshwater. The lake plays a significant role in influencing regional meteorology, as well as being very important to the surrounding region as a source of clean and abundant water and a medium for inexpensive, waterway transportation. It is unusual, when compared to the other Laurentian Great Lakes, in that human impact has been limited. First, Lake Superior is upstream of the other Laurentian Great Lakes and receives runoff from its own catchment basin only. Lake Superior’s catchment basin area is relatively small compared to the lake surface area with a ratio of 1.55 (Cotner et al., 2004). Second, development within its basin is not significant: only 3% of the Superior basin is used for agriculture as compared to 27–67% for the other Great Lake basins; over 90% of its basin is covered with forest, which is far less abundant elsewhere (Sea Grant College Program, 1985). Also, the amount of water withdrawn for consumption from Lake Superior is at most a small fraction of the amounts withdrawn from the other lakes (The Great Lakes Commission, 2006).

While the disturbanse of Lake Superior has been minor compared to the other Laurentian Great Lakes, recent work by Austin and Colman (2007) demonstrates that the thermal characteristics of Lake Superior have been changing over the past quarter century. Their compilation of available summer surface water temperature measurements shows a warming trend (~0.11 °C/yr over the last quarter century) in the lake that is in excess of the regional atmospheric warming rates (~0.06 °C/yr). This warming is hypothesized to be the result, in part, of decreasing winter lake ice cover, as determined from the spatial and temporal average of ice cover between December and May (Assel, 2003). The declining annual ice cover leads to earlier ice-out and spring overturn, as lake albedo is reduced and shortwave radiation absorption over the late winter and early spring is increased. An earlier overturn provides a longer warming season and the lake is able to warm significantly more than if the season had been delayed by a strong ice cover.

A greater warming of surface lake waters over the ambient surface water temperature difference and wind speed, and a significant upward trend in wind speed (Desai et al., 2009).

It is not entirely clear how these trends will affect the Lake Superior thermal structure in the future. On one hand, warmer air tends to strengthen summertime stratification. However, stronger winds would impart larger kinetic energy to the lake and tend to increase mixing and deepen the mixed layer depth. Austin and Allen (2011) found the impact of recent changes in wind speed and air temperature on summer water temperatures to be opposite and of the same
order of magnitude. Their estimates, however, relies upon an assumption of independence of the effects of air temperature and wind speed.

There is significant uncertainty in our knowledge of Lake Superior’s biogeochemistry as well. For one, the carbon budget of Lake Superior cannot be closed at the present time. The main sink of organic carbon in Lake Superior is respiration, which has been estimated by $^{14}$C uptake experiments. Compilations of estimates of respiration and production suggest that Lake Superior is net heterotrophic (Cotner et al., 2004; McManus et al., 2003; Urban et al., 2005); organic carbon consumption by respiration exceeds production by photosynthesis. Presumably, heterotrophy is also fueled by external sources of organic carbon from atmospheric deposition and runoff from the watershed. However, the sum of all known inputs of carbon to the lake from rivers, atmosphere, and photosynthesis (0.4–0.9 Tg C yr$^{-1}$, 0.02–0.41 Tg C yr$^{-1}$ and 2.0–8.2 Tg C yr$^{-1}$, respectively, Cotner et al., 2004; Urban et al., 2005) is only about half of the sum of all known outputs by outflow, sedimentary burial, and respiration (0.1 Tg C yr$^{-1}$, 0.06–2.0 Tg C yr$^{-1}$ and 13–81 Tg C yr$^{-1}$, respectively). Respiration rates have the largest range of uncertainty.

There are other unexplained features of nutrient and ecosystem dynamics in Lake Superior. Currently phosphate concentrations are very low in the lake. Typical Lake Superior soluble reactive phosphorus concentrations are in the range of <0.1 to 10 nmol kg$^{-1}$ (Anagnostou and Sherrell, 2008), which is two to four orders of magnitude lower than typical values in the ocean (which are commonly reported in μmol kg$^{-1}$). It is also lower than in the other Laurentian Great Lakes. For example, measurements of soluble reactive phosphorus in Lake Michigan have ranged from 20 to 330 nmol kg$^{-1}$ (Brooks and Edgington, 1994; Tarapach and Rubitschun, 1981) and from 20 to 419 nmol kg$^{-1}$ in Lake Erie (Holland et al., 1995; Makarewicz et al., 2000). Phosphorus appears to limit summer production, though iron may also play a role (Sterner et al., 2004). Recent measurements of dissolved organic phosphorus (DOP) show the presence of a sea-sonally highly dynamic pool (Baehr and McManus, 2003), suggesting the possibility that DOP may be fueling production in Lake Superior as well as in the Sargasso Sea (Lomas et al., 2010). Nitrate limits production in many parts of the world ocean, but it is in constant excess in Lake Superior. In fact, nitrate seems to be on a century-long trend of buildup from anthropogenic sources and from changing biogeochemical cycling (Bennett, 1986; Sterner et al., 2007). A further puzzle in ecosystem dynamics includes the formation of a pronounced deep chlorophyll maximum at 25–35 m every year during midsummer (Barbiero and Tuchman, 2004).

The primary goal of this work is to document the development of a realistically configured, 3-dimensional numerical model of Lake Superior, which includes models of hydrodynamics, ice dynamics and thermodynamics and the ecosystem. Secondly, we evaluate the ability of the model to reproduce interannual trends in surface water temperature and ice cover for the period 1985 to 2008. Finally, we investigate accompanying trends in annual primary productivity due to temperature and ice cover for the period 1985 to 2008. Finally, we investigate accompanying trends in annual primary productivity due to warming. Also, uncertainty in the carbon budget can be assessed by sampling the 3-dimensional model and determining how much sampling is needed to determine the lake-wide characteristics. Furthermore, sensitivity experiments with a multi-compartment ecosystem model are expected to elucidate the controls on the deep chlorophyll maximum.

There have been several numerical modeling studies of Lake Superior circulation. Lam (1978) used a hydrodynamic model with four layers in the vertical and 10 km horizontal resolution to simulate water circulation during the stratified season of 1973. As part of the Keweenaw Interdisciplinary Transport Experiment in Superior, a non-orthogonal coordinate model was created for Lake Superior (Chen et al., 2001, 2004; Zhu et al., 2001). The main focus of publications based on this model was coastal circulation dynamics in the region of the Keweenaw Peninsula. Most recently, Bennington et al. (2010) use a three-dimensional hydrodynamic model with imposed ice coverage to elucidate climatological circulation structures, the mechanisms that control them and their interannual variability. The Great Lakes Coastal Forecasting System (Schwab and Bedford, 1999) provides modeled nowcasts and forecasts of water temperature and circulation in the Great Lakes including Lake Superior. This modeling effort provides important information for lake users but there has been no published analysis of output from the model. Significantly, none of the models listed here includes dynamic and thermodynamic ice. By explicitly modeling water and ice, we achieve consistency between the physical fields of the lake (e.g., simulating ice where sub-freezing temperatures predict it) and the power to make future projections and conduct climate sensitivity experiments. The role of ice cover in affecting the air–lake flux of heat and gas as well as biogeochemical cycling makes a dynamic and thermodynamic model of ice a critical component for realistic simulation of Lake Superior.

Here we describe a 3-dimensional model of Lake Superior that is based on The Regional Oceanic Modeling System (ROMS, version 3.2). The second section describes the model, including the dynamic and thermodynamic ice model and the biogeochemical model, as well as the atmospheric boundary conditions used to force the model. The third section presents model results from runs covering 1985–2008 with a specific focus on 2005 and compares them to data where available. The fourth section offers conclusions.

**Description of model and atmospheric forcing**

**Hydrodynamic model**

ROMS is a free-surface primitive equation ocean model that utilizes a terrain-following vertical coordinate and a split-explicit time stepping scheme. The algorithms of the ROMS computational kernel are described in detail in Shchepetkin and McWilliams (2005). ROMS has been successfully applied in many regions around the globe, some including biogeochemical and sea–ice studies (e.g. Budgell, 2005; Dinniman et al., 2003; Fennel et al., 2006; Gruber et al., 2006). The Lake Superior model is implemented using realistic lateral and bottom boundaries (Fig. 1). The rectilinear horizontal grid has a resolution of 5 km and there are 20 sigma levels in the vertical, resulting in vertical resolution between less than one and 40 m. The level 2.5 closure turbulence model presented in Mellor and Yamada (1982) is used to calculate vertical mixing coefficients. A closed basin model is used with no input from tributaries and the surrounding watershed or drainage of water to the St. Marys River. As in Bennington et al. (2010), the closed based model is an appropriate first step for modeling Lake Superior, which has a large volume and long residence time of 178 years (Quinn, 1992). Future inclusion of tributary input will likely increase the accuracy of the ecosystem.
model in near shore regions of riverine input. In our application to Lake Superior, salinity is set to zero and temperature is the only state variable. To improve the behavior of the model in the vicinity of the 3.98 °C density maximum, we implemented an equation of state developed expressly for freshwater systems (Chen and Millero, 1986).

**Ice model**

The ice model used for the Lake Superior implementation is demonstrated by Budgell (2005) in an application to the Barents Sea and further described by Hedström (2009). The main features of this ice model are elastic–viscous–plastic (EVP) ice rheology, ice thermodynamics using single ice and snow layers, and a molecular sublayer adjacent to the base of the ice. The ice and hydrodynamic models are coupled using the same grid and timestep.

The dynamics of the ice model are based on the work of Hunke and Dukowicz (1997) and Hunke (2001). Ice momentum is determined by stress from air and water, tilt of the water surface, the Coriolis force, and internal ice stress (Hedström, 2009). A split timestep is used in calculating ice momentum with the internal ice stress updated more frequently to resolve internal dynamics. The EVP ice rheology follows the rheology of Hibler (1979) but uses Young’s Modulus as a modifiable coefficient to minimize the elastic term and allow for efficient solutions. The ice tracers, including internal ice temperature, surface melt ponds, ice thickness and concentration, and snow thickness are advected according to the calculated ice momentum.

The ice thermodynamics follow Mellor and Kantha (1989) and Häkkinen and Mellor (1992). Ice melting and freezing are calculated on all sides of the ice (top, bottom and sides, Hedström, 2009; Mellor and Kantha, 1989). The factors in changing effective ice volume and ice concentration are the freezing rate at the air–water boundary ($W_{f, a}$), the rate of freezing at the ice–water boundary ($W_{f, w}$), the rate of frazil ice growth ($W_{fr}$), the melt rate at the ice/snow surface ($W_{m, s}$), and the runoff rate for surface meltwater ($W_{m, o}$). Frazil ice formation is modeled after Steele et al. (1989). Energy fluxes in the snow–ice system are calculated using single ice and snow layers (Semtner, 1976). A molecular sublayer at the ice–ocean interface is used to improve freezing and melting rates. Fluxes of sensible and latent heat and incoming long- and shortwave radiation are based on those of Parkinson and Washington (1979). We modify the ice model for the Lake Superior application by setting the ice salinity to zero.

**Biogeochemistry and ecosystem model**

The biogeochemical model modified for the Lake Superior implementation is described by Fennel et al. (2006). We use phosphorus as the limiting nutrient in Lake Superior, which allows us to further simplify the architecture of the Fasham et al. (1990) type model. There are six state variables: phosphate, phytoplankton, chlorophyll, zooplankton, and large and small detritus (Fig. 2). Fluxes between the pools are shown as arrows. Ice:freeze/melt rates contributing to ice volume and concentration changes are shown with arrows. $W_{f, a}$: melt rate at ice/snow interface, $W_{f, w}$: freeze rate at water/air interface, $W_{fr}$: frazil ice formation rate, $W_{m, s}$: freeze rate at ice/water interface, $W_{m, o}$: runoff rate of surface meltwater, after Hedström (2009) Fig. 7.

The time rate of change of phytoplankton is a function of zooplankton grazing on phytoplankton, mortality of phytoplankton, coagulation of phytoplankton with small detritus to form large detritus and phytoplankton growth rate, itself a function of temperature, light, and nutrient limitation (see Supplemental Materials for governing equation). Temperature in general is positively related to the metabolic rates, and our temperature dependence on growth rates follows the Q10 relation (Kishi et al., 2007). Light availability is modified by the amount of light in the photosynthetically active portion of the spectrum, attenuation due to water and attenuation due to chlorophyll presence. The relationship between available light and rates of photosynthesis follows Platt et al. (1980). Phosphorus limitation follows Michaelis–Menten uptake kinetics (Michaelis and Menten, 1913). Phytoplankton sinks at a relatively slow rate and may coagulate with small detritus to join the large detritus pool. Zooplankton grazing rates are characterized using a Holling-type s-shaped curve (Holling, 1959, 1962, 1965). Zooplankton time rate of change is a function of rates of zooplankton grazing on phytoplankton and efficiency of assimilation of the grazed material, basal metabolism excretion rates, assimilation related excretion rates, and zooplankton mortality.

The amount of chlorophyll associated with a given phytoplankton mass varies nonlinearly. A portion of phytoplankton growth is allotted to chlorophyll synthesis following the formulation of Geider et al. (1996, 1997). The fraction allocated is a function of nutrient and light availability. This takes into account the process of photoacclimation in which phytoplankton increase or decrease the amount of resources used in synthesis of light-harvesting cellular components depending upon environmental conditions. This is a potentially important process in the deep chlorophyll maximum. Chlorophyll sinks include grazing by zooplankton, mortality of phytoplankton, and coagulation of phytoplankton with small detritus to form large detritus.

Two size classes of detritus are used in the model. The small class sinks at a characteristic slower rate and represents both the dissolved organic phosphorus pool and minute slowly sinking particulates while the large detritus pool sinks at a faster rate. Both classes of detritus are subject to horizontal advection, and so the limited sinking rates, especially for the small detritus, allow for a horizontal transport.
or seston, however, is consistently elevated and can reach as high as 106:16:1. The ratio of carbon to phosphorus (C:P) ratio in Lake Superior is usually assumed to follow the Redfield ratio of carbon, nitrogen, and phosphorus in organic matter. Small detritus and phytoplankton are immediately remineralized. Upon reaching the bottom boundary, detritus sources are coagulation of small detritus and phytoplankton mortality and coagulation. Losses are remineralization and sinking. Large detritus through excretion and mortality and through phytoplankton via mortality. Downward shortwave radiation was determined by combining the climatological average monthly cloud cover without interannual variability. The half-saturation concentration value for the state variables were chosen to according numbers from Table 2.

<table>
<thead>
<tr>
<th>Table 1</th>
<th>Biological parameters.</th>
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<tbody>
<tr>
<td>Parameter</td>
<td>Units</td>
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<tr>
<td>Light attenuation by water</td>
<td>m$^{-1}$</td>
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<tr>
<td>Light attenuation by chlorophyll</td>
<td>m$^{-1}$</td>
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<tr>
<td>PAR fraction</td>
<td>Nondimensional</td>
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<tr>
<td>Phytoplankton growth at 0°C</td>
<td>molc gChl$^{-1}$ d$^{-1}$</td>
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<tr>
<td>Half-saturation conc. for PO$_4$ uptake</td>
<td>mmol P m$^{-3}$</td>
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<tr>
<td>Half-saturation conc. for phytoplankton uptake</td>
<td>(mmol P m$^{-3}$)$^{-1}$</td>
</tr>
<tr>
<td>Maximum chlorophyll to phytoplankton ratio</td>
<td>mgChl mgC$^{-1}$</td>
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<tr>
<td>P-I curve initial slope</td>
<td>molc gChl$^{-1}$</td>
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<tr>
<td>Photosynthetic parameter</td>
<td>molc m$^{-3}$d$^{-1}$</td>
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<tr>
<td>Photoinhibition parameter</td>
<td>°C$^{-1}$</td>
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<tr>
<td>Temperature coefficient</td>
<td>molc molP$^{-1}$</td>
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<td>Phytoplankton mortality rate</td>
<td>d$^{-1}$</td>
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<td>Zooplankton assimilation efficiency</td>
<td>d$^{-1}$</td>
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<td>Zooplankton basal metabolism excretion</td>
<td>d$^{-1}$</td>
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<tr>
<td>Zooplankton carbon to phosphorus ratio</td>
<td>molc molP$^{-1}$</td>
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<tr>
<td>Zooplankton maximum grazing rate</td>
<td>(molP m$^{-3}$)$^{-1}$ d$^{-1}$</td>
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<td>Zooplankton mortality rate</td>
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<td>Large detritus remineralization rate</td>
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<td>Small detritus remineralization rate</td>
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<td>Phytoplankton sinking rate</td>
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<td>Large detritus sinking rate</td>
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The model is initialized with waters at a uniform temperature of 4°C (close to the temperature of maximum density), no ice, uniform surface topography and no momentum on 1 January 1985. Biogeochemical state variables are initialized at the values given in Table 2. The model is spun up for two years using the 1985 annual, realistic atmospheric forcing with three hour time resolution (described below) allowing the model to come into equilibrium. The forcing for 1985 to 2008 is then applied with each year being initialized from the end state of the previous year to produce results for analysis.

### Atmospheric forcing data

The forcing applied to the model was developed by using interpolated data from the National Oceanic and Atmospheric Administration (NOAA) National Data Buoy Center (NDBC) array of open-lake buoys and Coastal Marine Automated Network (CMAN) stations. The number of these stations providing data varied over the course of the 25 year simulation, with the number of stations providing data increasing monotonically from 7 in 1985 to 18 in 2008. As this data exists only on the US portion of the lake, there is no coverage in the far northern portion of the lake. In addition, the open-lake buoys are typically recovered in November and re-deployed the following spring so that they are not on the lake during the ice-cover season, thus there are no direct measurements over the open lake during the winter.

The available data consists of wind speed and direction and air temperature. The wind speed data was adjusted to 5 m using a power law adjustment (Hsu et al., 1994) with $p = 0.11$. All available data was used to construct interpolated wind velocity and air temperature fields over the lake, using objective analysis with a correlation length scale of 100 km. The field was relaxed to the mean of available data in regions distant from the available data.

Although there is one site (ROAM4) where a historical record of humidity is available, we chose to impose a uniform, constant relative humidity of 80% over the entire domain (note that this implies that the specific humidity will vary with air temperature). A separate run, in which humidity from the single available record was applied uniformly, revealed no significant difference from a run otherwise identical but with constant humidity (not shown).

Both shortwave and longwave radiation were determined using climatological average monthly cloud cover without interannual variability. Downward shortwave radiation was determined by combining the...

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monthly cloud cover estimate with an astronomical prediction of clear-sky radiation and a quadratic cloud cover correction (Barry and Chorley, 1976):

$$CC = 1 - 0.65C^2$$

Where C is the observed cloud fraction and CC is the cloud correction factor so that

$$Q_{SW,FC} = (1 - CC)Q_{SW,CLEARSKY}.$$  

Downward longwave radiation was set using a regression of directly measured longwave radiation at one location in Lake Superior (Austin and Allen, 2011) to cloud cover and air temperature:

$$Q_{LW,DOWN} = 323Wm^{-2} + 4.7Wm^{-2}C^{-1}T_{AIR} - 72Wm^{-2}CC$$

where $T_{AIR}$ is in °C. Upward longwave radiation is determined in the model as a function of the surface water temperature, and a constant albedo of 0.93 (Payne, 1972) is used to determine the upward shortwave term. Surface water temperature restoring to observed values is not used to correct heat fluxes in this model.

Results and discussion

Physical results

Lake Superior, similar to other deep temperate lakes, experiences twice annual mixing of the water column during the spring and fall with a period of relatively strong stratification during the summer and weaker, deeper stratification during the winter months. The duration of the periods of mixing and stratification play an important role in lake biogeochemistry, as they affect vertical distribution of nutrients and phytoplankton. We compare model output to surface water temperature observations and twice annual vertical water column temperature data.

Surface water temperature observations from NDBC moored buoys are compared to modeled surface water temperatures from corresponding locations in the model grid for 2005 (Figs. 3A, B and C). The three Lake Superior NDBC buoys are located in the western, central, and eastern portions of the lake (squares, Fig. 1). Due to removal of the buoys during the winter season, observational records span from early spring (April or May) to late fall (November), barring absence of data due to technical difficulties. In general, the annual cycle of temperature in the model captures the extent and timing of the summer stratified season. Timing of vernal onset of stratification and fall cool down are matched well at the western buoy, though late stratified season temperatures at the central and eastern buoys tend to be cooler than those seen in observations. Following Wang et al. (2010), we use the root mean square error (RMSE), defined as

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (x_i - y_i)^2}$$

where x and y are modeled and observed values, respectively, to assess the absolute error of the modeled time series compared to observed. The RMSEs at the western, central and eastern buoy locations for 2005 are 1.52 °C, 1.33 °C and 1.56 °C, respectively. These values are similar to those obtained for annual cycles of lake surface water temperature in other modeling studies of the Great Lakes, e.g. 0.7–2.5 °C in Lake Michigan (Beletsky and Schwab, 2001), 0.95–1.43 °C in Lake Ontario (Huang et al., 2010) and 1.039 °C in Lake Erie (Wang et al., 2010). The model does a fair job of reproducing surface water temperatures at all three locations for the period of 1985 to 2008 (Figs. 4A, B and C). The mean RMSEs at the western, central and eastern buoy locations for 1985–2008 are 2.12 °C, 1.77 °C, and 1.69 °C, respectively. The minimum and maximum RMSE for these locations during the 1985–2008 period are 0.50/6.32 °C, 0.90/3.57 °C, and 0.82/2.97 °C, respectively. These occur in the years 2007/1996, 1997/2001, and 1997/2001. The RMSE for each year at the three locations is listed in Supplemental Materials (Table S1). Over the 1985 to 2008 period a general trend of warmer maximum surface water temperatures at the western buoy location than the central or eastern is present in both the model and observations (Figure S1). Though the model tends towards higher maximum water temperatures, a clear spatial trend is seen. In their modeling study, Bennington et al. (2010) also note that western arm of Lake Superior is warmer than the eastern arm. The trend towards higher maximum surface water temperatures in the model is likely due to a shallow mixed layer depth that precludes penetration of heat to greater depth and thus increases the surface water temperature. This issue is noted in a study of Lake Erie by Wang et al. (2010), and its cause is described in greater detail below.

Typical surface water temperature spatial patterns as seen in 2005 are shown in Fig. 5B. Early spring surface water temperatures are uniform to within a few degrees Celsius in the model. This homogenous
state in the early spring is verified by vertical temperature profiles (Fig. 5A, gray dots) taken by the Environmental Protection Agency in spring 2005 at the nineteen stations indicated in Fig. 1 (asterisks). Vertical profiles of temperature at the EPA sampling locations from the model (Fig. 5A, solid lines) show slightly warmer surface temperatures with a nearly isothermal water column throughout the lake. Upwelling, key to biogeochemical processes, can be seen along the northwest coast in the map of 2005 model summer surface water temperatures (Fig. 5D). It shows characteristic Lake Superior thermal patterns, as noted by Bennett (1978), of summertime upwelling along the northwestern shore and warmer waters along the south shore. A comparison of model (Fig. 5C, lines) and observed (gray dots) vertical thermal structure during the summer shows good reproduction of summer surface water temperatures with the model. The lesser variability among the modeled temperatures as compared to observations is possibly due to the fact that the observed temperatures represent measurements taken throughout the day and night unlike the modeled temperatures. The modeled mixed layer depth is shallow in comparison with observations. This issue has been noted in other modeling studies of the Great Lakes (Beletsky and Schwab, 2001; Huang et al., 2010) and of the Bering Sea (Hu and Wang, 2010) note that wind-wave mixing inclusion is necessary to obtain greater upper mixed layer depth and that use of the level 2.5 closure turbulence model, as was done in this study, is not sufficient to remedy the problem. Wind-wave mixing parameterization may be included in the future to increase the accuracy of the mixed layer depth though it is not within the scope of the current study.

Increasing summer surface water temperatures in Lake Superior over the past century and especially the last 30 years have been noted by Austin and Colman (2007, 2008). Fig. 6 plots the surface water temperature averaged over the stratified season (July–September) for the model and observations at the three buoy locations for 1985 to 2008 as well as a linear fit to the data. Both the buoy temperature data and model output concur with the positive trend at all three locations. NDBC buoy data shows a rate of increase of surface water temperature of 0.15 ± 0.05, 0.12 ± 0.07, and 0.12 ± 0.08 °C y⁻¹ at the western, central, and eastern buoys, respectively (Fig. 6 West, Central, and East). An average of temperatures at the three buoys shows a positive trend of 0.14 ± 0.06 °C per year (Fig. 6 Spatially Averaged). Model space- and time-averaged surface water temperatures are consistently warmer than in observations for the first ten years, when the number of meteorological data used to create the surface forcing fields was relatively small. Thus model temperatures show slightly slower rates of increase: 0.08 ± 0.06, 0.07 ± 0.06, and 0.05 ± 0.06 °C per year at the western, central, and eastern buoys, respectively. The average of the west, central and east modeled rate of temperature increase is 0.07 ± 0.06 °C y⁻¹. An average of modeled temperatures from the entire lake surface, which is representative of overall model behavior, gives a value of 0.10 ± 0.05 °C y⁻¹. These values are all comparable to the rate of increase for the summer (JAS) period reported for 1979 to 2006 by Austin and Colman (2008) of 0.11 ± 0.06 °C y⁻¹.

Model ice cover is compared to two data sets: NOAA’s Great Lakes Ice Atlas (Assel, 2003) and the Interactive Multisensor Snow and Ice Mapping System (IMS) Daily Northern Hemisphere Snow and Ice Analysis at 4 km (National Ice Center, 2008). The Great Lakes Ice Atlas contains composite ice charts for the entire surface area of the Laurentian Great Lakes from 1973 to 2002 with a recent update to 2005 in Assel (2005). Data covers the lake-ice season (December to April/May) and frequency of the data ranges from every three to four days to every week. Comparison with model output is performed using the spatially average daily ice-cover time series for Lake Superior, an analysis product in the Great Lakes Ice Atlas. The IMS database is used to provide data from 2005 to 2008. IMS ice-cover data has daily resolution and covers the entire northern hemisphere at a spatial resolution of four kilometers (2004 and onwards). Each 4 km grid cell is evaluated and designated as being land, snow, ice or water. To compare our model output to this binary format of determining ice coverage for a grid cell, we assign ice cover in each model grid cell in a similar binary manner based on an ice cover greater than 30%. Though there is no systematic data set available for thickness of ice cover on Lake Superior, analyses of modeled ice thickness are presented.

The annual cycle of ice cover and spatially averaged ice thickness during 2005 are shown in Figs. 8A and B. Observed ice cover from the IMS Daily Northern Hemisphere Snow and Ice Analysis and the Great Lake Ice Atlas are both available for 2005. Fig. 7A compares time series of the percent of Lake Superior’s surface area covered by ice calculated from the IMS (asterisks) and the Great Lakes Ice Atlas (dots) with modeled percent ice cover (line). The domain-averaged ice thickness is calculated as the average thickness of all ice cover present on a given day. The Great Lakes Ice Atlas and IMS observations are largely consistent with each other as seen in Fig. 7A. An early increase in ice cover and thickness occurs from mid-January to the

beginning of February in response to a basin-wide cold air outbreak (see Supplemental Material Figure S2). Ice begins to form in the periphery of the lake (Fig. 9). During an extended period of sub-zero air temperatures from early to mid-March ice cover quickly increases to a maximum of 58% lake surface area coverage on March 18. Ice thickness follows a similar though slightly lagging increasing trend to reach a maximum of 7 cm on March 23. Both ice cover and thickness subsequently decrease rapidly from late March through April concurrent with basin-wide steadily increasing air temperatures. Ice melt timing in the model lags the observations. This is discussed further in the following paragraph. The RMSE of the modeled percent ice cover compared to that calculated from the IMS data set is 7.8%. In comparison with the Great Lakes Ice Atlas time series, it is 8.2%.

The percent ice cover of Lake Superior from 1985 to 2008 is presented in Fig. 8A. Observational data from 1985 to 2004 is from the Great Lakes Ice Atlas. Observational data from 2005 to 2008 is from the IMS. The variability in the overall magnitude of ice cover from year to year is reproduced well by the model. On this lake-wide scale, the timing of the onset of ice cover compares well between the data and model. Ice-cover melting, however, tends to be delayed in the model as compared with observations, especially in years with large percent ice cover. This may be due to a deficiency in near-surface vertical mixing because of the lack of wind-wave mixing parameterization in the model as noted earlier. This would allow surface water temperatures to remain colder than expected, thus delaying ice-cover melting. RMSE values for ice cover for each year are given in Table S2 in Supplemental Materials. The average RMSE for the 1985 to 2008 period is 16.9%. The maximum RMSE is 41.3 occurring in 1985 and the minimum is 3.8 occurring in 1998. The RMSE tends to be high in years with greater overall ice coverage when the lag in modeled ice melt in comparison with observations is relatively high. Domain-averaged ice thickness in meters is presented in Fig. 8B. Increases in ice thickness are strongly correlated with cold air outbreaks, as noted for year 2005 above. Years with high ice thickness (e.g. 1994 and 1996) exhibit extended periods of sub-zero air temperatures and co-occurring ice thickness increase. Histograms of ice thickness for each year are available in Supplemental Materials (Table S3, after Wang et al., 2010). The fraction of ice cover with thicknesses in the ranges of 0–5 cm, 5–15 cm, 15–30 cm, and greater than 30 cm are given for each month (December to April). Though there are currently efforts to create airborne and satellite ice thickness retrieval algorithms, existing measurements of ice thickness on Lake Superior are scant and not readily available (pers. comm., George Leshkevich, 2011). Therefore, information on ice thickness from the model will be useful for future comparison with satellite or other observations.

Figure S3 in supplementary materials presents a map of observed and model ice cover and environmental conditions for January 26, 2005. The observed ice cover is from the IMS Daily Northern Hemisphere Snow and Ice Analysis. Geographic distribution of the ice cover is similar between observations (Figure S3A) and model (Figure S3B) with ice cover along the southwestern, southeastern shores and in the northern bays, though the model produces more extensive coverage along the southeastern shore. Zero degree waters are present only along the coastal regions with warmer water over the rest of the lake surface (Figure S3C). Ice can, therefore, only form along a thin region near the shore, but the model ice extends into warmer waters. The presence of ice in warmer waters therefore is explained by advection of ice, indicated by a predominantly east-to-west ice velocity (black arrows, Figure S3B) driven by sustained northwesterly winds (Figure S3D). In other words, along the southern and eastern shores the ice moves away from freezing coastal waters, allowing more ice to form along the shoreline and adverting the ice away in a mechanism similar to that of coastal polynya found in polar seas. The size of the ice cover in this situation is determined by the relative rates of new ice formation nearshore and of ice melting along the outward ice edge. The regular presence of coastsally formed ice, especially in years with less than complete ice cover, can also be seen in a comparison of the spatial distribution of ice cover as observed (left column,

Fig. 7. A: The percentage of lake surface area covered by ice for 1985 to 2008. Model output is shown as a solid line and observations from the NOAA Great Lakes Ice Atlas (dots) of percentage of lake surface area covered by ice during 2005. B: Domain-averaged ice-cover thickness in meters during 2005.

Fig. 8. A: The percentage of lake surface area covered by ice for 1985 to 2008. Model output is shown as a solid line and observations from the NOAA Great Lakes Ice Atlas (1985–2004) and the Interactive Multisensor Snow and Ice Mapping System Daily Northern Hemisphere Snow and Ice Analysis at 4 km (2005–2008) are shown as dotted lines. B: Domain-averaged ice thickness in meters for 1985–2008.
Ice cover first forms in the shallow northern bays, then along the relatively shallow and bathymetrically gently sloping southwestern shores and finally in Whitefish Bay (Jan 12 panels, Fig. 9). Ice cover begins increasing in extent in reaction to a cold air outbreak (Feb 24 panels, Fig. 9, Figure S2). Ice cover reaches a maximum in mid-March due to continued sub-zero air temperatures following the late February cold air outbreak (not shown). Ice cover occupies nearly the entire coastline with no coverage in the central and eastern basin offshore waters. As ice cover decreases in late March in response to warming air temperatures (Mar 21 panels, Fig. 9), the width of ice cover along the coastline decreases with ice cover in the central and eastern basins melting first in the offshore waters. By April, ice cover persists mainly in the shallow northern bays (not shown).

Annual ice-cover magnitude has been shown to be decreasing over the past several decades (Austin and Colman, 2007). Figure S4 shows the average percent of lake surface area covered by ice for each year’s winter season. The model tends towards slightly greater ice coverage and is decreasing at a rate of 1.20±0.29%/yr for 1985–2008. The observations show a rate of decrease of 0.80±0.20%/yr. These values are comparable to the value of 0.42±0.20%/yr reported by Austin and Colman (2007) for the period of 1979–2006.

Mean annual water current magnitudes and directions at the surface (<20 m) and at depth (>75 m) from the model for 2005 are presented in Fig. 10. Average annual surface current speed and average annual deep current speed are on the order of 0.50 cm s⁻¹ and 0.36 cm s⁻¹. Winter currents both at the surface and at depth tend to dominate the annual average values, because winter surface currents are stronger than summer currents due to greater wind speeds during the fall and winter. Though using different atmospheric boundary conditions we find that, similar to results in Bennington et al. (2010), winter surface currents tend to reflect wind directions that have a strong northerly component. Winter currents at depth are stronger than summer due to the strength of the surface currents and the lack of strong density stratification. Weaker stratification during the winter allows wind momentum to be transferred more readily into deeper waters than during the summer. Topography (see Fig. 1) is reflected in the distribution of cyclonic circulation at the surface and at depth above the deep Eastern and Western basins (Bennington et al., 2010). Current directions also are roughly consistent with those presented in Beletsky et al. (1999).

Biogeochemical results

Surface maps of modeled temperature, phosphate, and chlorophyll concentrations from August 22, 2005 show mechanistically consistent spatial patterns (Fig. 11). Upwelling, indicated by cooler water temperatures, is clear along the northwest shore (Fig. 11A).
presence of upwelling is also apparent in elevated surface phosphate concentrations (Fig. 11B). A similar spatial pattern in chlorophyll concentrations show the response of phytoplankton to waters with relatively higher nutrient concentration being brought to the photic region of the water column through upwelling (Fig. 11C). These relationships demonstrate internal consistency within the biogeochemistry and ecosystem model. They also show that phosphorus exerts primary control on phytoplankton growth in the model.

The EPA measures chlorophyll concentration with depth annually at nineteen sites (asterisks, Fig. 1). Fig. 12 compares model chlorophyll concentrations at the same locations and summertime sampling dates with the EPA data. The deep chlorophyll maximum (DCM) is a ubiquitous feature in Lake Superior during the summer months. The depth and magnitude of the DCM are reproduced well in modeled chlorophyll values. Chlorophyll in the model displays less spatial heterogeneity than the observed chlorophyll does. This may be due to the horizontal resolution of the model grid (5 km by 5 km) and the fact that the observed values represent measurements taken at multiple times throughout the day and night. Surface chlorophyll values in the model tend to be slightly higher than those observed. This could be due to the absence of a phytoplankton photoinhibition mechanism in the ecosystem model. The model also displays lower overall chlorophyll values at sub-thermocline depths.

Productivity in Lake Superior has limited seasonal variability. Sterner (2010) notes only small change in algal biomass and chlorophyll levels in measurements spanning April to November which covers conditions from an isothermal less than 2 °C water column (April) through fully developed summer stratification with surface temperatures of 18.38 °C. Sterner states an annual range of productivity of 200–350 mg C m−2 d−1. An earlier study by Munawar and Munawar (1978) on diversity and biomass of phytoplankton throughout Lake Superior also noted a lack of clear seasonal trends in phytoplankton biomass that set it apart from the other Great Lakes. The model exhibits a seasonal range of productivity from approximately 20 to 700 mg C m−2 d−1. That the model has a stronger seasonal variability than indicated by available observations suggests that the dissolved pool of organic matter may be too small vis-à-vis the particulate pool. As noted above, we attempted to implicitly account for the purportedly strong microbial loop by selecting a low half-saturation concentration of phosphate uptake by phytoplankton and high rates of remineralization of detritus. As in most marine ecosystem models, the selection of these poorly constrained biological parameter values is delicate and difficult. A more judicious selection of biological parameters as well as possibly different ecosystem construction are areas of future improvement. It is worth noting that by removing seasonal peaks in surface phosphate concentration, a strong microbial loop and a larger pool of dissolved organic matter would tend to diminish the appearance of phosphate controlling phytoplankton growth. This may explain why temperature and light can come out statistically as dominant controls on primary production (Sterner, 2010). Three other factors that may affect the seasonality of productivity in the model are ice-cover presence which has been noted to last longer in the spring in the model compared to observations and which affects the amount of light experienced by the ecological model, the use of a single class of phytoplankton in the model which does not allow for species succession throughout the year, and the use of a constant carbon to phosphorus ratio for phytoplankton.

The average annual gross primary productivity from the model for the 1985 to 2008 period is approximately 6.2 Tg C yr−1 (Figure S5). This value is within the ranges offered by Cotner et al. (2004, 5.3–8.2 Tg C yr−1) and Urban et al. (2005, 2.0–6.7 Tg C yr−1). Model results for 2006 to 2008 range from 7.1 to 7.8 Tg C yr−1 and are similar to the more recent value of 7.6 to 9.73 Tg C yr−1 from Sterner (2010). Much as the annual surface water temperatures and annual ice cover show large variability, so does total annual gross primary production. The interannual range for this period is about 4.1 Tg C with more productivity during warmer years with less ice cover. Years with high ice cover have reduced levels of annual gross primary production possibly owing to, as mentioned above, the tendency in the model to retain ice in the spring past the date of ice-out indicated by observations as well as the impact of ice on light experienced by the ecological model. A fit to these values shows gross primary productivity increasing at a rate of 0.07 ± 0.03 Tg C yr−1 over this time period (Figure S5).

Gross primary production is strongly correlated with annual average surface water temperatures and average percent wintertime ice cover (r² = 0.98, r² = 0.85, respectively, Fig. 13). Two key factors in Lake Superior primary productivity are water temperature and light availability according to Sterner (2010). Therefore, increased surface water temperatures may allow for greater rates of primary productivity. At the same time, stronger thermal stratification reduces the depth to which phytoplankton are mixed in the water column, increasing light availability for primary production. A longer stratified season can thus yield greater annual primary productivity by allowing phytoplankton to experience warmer temperatures and greater light intensity for a larger portion of the year, assuming that nutrients do not become the limiting growth factor.

Conclusions

We present a new realistically configured three-dimensional model for Lake Superior including for the first time prognostic models of ice and biogeochemistry. For the simulation period of 1985 to 2008, the new model is able to reproduce many physical and biological characteristics of Lake Superior as well as long-term interannual trends in water temperature and ice cover.

The annual surface water temperature cycle is well represented by the model with average root mean square errors of 2.12 °C, 1.77 °C, and 1.69 °C in comparison with observations at the western, central, and eastern NOAA buoy locations. Large-scale spatial patterns in surface water temperatures, e.g. higher overall water temperatures in the western arm versus the central and eastern basins, are reproduced by the model. The mixed layer depth tends to be shallower in the model in comparison to observations, possibly because the model lacks wind-wave mixing parameterization, which may be included in the future. A repercussion of the shallow thermocline is relatively high summer maximum surface water temperatures. However, the trend of increasing summertime surface water temperatures in the model during the period 1985–2008 is consistent with observations.

Interannual variability of ice-cover magnitude simulated by the model is consistent with observations. Focus on the 2005 shows
good reproduction of timing of ice formation and the magnitude and timing of peak ice cover as considered against two sets of ice-cover observations. Melting of ice cover in the model is delayed in comparison with observations. This is also likely linked to the shallowness of the mixed layer depth and can be improved in the future. The rate of decrease of wintertime ice-cover magnitude from 1985 to 2008 in the model is similar to but greater than observations.

Spatial patterns of biogeochemical variables show internal and therefore mechanistic consistency within the model, although an improved representation of the microbial loop and dissolved phase of organic matter is an area of future model development. Vertical chlorophyll profiles, including the deep chlorophyll maximum in the stratified season, are reasonably well simulated when compared to observations. Average total annual gross primary production for 1985–2008 is comparable to several recent estimations of productivity including that of Sterner (2010). Long-term interannual gross primary productivity rates are highly variable but show an increasing trend for the period 1985–2008 that is strongly correlated with increasing annual average surface water temperatures and decreasing winter ice cover.

This new model is the first to explicitly model the dynamics of water, ice, and biogeochemistry of Lake Superior. The model is internally consistent, responds well to the data-based forcing fields, and overall reproduces lake observations well. These attributes make this model a useful tool for elucidating mechanisms controlling the physical state and biogeochemical cycling of the lake today and how these may change in the future under global climate change.

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