The role of stratification on lakes' thermal response: The case of Lake Superior

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Abstract

During the last several decades, the Great Lakes region has been experiencing a significant rise in temperatures, with the extraordinary summer warming that affected Lake Superior in 1998 as an example of the marked response of the lake to increasingly warmer atmospheric conditions. In this work we combine the analysis of this exceptional event with some synthetic scenarios, to achieve a deeper understanding of the main processes driving the thermal dynamics of surface water temperature in Lake Superior. The analysis is performed by means of the lumped model *air2water*, which simulates lake surface temperature as a function of air temperature alone. The model provides information about the seasonal stratification dynamics, suggesting that unusual warming events can result from two factors: anomalously high summer air temperatures, and increased strength of stratification resulting from a warm spring. The relative contribution of the two factors is quantified using the model by means of synthetic scenarios, which provide a simple but effective description of the positive feedback between the thermal behavior and the stratification dynamics of the lake.

1. Introduction

Recent studies have demonstrated that lakes are highly sensitive to changes in environmental conditions, thus representing a valuable proxy to evaluate the effects of a changing climate [*Quayle et al.*, 2002; *Adrian et al.*, 2009; *Williamson et al.*, 2009]. As a consequence, many climate change studies have focused on long-term trends observed in lakes, with particular emphasis on the analysis of water temperature dynamics of large lakes [e.g., *Livingstone* 2003; *Verburg et al.*, 2003; *Vollmer et al.*, 2005; *Coats et al.*, 2006; *Hampton et al.*, 2008]. Observational evidences revealed that inland water bodies are rapidly warming throughout the world, with Lake Surface water Temperature (LST) increasing at rates up to an order of magnitude higher than those found for the global ocean [*Schneider et al.*, 2009]. Furthermore, it has been shown that lakes warming is in some case larger than that observed for the surrounding air temperature [*Austin and Colman* 2007; *Lenters et al.*, 2012], especially at mid-latitudes including North America and North Europe [*Schneider and Hook*, 2010].

Of particular interest is the warming trend that the Laurentian Great Lakes have been experiencing in the last century [e.g., *McCormick and Fahnenstiel*, 1999]. For example, by using a 100-year long time series of water temperature measured at Lake Superior outlet as a proxy of the offshore LST, *Austin and Colman* [2008] estimated a mean rate of warming of about 0.027°C yr^{-1} over the last century (i.e., data covering the period 1906-2005), with a dramatic increase up to 0.11°C yr^{-1} taking place starting in the 1980's. This recent trend has been also confirmed by analyzing in situ measurements from offshore buoys [*Austin and Colman*, 2007]. Notice that these values refer to the three-month summer period July, August and September (JAS), which are the months with the largest LST increases [*Lenters* 2004; *Austin and Colman*, 2008]. During the last several decades, similar summer warming trends have been also observed for other lakes in North America, as is the case of Lake Michigan and Lake Huron

[*Austin and Colman*, 2007], and some smaller lakes between California and Nevada [*Schneider et al.*, 2009]. However, none of these lakes have been showed to warm as rapidly as Lake Superior.

In 1998 uncommonly high air temperatures throughout the year determined an exceptional warming of Lake Superior, with summer LST difference between 1998 and 1997 being higher than the corresponding air temperature difference. This extraordinary event can be explained as a combined consequence of a particularly mild, nearly ice-free winter in part due to a significantly strong El Niño event [*Assel et al.*, 2000; *Van Cleave et al.*, 2014], and an anomalously warm summer season [*Austin and Colman*, 2007]. More generally, it can be seen as a remarkable example of the amplified response of a lake to increasing air temperature, and developing a phenomenological understanding is of paramount importance for a comprehensive description of lake behavior under evolving climate conditions. In addition, as water temperature plays a primary role in controlling a wide range of geochemical and ecological processes, an in-depth analysis of LST dynamics can also provide significant indirect information concerning possible influences on lake water quality and ecosystem functioning [e.g., *Wetzel*, 2001; *Winder and Sommer* 2012; *De Senerpont Domis et al.*, 2013]. This is even more relevant considering that an enduring and rapid rising of Lake Superior water temperature could substantially affect the lake ecosystem [e.g., *Magnuson et al.*, 1997; *Cline et al.*, 2013].

Recognizing the main processes affecting the thermal dynamics of LST during an exceptional event like the 1998 summer warming of Lake Superior can provide a deeper understanding of the thermal response in more general contexts. A fundamental question, in this perspective, concerns the contribution to LST variation which is attributable to the increased heat flux in the summer period as opposed to the influence of previous conditions of the lake. To address such an issue, we exploited *air2water*, a simple model [*Piccolroaz et al.*, 2013; *Toffolon et al.*, 2014] that simulates LST relying solely on air temperature, to isolate the relative contributions of two factors: external forcing and thermal structure of the lake. After introducing the model in the next section, we show that these factors are sufficient to suitably reproduce the LST dynamics, and then we analyze some synthetic scenarios to isolate their relative importance. Wider implications of the results and conclusions are finally presented in the last two sections.

2. Material and methods

2.1 Study site and available data

Lake Superior (Figure 1) is the largest of the five Great Lakes of North America, and the largest freshwater basin on Earth by surface area (surface area 82 103 km^2; volume: 12 000 km^3; maximum depth: 406 m). Long-term data of air and surface water temperature are available and are freely distributed by the National Oceanic and Atmospheric Administration (NOAA).

Two different sources of data have been used in this work: daily in situ measurements of air temperature provided by the National Oceanic and Atmospheric Administration's (NOAA) National Data Buoy Center (NDBC, webpage: http://www.ndbc.noaa.gov/), and daily LST retrieved from satellite imagery provided by NOAA Great Lakes Environmental Research Laboratory (GLERL, webpage: http://www.glerl.noaa.gov/). Air temperature data adopted in this study are measured at the STDM4 – Stannard Rock station, which belongs to the NOAA NDBC Coastal Marine Automated Network (C-MAN) and is installed at about 35 m above the lake level on a lighthouse located in the South-Eastern part of the lake (see Figure 1). The values of LST freely downloadable by the GLERL website refer to satellite-derived LST averaged over the whole lake, do not present significant gaps, and provide information during the entire year. Local LST values of the GLERL dataset are in overall good agreement with LST measured by offshore buoys (NDBC network) [*Schwab et al.*, 1999], making the first dataset preferable compared to in situ NDBC measurements, which are characterized by systematic gaps from October to April when devices are removed to prevent damage from ice. We remark that LST data during winter time are of pivotal importance in order to investigate the role of ice in controlling the timing and intensity of LST warming in summer. Both air temperature and LST data have been downloaded for the period between1994 and 2011.

2.2 air2water: a simple model to predict LST

The analysis presented in this work has been performed by means of *air2water* [*Piccolroaz et al.*, 2013], a simple lumped model that allows for estimating LST using air temperature as the only meteorological forcing. *air2water* is derived from the volume-integrated heat equation applied to the upper layer of the lake

$$\rho c_p V_s \frac{dT_w}{dt} = A\Phi_{net}, \qquad (1)$$

where ρ is water density, c_p is the specific heat capacity, V_s is the surface volume of water that is involved in the heat exchange with the atmosphere, T_w is LST, t is time, A is the surface area of the lake and Φ_{net} is the net heat flux into the upper water volume (accounting for the main fluxes entering and exiting V_s: short and long wave radiation, sensible and latent heat fluxes). After introducing appropriate simplifications, which are summarized in Appendix A (for a thorough discussion we refer to *Piccolroaz et al.*, [2013] and *Toffolon et al.*, [2014]), the equations of the model in its full (8-parameters, from a_1 to a_8) version reads as follows:

$$\frac{dT_w}{dt} = \frac{1}{\delta}\left\{a_1 + a_2 T_a - a_3 T_w + a_5 \cos\left[2\pi\left(\frac{t}{t_y} - a_6\right)\right]\right\}, \qquad (2)$$

$$\begin{cases} \delta = \exp\left(-\frac{T_w - T_h}{a_4}\right) & \text{for } T_w \geq T_h \\ \delta = \exp\left(-\frac{T_h - T_w}{a_7}\right) + \exp\left(-\frac{T_w}{a_8}\right) & \text{for } T_w < T_h \end{cases} \qquad (3)$$

where T_a is air temperature, δ is a dimensionless number given by the ratio between the volume V_s of the surface layer introduced in equation (1) and a reference volume V_r, and T_h is a reference value of the deep water temperature, which is approximately 4°C for deep dimictic lakes. We note that V_s (hereafter referred to as the reactive volume) varies in time due to thermal stratification, while V_r is the maximum volume affected by the surface heat flux when the lake experiences the weakest stratification conditions. In our formulation these two volumes and the surface heat flux are not estimated separately, and the parameter δ is used to implicitly account for temporary reduction or enhanced efficiency of the heat exchange with the atmosphere (for instance in the case of ice cover), as will be discussed later on.

The model parameters a_1 to a_8 account for a series of different processes and are defined within a physically reasonable range of variation, and are obtained through calibration against LST measurements. The ordinary differential equation (2) is solved numerically using the Runge-Kutta fourth order scheme, with a daily time step. In spite of the simple formulation and the limited number of parameters, *air2water* is able to satisfactorily capture seasonal variations and inter-annual dynamics in LST (see *Toffolon et al.*, [2014] for an application of the model to 14 temperate lakes with different morphological characteristics), thus representing an appealing tool for both conceptual studies and real case analyses. The fact that the model is data-driven, while being physically based, allows for the direct acquisition of information about the studied system during the calibration phase, which is performed via an automatic optimization procedure. Besides predicting LST, the model also estimates the seasonal evolution of the upper volume of water affected by the surface heat budget, through the evaluation of the volume ratio δ (well-mixed $\delta \rightarrow 1$, stratified $\delta \rightarrow 0$, ice covered $\delta > 1$ [*Piccolroaz et al.*, 2013]). The model has been successfully applied using different sources of data (i.e., LST measured at buoys or retrieved from satellite) and considering different case studies [*Piccolroaz et al.*, 2013; *Toffolon et al.*, 2014].

3. Results

3.1 Model performances

Model parameters have been calibrated considering the historical series of air temperature and LST available for the period 1994-2011. A general good agreement between measured and simulated series has been obtained, with a Kling Gupta Efficiency (KGE) index [*Gupta et al.*, 2009] of 0.98 and a root mean square error of about 1.1°C. We recall that KGE ranges from -∞ to 1: the closer to 1, the better the model performances. The mean deviation between simulated and observed LST is equal to -0.0004°C, suggesting the absence of a significant bias. We notice that the performance achieved by *air2water* is fully comparable to that obtained with more complex process-based models [e.g., *Thiery et al.*, 2014], which however require a significantly larger amount of input data.

Figure 2a shows air temperature and LST records for the summer season (averages over JAS). Detecting long-term trends by means of linear regressions is difficult and may lead to results that are not statistically significant. Anyway, it is interesting to note that a significant warming of about 0.098°C yr^{-1} (R^2 = 0.17, p-value = 0.09) and 0.107°C yr^{-1} (R^2 = 0.08 , p-value = 0.27) can be observed for measured air temperature and LST, respectively. This result differs from previous analyses [*Austin and Colman*, 2007; *Schneider and Hook*, 2010], which found that LST increased faster than air temperature based on meteorological stations located within a 500 km radius from the lake. Notice that in the present work we refer to air temperature data retrieved at about 35 m above the lake surface from a single station at an offshore location (i.e., STDM4 C-MAN station), which is more representative of the real lake conditions, while being fully representative of the typical seasonal thermal pattern of the atmosphere. In fact, the marked time lag between the temporal variations of air and water temperatures is clearly demonstrated in Figure 2b for the two years 1997 and 1998. Figure 2 also shows the performance of the model, which behaves properly both in detecting the long-term LST trend (0.100°C yr^{-1}, R^2 = 0.13 , p-value =0.14) and the associated intra- and inter-annual variations. In particular, the two years have been characterized by substantial differences (Figure 2b): 1997 being particularly cold, especially in summer, and 1998 showing unusually warm temperatures during the whole year (as already discussed above). These marked differences are also evident in Figure 2a, where both JAS air temperature and JAS LST are positioned below and above the corresponding trend lines, respectively for 1997 and 1998. In this perspective, this two-year period constitutes an interesting example of inter-annual climate variability, which is worth being examined to characterize the general thermal dynamics of the lake.

In Figure 3 we show the capability of *air2water* to reliably reproduce the temporal evolution of the reactive surface volume. This is done by comparing the simulated dimensionless volume ratio (δ_{sim}) (see Section 2.2) with an independent estimate of the same variable (δ_{est}) obtained from the analysis of water temperature profiles measured at a mooring station deployed in the central part of the lake [*Titze and Austin*, 2014]. Water temperature data cover the period 2008-2011 with hourly resolution, and are available at different depths, from surface down to 250 m depth. Following the same procedure adopted in *Toffolon et al.*, [2014] for the case of Lake Constance, we used the measured vertical profiles of temperature to estimate the volume of the surface well-mixed layer, assuming that this is a reasonable approximation of the reactive volume V_s. We first identified the thickness of the surface well-mixed layer as the smallest depth where water temperature difference with respect to surface is lower than a threshold of 1°C. Then we converted this depth into the corresponding volume of water on the basis of the hypsometric curve of the lake. Finally, we calculated δ_{est} by normalization to a reference volume, V_r, here assumed to be the entire volume of the lake. Despite the temperature threshold and the reference volume are arbitrary and may influence the evaluation of δ_{est}, the overall comparison between simulated and estimated δ (Figure 3) clearly shows that the simple parameterization (2b) is able to correctly reproduce seasonal and inter-annual (see e.g., the anticipated stratification in summer 2010) patterns of stratification, thus indicating its suitability to be used for the purposes of this work. In order to make the comparison between δ_{sim} and δ_{est} fair, we have calibrated the model locally using

LST retrieved from the closest NDBC buoy (i.e., station 45001, located at 2 km from the mooring station, and for which a 27-year long dataset is available during the period 1985-2011) instead of the lake-averaged, satellite-retrieved LST. We note that this longer LST series was required to achieve a more robust calibration of the model than the one that could be obtained relying only on the 4-year data measured at the thermistor chain. Model calibration over the 27-year period yielded KGE = 0.98, a root mean square error of 1.6°C, and mean deviation of -0.0086°C. In addition, δ_{sim} in Figure 3 has been calculated through equation (3) with the same surface T_w used to evaluate δ_{est}, and the values of the parameters a_4, a_7 and a_8 derived from point calibration of the model.

Although δ_{sim} is defined as the dimensionless reactive volume, it implicitly accounts for possible increase or decrease of heat fluxes due complex processes that are not explicitly included in the simple formulation of the model. For instance, this is the case of the insulating effect of ice cover that results in a fictitious larger reactive volume (i.e., δ>1 as discussed in *Piccolroaz et al.*, [2013]), or the increased effective heat fluxes due to unstable atmospheric boundary layer in late summer [*Blanken et al.*, 2011; *Lofgren and Zhu*, 1999] that can be partially explained with the lower values of δ_{sim} compared to δ_{est} in Figure 3. These results indicate that *air2water* is able to accurately simulate thermal and stratification dynamics of the lake, without the need to introduce a complex description of the air-water interface processes based on the quantification of the single heat flux components. This should be seen as a major advantage of the proposed formulation rather than a limitation, as it is generally difficult to find complete datasets of all meteorological variables (e.g., solar radiation, cloudiness, humidity, etc.) covering long-term periods, compared to the relatively larger availability of air and water temperature measurements.

3.2 Assessing the roles of air temperature and stratification

The analysis of the heat balance equation is a good starting point for understanding the influence of stratification, in general, and for pointing out the significant differences between LST in 1997 and 1998 (Figure 2), as a particular case. Looking at equation (1), it is evident that the warming rate of the lake is directly proportional to Φ_{net} and inversely proportional to V_s. The lake warms faster if the heat flux is high and the volume that directly participates in the heat exchange with the atmosphere is small (i.e., the lake is stratified). This is a central feature of the thermal dynamics of lakes.

In order to understand the role of the main factors controlling LST, in Figure 4 we compare the model results obtained for 1997, 1998 and for the mean year (corresponding to the overall period 1994-2011). The analysis of temperature as a function of the day of the year starting from 1 January (Figure 4a) shows again that 1997 and 1998 were respectively colder and warmer than the mean year both concerning air (thin lines) and water (thick lines) temperatures. Figure 4b shows the variation of the volume ratio δ calculated for the same three annual cycles. The nearly ice-free winter that occurred in 1998 is reproduced by the model with values of δ always ~ 1 (we recall that δ > 1 accounts for the insulating effect due to the presence of ice). This is confirmed in Figure 4a, where simulated LST is shown to be consistently greater than 0°C in winter 1998 and did not drop beneath ~2°C from the end of January to the end of April (contrary to the mean year). Thus, direct thermal stratification in 1998 started about 30 days earlier (start of May) than in 1997 (start of June), and about 20 days earlier compared to the mean year (end of May). Moreover, a significantly faster increase of LST characterized the lake in summer 1998: starting from June (in 1997 during the same period the lake was still inversely stratified, i.e., LST < 4°C) the lake reached a sufficiently strong thermal stratification that caused the surface mixed layer to get significantly shallower at mid-July (i.e., δ << 1). Strong stratification conditions, much stronger than those usually characterizing the lake (i.e., $\delta_{1998} < \delta_{my}$, where the subscript '$my$' stands for mean year), lasted for about 2.5 months, until the start of October.

Later on, stratification progressively weakened, but remaining always slightly stronger than in 1997 and in the mean year. As a consequence of the smaller surface volume in September 1998, the decrease of LST was faster in 1998 than in 1997.

As a whole, the combination of an exceptionally high air temperature and a significantly longer period of thermal stratification in summer 1998 resulted in a higher heat input to the lake acting on a smaller water volume, and eventually in the significant warming of LST. The onset of stratified conditions was anticipated, consistently with the observed tendency towards a longer ice-free season in North American lakes (earlier occurrence of ice-departure dates, see e.g., *Anderson et al*., [1996]; *Schindler et al.*, [1996]; *McCormick and Fahnenstiel* [1999]). This fact established a positive feedback to LST warming through an earlier reduction of the surface volume (lower values of δ) and hence a faster increase of LST, which in turn contributed to further decrease δ during summer months.

Aimed at understanding the feedback between net heat flux and thermal stratification and evaluating their distinct contributions to LST dynamics, we applied *air2water* under six different synthetic conditions, which are summarized in Table 1. In all cases, we considered the same model parameter set, as identified by calibration over the period 1994-2011. The six cases are described in the following paragraphs. In the analysis of the results we always refer to JAS as summer period to be consistent with previous analyses [*Austin and Colman*, 2008; *Van Cleave et al.*, 2014], although we will discuss the distinct role of the different months, and especially of July, on the average value.

Test 1 is obtained by combining air temperature series measured in 1998 and δ as simulated for 1997 (i.e., δ is not calculated by the model but externally imposed). The resulting annual cycle of LST is shown in Figure 4a. Although the external forcing (i.e., air temperature) is the same as in 1998, LST exhibits a significantly different behavior compared to that simulated for 1998, solely as a consequence of the different stratification conditions that have been imposed. The timing is similar to that simulated for 1997 (e.g., summer peak around the 20th of August) because it is controlled by the value of δ; moreover, until the end of August LST is generally much lower than in 1998. The mean LST during JAS is about 1.7°C colder than in 1998, with most of the difference occurring in July (almost 5°C, see Table 2). In winter, LST for Test 1 is similar to 1998, and the two series start to diverge only when the stratification begins to play a role. In fact, the lower temperatures in summer for Test 1 can be fully attributed to the slower warming caused by the larger volume of water involved in the heat exchanges, and hence to a weaker and postponed thermal stratification of the lake (i.e., larger values of δ) compared to 1998. Finally, Test 1 shows a slower cooling of LST in autumn with respect to 1998. This indicates a higher thermal inertia of the lake, coherently with the occurrence of larger values of δ, thus larger volumes of water participating to the heat exchanges with the atmosphere.

Test 2 is the reciprocal of Test 1 (see Table 1), being obtained by combining air temperature series measured in 1997 with δ simulated for 1998. The analysis of results, which are shown in Figure 4a and summarized in Table 2, leads to similar, and in some cases complementary, considerations as those made for Test 1: i) the timing of LST is driven by δ, thus is consistent with that simulated for 1998; ii) the mean LST during the JAS period is about 1.7°C warmer than in 1997, but it is colder than in 1998 and Test 1; iii) July is the month characterized by the largest difference with respect to thermal conditions in 1997; iv) from June to September the mean monthly LST is always colder than in Test 1 with the exception of July, when the presence of a strong stratification (i.e., small values of δ) determines a faster warming of the lake; and v) in autumn LST decreases faster than in 1997 due to the reduced thermal inertia of the system (lower values of δ).

The combined analysis of Test 1 and Test 2 provides interesting elements for an approximate quantification of the specific role that net heat flux and stratification play in controlling LST dynamics. Results in Table 2 suggest that the difference between mean summer (JAS) LST in 1998 and 1997 (i.e., about 4.2°C) is attributable to a warmer T_a for about 60% (the difference between mean summer LST in Test 1 and 1997 is about 2.5°C), and to a stronger stratification for the remaining 40% (the difference between mean summer LST in Test 2 and 1997 is about 1.6°C). We notice that this proportion is valid only for the comparison between 1997 and 1998, and may change in other cases due to the inherent inter-dependence of the two effects and the high non-linearity of the processes involved. However, the results of this simple analysis provide a clear indication that air temperature and thermal stratification play a nearly balanced role in regulating LST behavior.

3.3 Assessing the role of the history of the system

Two additional synthetic tests have been built as combinations of T_a observed in 1997 and in 1998 (see Table 1), aimed at understanding the relative contribution of winter/spring and summer seasons to the 1998 summer warming. In particular, Test 3 has been defined assuming T_a from 1997 for the period January-June and October-December, and T_a from 1998 for the remaining period (i.e., JAS). Thus, this synthetic year is characterized by a warm summer and cold conditions during the rest of the year, with steeper rising and falling limbs during June and October, respectively (see Figure 5a). The second synthetic year (Test 4) has been constructed as the opposite to Test 3, thus is characterized by a cold summer (T_a from 1997) and warm conditions during the rest of the year (T_a from 1998), with a flatter transition during later spring and early autumn (see Figure 5a). Unlike the previous tests, δ is calculated by the model rather than being externally imposed.

Results for Test 3 (Figure 5) show that water temperature remains low from January to June (when the forcing coincides with that observed in 1997), but the lake starts warming as soon as air temperature rises in summer, and eventually in August and September it reaches temperatures that coincide with those obtained in 1998 (see Table 2). This is a consequence of the fact that the late summer/early autumn period is characterized by a strong thermal stratification, thus very small values of δ, which determines a fast adaptation of LST to air temperature [*Toffolon et al.*, 2014], fully overcoming the low temperatures resulting from the colder winter months. On the contrary, the results of the second synthetic year (Test 4, Figure 5) shows that, although LST coincides with that obtained in 1998 from January to June because the external forcing is the same, it starts deviating from the trend observed in 1998 as soon as the colder summer begins. The abrupt warming of the lake is absent, as is suggested by the fact that water temperature does not reach the same maximum of 1998, not even that of the mean year. Nevertheless, LST in summer is always higher than that obtained in 1997 (with the exception of September, when LST coincides in the two cases, see Table 2), coherently with the occurrence of lower (or at least equal) values of δ throughout the whole year.

The comparison between the mean summer values of LST reported in Table 2 shows that the lake in Test 3 is about 2.6°C warmer than in 1997, which allows one to conclude that the exceptionally high air temperatures registered during the JAS period in 1998 alone contributed to about 60% of the whole LST difference between 1998 and 1997 (i.e., nearly 4.2°C). Analogously, from Test 4 we can infer that the occurrence of a warm winter/spring period in 1998 alone explained about 40% (i.e., about 1.7°C) of the total mean summer LST difference between the two years. It is necessary to notice that although the two contributions sum to almost 100%, this is purely due to how scenarios have been constructed, and should not be taken as general rule.

The thermal response of lakes is strictly dependent on the sequence of meteorological and climatic conditions, thus making difficult to analyze the independent contributions of single periods of the year. This is especially true for deep lakes during non-stratified or weakly stratified conditions, when, thanks to a high thermal inertia (large volume of the surface layer, i.e. large δ in our model), the system is able to retain a historical memory of the past conditions, with a significant influence on the ensuing thermal dynamics. Conversely, during the stratification period, the response time of LST to changes in air temperature is shortened considerably due to the low thermal inertia [*Toffolon et al.*, 2014]. Hence, the adaptation of LST to air temperature is more rapid and its variation more intense, with the inertial effect being significantly reduced during strong stratification conditions.

The behavior discussed above is quantitatively analyzed in the last two synthetic tests (Figure 6), which rely on an ensemble of 365 air temperature cycles dynamically reconstructed on the basis of two reference years: a warm year and a cold year. The air temperature in the colder year has been fixed as in the mean year 1994-2011 (T_{my}), while the warmer year has been defined as $T_{my} + \Delta T_a$, where the increment ΔT_a has been assumed equal to the average difference between 1998 and the mean year, which is approximately 2°C.

The 365 annual cycles of air temperature used in Test 5 have been obtained by combining the first part of the warm year with the remaining part of the cold year, progressively delaying by one day the transition between the warm and cold conditions, from January 1 to December 31 (see Figure 6a for a schematic illustration). Test 5 is thus aimed at quantifying the effect that a lasting warm winter may produce on the annual evolution of LST. Test 6 is the opposite case of Test 5 (see Figure 6b) and is aimed at evaluating the possible effect of an anticipated warm summer. Therefore, Tests 5 and 6, in addition to Tests 3 and 4, contributes to a comprehensive overview of the possible effects that different air temperature conditions, occurring at different times of the year, may have on LST dynamics.

We focused on the analysis of LST changes during five different periods of the year: June, July, August, September, and the entire summer period JAS. For each of these periods, we evaluated the difference ΔT_w between the period-averaged LST of the test and of the mean year, and we plotted it as a function of the i-th day of the year when the transition between the two reference years takes place (Figure 6c-g):

$$\Delta T_w|_{t_1}^{t_2}(i) = \frac{1}{(t_2-t_1)}\left[\int_{t_1}^{t_2} T_w^{test(i)}\, dt - \int_{t_1}^{t_2} T_w^{my}\, dt\right], \quad (4)$$

where t_1 and t_2 are the limits of the averaging period (delimited by vertical lines in Figure 6c-g), T_w^{my} is the LST calculated for the mean year, and $T_w^{test(i)}$ is the LST calculated for each case i of the set of 365 annual cycles of air temperature constituting the two tests (Figure 6a-b). Continuous ascending and descending curves in Figure 6 refer to Test 5 and Test 6, respectively.

These plots provide an immediate picture and a quantitative evaluation of the effects that a progressive shift of the transition between the two reference years may have on the mean LST. In particular, we analyzed five target periods of the year previously identified (i.e., the single months June, July, August, September, and the summer period JAS, see Figure 5 from subplot c to subplot g). In order to correctly interpret the figure, we suggest to read the ascending curve from left to right (i.e., LST increases for a progressively lasting warm winter), and the descending curve from right to left (i.e., LST increases for a progressively anticipated warm summer). Table 3 supports Figure 6 presenting the total ΔT_w associated with each target period (i.e., ΔT_w obtained when the transition between the two reference years occurs at the end of the averaging time window, i.e., at time t_2), as well as the relative contributions to the total ΔT_w of different periods of the year (winter, spring and the target period itself).

The analysis of the results highlights interesting differences between the five periods, mainly due to the stratification conditions of the lake, which significantly vary during the year. Notice that the stratification during the warm year can be approximated by the evolution of δ during 1998 shown in Figure 4 (see also the following discussion). The mean LST in June and July (Figure 6c-d) is strongly affected by the conditions that the lake experienced during the first half of the year, as can be seen by the fact that ΔT_w shows a significant continuous increase starting from January. Thermal inertia in both the cold (mean year) and warm (mean year + 2°C) years is always relatively large (i.e., not so small values of δ), and the system keeps memory of the past conditions to the extent that the previous state controls the mean LST in June and July. Thus, warmer air temperatures during winter and/or spring may induce an anticipation of the stratification, with substantial repercussions on the values of LST. In Test 5 and 6, an amplified warming of LST is observed with respect to air temperature, ΔT_w being up to 110% and 215% of ΔT_a (2°C), respectively in June and July (Table 3). This dramatic effect in July results from an earlier onset of strong stratification (Figure 4b), which makes LST warming much faster in the warm year than in the cold year (compare the rising limbs of 1998 and the mean year in Figure 4a). The role played by previous lake conditions is clear: warmer air temperature during the period January to June (i.e., winter and spring months in Table 3) explains around 71% of the total simulated ΔT_w in July for Test 5 (Figure 6d). Similar considerations can be made for June, but the memory effect is even higher: warmer air temperature during the period January to May explains around 79% of total simulated ΔT_w for Test 5. A similar analysis can be repeated for Test 6, showing that an anticipated warm period explains 86% and 74% of ΔT_w in June and July, respectively (which correspond to the complement to 100% of the values in Figure 6d,e).

Differently, in August and September the dependence on past conditions is completely negligible (Figure 6e-f and Table 3), with the mean LST being essentially controlled by the values of air temperature observed during the target periods (73% and 75% of the total variation, respectively for the two months). The reason is that the lake is always strongly stratified from August to September, thermal inertia is reduced (causing a short historical memory of the system), and hence LST responds much faster to current air temperature modifications, thus being substantially disconnected from past thermal conditions. Consequently, air temperature decline beginning from August causes LST to decrease at a similar rate as air temperature in the warm year because of the smaller thermal inertia (i.e., stronger stratification), while the larger thermal inertia in the cold year allows the lake to retain more heat with a consequent slower decrease of LST. The overall resulting effect is a weaker increase of LST compared to air temperature, being ΔT_w equal to 80% of ΔT_a in August, and 63% of ΔT_a (see Table 3) in September, respectively. Analogous considerations were already discussed in Section 3.2 when presenting results of Tests 1 and 2.

Concerning the entire JAS period, results shown in Figure 6g are coherent with those of Test 3 and 4, with the two periods January-June and JAS contributing almost equally to LST changes in summer (JAS air temperature explains 56% of total ΔT_w for both Test 5 and 6, see Table 3). In light of the previous discussion on the contribution of the individual months, it is interesting to note that the JAS-averaged LST is affected by winter and spring conditions only because of the presence of July in the period.

Furthermore, the simultaneous comparison of Test 5 and 6 allows us to identify an intersection point. This represents the day of the year in which the effect of a warm winter with a cold summer is comparable to that of a cold winter with a warm summer. Considering June and July, the intersection time is located about one month before the start of the target period, while for August and September the intersection is within the period, suggesting again that in these months LST dynamics are chiefly controlled by the concurrent air temperature signal.

As a final note, we recall that the warm year characterized by T_{my} + 2°C was chosen as an approximation of the conditions in 1998. In order to show the actual difference between the mean year and 1998, we have reported this case in Figure 5 using dashed lines (Test 5* and Test 6*). Neglecting small variations due to the more irregular pattern of air temperature difference, the results are essentially the same: June and July are affected by previous thermal conditions, while LST in August and September depends almost exclusively on the air temperature in that period. Interestingly, in Figure 5 (subplots c, d and g) it is possible to recognize the effect of the exceptionally warm air temperature values in February (nearly 6°C warmer than in the mean year, on average) on the mean LST in June, July and, to a minor extent, also on JAS.

4. Discussion

Prediction of LST is crucial because it exerts a strong control on lake biogeochemistry and ecology, influencing water quality parameters, chemical reaction rates, presence of pathogens, photosynthesis by algae and aquatic plants, and the habitat for macroinvertebrates and fishes [e.g., *Wetzel*, 2001]. For instance, higher temperatures increase algal photosynthesis and the metabolic rates of most aquatic animals, thus requiring more food and oxygen, which is contrasting with the reduced oxygen flux from the atmosphere to the lake [*Winder and Sommer*, 2012]. The surface layer of lakes is indeed rich in biodiversity, and at the same is very sensitive to thermal alterations, whereas the deep waters are substantially not affected during the periods of strong stratification, which dramatically reduces the vertical fluxes across the thermocline [e.g., *Imberger*, 1998]. This isolation of the surface layer from below strengthens with stratification (larger temperature gradients) even though the epilimnion may become thicker. Thus, the reactive volume shrinks and responds more rapidly to the heat exchanged with the atmosphere. The process is governed by complex mechanisms, which are retained in our formulation only in a simplified, yet effective, way. In particular, *air2water* does not need to reconstruct the individual terms of the heat budget, nor the vertical mixing process in the water body. In its lumped formulation, it directly provides the relevant information that is LST and a metric for thermal stratification. Through the calibration phase, the model assimilates the dominant features of the examined lake, with the formulation remaining general and the parameters being specific of the case study. Interestingly, a few parameters capture the thermal behavior (for instance, the single parameter a_4 controls summer stratification), thus leading to a synthetic description and, potentially, to a classification of lake thermal properties (in this respect, see the attempt done in *Toffolon et al.* [2014]).

The simplicity and robustness of the model suggests its possible use in long-term predictions. This is particularly relevant in a future perspective, since lake temperatures are expected to be affected by warming trends as a result of climate change [e.g., *Mortsch and Quinn*, 1996; *Stefan et al.*, 1998]. Some studies investigated the effect of varying meteorological forcing (including air temperature) on lake thermal dynamics by means of process-based one-, two- and three-dimensional numerical models [*Leon et al.*, 2005; *Yamashiki et al.*, 2010; *Wahl and Peeters*, 2014]. Three-dimensional (3D) models are especially designed to describe the individual processes, but require large computational times and are usually applied for short-term simulations. Moreover, they require detailed time series of meteorological data as input (e.g., wind speed, humidity, cloudiness, etc., in addition to air temperature), which are often not available or not provided with the needed time resolution.

In order to overcome these limitations, regression models have been widely used in climate change impact assessment [e.g., *Dokulil*, 2014], extrapolating LST from air temperature measurements on the basis of linear or nonlinear regression relationships. These models are indeed attractive because of their simplicity and limited requirement of meteorological data, but their use may be questionable in a climate change context especially when it is necessary to extrapolate temperature values beyond the limits of the measured time series.

In this perspective, *air2water* represents a valuable alternative tool to regression models, which require the same data in input but are not able to address some fundamental processes (e.g., the hysteresis cycle between air and water temperature). Furthermore, it can be used in place of process-based models when meteorological data are not sufficient for a proper calibration during a reference climate scenario. In this respect, we note that downscaling climate projections from the coarse resolution of the climate models to a finer scale suitable for the predictive lake model is a complex issue. In order to apply the downscaling procedure, a significantly large amount of historical data is required for all the meteorological forcing, with the drawback that the downscaling of some variables (especially precipitation, cloudiness, wind and radiative fluxes) is usually associated with large uncertainties [e.g., *Dettinger*, 2013]. Differently, *air2water* requires as an input variable a quantity whose downscaling procedure is very robust, i.e. air temperature, and thus can be seen as a valuable tool in climate change impact studies, allowing for predictions of future trends of lake surface water temperature. Finally, the possibility of coupling *air2water*, as a lumped lake model, in atmospheric circulation and weather prediction models has also been evidenced by *Toffolon et al.*, [2014].

5. Conclusions

The present analysis contributes to the understanding of the conditions leading to extreme warming of lake surface temperature (LST). These events typically occur for a positive combination of two factors: i) warm winter and spring seasons anticipate the onset of direct stratification, thus reducing the volume (and hence the thermal inertia) of the lake surface layer; ii) with a relatively thin layer reacting to the surface heat flux, a warm summer season can determine a pronounced warming of LST, which rapidly adapts to air temperature conditions in July, August and September (JAS). Such a description is confirmed by the analysis of the exceptional warming of Lake Superior in summer 1998, which was determined by the concurrence of both factors.

The *air2water* model was shown to be able to capture the positive feedback between LST and stratification. Therefore, we analyzed some synthetic scenarios in order to isolate the relative contributions of the different factors, showing that the increase of LST during summer 1998 is almost equally imputable to what happened in January-June (and hence to the stratification conditions at the beginning of the considered period) and to air temperature in JAS. This result is in line with *Austin and Colman* [2007] who based their analysis on a different method relying on long-term trends. The model also suggests that July is the month where the increase of LST with respect to a warmer air temperature is maximum, and strongly dependent upon the previous months, while LST in August and September is affected only by concurrent air temperature. Given that the JAS period is often considered in statistical analyses of Lake Superior, our results suggest the opportunity to use a more appropriate index to characterize the changes in the thermal behavior of the lake in summer. In this respect, we recommend future analyses to separate the contribution of the different summer months on the averaged warming, since the mechanisms that control LST in July are inherently different from those in August and September.

As a whole, the results point out that the dynamics of thermal stratification of the lake are crucial for the seasonal evolution of surface water temperature, and should be carefully considered in this kind of analyses. In this regard, despite the simplicity of the model, we demonstrated that it is able to satisfactorily reproduce the main processes controlling the response of LST, and can be effectively used to perform sensitivity analyses aimed at evaluating the role exerted by air temperature in controlling the seasonal behavior of stratification and LST. This possibility is especially relevant in climate change studies, where the scenarios for water temperature (when available) contain much more uncertainties than those for air temperature. Thus, *air2water* may contribute to reconstruct first approximations of the future dynamics of LST as one of the main drivers of ecology and biogeochemistry in lentic waters.

Appendix A: Net heat flux at the lake-atmosphere interface

The net heat flux per unit surface Φ_{net} in equation (1) can be decomposed in the following terms (defined as positive when directed to the lake surface layer):

$$\Phi_{net} = \Phi_S + \Phi_A + \Phi_W + \Phi_L + \Phi_C + \Phi_P + \Phi_I + \Phi_D \,, \qquad \text{(A1)}$$

where Φ_S is the net short-wave solar radiation actually absorbed by the water volume, Φ_A is the net long-wave radiation emitted from the atmosphere towards the river, Φ_W is the long-wave radiation emitted from the water, Φ_L is the latent heat flux due to evaporation/condensation, Φ_C is the sensible heat flux due to convection, Φ_P is the heat flux due to precipitation, Φ_I is the effect of the throughflow by inlets and outlets, and Φ_D is the heat flux exchanged with deep water.

Following *Piccolroaz et al.*, [2013], which the reader is referred to for further details, we linearize all the terms composing Φ_{net} as a function of T_w and T_a as follows:

$$\Phi = \Phi_0 + \left.\frac{\partial \Phi}{\partial T_a}\right|_{T_{a0}} (T_a - T_{a0}) + \left.\frac{\partial \Phi}{\partial T_w}\right|_{T_{w0}} (T_w - T_{w0}) \,, \qquad \text{(A2)}$$

where Φ is a generic flux term present in (A1), T_{w0} and T_{a0} are reference values (e.g., long-term averages) of LST and air temperature, respectively, and Φ_0 is the part of the heat flux that is independent of variation of air and water temperatures, but that can vary in time. We further assume that, for the purposes of the present analysis, the term $\Phi_0 + \left.\frac{\partial \Phi}{\partial T_a}\right|_{T_{a0}} + \left.\frac{\partial \Phi}{\partial T_w}\right|_{T_{w0}}$ can be approximately described by the sum of a constant value and a sinusoidal function of time with a period of one year.

Hence, substituting (A1) and (A2) into equation (1) we obtain:

$$\frac{dT_w}{dt} = \frac{A}{\rho c_p V_s} (\hat{a}_1 + \hat{a}_2 T_a - \hat{a}_3 T_w + \hat{a}_t), \qquad \text{(A3)}$$

where $\hat{a}_1$, $\hat{a}_2$ and $\hat{a}_3$ are coefficients that can be directly derived by the heat flux terms once suitable empirical relationships are adopted [e.g., *Martin and McCutcheon*, 1998], and $\hat{a}_t$ is the sinusoidal term. We also introduce the dimensionless ratio $\delta = V_s/V_r$, where the reference volume V_r is left unspecified. Thus, equation (A3) can be rewritten as:

$$\frac{dT_w}{dt} = \frac{V_r}{V_s} \left(\frac{A\hat{a}_1}{\rho c_p V_r} + \frac{A\hat{a}_2}{\rho c_p V_r} T_a - \frac{A\hat{a}_3}{\rho c_p V_r} T_w + \frac{A\hat{a}_t}{\rho c_p V_r} \right), \qquad \text{(A4)}$$

which it is straightforward to reformulate as in equation (2) by introducing δ and the parameters a_1, a_2, a_3, a_5 and a_6.

In order to account for the strong seasonal variations of the reactive layer volume, we assume that δ is a function of the difference between LST and the deep water temperature T_h as specified in equation (3), with the introduction of three additional parameters: a_4 to quantify the effect of direct stratification, and a_7 and a_8 to account for inverse stratification and the effect of ice cover (we impose $T_w \geq 0$ as a lower limit for simulated LST).

Finally, we note that the last two terms of equation (A1) are not explicitly considered in the analysis, but their effect is implicitly retained by the other parameters through the calibration procedure. We refer to *Toffolon et al.*, [2014] for a more extensive discussion of the physical interpretation of the parameters.

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Tables

Table 1: Synthetic scenarios obtained combining different periods of air temperature and choosing different procedures for estimating the volume ratio δ.

Scenario	T_a	δ
Test 1 (T_a 1998 & δ 1997)	1998	1997
Test 2 (T_a 1997 & δ 1998)	1997	1998
Test 3 (steeper T_a)	1997: Oct-Jun 1998: Jul-Aug	Model
Test 4 (flatter T_a)	1998: Oct-Jun 1997: Jul-Aug	Model
Test 5 (ensemble of 365 cases) (lasting warm winter)	T_{my}+2°C: DOY=1,i [a] T_{my}: DOY=i+1,365	Model
Test 6 (ensemble of 365 cases) (anticipated warm summer)	T_{my}: DOY=1,i T_{my}+2°C: DOY=i+1,365	Model
Test 5* (ensemble of 365 cases) (lasting warm winter)	1998: DOY=1,i T_{my}: DOY=i+1,365	Model
Test 6* (ensemble of 365 cases) (anticipated warm summer)	T_{my}: DOY=1,i 1998: DOY=i+1,365	Model

[a] DOY stands for day of the year

Table 2: Simulated annual maximum, mean summer (JAS) and mean monthly (June, July, August and September, respectively) LST for years 1997 and 1998, and for the synthetic scenarios Test 1-4 reported in Table 1.

Cases	1997	1998	Test 1	Test 2	Test 3	Test 4
Period	T_w [°C]					
maximum	15.17	19.14	17.61	17.25	18.76	16.55
JAS	11.97	16.19	14.48	13.61	14.58	13.63
Jul	8.65	15.50	10.76	12.86	10.62	12.67
Aug	14.02	17.69	16.81	14.77	17.55	14.88
Sep	13.28	15.35	15.73	13.10	15.35	13.30

Table 3: Period-averaged LST difference between the synthetic year and the mean year for Test 5 and Test 6, respectively, considering different target periods (i.e., June, July, August, September and JAS). The separate effects associated to winter and spring seasons and that of the target period are also reported.

Target period	Test	Winter (JFM [a])	Spring (AMJ [b])	Target period	Total
		ΔT_w [°C] (referred to the mean of the target period)			
Jun	5	0.67 (30.4%)	1.05 [c] (48.1%)	0.47 (21.5%)	2.19
	6	0.88 (40.1%)	1.00 [c] (45.9%)	0.31 (14.0%)	
Jul	5	0.96 (22.2%)	2.10 (48.8%)	1.25 (29.0%)	4.31
	6	0.80 (18.7 %)	2.37 (55.0%)	1.13 (26.3%)	
Aug	5	0.08 (5.1%)	0.07 (4.1%)	1.18 (73.0%)	1.62
	6	<0.01 (0.1%)	0.03 (2.0%)	1.18 (72.9%)	

Sep	5	0.00 (0.0%)	0.00 (0.0%)	0.96 (75.3%)	1.27
	6	0.00 (0.0%)	0.00 (0.0%)	0.95 (75.0%)	
JAS	5	0.34 (14.3%)	0.70 (29.4%)	1.34 (56.3%)	2.38
	6	0.26 (10.8%)	0.78 (32.9%)	1.34 (56.3%)	

[a] January, February and March

[b] April, May and June

[c] For the case of June spring months are only April and May (AM).

Figures

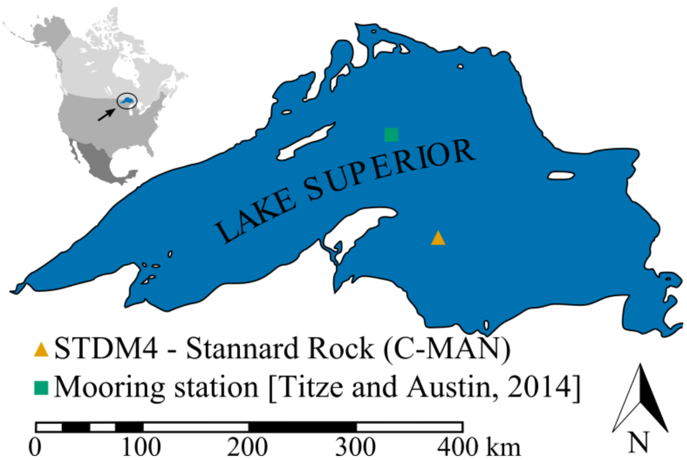

Figure 1: Lake Superior with the location of the air temperature station (STDM4 – Stannard Rock) and the moored thermistor chain [Titze and Austin, 2014] used in this work.

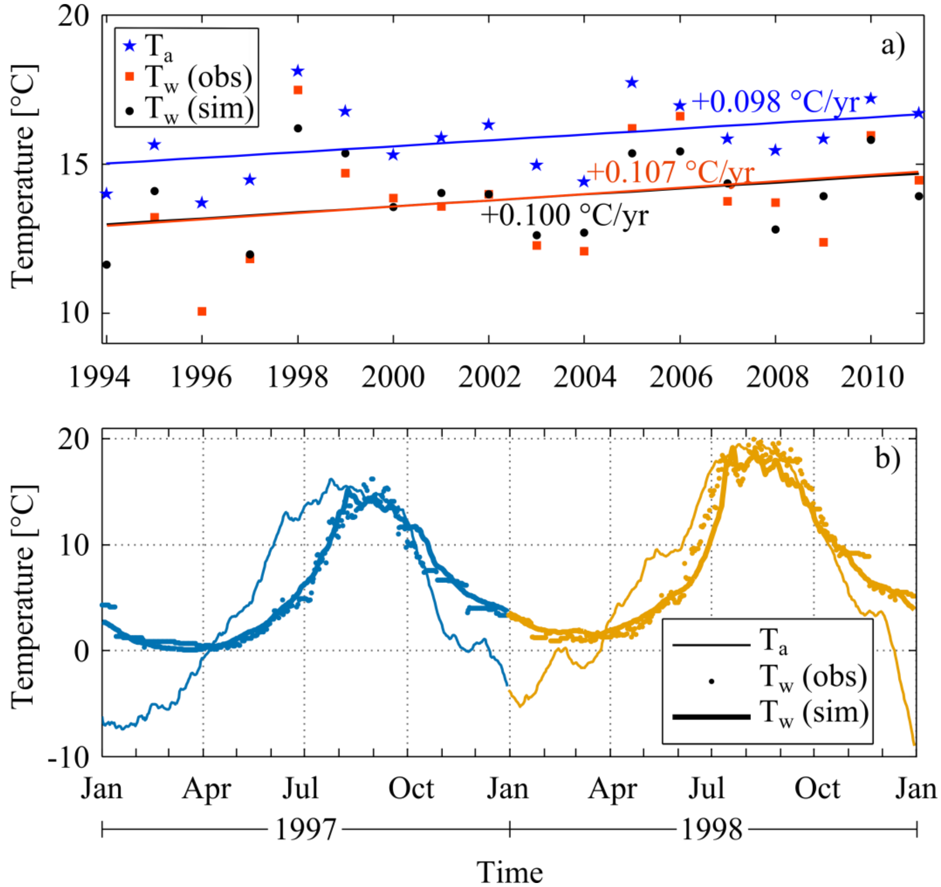

Figure 2: Comparison between air temperature T_a (observed) and lake surface temperature T_w (observed and simulated): (a) long-term trends of mean summer values (JAS) within the period 1994-2011; and (b) daily values in 1997 and 1998. LST is retrieved by satellite imagery (GLERL dataset). For representation purposes, air temperature has been filtered with a 30 days moving average in (b).

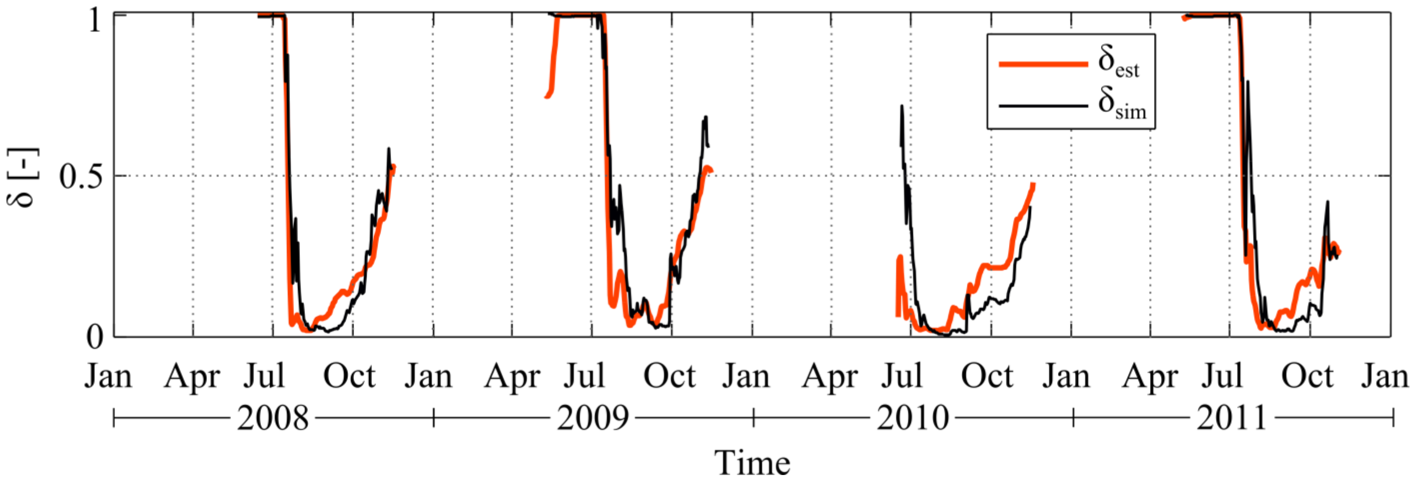

Figure 3: Comparison between δ simulated by *air2water* (δ_{sim}) and estimated from the analysis of water temperature profiles measured at the mooring station indicated in Figure 1 (δ_{est}). For representation purposes δ_{est} has been filtered with a 7 days moving average.

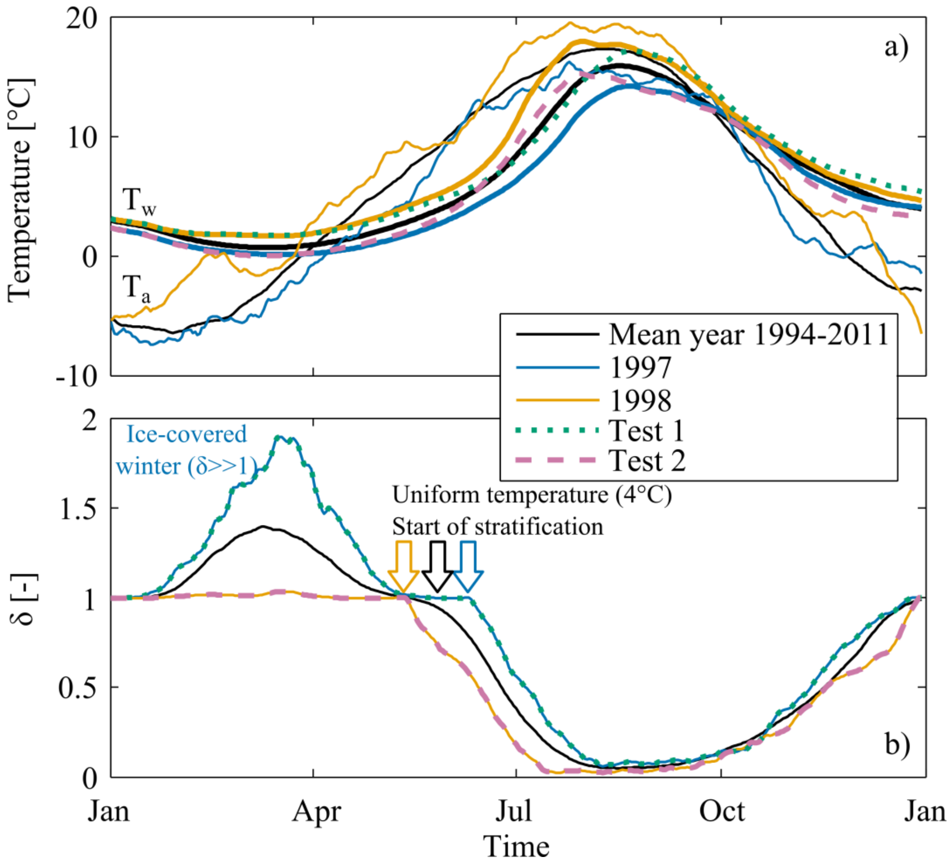

Figure 4: Annual cycle of (a) observed T_a (thin line) and simulated T_w (thick line), and (b) volume ratio δ, considering 1997, 1998, mean year 1994-2011, Test 1 (dotted line), and Test 2 (dashed line). The value of δ is imposed in the two tests (see Table 1). For representation purposes, all temperature series have been filtered with a 30 days moving average.

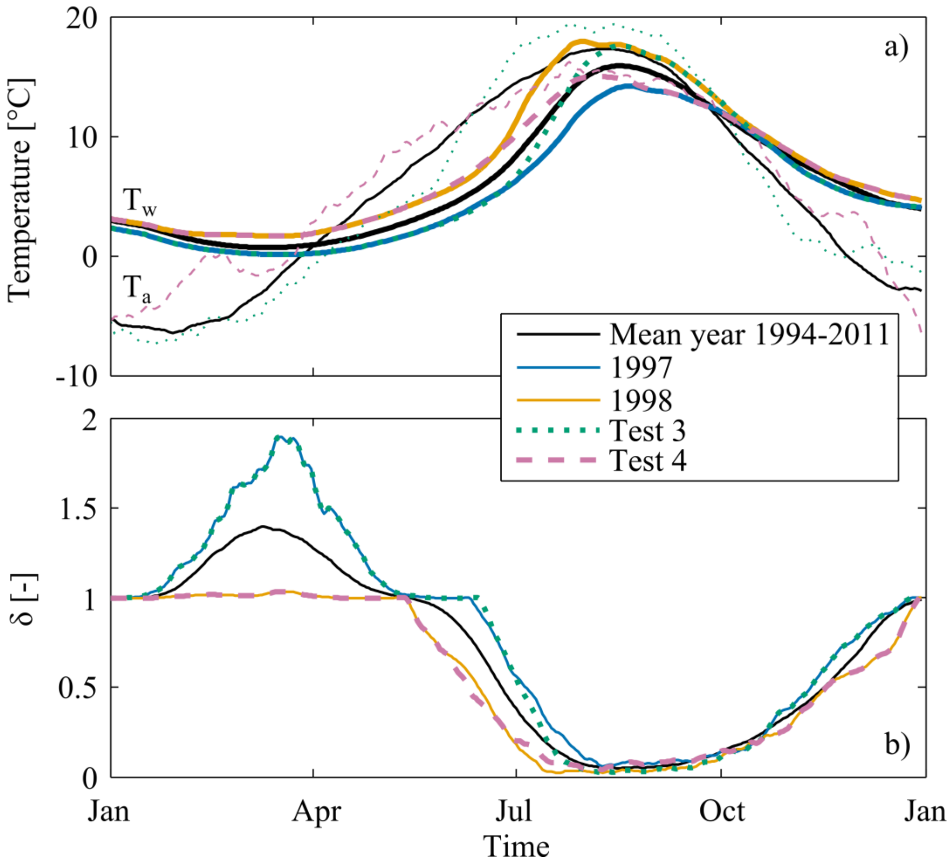

Figure 5: Annual cycle of (a) reconstructed T_a (thin line, see Table 1) and simulated T_w (thick line), and (b) simulated volume ratio δ, considering 1997, 1998, mean year 1994-2011, Test 3 (dotted line), and Test 4 (dashed line). The value of δ is calculated in all cases. For representation purposes, all temperature series have been filtered with a 30 days moving average.

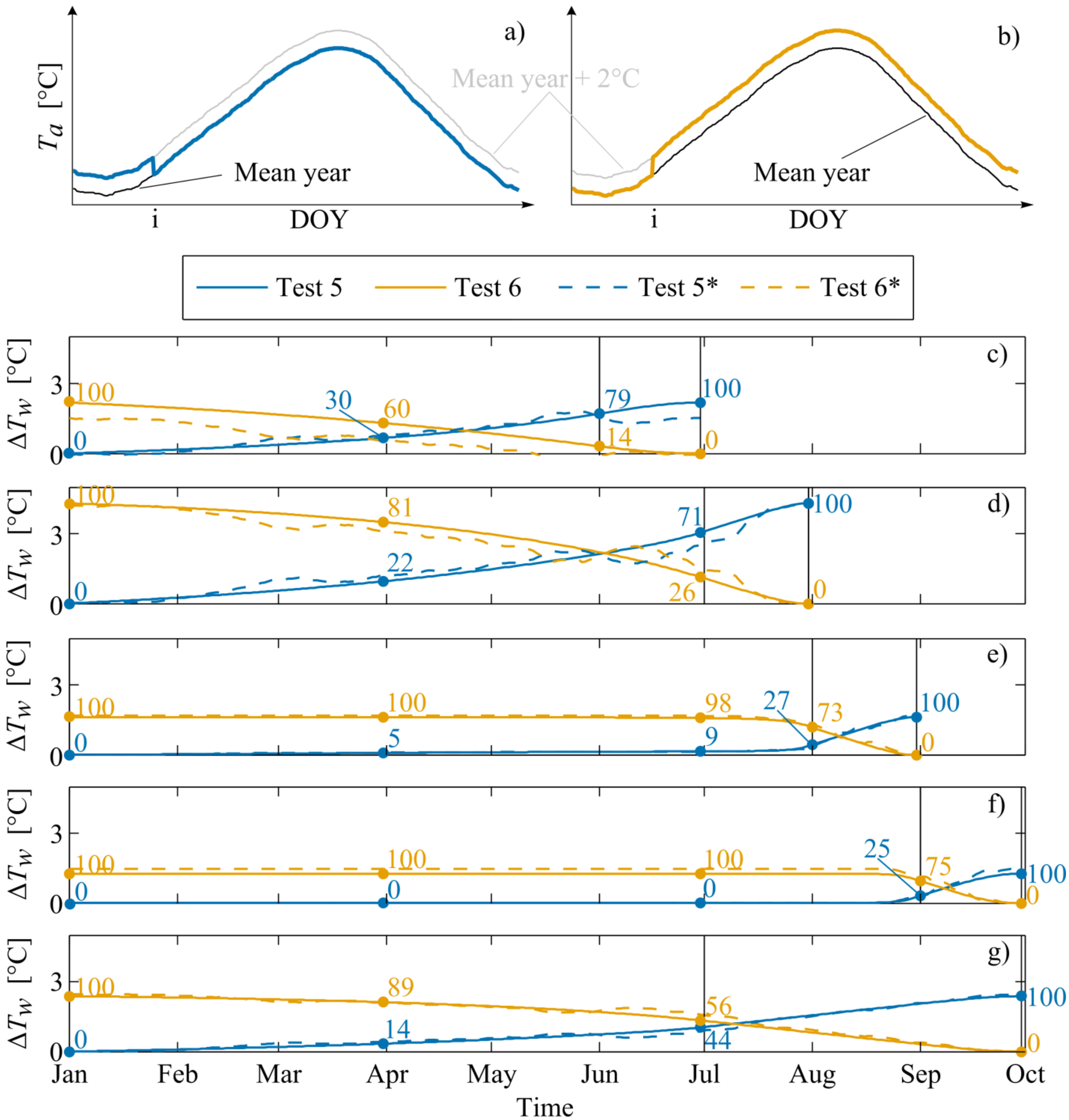

Figure 6: Analysis of Test 5 and Test 6, composed by a set of cases depending on the day of the year (DOI) where the transition occurs (see Table 1): (a) reconstructed T_a for Test 5 and (b) for Test 6, for a given day i; (c)-(g) period-averaged LST difference ΔT_w as a function of i (vertical lines denote the limit of the period considered for averaging: June, July, August, September and JAS, respectively from subplot c to subplot g).