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- Stratification onset in lakes can be estimated from surface water temperature measurements

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A novel method for estimating the onset of thermal stratification in lakes from surface water measurements

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Abstract High-frequency surface water temperature measurements were analyzed for 17 annual data series from seven lakes to assess whether the onset of thermal stratification can be determined from time series of surface water temperature measurements alone. Current methods for estimating the start of thermal stratification require depth-resolved temperature measurements, whereas many existing high-frequency measurements are often limited only to the lake surface. In this study, we show that the magnitude of the diel surface water temperature range can be used to estimate the onset of thermal stratification. We assess the accuracy of using the diel range as an estimate of the onset of thermal stratification by applying two methods based on the calculation of (1) the absolute difference in the diel surface temperature range and (2) the magnitude of the diel range from wavelet analysis. Our study shows that the onset of thermal stratification can be accurately estimated by wavelet analysis with a root mean square error of 2.1 days and by the observed diel temperature range method with a root mean square error of 11.8 days. This approach enables existing, and future, high-resolution surface water data sets to be used to estimate the onset of lake stratification. Furthermore, the continuously increasing observational powers of satellites may eventually result in surface water temperature being measured at a sufficiently high temporal resolution at the spatial scales of small lakes to allow the onset of thermal stratification to be estimated remotely.

1. Introduction

Thermal stratification is a natural phenomenon that occurs in many lakes and reservoirs as a result of the thermal expansion properties of water. The first-order paradigm of thermal stratification is well established, where the vertical thermal structure of the water column is determined by the balance between turbulence, which acts to enhance mixing, and buoyancy forces, which acts to suppress turbulence and result in a vertical layering. The epilimnion, also known as the surface mixed layer, is defined as that part of the water column immediately below the water surface, which is directly influenced by the momentum and turbulence introduced by the surface wind stress and buoyancy flux. The hypolimnion, the coolest and most dense layer, lies in contact with the bottom of the lake and is separated from the epilimnion above by a temperature-driven density gradient known as the thermocline. The strength and extent of thermal stratification is determined by extrinsic features of the lake, such as inflows [e.g., *Rimmer et al.*, 2011] and meteorological conditions [*Imberger*, 1985], and by intrinsic factors such as basin morphometry, surface area [*Fee et al.*, 1996; *Gorham and Boyce*, 1989], degree of exposure to wind [*France*, 1997], and water clarity [*Mazumder and Taylor*, 1994]. For many lakes of sufficient depth, the water column evolves seasonally from being isothermal in the early spring, developing stratification as the weather warms and then overturning sometime in the autumn, although the timing and duration of this stratification may vary enormously between lakes. A detailed review of thermal stratification is given by *Boehrer and Schultze* [2008].

A lake can be considered to be stratified when the temperature difference between the epilimnion and the hypolimnion is greater than 1°C [e.g., *Stefan et al.*, 1996; *Foley et al.*, 2012]. The onset of thermal stratification has an important influence on lake ecology as it separates processes of production and nutrient depletion in the epilimnion from processes of decomposition and nutrient regeneration in the hypolimnion and sediment. The reduction in surface mixed layer depth that occurs as the epilimnion is formed, for example, increases light availability per unit volume to phytoplankton [*MacIntyre*, 1993] which can trigger the spring bloom [*Bleiker and Schanz*, 1997; *Gaedke et al.*, 1998; *Huisman et al.*, 1999]. An earlier onset of thermal stratification can lead to an increase in the spring peak biomass of phytoplankton which can lower summer

Table 1. The General Characteristics of the Lakes Studied in This Investigation and the Years Studied, Lakes Are Shown in Descending Order According to Their Surface Area[a]

Lake	Latitude (°N), Longitude (°E)	Area (km^2)	Maximum Depth (m)	Mean Depth (m)	Average Onset of Stratification (Day of Year)	Years Investigated (Total Number of Years)
Rotorua	−38.08°, 176.27°	79.8	22	10	79	2008–2009 (1)
Lake Mendota	43.11°, −89.42°	39.4	25	12	127	2009 (1)
Windermere South Basin	54.35°, −2.94°	6.7	42	17	91	2007–2009, 2011, and 2012 (5)
Bassenthwaite Lake	54.65°, −3.22°	5.3	19	5	92	2010 and 2012 (2)
Llyn Tegid	52.88°, −3.63°	4.1	42	24	80	2009 and 2011 (2)
Esthwaite Water	54.36°, −2.96	1.0	16	6	81	2005, 2007, and 2009 (3)
Blelham Tarn	54.36°, −2.98°	0.1	15	7	83	2008, 2009, and 2011 (3)

[a]Note that the day of year for Rotorua has been altered to be comparable with Northern Hemisphere times (i.e., day of year + 182).

biomass of zooplankton [*George and Taylor*, 1995]. Consequently, phenological change in plankton seasonality can be influenced by the change in timing of stratification [*Thackeray et al*., 2008; *Winder and Schindler*, 2004].

The duration of thermal stratification restricts the supply of oxygen to the hypolimnion and sediment [*Foley et al*., 2012], leading to deoxygenation in productive lakes and potential release of phosphorus from the sediment into the water column [*Mortimer*, 1941]. Reduced oxygen concentrations at depth can also reduce the ecological niche of many species such as fish [*Jones et al*., 2008; *Elliott and Bell*, 2011], and stratification can affect the vertical distribution of other species by providing different physical and chemical conditions at different depths and by reducing rates of water movement so that motile organisms can accumulate at preferred depths [e.g., *Clegg et al*., 2007; *Mellard et al*., 2011]. Stratification can also influence the role of lakes in the global carbon cycle by affecting metabolism and the flux of gases between the lake and the atmosphere [*Coloso et al*., 2011], especially the potent greenhouse gas methane that is produced in anoxic parts of a lake [*Bastviken et al*., 2011].

Recent developments in aquatic sensor technology have made it possible to monitor conditions in lakes automatically from in situ platforms. Many such platforms have been deployed worldwide over the last two decades, and vertical temperature profiles are now frequently measured. Many lake stations are integrated into networks such as the Global Lake Ecological Observatory Network (GLEON; http://www.gleon.org) and the Networking Lake Observatories in Europe (NETLAKE; https://www.dkit.ie/netlake). This unprecedented increase in the deployment of instrumental buoys has led to an increased volume of data being collected for lakes around the world [*Porter et al*., 2009].

Historically, high-frequency depth-resolved data sets [e.g., *Pilotti et al*., 2013] have been rare. Traditional monitoring of depth-resolved temperature measurements has typically involved weekly or fortnightly sampling, although high-frequency monitoring of surface temperatures have been made [e.g., *Maberly*, 1996; *Livingstone and Kernan*, 2009]. In the following, we assess the feasibility and accuracy of using two related methods for estimating the onset of thermal stratification from high-frequency surface water temperature measurements based on the diel range in lake surface water temperature. We propose that the magnitude of the diel range in lake surface water temperature can be influenced by thermal stratification to the extent that important information about the vertical thermal structure of lakes may be gleaned from surface water temperature measurements alone. This method is applied to seven lakes, some with up to 3 years of data, to test whether the onset of thermal stratification can be estimated accurately across a geographical and morphological range of lakes.

2. Material and Methods

2.1. Study Sites

Surface water temperature measurements (actually, near-surface water temperatures; 0–1 m depth) were analyzed from seven temperate lakes that range in surface area from 0.1 to 79.8 km^2 and cover maximum depths of 15–42 m. The study sites encompassed five lakes from the United Kingdom, one lake from the United States of America and one lake from New Zealand (Table 1). None of the data series include times when the lakes were ice covered.

2.2. Time Series of Temperature Measurements

Water temperature measurements from each lake were collected by several instruments, monitored, and maintained by different organizations. The lakes situated in the United Kingdom are part of the United Kingdom Lake Ecological Observatory Network and are maintained by the Centre for Ecology & Hydrology (CEH; Bassenthwaite Lake, Blelham Tarn, Esthwaite Water, and Windermere) and Natural Resources Wales (NRW; Llyn Tegid). Water temperatures were recorded by an Automatic Water Quality Monitoring Station (AWQMS) located at the deepest point on each lake with up to 12 stainless-steel sheathed platinum resistance thermometers with relative accuracies to within 0.1°C. Data were recorded at 4 min intervals; 15 min averages were then computed from the high-resolution data. To calculate the 15 min averages, linear interpolation was first used to yield 1 min data, which was then averaged to 15 min intervals. Water temperature measurements from Rotorua were measured by a high-frequency water quality monitoring buoy that collects data at 15 min intervals. Temperature measurements cover an 8 month period from July 2008 to May 2009 and were accurate to within 0.1°C. The day of year for Rotorua was altered to be comparable with Northern Hemisphere times (i.e., day of year + 182). The instrumental buoy on Lake Mendota is maintained by the NTL-LTER program which studies lakes in the north and south of Wisconsin. The instrumented buoy is equipped with a thermistor chain with temperature measurements accurate to within 0.1°C. Data are collected every minute and the 15 min water temperature averages were then computed from the high-resolution data. Temperature measurements were recorded at several depths on each lake. Surface water temperature measurements were considered as those measured at a depth of approximately 1 m below the water surface.

2.3. Magnitude of the Diel Surface Water Temperature Range

The magnitude of the diel temperature range was evaluated by two methods: (1) by calculating the absolute difference between the maximum and minimum daily lake surface water temperature measurements and (2) by calculating the magnitude of the diel cycle in lake surface water temperature using wavelet analysis [*Torrence and Compo*, 1998]. Wavelet analysis was used during this investigation to calculate the magnitude of the diel cycle in lake surface water temperature as it performs a time scale decomposition of a signal by estimating its spectral characteristics as a function of time [*Torrence and Compo*, 1998]. This approach estimates how the different scales (periods) of the time series changes over time and the relative power (i.e., variance) of that signal. Significant features of the spectra are determined by comparing wavelet coefficients for the diel temperature cycle against a red-noise-background spectrum, which is observed in many geophysical time series [*Torrence and Compo*, 1998].

The continuous Morlet wavelet transform was used as the wavelet base function as it provides a good balance between time and frequency localizations, which is desirable for feature extraction purposes [*Grinsted et al*., 2004]. In order to minimize biases due to edge effects, the data were padded with zeros to the next power of two. The cone of influence reflects the consequent loss in statistical power near the start and end of the time series. Regions where edge effects become important, as shown by the cone of influence, were excluded from this analysis. Prior to computing the wavelet spectra, the temperature measurements were normalized to have zero mean and unit variance.

As the wavelet spectrum contains a large amount of information, the wavelet coefficients were condensed by averaging the power (i.e., variance) at every scale over the entire time series. This is referred to as the global wavelet transform (GWT) and results in a graph of variance versus scale, where similarly to traditional spectral analysis, time information is lost. The GWT was used to identify the dominant frequency components and to quantify the dominance of the diel cycle in lake surface water temperature. The GWT was corrected by scale; that is, the spectrum was divided by the corresponding scale [*Liu et al*., 2007]. The MATLAB functions of *Torrence and Compo* [1998] were used to compute the power spectrum for our time series and these can be downloaded from: http://paos.colorado.edu/research/wavelets/software.html. For a more detailed view of wavelet analysis, significance testing, and the cone of influence, see *Torrence and Compo* [1998] where a practical guide to wavelet analysis is provided.

2.4. Thermal Stratification

The onset of thermal stratification was defined from the depth-resolved temperature measurements as the time when the temperature difference between the surface and the bottom of the lake first exceeded 1°C. The onset of stratification from the wavelet spectra was estimated to be the time when the power of the

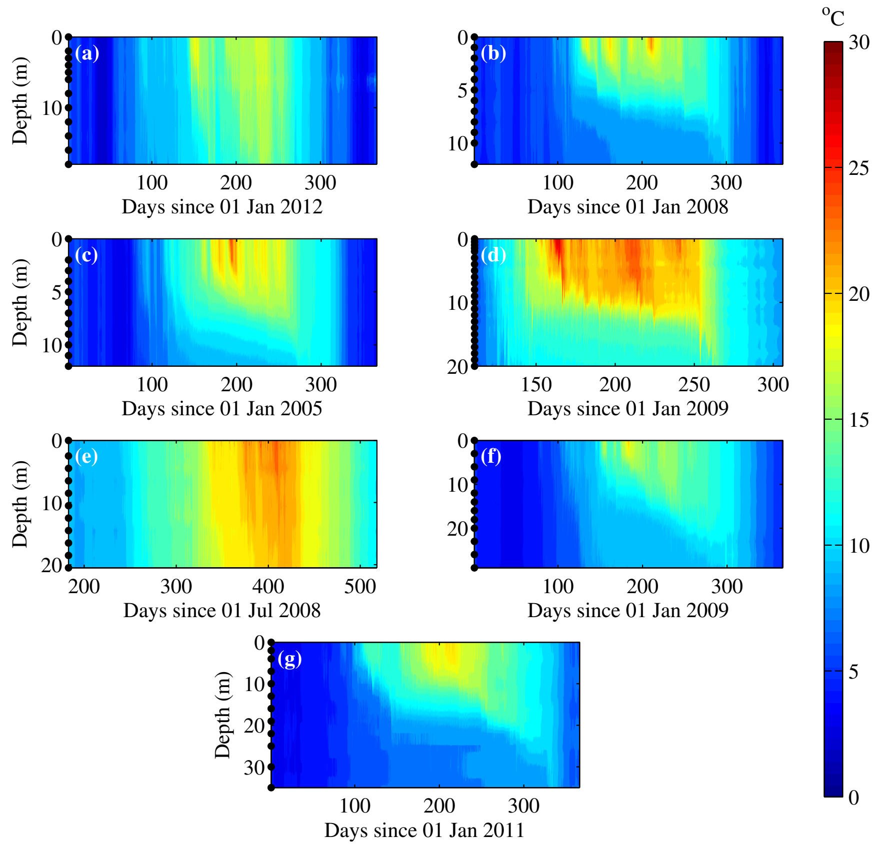

Figure 1. Examples of high-frequency (hourly) water column temperature profiles for (a) Bassenthwaite Lake, 2012; (b) Blelham Tarn, 2008; (c) Esthwaite Water, 2005; (d) Lake Mendota, 2009; (e) Rotorua, 2008–2009; (f) Llyn Tegid, 2009; and (g) Windermere, 2011. Thermistor depths are shown by the black filled circles. Note the different depth scales for each lake.

wavelet signal became significant, that is, when it first exceeded 1. This denotes the time that the wavelet coefficients became a significant feature of the power spectra when compared to background noise [*Torrence and Compo*, 1998]. To estimate the onset of thermal stratification from the diel range in surface water temperature, we used a threshold of 1°C for the diel range. In order to avoid the detection of transient stratification events, in all cases we defined the onset of stratification to occur only when the criterion mentioned was first maintained for a period of at least 48 h.

3. Results

3.1. Temperature Profiles

The lakes included in this analysis varied greatly in terms of timing, duration, and strength of thermal stratification (Table 1). Each of the seventeen time series of water column temperature, however, demonstrated a period of thermal stratification in the summer, and periods of isothermal conditions in winter (Figure 1). During the analysis period, Blelham Tarn, Esthwaite Water, Lake Mendota, Llyn Tegid, and Windermere mixed twice per year. Bassenthwaite Lake and Rotorua were polymictic, with short periods of defined stratification that seldom lasted longer than a week before the occurrence of convective and wind-driven destratification events vertically mixed the water column. Surface mixed layer depths were typically quite shallow at the onset of stratification, varied continuously, but deepened as overturn approached. For some lakes, such as Windermere (Figure 1g), this deepening was quite gradual throughout the summer and autumn while for others, such as Blelham Tarn, it took place abruptly, only a couple of weeks before overturn (Figure 1b).

3.2. Wavelet Transform of Surface Temperature Measurements

The continuous wavelet power spectrum of surface water temperature (Figure 2) revealed a statistically significant 24 h cycle in all of the time series investigated. The dominance of the diel cycle was clearly

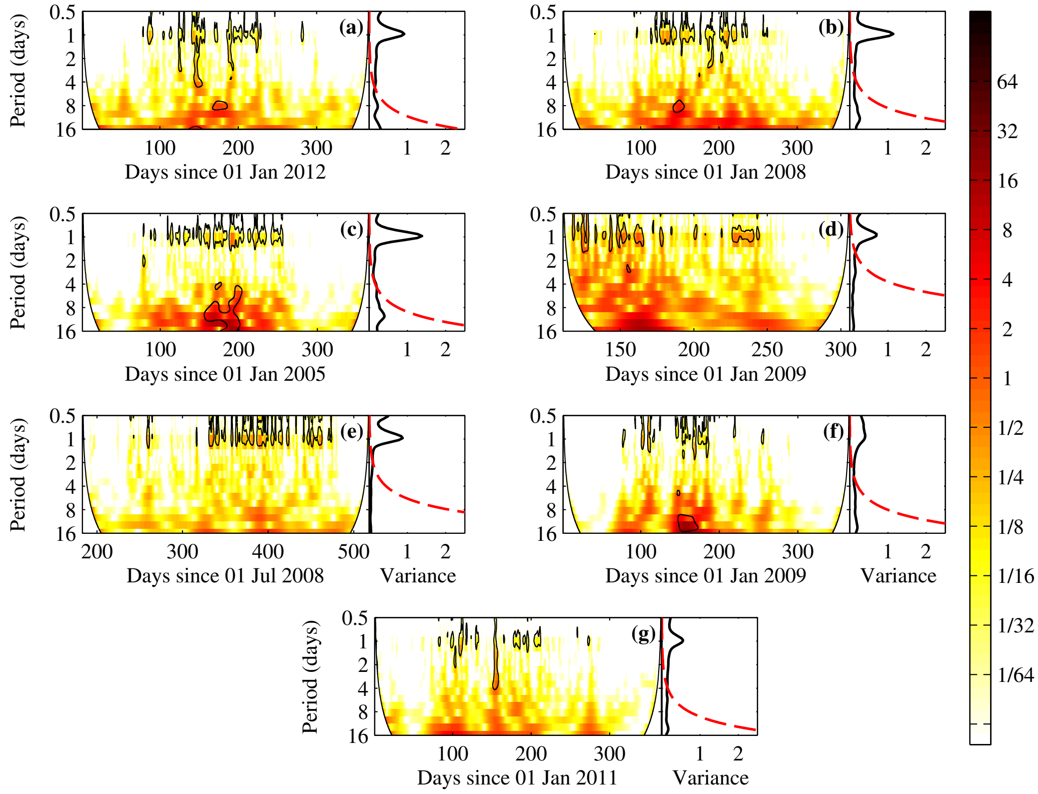

Figure 2. Wavelet power spectrum of high-resolution (15 minute) surface water temperature for (a) Bassenthwaite Lake, 2012; b) Blelham Tarn, 2008; (c) Esthwaite Water, 2005; (d) Lake Mendota, 2009; (e) Rotorua, 2008-09; (f) Llyn Tegid, 2009; and (g) Windermere, 2011. The left side of each panel shows the continuous wavelet spectrum and the solid black lines represent the features of the spectra that are significant ($p < 0.05$). The continuous wavelet spectra are shown in base 2 logarithm, and illustrate how the strength of the periodicities change with time. The right side of each panel illustrates the global wavelet spectra where the black line encloses the time-averaged spectra and the dashed red line shows the 95% significance level. The power values are coded from white for low power to dark red for high power, as shown in the color bar.

illustrated in the global wavelet transform (Figure 2), where a peak in the power spectra was calculated at a period of 24 h. The time-averaged power spectrum (i.e., GWT) at diel time scales varied among the lakes as a result of the different magnitudes of the diel surface water temperature cycle. The diel signal followed a pronounced seasonal cycle which was significant during the summer when the surface water temperature was high, as illustrated by the black contour lines overlaying the wavelet spectra (Figure 2).

3.3. Correlation Between Observed Diel Temperature Range and Wavelet Power

The observed diel surface temperature range was highly correlated with the wavelet power at a period of 24 h (Figure 3). The statistical dependence (evaluated with the Spearman rank correlation, r_s) between the observed diel surface temperature range and the wavelet power was high ($p < 0.001$) for all of the lakes. The relationship between these variables, however, was drastically different at times when the observed diel temperature range was less than 1°C where wavelet power shows a strong dependence on the observed temperature range, unlike those periods where the diel temperature range was greater than 1°C. The heteroskadastic relationship is evident among all of the lakes (Figure 3) where the variability between the wavelet power at a period of 24 h and the observed diel surface temperature range increased at higher values. During the stratified period, the observed diel temperature range closely followed the wavelet power (Figure 4), where a sharp increase or decrease in observed diel temperature range was reflected in an increase or decrease in the wavelet power.

3.4. Estimating the Onset of Thermal Stratification

The onset of thermal stratification was accurately predicted from the wavelet power at a period of 24 h and generally well predicted using the observed diel surface temperature range (Figure 5). Using the wavelet

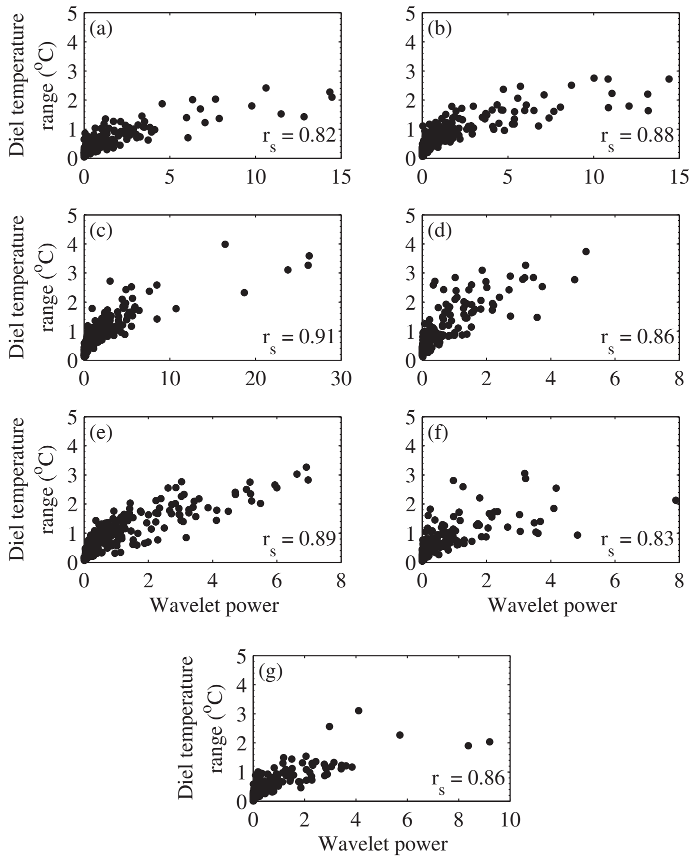

Figure 3. Example correlations between observed diel surface temperature range and the wavelet power at a period of 24 h (black) for (a) Bassenthwaite Lake, 2012; (b) Blelham Tarn, 2008; (c) Esthwaite Water, 2005; (d) Lake Mendota, 2009; (e) Rotorua, 2008–2009; (f) Llyn Tegid, 2009; and (g) Windermere, 2011. A nonparametric test (Spearman rank correlation) was used to evaluate the statistical dependence between each paired variable. Correlations are significant at the $p < 0.001$ level. Note the different scales for each x axis.

power method allowed prediction of the onset of stratification with a RMSE of 2.1 days. The observed temperature range method was less accurate but still allowed prediction of stratification onset with a RMSE of 11.8 days on average.

3.5. Frequency of Temperature Measurements Needed to Estimate Stratification

In order to determine the effect of sampling frequency on the accuracy of estimating stratification, the high-resolution surface temperature measurements were downsampled to produce data series with frequencies ranging from 2 to 8 h. Accuracy of predicting the onset of stratification declined with lower-frequency data (Figure 6). Using the wavelet method the accuracy dropped from having a RMSE of 2.1 days for the 15 min temporal resolution data to an RMSE of approximately15 days for the 8 h temporal resolution data. The greatest loss in accuracy for the wavelet method is between a sampling resolution of 1 and 2 h where, on average, the accuracy of the method dropped from 2.5 to 7 days. The observed diel surface temperature range approach was also sensitive to sampling frequency. Downsampling to a temporal resolution of 8 h increased the residual error to about 24 days (Figure 6).

4. Discussion

There are sound theoretical reasons why the diel cycle in lake surface water temperature can be influenced by thermal stratification to the extent that important information about the vertical thermal structure of the lake may be gleaned from surface water temperature measurements alone. The seasonal and diel variation in surface temperature depends on the surface heat flux and surface mixed layer depth [e.g., *Frempong*, 1983]. A considerable increase in the diel surface temperature range will,

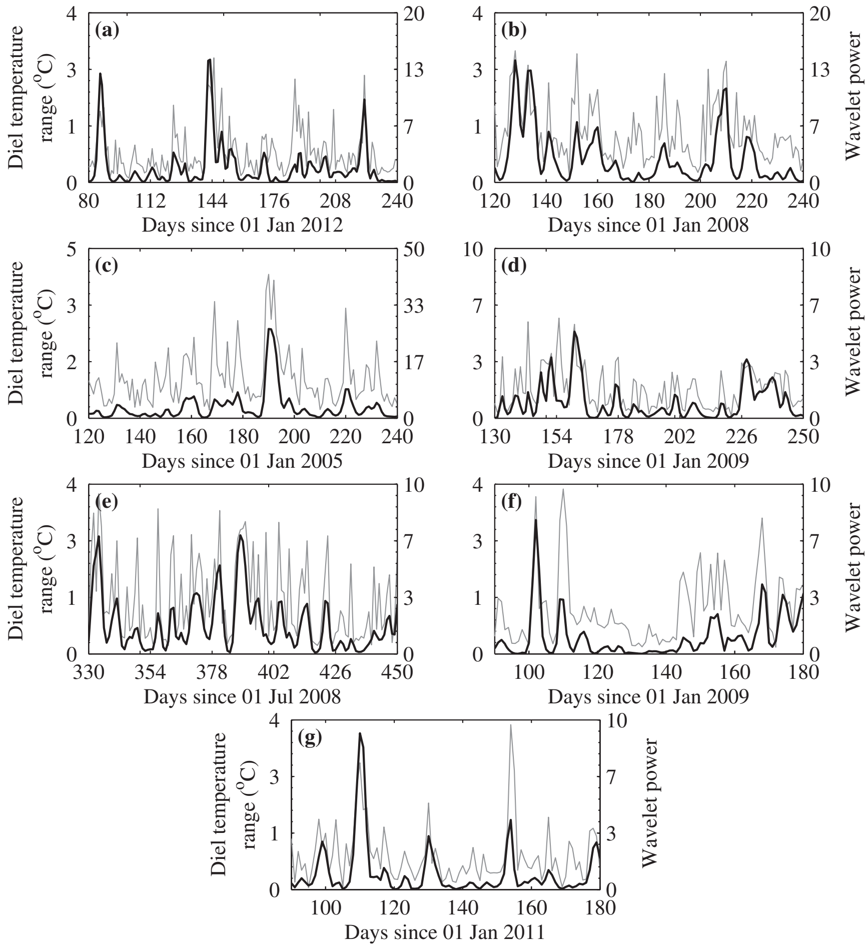

Figure 4. Example comparison of the observed diel surface temperature range (gray) and the wavelet power at a period of 24 h for (a) Bassenthwaite Lake, 2012; (b) Blelham Tarn, 2008; (c) Esthwaite Water, 2005; (d) Lake Mendota, 2009; (e) Rotorua, 2008–2009; (f) Llyn Tegid, 2009; and (g) Windermere, 2011. Note the different scales for each of the lakes.

therefore, occur when the surface heat flux is large and the depth of the surface mixed layer is shallow [e.g., *Alexander et al*., 2000], as is the case during the onset of thermal stratification. As the onset of thermal stratification is typified by a change from an isothermal lake to a lake with a relatively shallow mixed depth [e.g., *Körtzinger et al*., 2008], the timing of this onset can be estimated by measuring changing surface water temperature over time.

The applicability of any definition of stratification is compromised by periods of transient stratification. Such periods are common throughout the year in polymictic lakes, such as Bassenthwaite Lake or Rotorua, where stratification is weak and readily broken down by wind and convective mixing. Transient periods of thermal stratification, however, also exist in other lakes, particularly prior to the onset of continuous thermal stratification, where periods of high net incoming radiation and low wind forcing may cause the lake to become temporarily stratified. As such, any two different definitions of stratification will not produce the same onset date in all situations.

An alternative method to estimate thermal stratification without knowing water temperature at depth is to use a numerical lake physics model [*Peeters et al*., 2002]. Such numerical process-based models, however, require detailed and local time series of meteorological measurements. Traditionally, relatively few lakes have sufficient data, and lake modelers often use meteorological measurements from local weather stations, introducing inaccuracies in the driving variables for the model and consequently reducing the accuracy in determining stratification timing. Other sources of uncertainty include observational uncertainty

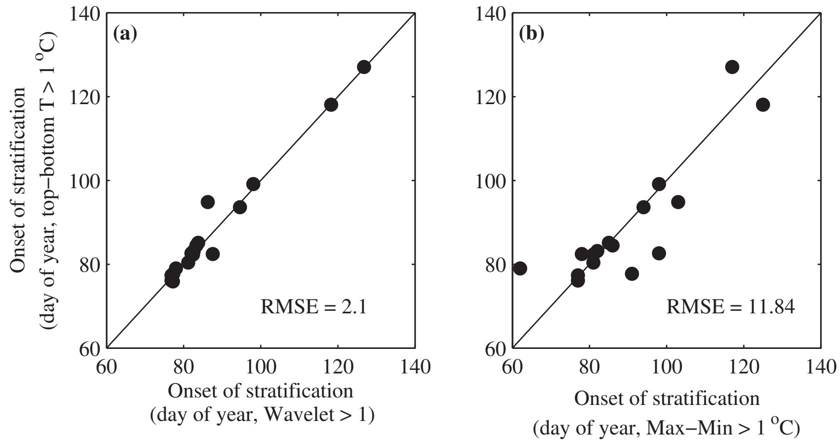

Figure 5. Comparison of the day of year when the observed temperature difference between the lake surface and bottom first exceeded 1°C with (a) the day of year when the wavelet power at the 24 h scale became significant and (b) the day of year when the diel surface temperature range exceeded 1°C. The root mean square error (RMSE) for each method is shown. The 1:1 linear relationship is shown by the solid black line. Note that the day of year for Rotorua has been altered to be comparable with Northern Hemisphere times (i.e., day of year + 182).

such as the accuracy of the sensors, parameter uncertainty and model uncertainty, all of which will influence the accuracy of the model.

Although long-term vertical temperature profile records do exist, they are often relatively sparse, thus limiting the generalness of their results. Where they do exist, such data sets have provided a valuable source of information on the immediate physical effects of climate change on lakes [*Livingstone*, 2003]. Long-term studies in Lake Constance, for example, revealed that an earlier onset of thermal stratification led to an earlier onset of the spring phytoplankton bloom [*Peeters et al*., 2007]. Although these data sets provide valuable information on the effect of climate change on the thermal regime in specific lakes, such data sets are too sparse to be generally applicable.

The approach presented here has the potential to be applied to other high-frequency data sets that are restricted to surface temperature measurements alone [e.g., *Livingstone and Kernan*, 2009]. This method was developed, however, using a limited number of lakes, none of which had a maximum depth of less than 15 m. It is expected that the method would also work in shallower lakes that stratify, but possibly with some loss of accuracy. By using the wavelet method for lakes that stratify, however, we have shown that low-cost sensors measuring surface water temperatures at 30 min intervals can provide an improvement in the accuracy of estimating stratification when compared to traditional monitoring of depth-resolved temperatures at fortnightly intervals.

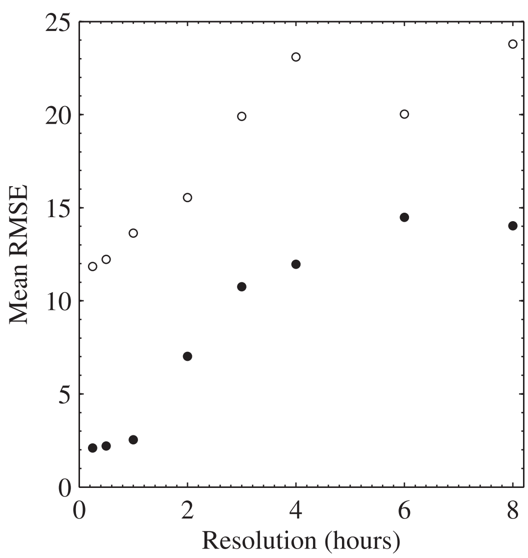

Figure 6. Comparison of the root mean square error (RMSE) associated with estimating the onset of thermal stratification from observed diel temperature range (open circles) and wavelet power (closed circles) for different frequencies of data collection.

4.1. Outlook

In the future, this approach may also be applicable to surface temperature measurements obtained from satellites. Remote sensing has the potential to retrieve such measurements, but is currently limited by the sampling frequency of sensors. Two measurements per day is the minimum required for wavelet analysis to capture a diel signal, as the sampling frequency necessary to capture any signal must exceed twice the frequency of that signal. The timing of these observations is also important; the method is most effective if the observations are equally spaced because even at a low frequency, the diel cycle would still be resolved to a reasonably high accuracy. New techniques applied to the Along Track Scanning Radiometer (ATSR) series of sensors have recently generated accurate and consistent lake surface temperature time series for greater than 250 large lakes globally [*MacCallum and Merchant*, 2012] from 1991 to 2009. In addition, the MODIS (Moderate Resolution Imaging Spectroradiometer) instruments on the Terra and Aqua polar-orbiting satellites provide information on sea surface temperature and land surface temperature measurements [*Oesch et al*., 2008; *Reinart and Reinhold*, 2008]. MODIS can produce sea surface temperature over certain regions approximately 3 times per day. Lake surface water temperature retrieval, however, is currently limited to 1 km^2, and therefore, not possible for small lakes [*MacCallum and Merchant*, 2012]. One potential issue with satellite measurements, however, is that they record the skin temperature rather than the temperature at 1 m. This represents a temperature within a millimeter of the air-water interface and can differ from the bulk temperature by as much as a few degrees [*Minnett*, 2003]. Although several techniques are currently used to infer bulk temperatures from skin temperature [e.g., *Wilson et al*., 2013], further analysis would be required to establish whether the methods described here can be successfully used with satellite measurements of temperature. Nevertheless, this method can be used to leverage the increasing number of high-frequency surface temperature measurements on lakes to provide an improved understanding on the recent trends in the onset of thermal stratification for lakes from around the world.

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