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Calibration and validation of lake surface temperature simulations with the coupled WRF-lake model

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Abstract A one-dimensional (1-D) physically based lake model was coupled to the Weather Research and Forecasting (WRF) model version 3.2 developed by the National Center for Atmospheric Research to dynamically simulate physical processes of lakes and their effects on weather and climate at local and regional scales. Our study area is focused on the Great Lakes. This coupled model realistically reproduces the lake surface temperature (LST) at a buoy station in a shallow lake (Lake Erie) while generating strong LST biases ranging from −20 to 20 °C at a buoy station in a deep lake (Lake Superior). Through many sensitivity tests, we find that the biases in the deep lake LST simulations result from the drastic underestimation of heat transfer between the lower and upper parts of the lake through unrealistic eddy diffusion. Additional tests were made to calibrate the eddy diffusivity in WRF-Lake. It is found that when this parameter is multiplied by a factor ranging from 10^2 to 10^5 for various lake depths deeper than 15 m, the LST simulations for the deep lake buoy station show good agreement with observations, and the bias range reduces to ±4 °C. Essentially, the enlarged eddy diffusivity strengthens heat transfer within the lake columns in the deep lake, which is significantly underestimated in the lake model without calibration. Validation simulations with the calibrated eddy diffusivity were carried out for the whole of Lake Superior and Lake Erie. The LST simulations still have a substantial bias reduction when compared with those produced with the original eddy diffusivity, indicating that the

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calibrated parameter is representative. In addition, the improved 1-D lake model with WRF reasonably reproduces the remotely sensed LST geographic distribution.

1 Introduction

Lake-atmosphere interactions are important to local and regional weather and climate in lake-dominant areas (Bates et al. 1993; Swayne et al. 2005; Leon et al. 2007; Rouse et al. 2005; Samuelsson et al. 2010; Subin et al. 2012; Notaro et al. 2013; Vavrus et al. 2013; Wright et al. 2013). Lake-atmosphere interactions can lead to the production of lake effect precipitation during early winter or spring when cold air masses are warmed and moistened by the underlying water, generating heavy snowfall in the downwind regions (Eichenlaub 1979; Braham and Dungey 1984; Niziol et al. 1995; Scott and Huff 1996). For example, a severe early winter snowstorm occurred from November 9 to 14, 1996, in the Great Lakes region and led to hundreds of thousands of customers losing electric power (Schmidlin and Kosarik 1999). This storm dumped nearly 178 cm of snow on the ground. The precipitation amount, extent, and intensity depended on the air-lake temperature difference and the over-water fetch. An early study by Lavoie (1972) used a simple numerical model to examine lake-atmosphere interactions with some success, showing that the temperature difference between the lake and lower atmosphere is the most important indicator of the intensity of lake-effect precipitation. An observational study by Holroyd (1971) indicated that a 13 °C temperature difference between the lake and the 850-mb level of the atmosphere was a necessary condition for lake-effect snowfall. Some researchers have incorporated one-dimensional (1-D) physically based lake schemes with weather and climate models to investigate the impact of lakes on weather and climate at local or regional scales (Lavoie 1972; Hostetler 1993; Bates et al. 1993; Samuelsson et al. 2010).

Over the last three decades, various 1-D lake models with different degrees of sophistication in physical processes have been developed (Henderson-Sellers 1985; Ljungemyr et al. 1996; Goyette et al. 2000; Tsuang et al. 2001). Stepanenko et al. (2010) conducted the Lake-Model Intercomparison Project with these 1-D lake models ranging from the simplest one-bulk-layer models to complex finite-difference models with a turbulence closure scheme. Their results indicated that these models could realistically simulate water mixing processes and temperature profiles in shallow lakes that were mostly less than 50 m deep (Boyce et al. 1993; Peeters et al. 2002; Yeates and Imberger 2003; Mironov et al. 2010). However, problems arose when these models were used to simulate energy exchanges within deep lakes that were mainly more than 50 m deep. For instance, none of these models was able to realistically reproduce the observed lake surface temperature (LST) in Lake Michigan, with an average depth of 85 m. To eliminate the errors from the simulated atmospheric forcing, observational data were used to drive two 1-D lake models for the Great Lakes (Martynov et al. 2010); the results showed that both models performed poorly in simulating water temperature in deeper lakes (e.g., Lake Superior, with an average depth of 147 m), strongly indicating that the simulated temperature errors resulted from unrealistic lake process simulations.

Thus, there is a need to fully understand physical processes, especially in deep lakes, in order to improve simulations and predictions of lake thermal conditions and lake-atmosphere interactions. For this study, we coupled a 1-D physically based lake model with an advanced regional climate model to examine lake process simulations at a regional scale by comparing simulations for a shallow lake and a deep lake in the Great Lakes. Our special focus is on improving and gaining a better understanding of deep lake process simulations through a large number of modeling experiments with our coupled model. This paper is arranged as follows:

model descriptions are presented in Section 2, model configuration and data introduction are included in Section 3, results and analysis are given in Section 4, and the last section contains conclusions and discussion.

2 Model descriptions

2.1 The 1-D lake model

The lake model used in this study is a 1-D mass and energy balance model that was retrieved from the Community Land Model (CLM) version 3.5 (Oleson et al. 2004). This lake model is described in Zeng et al. (2002) and uses the concepts in Henderson-Sellers (1985), Henderson-Sellers and Davies (1989), Hostetler (1993), Hostetler et al. (1994), and Bonan (1995), along with some of the modifications in Subin et al. (2012). The lake depth is originally set to 50 m for all lakes and is divided into 10 layers. However, such a fixed lake depth model setting could cause significant biases in lake thermal process simulations as discussed in the remaining sections, especially for deep lakes (e.g., depth > 50 m). Therefore, actual lake depth data at 1 km resolution (Kourzeneva 2010) are used in our study, and the top lake layer is always set to 0.1 m regardless of the lake depth in order to reflect the diurnal cycle of surface variables; the thickness of the lake layer then gradually increases from the second layer to the tenth layer at the bottom. The lake temperature for each layer is computed based on a Crank-Nicholson thermal diffusion solution, and the lake surface heat and water fluxes are calculated assuming a freely varying (infinitesimal skin) surface temperature, with aerodynamic resistances computed as for nonvegetated surfaces in CLM (Oleson et al. 2004). There are also 10 layers of soil on the lake bottom, 5 layers of snow on the lake ice, and a parameterization of the fraction of ice on the lake surface added by Subin et al. (2012), in addition to correction of several errors in the calculation of surface fluxes and eddy diffusivity occurring in the original CLM3.5 code (Oleson et al. 2004). Energy transfer between the lake layers is controlled by temperature differences and molecular and eddy diffusion. The molecular diffusivity in the model is set to a constant (1.433×10^{-7} m^2/s), and the eddy diffusivity (k_e) is parameterized mainly as a function of near-surface wind stress and lake density gradient (Henderson-Sellers et al. 1983; Henderson-Sellers 1985). When the LST is below the freezing point, the eddy diffusivity is set to zero. At the lake bottom, the heat flux exchange between the lake and soil is calculated based on the energy transfer equation. However, there is no lake scheme in any of the release versions (up to Version 3.4.1) of WRF, which is one of the most advanced regional climate models in the world. For this study, the lake model discussed above is coupled with WRF (hereafter WRF-Lake) to explicitly simulate and predict lake processes and lake-atmosphere interactions in regional climate systems.

3 Model configuration and data

In this study, we focus on two lakes in the Great Lakes region: Lake Superior, with an average depth of 147 m as mentioned previously and a maximum depth of 406 m; and Lake Erie, with an average depth of 19 m and a maximum depth of 64 m. The former represents deep lakes, and the latter represents shallow lakes. In this study, we focus only on lake water processes; lake ice and its related snow processes are not included and will be addressed elsewhere. Thus, our study period is 1 September 2001 to 31 December 2002, an ice-free period in all of the Great Lakes. To achieve realistic LST simulations, lake profile initializations are very important, especially for deep lakes. The lake temperatures in the top layer for 1 September 2001 are initialized with the Moderate Resolution Imaging Spectroradiometer (MODIS) LST, and from the second layer to the bottom layer, the initial temperature values are assigned based roughly on the shape of the observed lake temperature profile for 1 September 2008 for Lake Superior, which was obtained from the University of Minnesota (http://www.seagrant.umn.edu/superior/processes). Through this method, we found that the layers of a lake column deeper than 50 m were mostly initialized at 4 °C for Lake Superior and Lake Erie for the start time of the simulations. Our results show that there is no clear convergence or divergence between observations and simulations (discussed in Section 4), indicating our lake temperature initial conditions may be reasonable. Originally, we planned to use the simulations of the first three months (September, October, and November 2001) as a model spin-up. However, our simulations agree very well with observations for these three months, and thus we take the results for the entire study period (1 September 2001 through 31 December 2002) for time series analysis.

Our two simulation domains are 60 × 40 model grids at a 10 km resolution and are centered at 47.59°N, 88.20°W on Lake Superior and at 42.25°N, 81.25°W on Lake Erie, respectively (Fig. 1). We performed a series of sensitivity tests with WRF and found an optimal combination that produced realistic precipitation and temperature simulations (figures not shown). In this optimal combination, we used the Noah land surface scheme, the Lin microphysics scheme (Lin et al. 1983), the Kain-Fritsch scheme (Kain and Fritsch 1993) for parameterizing cumulus clouds, the Yonsei University scheme for boundary layer processes (Hong and Pan 1996), the Rapid Radiative Transfer Model (RRTM) based on Mlawer and Clough (1997) for calculating longwave radiation, and the Dudhia scheme for calculating shortwave radiation (Dudhia 1989).

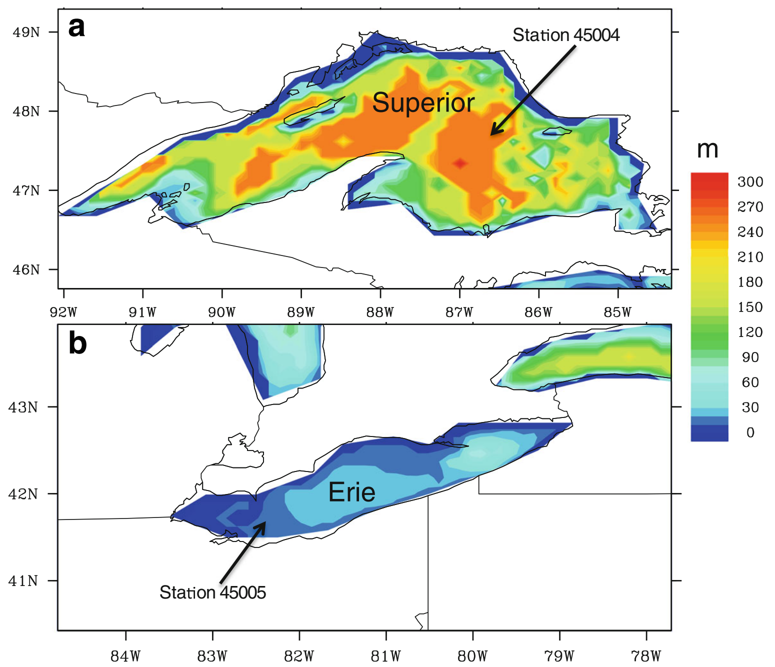

Fig. 1 Lake depth observations: (**a**) Lake Superior (deep lake) and the location of buoy station 45004: 47.584 N, 86.587 W; water depth: 227.4 m; (**b**) Lake Erie (shallow lake) with the location of buoy station 45005: 41.677 N, 82.398 W; water depth: 12.6 m

The initial and lateral boundary conditions of WRF-Lake were provided by the North American Regional Reanalysis (NARR) data at 32 km resolution and were updated every 3 h. We also used buoy LST observations from the National Data Buoy Center (NDBC) and the MODIS LST for model calibration and validation. The buoys are usually removed from the sites in late fall and replaced in early spring; thus there are no buoy observations over wintertime, but the gap is filled by the National Aeronautics and Space Administration's Moderate Resolution Imaging Spectroradiometer (MODIS) satellite LST data, which cover our entire study period.

4 Results and analysis

4.1 Initial simulations for deep and shallow lakes

We first select two buoy stations whose temperature measurements partially cover our study period (1 September 2001 through 31 December 2002) in order to evaluate the coupled WRF-Lake's ability to simulate the LST. One station is in Lake Superior (Station 45004), and the other is in Lake Erie (Station 45005; Fig. 1). The simulated daily LSTs (blue line in Fig. 2) are compared against daily buoy observations (black line) and the 8-day averaged MODIS data (green stars). WRF-Lake appears to quite accurately reproduce the observed LSTs in the shallow lake, Lake Erie, where the simulated bias and root-mean-square-error (RMSE) against the buoy data are −0.55 °C and 1.76 °C, respectively; against the MODIS data they are 0.98 °C and 2.29 °C, respectively. However, for Lake Superior, a deep lake, the coupled WRF-Lake generates a 40 °C bias range from −20 °C during the winter up to 20 °C during the summer, due to unrealistic winter ice development and early summer stratification, and the simulated RMSE is also more than 7 °C, when compared with the MODIS data. These large errors should be reduced to a reasonable level before the coupled model can be used to study and predict the physical process in lakes and lake-atmosphere systems. Based on our simulations, WRF-Lake can reasonably simulate land surface temperatures in the areas near Lake Superior and Lake

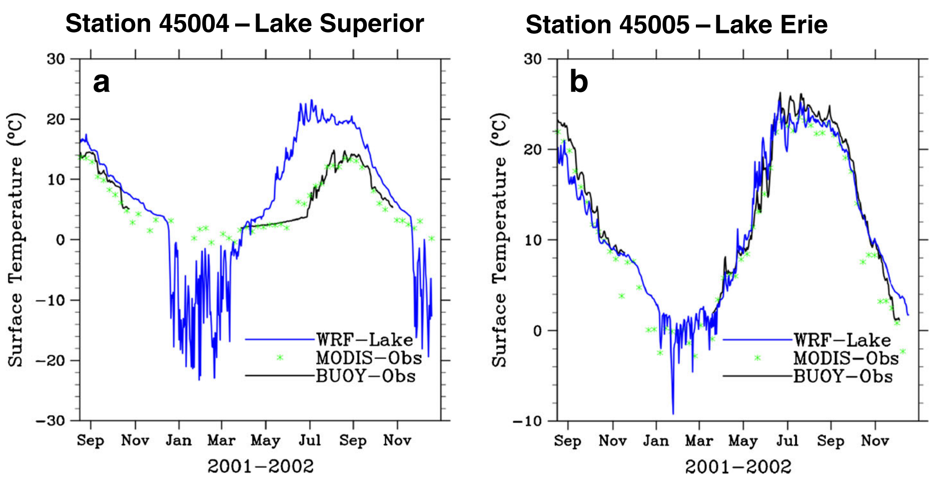

Fig. 2 Time series of observed daily buoy LST (*black line*), MODIS LST (*green stars*), and WRF-Lake simulations (*blue line*) at (**a**) Station 45004 (Lake Superior) and (**b**) Station 45005 (Lake Erie) for the period of 1 September 2001 through 31 December 2002. Unit: °C

Erie when compared to the MODIS surface temperatures (figure not shown), suggesting that the atmospheric forcing generated by WRF is within a plausible range. Thus, the errors seen in the LST simulations for the deep lake likely result from unrealistic simulation of lake mechanisms in the model. Similar large biases in deep lake LST simulations are seen in Martynov et al. (2010) and Stepanenko et al. (2010) using offline lake models forced by observed atmospheric data, further confirming that the deep lake processes need to be closely investigated.

4.2 Atmospheric forcing for deep and shallow lakes

To understand the lake process simulations, we first need to examine the near-surface atmospheric forcings. Figures 3a and b show the comparison of the 30-year climatologies of the observed air temperatures at a height of 4 m and LSTs in Lake Superior (Station 45004) and Lake Erie (Station 45005). The pattern of 4 m height temperatures follows that

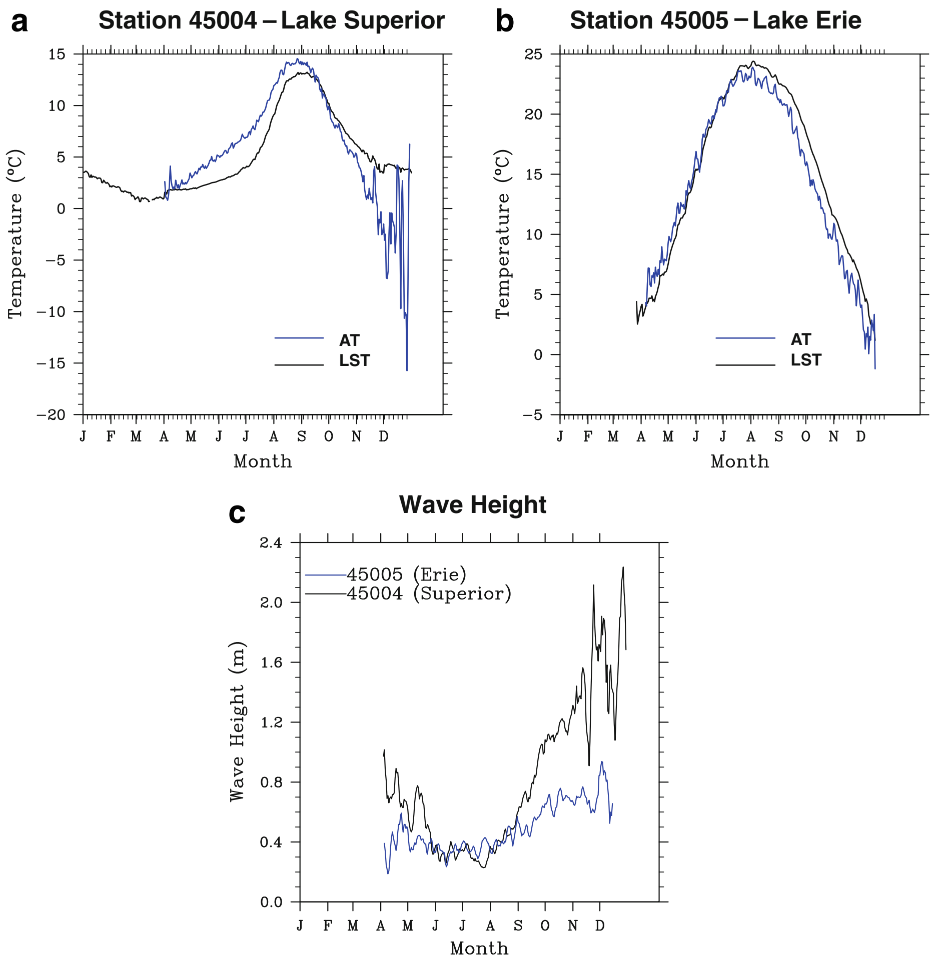

Fig. 3 Thirty-year climatology (1981–2010) of observed daily LST (*black line*, unit: °C) and near-surface air temperature at a height of 4 m (AT, *blue line*, unit: °C) for (**a**) Station 45004 (Lake Superior) and (**b**) Station 45005 (Lake Erie). Also, (**c**) wave height climatology for the same period for both buoy stations

of the LST in Lake Erie very closely, while there are large discrepancies between the two variables in Lake Superior, especially during the summer and winter. This phenomenon indicates that for the shallow lake the lake-atmosphere is well coupled, and the LST variation follows the changes in the atmospheric forcing. In other words, if an accurate atmospheric forcing is generated over the shallow lake in our coupled WRF-Lake model, the LST can be realistically reproduced. For the deep lake, atmospheric forcing is apparently not the only factor that controls changes in LST. One hypothesis is that the deep part of the lake often acts as an energy sink or source to modulate changes in LST. Thus, understanding heat transfer within the deep lake may be important to estimate the LST in Lake Superior.

Figure 3c shows the observed wave height climatology derived from data over the 30-year period from 1981 to 2010 at the two buoy stations (Stations 45004 and 45005) in Lake Superior and Lake Erie, respectively. This figure indicates that the wave height in Lake Superior is much higher than that in Lake Erie; the average wave height in Lake Erie is below 1 m, while it more than doubles in Lake Superior. These large differences occur in the spring, fall, and winter. The differences in wave height indicate that turbulent water mixing in the deep lake is much stronger than in the shallow lake. Based on these observations, we hypothesize that heat transfer through water mixing in the deep lake is stronger than in the shallow lake, and the large simulated LST biases (Fig. 2a) result from the insufficient estimation of heat exchange within the deep lake in our coupled WRF-Lake model.

4.3 Calibration of lake eddy diffusion

As we discussed in Section 2.1, two parameters control heat transfer within lakes: molecular and eddy diffusivities. Adjusting these two parameters could lead to changes in LST simulations. Martynov et al. (2010) found a large bias in their deep lake LST simulations using a lake model similar to the one we have coupled to WRF. They increased molecular diffusivity in an attempt to strengthen heat flux transfer in the deep lakes. However, the simulated changes in LST produced with these increased molecular diffusivity values did not follow the observed LST patterns. We have also done sensitivity tests with different molecular diffusivity values and produced similar biased patterns. These results tell us that the large biases in LST simulations shown in Fig. 2a are not related to molecular diffusion. Therefore, we performed additional sensitivity tests by changing the eddy diffusivity (k_e). In order to have a clear perception of k_e scaling in the lake model, we have examined the k_e values in the lake column. It is shown that the original k_e values at Station 45004 range from around 1×10^{-4} to 5×10^{-4} m^2/s, which are on the same order as those discussed in Sweers 1970; Csanady 1964, and Csanady 1966. We then increased k_e by a factor of 10^3, and the corresponding WRF-Lake results show that the simulated LST pattern (red line in Fig. 4) starts to approach the observations. We then enlarged k_e by a factor of 10^5, and the resulting LST simulations (purple line in Fig. 4) approach the observations very closely. In particular, the enormous cold biases occurring in the winter disappear. Moreover, an observed temperature drop is seen in August, and WRF-Lake is able to simulate this drop, but the simulations do not match well with the observations in either shape or magnitude when k_e is increased by a factor of 10^3 or 10^5. Especially, in the latter case, the temperature is underestimated by the model, implying that the simulated turbulent water mixing in the lake may be too strong for that month. Through these tests, it is apparent that a single value of eddy diffusivity may not be able to sufficiently capture complex turbulent mixing processes in the deep lake. Thus, we performed many additional model tests with different eddy diffusivity values to produce better LST simulations than those shown in Fig. 4. Based on the experience and knowledge gained from these modeling tests, we set eddy diffusivity as a function of lake depth and LST as shown in Table 1, where the LST at the previous time step was used to set the factor value for k_e at the next

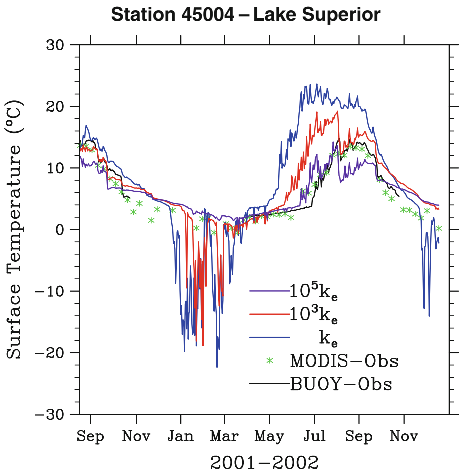

Fig. 4 Time series of daily LST (unit: °C) at Station 45004 (Lake Superior) from MODIS data (*green stars*), buoy observations (*black line*), and WRF-Lake simulations with three different eddy diffusivities (*blue, red, and purple lines*) for the period of 1 September 2001 through 31 December 2002

time step in the model. Based on our simulations for these two lakes, we found that when the lake is deeper than 15 m, there is a clear divergence between observations and simulations with the original k_e (figure not shown), indicating a limit of the original k_e at lake depths greater than this value. Table 1 shows that an increase in eddy diffusivity is made for nonfreezing lakes deeper than 15 m. However, we believe that the criteria for distinguishing deep and shallow lakes are still model dependent. Specifically, for this lake model, a greater eddy diffusivity is needed when the lake depth is deeper than 15 m.

In general, when the lake is deeper and the LST is equal to or lower than 4 °C but greater than the freezing point, k_e is multiplied by a larger factor, and vice versa. Under this LST range, which often occurs during the cold season, stratification in the upper part of the lake is usually weak, and the turbulent water mixing driven by the near-surface wind stress can easily reach the lower part of the lake or even its bottom, indicating a large eddy diffusivity value. When the LST increases from 4 °C, which occurs in the Great Lakes mostly during late spring and summer, there is an increase in the epilimnion, defined as the depth of the warm water layer at the top of the lake. Strongest lake stratification over the year usually occurs during this period of time. Thus, lake stratification in the warm seasons greatly limits water mixing, indicating a small eddy diffusivity value.

We applied the calibrated values of eddy diffusivity shown in Table 1 to WRF-Lake and performed one additional simulation for the period of 1 September 2001 through 31 December 2002. Figure 5 shows that with these calibrated eddy diffusivity values, WRF-Lake quite reasonably reproduces the LST observations (red line in Fig. 5). The bias range decreases from

Table 1 Calibrated eddy diffusivities for different lake depths under the three LST ranges. k_e is the original eddy diffusivity (unit: $m^2\ s^{-1}$)

Depth	LST	> 4 °C	0–4 °C	≤ 0 °C
≥ 150 m		10^2k_e	10^5k_e	0
15~150 m		10^2k_e	10^4k_e	0
≤ 15 m		k_e	k_e	0

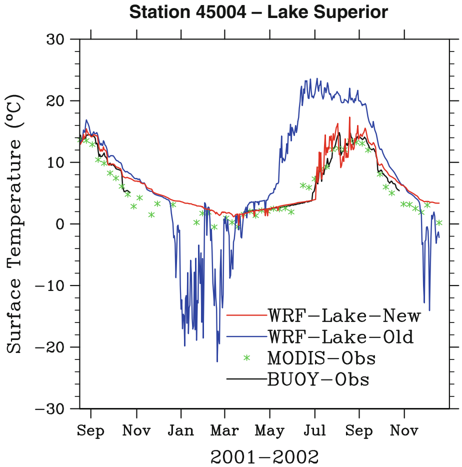

Fig. 5 Time series of daily LST (unit: °C) at Station 45004 (Lake Superior) from MODIS data (*green stars*), buoy observations (*black line*), and simulations by the original WRF-Lake (*blue line*) and the calibrated WRF-Lake (*red line*) for the period of 1 September 2001 through 31 December 2002

± 20 °C to about ±4 °C, and the RMSE also reduces to 2–5 °C from about 7 °C when compared against both buoy and MODIS observations. Clearly, the calibrated eddy diffusivity values in Table 1 drastically improve our LST simulations for Lake Superior. The same diffusivity values in WRF-Lake are also applied to Lake Erie, and slightly improved results are also seen when compared to those in Fig. 2b. We also draw the vertical temperature profile evolution for our study periods (Fig. 6). From this figure, we can clearly see that in the original lake model, lake stratification is very thin when compared with observations for 2008 and 2009 (obtained from the University of Minnesota, http://www.seagrant.umn.edu/superior/processes). Especially during the winter, the stratification reaches about 15 m in depth. After we multiply the original k_e by factors ranging from 10^2 to 10^5, the vertical heat transfer increases greatly, and the thermocline goes deeper in both summer and winter. Also, the winter cooling and summer warming are postponed, and vertical mixing is strengthened, resulting in more realistic LST simulations. However, these eddy diffusivity values are based on the modeling results, and they may not accurately reflect actual conditions, but we further validate these calibrated diffusivity values with additional simulations, as described in the following section.

4.4 Validation of the LST simulations

All of the above simulations are calibrated at the buoy stations in Lake Superior and Lake Erie, and it is still unknown whether the calibrated parameters are suitable for the rest of the two lakes. Thus, a validation process is vital for generalizing the use of the coupled model. Figure 7 shows the time series of the LST simulations with WRF-Lake and MODIS observations averaged over the whole of Lake Superior and Lake Erie. The model with the calibrated eddy diffusivity improves LST simulations to a great extent when compared with the model without calibration and the MODIS data. For Lake Superior, the bias range decreases from −18.2–14.0 °C to −6.3–5.2 °C, and the RMSE reduces from 6.2 °C to 1.5 °C. We also see improvements in the LST simulations in Lake Erie, because there are still many lake columns deeper than 15 m in that lake (Fig. 1). The bias range for this shallow lake decreases from ± 7.0 °C to ± 4.0 °C, and the RMSE reduces from 3.0 °C to 2.0 °C.

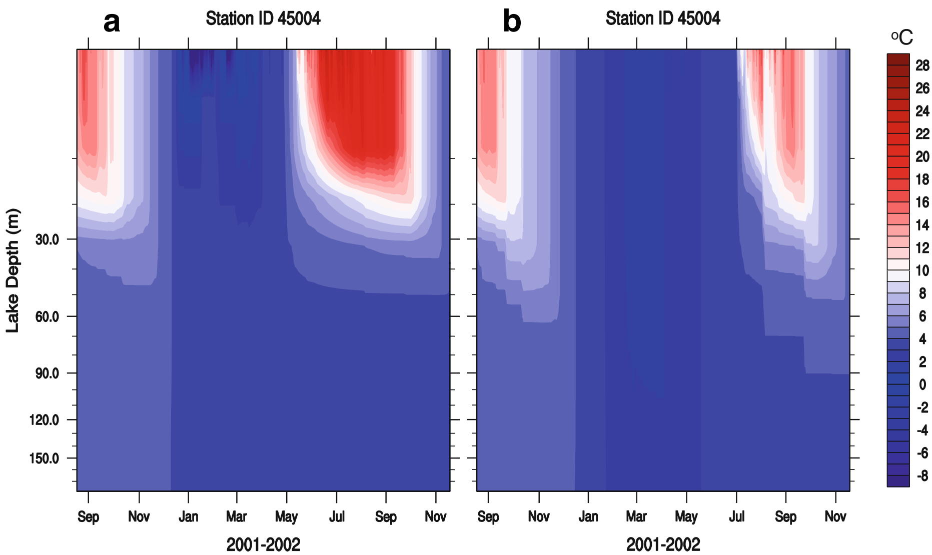

Fig. 6 Vertical water temperature profiles simulated by the original WRF-Lake (**a**) and calibrated WRF-Lake (**b**) for Station 45004 for the period of 1 September 2001 through 31 December 2002. Unit: °C

We have examined the geographic distribution of MODIS and simulated LSTs at a seasonal scale for Lake Superior and Lake Erie (figures not shown), respectively. It is evident that the calibrated WRF-Lake model produces very reasonable simulations for the spatial distribution of LST in both lakes when compared with the MODIS data. In addition, the biases for almost all seasons are reduced with the new eddy diffusivity values. The greatest improvements are seen in the summer for both lakes. The bias range decreases from −3.20–8.5 °C to −0.4–1.3 °C for Lake Superior, and −0.23–3.27 °C to 0.35–1.44 °C for Lake Erie. These validation simulations

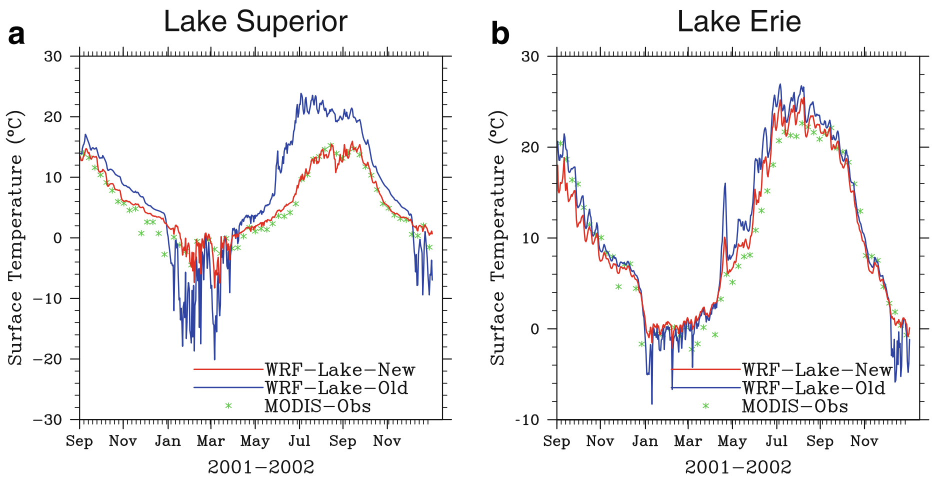

Fig. 7 Daily LST time series of MODIS (*green stars*) and simulations by the original WRF-Lake (*blue line*) and calibrated WRF-Lake (*red line*) for the whole of (**a**) Lake Superior and (**b**) Lake Erie for the period of 1 September 2001 through 31 December 2002. Unit: °C

clearly indicate that the calibrated eddy diffusivity values allow realistic simulations in both shallow and deep lakes.

5 Conclusions and discussion

A 1-D physically based lake model was coupled to WRF (version 3.2) to dynamically simulate lake processes and lake-atmosphere interactions. The coupled model realistically reproduces the LST at a buoy station in the shallow lake (Lake Erie), while it generates strong LST biases ranging from −20 °C to 20 °C at a buoy station in the deep lake (Lake Superior). Through a large number of sensitivity tests, we found that the biases in the deep lake LST simulations result from the drastic underestimation of heat transfer between the lower and upper parts of the lake through eddy diffusion. Additional tests were made to calibrate the eddy diffusivity in WRF-Lake. We found that when this parameter is multiplied by a factor ranging from 10^2 to 10^5 for various lake depths deeper than 15 m, the simulations for the deep lake station show good agreement with the observations. Essentially, the enlarged eddy diffusivity strengthens heat transfer within the lake columns in the deep lake, which is significantly underestimated in the model with the original diffusivity. Validation simulations with the calibrated eddy diffusivity values were carried out for the whole of Lake Superior and Lake Erie. A remarkable bias reduction in these simulations is still seen when compared with those simulations produced with the original eddy diffusivity, indicating that the calibrated parameters are representative. Very importantly, the improved 1-D lake model reasonably reproduces the observed spatial distribution of LST.

In this modeling exercise, the original eddy diffusivity is increased by up to several orders, and the augmented parameter very effectively helps produce realistic LST simulations. However, it should be realized that the model is simply being tuned to work for the deeper Great Lakes by lumping all 3-D processes into a 1-D proxy. The simulated vertical temperature profiles still need to be fully evaluated with high-quality observations. Nevertheless, we did not have access to long-term temperature profile observations for deep lakes at the time of this study to compare with our modeling results. Based on this study, it is obvious that a better understanding of the physical processes inside lakes are vital to producing realistic modeling results, and related field work should be strongly emphasized in the future.

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