

Using Satellite Observations to Assess the Spatial Representativeness of the GLNPO Water Quality Monitoring Program

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Abstract

The U.S. EPA's Great Lakes National Program Office (GLNPO) annual water quality survey (WQS) collects data at a relatively small number of stations in each lake. The survey was designed to measure conditions in the open-water regions of the lakes where an assumption of spatial homogeneity was thought likely to be met and the measured variables could be characterized by simple statistics. Here we use satellite observations to assess how well statistics based on samples collected in the GLNPO sampling network represent the lake-wide values of two variables, surface chlorophyll concentration and Secchi depth. We find strong linear relationships between the mean values calculated from the samples and the corresponding averages based on the subsets of the full satellite images. Although overall the means of the values from the sample locations agree well with means calculated from most of the non-coastal regions of the lakes, in terms of water depth, the GLNPO station averages best represent the regions of Lake Huron deeper than 30 m, of Lakes Michigan and Superior deeper than 90 m, and of Lake Ontario deeper than 60 m. When the lake regions are defined by distance offshore rather than by depth, the GLNPO station chlorophyll means in Lakes Huron, Ontario, and Superior are closest to the means for the area of the lakes > 10 km offshore. In Lake Michigan the closest correspondence is with the > 20 km offshore region. On a whole-lake basis in Lake Erie the GLNPO station chlorophyll averages are closest to the average calculated from the entire lake.

Keywords: Remote sensing, sampling design, statistical analysis, limnological networks

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Introduction

In 1983 the U.S. EPA's Great Lakes National Program Office (GLNPO) began an annual program of monitoring Great Lakes water quality. Intended in part to satisfy some of the monitoring requirements of the 1978 Great Lakes Water Quality Agreement which mandated "Implementation of a coordinated surveillance and monitoring program in the Great Lakes System... to assess compliance with pollution control requirements and achievement of the Objectives ... and to identify emerging problems" the new monitoring program replaced the United States' contribution to the original Great Lakes International Surveillance Plan (GLISP) which was based on intensive surveys (several per year) of each lake on a decadal rotating schedule (Barbiero et al., this issue). When started in 1983 the annual program included three ship-based surveys per year (spring, summer, and fall) of Lakes Michigan, Huron, and Erie; Lake Ontario was added in 1986 and Lake Superior added in 1993. The number of surveys was reduced to twice a year (spring and summer) in 1986. These surveys, which are on-going, are the primary means GLNPO uses to collect the water quality and biological data necessary to comply with the Clean Water Act (CWA) mandate for the Great Lakes (CWA Section 118 (c) (1) (B)).

In addition to making fewer surveys during the year, resource limitations necessitated reductions in the spatial scope of the annual program (Lesht and Rockwell, 1985). Sampling was restricted to the open waters of the lakes, which were defined generally as waters greater than 90 m deep or more than 13 km offshore (IJC, 1986). These regions were assumed to be homogeneous and thus could be characterized with fewer samples and simple statistical estimates, while still being representative of a substantial fraction of the lakes' volumes (Lesht, 1984). The total number of stations sampled in each lake as part of the annual program was much smaller than in the GLISP program. For example, the GLISP sampling scheme included 80 stations in Lake Erie compared to 20 used in the annual GLNPO WQS. Stations sampled as part of the GLNPO annual program were, with the exception of Lake Superior, a subset of the stations sampled in the GLISP program; Lake Superior stations were selected from the stations identified in the U.S. EPA's Environmental Monitoring and Assessment Program (EMAP) (U.S. Environmental Protection Agency, 1994). The station locations for each program are shown in Figure 1 and the general properties of each are compared in Table 1.

Our interest here is in testing the representativeness of samples taken at the WQS locations. To do so, we require information describing the underlying population, which in large bodies of water only can be obtained from high-resolution and synoptic data such as those available from satellite observations. Vos et al. (2003) used data from the SeaWiFS ocean color sensor to examine the spatial and temporal adequacy of traditionally sampled chlorophyll and total suspended material (TSM) concentrations in Lakes IJssel and Marken in The Netherlands. They concluded that the *in situ* program lacked suffi-

cient spatial and temporal frequency to fully resolve natural variability, but that data from one station in Lake IJssel could be used to represent the whole lake on a monthly average basis. Kallio et al. (2003) compared chlorophyll concentration estimated from an airborne spectral radiometer with *in situ* measurements done in Finland’s Lakes Lohjanjärvi and Hiidenvesi. In addition to evaluating the chlorophyll retrieval algorithm they used, Kallio et al. (2003) used the remote sensing data to identify likely locations for representative discrete samples. The notion of using satellite observations to direct the design of field sampling programs of a different type is one that was exploited by Frolov et al. (2014) who used MODIS ocean color observations to optimize planned paths for subsurface glider surveys. Similarly, in a study of Lake Geneva, Kiefer et al. (2015) found that satellite observations could be used to improve the representation of average chlorophyll concentration obtained from traditional sampling by guiding the addition of stations to existing sampling networks.

Our use of satellite data in the context of evaluating the spatial representativeness of the GLNPO sampling program is somewhat different from those described above. In our case, we are presented with a fixed sampling network (the GLNPO survey network) and the problem is to try and identify exactly what portions of the lakes being sampled are best represented by the stations in that network. In this study we assume that the satellite data, which are synoptic (entire lakes can be observed in a few minutes) and have high spatial resolution (~ 1 km raw pixel size for the sensors we use in this study), represent the “true” state of the lakes at a point in time (*i.e.* they represent the population to be sampled). Under this assumption and given a finite set of discrete locations (*e.g.* the GLNPO station locations), we then attempt to determine how well statistics (here we use the mean) calculated from samples drawn from the population at those locations represent the “true” state of the system. We also use these data to determine whether the data conform to the original intent of the program to represent the homogenous open-waters of the lakes.

Methods

Our primary goal in this paper is to use satellite data to examine how well the mean of the samples drawn from the GLNPO station locations agree with the mean value of the underlying “true” population where the definition of the population is varied using some descriptive characteristics of the lakes (*e.g.* water depth, distance offshore). We are assuming that the satellite images provide a snapshot of the full “populations” from which we will be drawing a finite number of samples. Of course, this assumption limits us in the number of different variables that can be analyzed. Here we focus on the concentration of chlorophyll-a in the surface water, which several studies (Lesht et al., 2012, 2013; Shuchman et al., 2013) have shown can be reliably retrieved from satellite observations of the

Great Lakes. We also examined satellite-estimated Secchi depth using a model developed by Binding et al. (2007). Other Great Lakes variables which could be studied by using satellite observations include surface temperature (Schwab et al., 1999) and possibly total suspended material (TSM) and dissolved organic carbon (DOC) (Shuchman et al., 2013) though retrievals of these latter two have not been fully validated with field observations.

The satellite data we use here are from the SeaWiFS (1998-2007) and MODIS (2002-2016) ocean color sensors. These data were extracted by lake and, for both sensors, we processed the original L1A data (raw radiances) to L2 (calibrated geophysical variables) and L3 (spatially binned and mapped) levels using Version 7.4 of NASA's SeaDAS system (Baith et al., 2001). The L3 satellite images were mapped onto an equidistant cylindrical projection with equal area 4 km² pixels (Campbell et al., 1995). We selected L3 files that were suitable for this analysis by checking to ensure that valid satellite values were available at every GLNPO station location in each lake following the procedures outlined in Lesht et al. (2016). During the period of sensor overlap (2002-2007) we used data from both sensors, treating each image as an individual sampling event.

Our estimate of surface chlorophyll-a concentration is based on retrievals made using the Great Lakes Fit (GLF) band-ratio algorithm, the derivation and verification of which are fully described in Lesht et al. (2013) and Lesht et al. (2016) and not repeated here. The Secchi depth (Z_{SD}) estimates we use are based on a power function model similar to the one presented by Binding et al. (2007), but fit to the Secchi data obtained from the GLNPO WQS matched to satellite images collected within a day of the field measurements.

Because the GLNPO WQS was designed to sample only open-lake areas, no stations were located in the lakes' major embayments, such as Green Bay in Lake Michigan and Georgian Bay, the North Channel, and Saginaw Bay in Lake Huron. Therefore we masked these regions from the satellite imagery before conducting our analyses. In addition to calculating the "true" lake-wide mean values of chlorophyll concentration and Secchi depth using the full (less bays) images we also calculated the mean values using subsets of the full images stratified both by depth and by distance offshore to represent different, easily defined, regions of the lakes potentially represented by the GLNPO program. Because chlorophyll concentrations typically conform to a log normal distribution (Campbell, 1995; Lesht et al., 2013) the chlorophyll concentration values were log transformed before calculating the means. The annual GLNPO sampling program includes a survey conducted in early spring before the lakes begin to stratify and a survey in late summer when the lakes are near maximum stratification. To determine if the relationships between the sample and population means change when the comparison is limited to the spring and summer seasons, in addition to using all available images, we repeated the above analysis using only the survey-matched images.

We assigned a depth value to each image pixel using the Great Lakes bathymetry data

from Schwab and Sellers (1980) (as updated in 1996) and transformed to match our image grid. We used the *distance* function of the R (R Core Team, 2014) **raster** package (Hijmans, 2016) to determine the distance of each pixel from the nearest point of land. For the deeper lakes (all but Lake Erie) we stratified by depths using the 15 m, 30 m, 45 m, 60 m, and 90 m contours. For all lakes we stratified by distances offshore using distances of 5 km, 10 km, 15 km, 20 km, and 25 km.

To quantify the overall differences between the means obtained from the GLNPO sample locations and the means calculated for the complete subsets, we calculated the mean absolute error (MAE) and the root mean squared error (RMSE) as:

$$MAE = \frac{\sum_{i=1}^N |\bar{x}_{subset,i} - \bar{x}_{GLNPO,i}|}{N} \quad (1)$$

and

$$RMSE = \sqrt{\frac{\sum_{i=1}^N (\bar{x}_{subset,i} - \bar{x}_{GLNPO,i})^2}{N}} \quad (2)$$

in which N is the number of images, $\bar{x}_{subset,i}$ is the mean value of variable x in the subset of image i , and $\bar{x}_{GLNPO,i}$ is the mean value of the samples drawn from the GLNPO network locations in image i . In the analyses below we use RMSE as a general metric to quantify the difference between the population and sample means; we note that RMSE is well correlated with other possible summary metrics (*e.g.*, MAE, r^2) which also are included in the tabulated statistics. Note that because our interest is in comparing the mean of the samples drawn from the GLNPO locations with the means calculated using the image subsets we do not exclude stations based on the subsetting criterion. Thus, for every image, the GLNPO station mean is the same for all the image subset means.

Results

Image recovery

The number of images that passed our screening, *i.e.* those for which valid data existed at every GLNPO sampling location, varied by lake. In total we used 122 images for Erie, 437 for Huron, 457 for Michigan, 517 for Ontario, and 88 for Superior. To determine if the seasonal (spring, summer) scheduling of the GLNPO sampling program might affect the comparisons, we further identified those images that were collected at roughly the times of the GLNPO field surveys (± 30 days). The total number of acceptable images matched to the surveys was 22 for Erie, 38 for Huron, 37 for Michigan, 38 for Ontario, and 29 for Superior. Broken down by season, the split for each lake was almost equal with

the numbers of spring/summer images being 11/11 for Erie, 20/18 for Huron, 18/19 for Michigan, 19/19 for Ontario, and 15/14 for Superior.

Characterization of the Sampling Networks

The areas and volumes of each lake for the whole lake (without major embayments) and for each water-depth-based subset (simply the areas and volumes of the indicated subsets) are listed in Table 2. Also listed are the sampling density for each lake and depth-based subset, simply the areas and volumes divided by the number of GLNPO sampling stations in each lake. Table 3 shows similar calculations for the distance-offshore subsets. The fraction of GLNPO stations in each depth- and distance-based subset for each lake is illustrated along with the relative fraction of lake volume and area in each subset in Figure 2. In all the lakes but Erie, over 50% of the volume of the lake is contained in waters greater than 90 m deep. In all the lakes, over 50% of the volume is contained in waters farther than 15 km offshore. The average water depth of each subset is given in Table 4.

Although our purpose here is not to compare the details of the current GLNPO network with the more extensive GLISP network, it is of interest to contrast some of their features. On average, the GLNPO stations are located in deeper water, are farther from shore, and are more distant from their nearest neighboring station than are the GLISP stations (Table 1). This reflects greater number of GLISP stations and the higher proportion of GLISP stations located in coastal areas which were explicitly excluded from the GLNPO network design (Lesht and Rockwell, 1985).

Secchi Depth Retrieval

Binding et al. (2007) and Binding et al. (2015) studied the relationship between measurements of Secchi depth and coincident satellite observations in the Great Lakes using Secchi data from Environment Canada and satellite data from the Coastal Zone Color Scanner (CZCS), SeaWiFS, and MODIS. Using data from lakes Erie and Ontario matched with CZCS and SeaWiFS images, Binding et al. (2007) fit the Secchi measurements to a model of the form $Z_{SD} = \alpha \cdot nLw_{\sim 550}^{\beta}$ where Z_{SD} is Secchi depth, $nLw_{\sim 550}$ is the water-leaving radiance in the green band (exact wavelength depends on the sensor), and α and β are empirically determined parameters. In a more recent study, Binding et al. (2015) added data from MODIS and included the upper lakes but used a different empirical model in the form of a third-order polynomial ($1/Z_{SD} = \alpha + \beta \cdot Rrs_{\sim 550} + \gamma \cdot Rrs_{\sim 550}^2 + \delta \cdot Rrs_{\sim 550}^3$) for the retrieval, where $Rrs_{\sim 550}$ is the remote sensing reflectance in the green band.

Based on a preliminary analysis of our data, we chose to apply a relationship of the form presented in Binding et al. (2007). The specific model we used is

$$Z_{SD} = 5.366 \cdot nLw_{555}^{-0.910} \quad (3)$$

in which nLW_{555} is the normalized water-leaving radiance at 555 nm. Our model fit was based on 985 observations (both SeaWiFS and MODIS) from all lakes between 1998 and 2015. The r^2 value of the fit was 0.827. These data and the model fit are plotted in Figure 3.

Dependence on Depth and Distance Offshore

Figure 4 illustrates the relationship between the mean chlorophyll concentration based on depth subsets of the image pixels and the sample means calculated from the image data extracted at only the GLNPO station locations for Lake Michigan (presented as an example; see Figs. S1-S14 for the other lakes). In this figure, each panel shows the results for a different definition of the full sample frame or “population.” In the case of Lake Michigan, although the slope of the regression (which may be interpreted in terms of the accuracy of sample mean) does not change substantially as the image subset moves toward deeper water, the intercept (bias) is reduced and the scatter decreases (as measured by increased values of r^2). This reflects the progressive elimination of pixels near the shore where chlorophyll concentration is generally higher (Warren et al., this issue) as the shallow depth limit of the subset increases.

The complete chlorophyll regression results for Lake Michigan are presented in Table 5 which, in addition to the slope, intercept, and r^2 value of the linear fit, includes RMSE, the MAE, and the bias, defined here as the mean of the image subset minus the mean of the GLNPO samples (see Tables S1- S16 for the other lakes). In contrast to the image subsets based on water depth, for chlorophyll the highest value of r^2 (0.984) and lowest values of MAE (0.039) and RMSE (0.057) are found when the > 20 km image subset averages are compared with the GLNPO sample averages. Because water depth and distance offshore are correlated, these two results cannot be considered independently. As shown in Table 4, the average depth of the pixels included in the > 20 km distance offshore subset is greater than the average depth of the pixels included in the > 60 m water depth subset and the lake area included in the > 20 km distance subset is larger than the area included in the > 90 m depth subset.

Using RMSE as a convenient summary measure of the degree to which the sample means represents the subset population means, the results for all lakes for both chlorophyll and Secchi, and for both depth- and distance-defined subsets are illustrated in Figure 6. With respect to water depth, the GLNPO sample averages for chlorophyll corresponds most closely with the > 90 m depth subset in Michigan, Ontario and Superior. In Lake Huron, the sample mean best corresponds to the image mean for the > 30 m depth subset though the results are almost the same for the > 45 m subset (Table S5).

The relationship between sampled-mean chlorophyll and image-mean chlorophyll by distance offshore subset depends on the bathymetric profile of each lake. In shallow Lake Erie, the minimum RMSE (0.211) is associated with the > 0 km (whole lake) subset (Ta-

ble S1) indicating that the distribution of GLNPO stations across the lake is well matched to the differences in values that are observed between the shallow western basin and deeper central and eastern basins. Means calculated using the > 10 km subset best match the GLNPO sampling means in Lake Ontario (Table S9). In deep, though steeply sloped Lake Superior the minimum RMSE is found with the > 10 km subset (Table S13). The GLNPO sample chlorophyll means correspond best to the > 15 km subset in Lake Huron (Table S5) and the > 20 km depth subset has the minimum RMSE for Lake Michigan though is only slightly better than for the adjacent > 15 km and the > 25 km subsets. Overall, with the exception of Lake Erie, the GLNPO sampling network chlorophyll means are closest to the means calculated from the > 15 km image subsets.

The relationship between mean Secchi depths calculated from the depth-subset images of Lake Michigan and the corresponding estimates based on samples from the GLNPO locations is shown in Figure 5 and the complete regression results in Table 6. As was the case for chlorophyll, the bias gets smaller and the r^2 value higher as the image-subset mean includes fewer shallow pixels. The minimum MAE and RMSE values are found for the > 90 m subset. The slope of the regression ranges between 0.971 and 1.00 for all subsets > 30 m. The highest r^2 value (0.981) and lowest RMSE (0.712) and MAE (0.559) values are found in the > 90 m subset. As was the case for chlorophyll, in Lake Michigan the lowest Secchi RMSE is found for the > 20 km distance subset. The Secchi sample mean also agrees best with the > 90 m image subset in Lake Superior but the best agreement in Lake Ontario is with the > 60 m subset. In Lake Huron (shallowest of the deeper lakes) the best agreement is with the > 45 m subset. The pattern of agreement between the GLNPO sample mean Secchi depth and the means of the distance offshore subsets in the other lakes is very similar to that found for chlorophyll. The RMSE for Secchi in Lake Erie increases rapidly as pixels near the shore are eliminated from the subsets. In Lakes Huron and Ontario, the minimum Secchi RMSE occurs with the > 15 km subset. In Lake Superior the minimum is found for the > 10 km subset.

Seasonal Dependence

Recalling that the definition of RMSE (Eq. 2) is based on the accumulated differences between the subset means and GLNPO sample means across all images, Figure 8 demonstrates how those differences change based on the time of year when the images were collected. That is, for each lake and subset the ordinate (y-axis) value is based on the comparison between the subset averages and sample averages across N images (N is the total number of images for that lake) and the abscissa (x-axis) value is based on the comparison across the M images that match the GLNPO survey times ($M < N$). If there were no difference between the RMSE obtained for all images and the RMSE obtained for the survey-matched images, the plotted points would fall on or near the 1:1 line. This ap-

appears to be the case when chlorophyll is used as the test variable (top row of the figure) for both the depth and distance subsets, though there is some deviation for the farther offshore subsets in Lake Erie. We find, however, that when Secchi is used as the test variable (bottom row of figure) the survey-matched for RMSE is somewhat higher than the RMSE obtained from all the images in Lake Michigan and somewhat lower in Lake Ontario for the depth subsets. Insofar as RMSE is a metric that represents the degree to which the spatial variability measured by samples collected at GLNPO network locations reflects the “true” spatial variability as measured by all the pixels in the subset, this suggests that the spatial variability in Secchi depth at the times of the surveys (spring and summer) in Lake Michigan is relatively higher than at other times of the year. In Lake Ontario the opposite appears to be the case.

Discussion

The emphasis of the original GLNPO WQS program was on substances related to chemical eutrophication and the response of the lakes to changes in phosphorus loads. Specifically, the program was intended to collect water quality data for use in nutrient-based lake eutrophication models which divided the lakes into a few large, well-mixed segments (Chapra and Sonzogni, 1977; Thomann, 1977; Rodgers and Salisbury, 1981) and to collect the long-term, annual data that would be required to estimate trends and assess the effectiveness of remedial actions (Lesht and Rockwell, 1985). A parallel program focused on the lakes’ biological communities was undertaken using the same basic network design (Barbiero et al., this issue). To satisfy the program needs under the constraint of visiting a limited number of stations, sampling was restricted to the well-mixed open-lake waters which were generally defined to be waters greater than 90 m deep or more than 13 km offshore (IJC, 1986), though instead of > 90 m deep, the cruise plan for the 1983 survey specifies stations locations > 30 m deep (Barbiero et al., this issue). These regions were assumed to be homogeneous and thus could be characterized by simple statistical estimates as well as being representative of a substantial fraction of the lakes’ volumes (Lesht, 1984; IJC, 1986).

We have attempted to assess the representativeness of the GLNPO WQS samples by comparing the average values of those samples to corresponding population averages based on values estimated from satellite observations. Our idea was that by using these comparisons it would be possible to find regions (subsets) of the lakes, defined in simple morphological terms (water depth and distance offshore), to which the GLNPO sample averages compare best. Our results show strong linear relationships between the subset population means and the GLNPO sample means for all lakes and subsets, suggesting that even though the GLNPO station locations were chosen to represent the offshore open-waters

of the lakes, they are proportional to population averages that include some nearshore areas. This reflects the relative domination of the larger offshore area when calculating a combined average. When accuracy is measured in terms of the RMSE and the slope of the linear relationship between the subset means and the GLNPO station means, with the exception of Lake Huron (discussed in more detail below) the GLNPO means accurately estimate the mean values of the offshore areas of the main lakes. Although the definitions of the best matching subset varies by lake, they generally conform to the criteria used when the program was designed.

Our analysis here is limited to surface chlorophyll concentration and Secchi depth, two variables that can be reliably retrieved from the satellite observations. Because chlorophyll concentration is related to phytoplankton biomass and because phytoplankton account for much of the absorption and scattering of light in the open waters of large lakes (Alikas and Kratzer, 2017), the two are highly correlated. Differences between the two variables result from the presence of other light absorbing and scattering substances. With very few minor exceptions, we find that the distance and depth subsets that best match the GLNPO station means are the same for both variables. Work done by El-Shaarawi and Kwiatkowski (1977), Kwiatkowski (1978), and Kwiatkowski (1980) using intensive survey data of lakes Huron, Ontario, and Superior shows that spatial distributions of variables such as chlorophyll, total phosphorus, dissolved reactive silica, and chloride are largely congruent and that the lakes could generally be divided into three types of regions or zones, a large homogeneous offshore zone, a narrow coastal nearshore zone, and point-source zones associated with specific locations particular to the lake being sampled. More recently, Yurista et al. (2016) showed that the Great Lakes can be characterized by distinct nearshore and offshore areas which are persistent across years. By comparing measurements of several water quality variables they concluded that the 30 m contour (or alternatively a distance 5 km from shore) was a reasonable dividing line between the two regions in the deeper lakes, but that 20 m was a more appropriate depth in Lake Erie. Based on these criteria, the GLNPO sampling network is located well within the offshore region.

Lake Erie

Lake Erie, of all the lakes, has the largest number of GLNPO stations (20) assigned to it. Because of differences in depths, Lake Erie is often segregated by basin (*e.g.* Fay and Herdendorf (1981), Fay et al. (1982), Lesht and Rockwell (1985), Witter et al. (2009)). The GLNPO station locations in Lake Erie are distributed among the three bathymetric basins in such a way that the station density is highest in the shallowest and most spatially variable (due to inputs from the Detroit and Maumee rivers) western basin (1 station per 180 km²), lowest in the largest and mid-depth central basin (1 station per 418 km²) and intermediate in the deepest and least variable eastern basin (1 station per 311 km²). This

distribution of stations (30% west, 50% central, 20% east) does not quite match the proportionate surface areas of the basins (14% west, 66% central, 20% east) but, based on our results, is a reasonable allocation.

Because Lake Erie is so shallow, we based our characterization of the population subsets for that lake on distance offshore only. We found that for both chlorophyll concentration and Secchi depth, the RMSE based on comparing the sampled and population means is lowest for the whole-lake (> 0 km) population subset. This subset also had the smallest bias for both variables. Because the western basin is smallest and shallowest, changing the population subset by increasing the distance offshore removes a larger fraction of western basin pixels from each image subset (see Table 2) thus modifying the weighting applied to the values from that basin. This effect is most clearly seen in the results for Secchi depth (Fig. S2) in which the progressive removal of nearshore (and shallower) pixels tends to increase the population subset average relative to the GLNPO station average. This effect is somewhat muted in the chlorophyll results (Fig. S1) because the range of retrieved mean chlorophyll values (~ 0 -7.5 mg/m³) is smaller than the range of retrieved mean Secchi depth values (~ 0 -12 m), though removing western basin pixels from the image averages also clearly increases the RMSE.

Analysis of Lake Erie data may be done basin-by-basin, but here we have focused on the whole-lake. Part of the reason for this choice is simplicity. Another part reflects our desire to evaluate the representativeness of the GLNPO network in terms of easily expressed lake subset definitions, in the case of Lake Erie by distance offshore. Given the distribution of stations we expect that conducting the same type of analysis on each basin individually would yield results similar to the whole-lake analysis in the western basin, but may be somewhat different in the central and eastern basins where, on average, the stations are located farther offshore. Yurista et al. (2016) suggested, however, that the boundary between the nearshore and offshore area in Lake Erie is only 5 km. If this is the case, we would see a better agreement between the GLNPO central basin station average and the > 5 km offshore subset than with the whole-central basin average.

Lake Huron

The GLNPO network includes fourteen stations in Lake Huron, the third largest of the Great Lakes by area. These stations are distributed along and on either side of the mid-lake axis and as a result the mean water depth at the stations (89 m, Table 1) exceeds the mean depth of the lake (71 m, Table 4) even though only five of the stations are in waters > 90 m deep. All, however, are > 15 km offshore. We find the lowest chlorophyll RMSE when the GLNPO station means are compared with the image subsets > 10 km offshore (0.050), > 15 km offshore (0.056), > 30 m depth (0.057), and > 45 m depth (0.058). As shown in Table 4 the average depth of the > 10 km subset is close to the average depth of

the GLNPO stations and between the average depths of the > 30 m and > 45 m subsets. When Secchi is used as the test variable, the best RMSE matches are with the > 15 km (0.557), > 20 km (0.586) and > 10 km (0.612) subsets. These Secchi RMSE values are lower than the minimum RMSE water depth subset (> 45 m, 0.695). Referring again to Tables 4 and 1, we see that the average depths for these subsets (range 86.8 m to 93.0 m) encompass the average depth of the GLNPO stations.

Lake Huron is the only lake for which the slopes of the regressions of the image subset chlorophyll means on GLNPO network chlorophyll means (Table S5, Fig. S3) are consistently less than 1, ranging between 0.716 (> 90 m subset) and 0.891 (> 15 km subset). Even though the GLNPO sample means in Huron are well correlated with the image subset means, the slope values < 1 suggest that the surface chlorophyll averages based on the GLNPO samples may slightly overestimate (~10%) the lake-wide true values. The overestimate of the lake-wide mean when the GLNPO stations are used probably results from the greater station density in the shallow southern region of the lake where chlorophyll concentrations are generally higher (Barbiero et al., 2012) than in the northern area of the lake. This explanation would be consistent with the decrease in slope and apparent separation of the comparison points as shallower pixels are eliminated from the deeper (> 60 m and > 90 m) subsets. The fact that the simple lake-wide station averages tend to exceed the true values suggests that the accuracy of the lake-wide means calculated from the GLNPO samples in Lake Huron may be improved by using a weighted averaging scheme based on station subsets by morphometric regions rather than by a simple average of all stations.

Lake Michigan

The eleven GLNPO stations assigned to Lake Michigan are distributed somewhat differently than in the other lakes. Morphometrically the lake is divided into two major basins separated by a ridge running roughly southwest-northeast (Thwaites, 1949). The five stations located in the southern portion of the lake are arranged in a crossing pattern centered roughly on the deepest point in the southern basin. The six stations in the northern part of the lake are arranged along and on either side of the lake axis, similar to the pattern used in Lake Huron. When water depth is used as the stratifying variable, the lake-wide chlorophyll mean determined from samples taken at the GLNPO station locations is most similar to the image mean obtained from the > 90 m depth subset (RMSE = 0.066). Overall, the minimum RMSE (0.057) is found for the > 20 km distance offshore subset. The average depth of the GLNPO stations (146 m) is slightly larger than the average depth of the > 90 m depth subset (144 m), but substantially larger than the average depth of the > 20 km distance subset (129 m).

All the GLNPO stations in Lake Michigan are located > 20 km offshore, so the fact that the means of the GLNPO stations match the means of the > 20 km offshore subset

is not surprising. The reason the average water depth for this subset is so different from the overall average depth of the stations results from the distribution of the stations and the morphology of the southern basin which gently slopes, almost symmetrically, to the maximum southern basin depth of ~160 m. The average depth of the southern basin in the > 20 km subset is 103.7 m compared with an average 183.1 m depth for the > 20 km subset in the northern basin. However, the area of the > 20 km subset in the southern basin (~18,700 km²) is more than twice the area of the > 20 km subset in the northern basin (~8,500 km²). Thus the average depth of the > 20 km subset is weighted more heavily by the southern basin.

Lake Ontario

Of the five lakes, Lake Ontario has the fewest number (8) of GLNPO stations and these are concentrated in the western three-quarters of the lake. Among the deeper lakes, we find the largest absolute differences between the depth-stratified image subset chlorophyll means and the GLNPO sample chlorophyll means in Lake Ontario (Fig. 6). This may be accounted for partly by the distribution of the GLNPO stations which does not include the deeper eastern basin of the lake, an area that is included in all the depth-stratified subsets. Although the overall comparison of the means is strongly linear, the absolute differences for individual images may be larger because the eastern basin is not included. Because the slope of the relationships for all the depth subsets are close to one, it does not appear that the eastern basin values are consistently higher or lower than the values in the rest of the lake. The lowest chlorophyll RMSE (0.178) is found for the > 10 km subset. Slightly higher RMSE values are found for the > 15 km (0.186) and > 60 m (0.209) subsets. The average depth of the eight GLNPO stations in Lake Ontario is 124 m, very close the average depths of the > 60 m subset (128 m) and > 10 km subset (124 m) which suggests that, as a general rule, the GLNPO sample chlorophyll mean corresponds best to that region of the lake with the same average depth as the stations being sampled.

Lake Superior

Although several of the nineteen GLNPO stations in Lake Superior are within 10 km of shore, the average station depth is 188 m. This is slightly deeper than the 184 m average depth of the > 90 m depth subset of which the GLNPO stations are most representative (RMSE (0.033), r^2 (0.978)). The average station depth also is deeper than the average depth of the lowest RMSE (0.045) distance subset (> 10 km) at 180 m. The steady decline in RMSE for both chlorophyll and Secchi as shallower pixels are eliminated from the image subsets corresponds to the increasing average depth of the subsets. In both cases the minimum RMSE occurs when the average subset depth approaches the average station depth.

Lake-wide Means and the Influence of Major Embayments

While we have shown that the GLNPO WQS stations produce data representative of the offshore waters of the main bodies of the lakes, the program specifically excludes large embayments, such as Green Bay in Lake Michigan and Georgian Bay, the North Channel, and Saginaw Bay in Lake Huron. Markedly different conclusions about both the levels of variables sampled and inter-annual changes in those variables might be reached if these embayments are included in the calculations. Figures 9 and 10 for example, show the monthly average surface chlorophyll concentration estimated from satellite observations of lakes Huron and Michigan made from 1998-2016. These figures demonstrate how the monthly average satellite chlorophyll concentrations for the time period depend on the spatial extent of the data set included in the average. In both figures, the top panel illustrates the monthly averages obtained when the input data are from the GLNPO station locations. The well-known disappearance of the spring bloom in these lakes during the 2002-2004 time period (Lesht and Wortman, 2007; Kerfoot et al., 2010) is evident. Although the general pattern is similar as the number of pixels included in the average is increased (the number of pixels included in the averages increases successively in the second, third, and bottom panels), the details of the extent and timing of temporal variations changes, with concentrations generally becoming larger as more pixels are added. When all lake pixels are used, including those from the major embayments (Saginaw Bay, Georgian Bay, and the North Channel in Lake Huron, Green Bay in Lake Michigan) the average concentrations are greatly increased throughout the year. Including different regions of the lakes in the averages may have an effect on the interpretation of the data. In the case of Lake Huron we see, for instance, that an apparent recent recovery in lake-averaged chlorophyll beginning in 2013 is evident in the averages that include shallower pixels and parts of the North Channel and Georgian Bay but is not seen in the averages based only on the GLNPO station locations. Similar plots for the other lakes are included in the supplementary materials (Figs. S15 - S19)

Small scale variations

Our analysis is based on the assumption that the satellite imagery we've used is of sufficient spatial resolution to capture the significant sources of variation that might be missed by the relatively sparse sampling provided by the GLNPO network. This might be a particular problem in our analysis because the distribution of phytoplankton and therefore chlorophyll concentration in surface waters is known to be spatially heterogeneous or patchy (Wroblewski and O'Brien, 1976; Levin and Segel, 1976). Gower et al. (1980) used satellite observations to examine phytoplankton patchiness in the ocean and concluded that the phytoplankton behaved as a passive scalar and the observed patchiness was related to mesoscale (10-100km) motions of the water. These scales are similar to the large-scale

motions typical of the Great Lakes (Boyce, 1974; Sterner et al., 2017). Satellite observations of chlorophyll concentration also were used by Mahadevan and Campbell (2002) to examine the relationship between variance and length scale in the ocean. They characterized patchiness by using the relationship $V \sim L^p$ in which V is the variance associated with length scale L and p is a parameter characterizing patchiness. Skákala and Smyth (2016) applied this relationship to satellite observations of chlorophyll in several regions of the continental shelf off the southwestern coast of the United Kingdom. They determined that characteristic fluctuation scales for chlorophyll were between 35 km and 104 km, much larger than the 1.1 km minimal pixel scale of the original data. Thus, although our satellite data were projected to 2 km grid, this scale should be small enough to represent the spatial variability of both the chlorophyll concentration and the closely related Secchi depth.

Conclusion

Conducted annually since 1983, the GLNPO WQS is a unique and valuable resource for study of the Great Lakes. Making optimal use of the WQS data requires an understanding of exactly what parts of the lakes are represented by the discrete samples collected during the surveys. Although the WQS was designed to sample the open water (*i.e.* not coastal) regions of the lakes, it has not previously been possible to determine the degree to which this goal has been met. In this study, we used satellite data to determine which regions of the lakes are best represented by the GLNPO data. With the exception of Lake Erie, the GLNPO network station locations conform to the original design criterion of being either in water deeper than 90 m (Superior) or farther offshore than 13 km (Huron, Michigan, Ontario). Our results confirm that for these lakes the mean values of chlorophyll and Secchi depth based on the GLNPO sample data agree with the corresponding means calculated for these subsets extracted from the higher resolution satellite imagery. In some lakes, the GLNPO sample averages represent even larger areas of the lake than originally assumed; in Lake Huron approximately 95% of the lake volume is deeper than 30 m, in Lake Michigan over 75% volume is more than 20 km offshore, and in Lake Ontario approximately 90% of the lake's volume is deeper than 60 m.

The question of the adequacy of the current GLNPO station network is not easily answered because the needs of the water quality and biological monitoring programs may change as different concerns arise and have to be addressed (Barbiero et al., this issue). When applied to its original purpose, our analysis suggests that the WQS data satisfy the goal of representing the state of the offshore open-waters of the lakes. Our analysis also shows, however, that if the desire is to calculate whole-lake values, the spatial extent of the data sets being used also must be considered, and having an accurate estimate of the open water values may not be sufficient. Satellite observations may be used both to supplement

the GLNPO sample data by expanding the areas of the lakes included in analyses and to assess possible modifications to or extensions of the existing network.

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Tables

			Stations						
			Depth (m)			Offshore (km)			Near
Lake	Network	N	Min	Max	Mean	Min	Max	Mean	Mean
Erie	GLISP	80	4.40	62.50	18.20	2.00	39.80	11.70	21.80
Erie	GLNPO	20	6.90	62.50	22.60	7.20	39.80	19.90	32.50
Huron	GLISP	72	7.00	185.80	48.60	1.00	58.40	15.80	26.70
Huron	GLNPO	14	50.90	139.80	89.10	15.20	58.40	34.40	52.30
Michigan	GLISP	93	0.10	256.00	56.30	1.00	74.00	13.80	17.80
Michigan	GLNPO	11	89.50	256.00	145.90	24.10	74.00	40.30	45.70
Ontario	GLISP	95	10.00	209.60	68.30	1.00	28.00	9.50	17.40
Ontario	GLNPO	8	48.30	193.70	123.50	16.00	28.00	21.30	33.40
Superior	GLISP	78	0.50	311.40	103.40	1.00	64.00	10.90	28.30
Superior	GLNPO	19	104.20	287.10	187.50	5.70	78.10	27.70	56.50
Superior	EMAP	37	100.20	327.80	193.90	5.70	78.10	31.10	35.40

Table 1: General properties of EMAP, GLISP, and GLNPO Great Lakes sampling networks. Depth refers to the water depth at the station, offshore to the distance of the station from the nearest point of land, and near to the distance from each station to its nearest neighbor.

	Erie	Huron	Michigan	Ontario	Superior
Area (km ²)					
> 0m	25312	39440	53460	19084	86928
> 15m	17112	35712	49396	17264	84148
> 30m	2252	31712	43472	15100	81044
> 45m	680	27004	39440	13408	78096
> 60m	88	21204	35308	11956	75200
> 90m	0	12136	25152	9180	68640
Density (km ² /Station)					
> 0 m	1266	2817	4860	2386	4575
> 15m	856	2551	4491	2158	4429
> 30m	113	2265	3952	1888	4265
> 45m	34	1929	3585	1676	4110
> 60m	4	1515	3210	1494	3958
> 90m	0	867	2287	1148	3613
Volume (km ³)					
> 0m	480.8	2812.2	4931.6	1728.4	13467.2
> 15m	401.9	2779.6	4893.1	1713.0	13446.1
> 30m	94.9	2689.3	4763.4	1664.0	13376.8
> 45m	35.8	2510.4	4611.9	1601.4	13265.9
> 60m	5.4	2205.7	4395.3	1526.0	13112.0
> 90m	0.0	1545.9	3615.8	1318.8	12616.4
Density (km ³ /Station)					
> 0m	24.0	200.9	448.3	216.0	708.8
> 15m	20.1	198.5	444.8	214.1	707.7
> 30m	4.8	192.1	433.0	208.0	704.0
> 45m	1.8	179.3	419.3	200.2	698.2
> 60m	0.3	157.6	399.6	190.8	690.1
> 90m	0.00	110.4	328.7	164.8	664.0

Table 2: Areas, volumes, and per GLNPO station densities of lake grids by water depth subset.

	Erie	Huron	Michigan	Ontario	Superior
Area (km ²)					
> 5km	20300	34556	47148	15400	76552
> 10km	14664	29212	39268	11180	63400
> 15km	10612	25008	32956	7988	53192
> 20km	6828	20380	27244	4524	43516
> 25km	4304	16684	22880	1908	35600
Density (km ² /Station)					
> 5km	1015	2468	4286	1925	4029
> 10km	733	2087	3570	1398	3337
> 15km	531	1786	2996	998	2800
> 20km	341	1456	2477	566	2290
> 25km	215	1192	2080	238	1874
Volume (km ³)					
> 5km	430.5	2730.3	4784.7	1658.3	12883.8
> 10km	333.4	2536.9	4423.8	1391.6	11385.1
> 15km	245.8	2298.1	3997.2	1070.8	9998.2
> 20km	155.5	1964.0	3503.5	641.3	8538.9
> 25km	94.3	1647.6	3032.0	281.6	7212.2
Density (km ³ /Station)					
> 5km	21.5	195.0	435.0	207.3	678.1
> 10km	16.7	181.2	402.2	174.0	599.2
> 15km	12.3	164.2	363.4	133.8	526.2
> 20km	7.8	140.3	318.5	80.2	449.4
> 25km	4.7	117.7	275.6	35.2	379.6

Table 3: Areas, volumes, and per GLNPO station densities of lake grids by distance offshore subset. Note that whole-lake values (> 0 km) are the same as those values shown for > 0 m in Table 2

Depth	Erie	Huron	Michigan	Ontario	Superior
> 0m	19.0	71.3	92.2	90.6	154.9
> 15m	23.5	77.8	99.1	99.2	159.8
> 30m	42.1	84.8	109.6	110.2	165.1
> 45m	52.7	93.0	116.9	119.4	169.9
> 60m	61.3	104.0	124.5	127.6	174.4
> 90m		127.4	143.8	143.7	183.8
> 5km	21.2	79.0	101.5	107.8	168.3
> 10km	22.7	86.8	112.7	124.5	179.6
> 15km	23.2	91.9	121.3	134.1	188.0
> 20km	22.8	96.4	128.6	141.9	196.2
> 25km	21.9	98.8	132.5	147.6	202.6

Table 4: Average depth (m) by subset for lake bathymetric grids.

Lake	Subset	Slope	Intercept	r^2	N	Bias	RMSE	MAE
Michigan	> 0m	0.965	0.163	0.883	457	0.131	0.164	0.139
Michigan	> 15m	0.966	0.122	0.898	457	0.091	0.129	0.105
Michigan	> 30m	0.989	0.068	0.922	457	0.058	0.099	0.077
Michigan	> 45m	1.002	0.044	0.938	457	0.046	0.085	0.065
Michigan	> 60m	1.007	0.028	0.954	457	0.034	0.071	0.053
Michigan	> 90m	0.994	0.038	0.959	457	0.033	0.066	0.048
Michigan	> 5km	0.962	0.111	0.904	457	0.076	0.116	0.092
Michigan	> 10km	0.972	0.061	0.934	457	0.035	0.080	0.060
Michigan	> 15km	0.983	0.028	0.953	457	0.012	0.062	0.044
Michigan	> 20km	0.984	0.008	0.960	457	-0.007	0.057	0.039
Michigan	> 25km	0.980	-0.003	0.958	457	-0.021	0.061	0.043

Table 5: Lake Michigan regression results for chlorophyll: Mean chlorophyll concentration (mg/m^3) of image pixel subsets versus mean chlorophyll concentration extracted from pixels at GLNPO station locations using data from all clear images. Results above the line are for the subsets of the image pixels stratified by depth and below the line for the image pixels stratified by distance offshore. Note that “> 0 m” depth image subset is the same as the “> 0 km” distance offshore image subset. Bias is the average value of the image subset minus the average value of the sampled locations.

Lake	Subset	Slope	Intercept	r^2	N	Bias	RMSE	MAE
Michigan	> 0m	0.810	1.834	0.911	457	-0.428	1.211	0.960
Michigan	> 15m	0.891	1.438	0.932	457	0.146	0.960	0.782
Michigan	> 30m	0.971	0.830	0.959	457	0.484	0.875	0.697
Michigan	> 45m	0.994	0.584	0.969	457	0.515	0.817	0.648
Michigan	> 60m	1.003	0.420	0.977	457	0.455	0.712	0.563
Michigan	> 90m	0.984	0.707	0.981	457	0.514	0.712	0.559
Michigan	> 5km	0.894	1.313	0.943	457	0.049	0.878	0.714
Michigan	> 10km	0.947	0.744	0.971	457	0.115	0.631	0.492
Michigan	> 15km	0.978	0.312	0.983	457	0.055	0.470	0.351
Michigan	> 20km	0.998	0.008	0.988	457	-0.017	0.400	0.299
Michigan	> 25km	1.010	-0.193	0.988	457	-0.073	0.411	0.313

Table 6: As Table 5 for Secchi depth (m).

Lake	Subset	Slope	Intercept	r^2	N	Bias	RMSE	MAE
Michigan	> 0m	1.088	0.059	0.925	37	0.136	0.155	0.136
Michigan	> 15m	1.084	0.021	0.926	37	0.094	0.120	0.099
Michigan	> 30m	1.098	-0.021	0.934	37	0.064	0.096	0.074
Michigan	> 45m	1.093	-0.028	0.947	37	0.052	0.082	0.065
Michigan	> 60m	1.079	-0.028	0.960	37	0.040	0.068	0.054
Michigan	> 90m	0.967	0.057	0.968	37	0.028	0.050	0.038
Michigan	> 5km	1.101	-0.007	0.932	37	0.081	0.109	0.086
Michigan	> 10km	1.105	-0.048	0.950	37	0.043	0.077	0.059
Michigan	> 15km	1.105	-0.070	0.962	37	0.022	0.061	0.046
Michigan	> 20km	1.099	-0.083	0.964	37	0.003	0.055	0.042
Michigan	> 25km	1.092	-0.090	0.961	37	-0.010	0.056	0.045

Table 7: Regression results for mean chlorophyll concentration (mg/m^3) of image subsets versus mean chlorophyll concentration extracted at GLNPO station locations in Lake Michigan using data from survey-matched images.

Lake	Subset	Slope	Intercept	r^2	N	Bias	RMSE	MAE
Michigan	> 0m	0.811	1.370	0.948	37	-0.868	1.396	1.155
Michigan	> 15m	0.885	1.104	0.963	37	-0.260	0.885	0.753
Michigan	> 30m	0.960	0.655	0.980	37	0.179	0.614	0.492
Michigan	> 45m	0.985	0.461	0.984	37	0.278	0.584	0.454
Michigan	> 60m	0.995	0.337	0.987	37	0.271	0.533	0.411
Michigan	> 90m	0.962	0.792	0.988	37	0.338	0.564	0.443
Michigan	> 5km	0.898	0.920	0.969	37	-0.292	0.829	0.710
Michigan	> 10km	0.958	0.433	0.983	37	-0.067	0.542	0.440
Michigan	> 15km	0.993	0.093	0.989	37	0.007	0.428	0.323
Michigan	> 20km	1.018	-0.158	0.992	37	0.051	0.394	0.308
Michigan	> 25km	1.033	-0.324	0.992	37	0.070	0.406	0.320

Table 8: As Table 7 for Secchi depth (m).

Figure Captions

Figure 1. Station locations of GLNPO (filled squares), GLISP (open squares), and EMAP (Superior only, open circles) monitoring networks. Positions for GLISP stations were obtained from GLISP planning documents (IJC, 1986) and EMAP stations from the EPA Archive (<https://archive.epa.gov/emap/archive-emap/web/txt/lستا94.txt>).

Figure 2. Percentages of lake areas (middle row) and volumes (bottom row) represented in the water-depth (left column) and distance-offshore (right column) subsets. Distribution (percent of total) of GLNPO stations (top row) in each lake by water depth and distance offshore. Note that change in lake area with distance offshore is nearly identical in Huron, Michigan, and Superior.

Figure 3. Secchi depth (Z_{SD}) versus normalized water leaving radiance at 555 nm (nLW_{555}) from GLNPO samples matched with satellite observations (1998-2015) fit to power law model Binding et al. (2007).

Figure 4. Mean chlorophyll concentration from selected image subsets versus mean chlorophyll concentration from image data extracted at GLNPO sample locations. Circles indicate images collected from January through June and triangles indicate images collected from July through December.

Figure 5. Mean Secchi depth from image subsets versus mean Secchi depth from image data extracted at GLNPO sample locations. Circles indicate images collected from January through June and triangles indicate images collected from July through December.

Figure 6. Root mean squared error (RMSE) of chlorophyll concentration (top row) and Secchi depth (bottom row) based on paired means of the image subsets (water depth and distance offshore) with corresponding means of samples extracted at GLNPO station locations using all clear images during the year.

Figure 7. Root mean squared error (RMSE) of chlorophyll concentration (top row) and Secchi depth (bottom row) based on paired means of the image subsets (water depth and distance offshore) with corresponding means of samples extracted at GLNPO station locations using clear images matched with GLNPO surveys (spring and summer).

Figure 8. Mean absolute error (RMSE) of chlorophyll concentration (top row) and Secchi depth (bottom row) calculated for all images and images matched with survey dates for both depth stratified (left column) and distance stratified (right column) subsets. Subsets

are identified by symbol shape, and lake by color.

Figure 9. Monthly average chlorophyll concentration in Lake Huron 1998-2016 estimated from four different sets of satellite image pixels. Top panel is based on averages of image data extracted from GLNPO station locations, second panel is based on averages of image data from pixels in water greater than 60 m deep, third panel is based on averages of image data from pixels in water greater than 30 m deep, the bottom panel is based on all pixels including major embayments.

Figure 10. Monthly average chlorophyll concentration in Lake Michigan 1998-2016 estimated from four different sets of satellite image pixels. Top panel is based on averages of image data extracted from GLNPO station locations, second panel is based on averages of image data from pixels in water greater than 60 m deep, third panel is based on averages of image data from pixels in water greater than 30 m deep, the bottom panel is based on all pixels including major embayments.

Figures

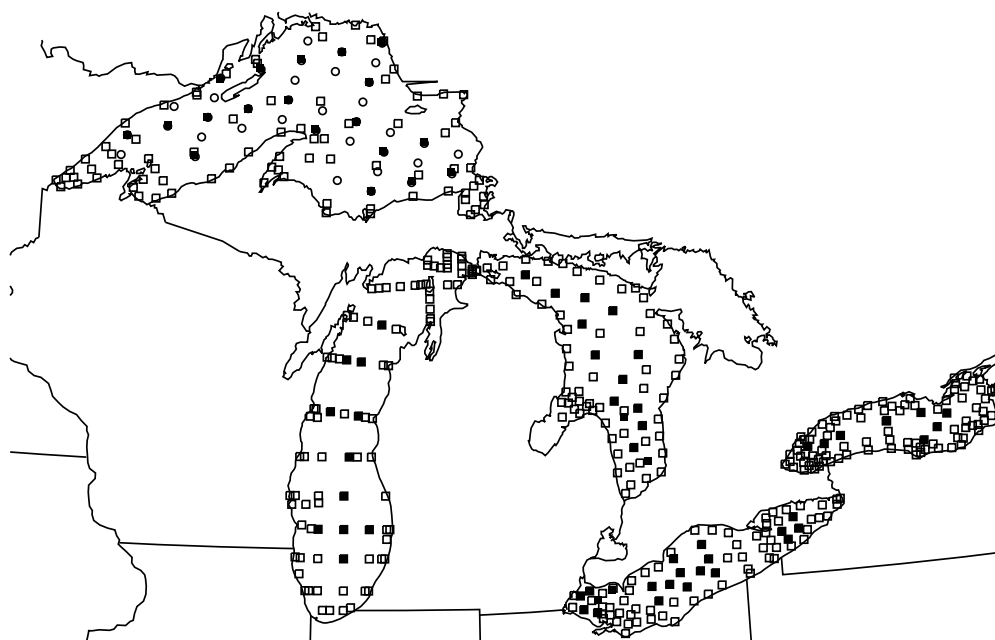


Figure 1

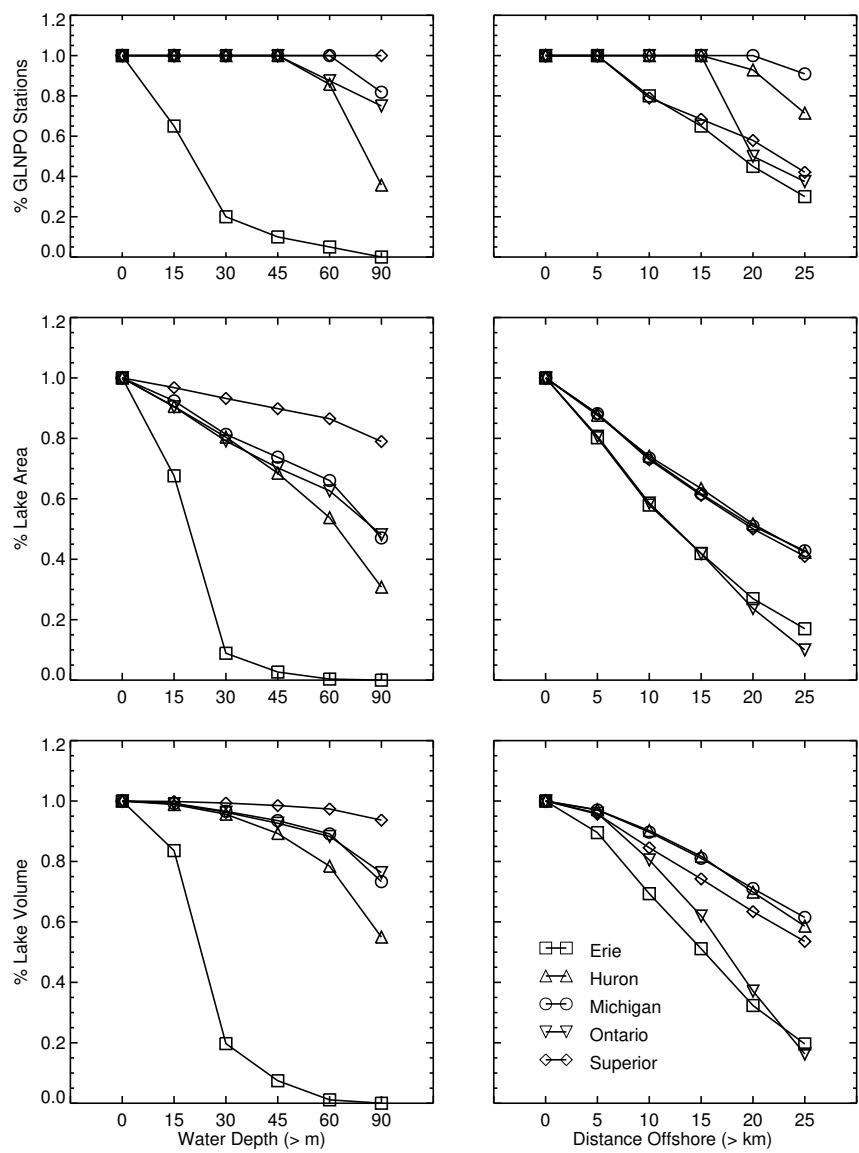


Figure 2

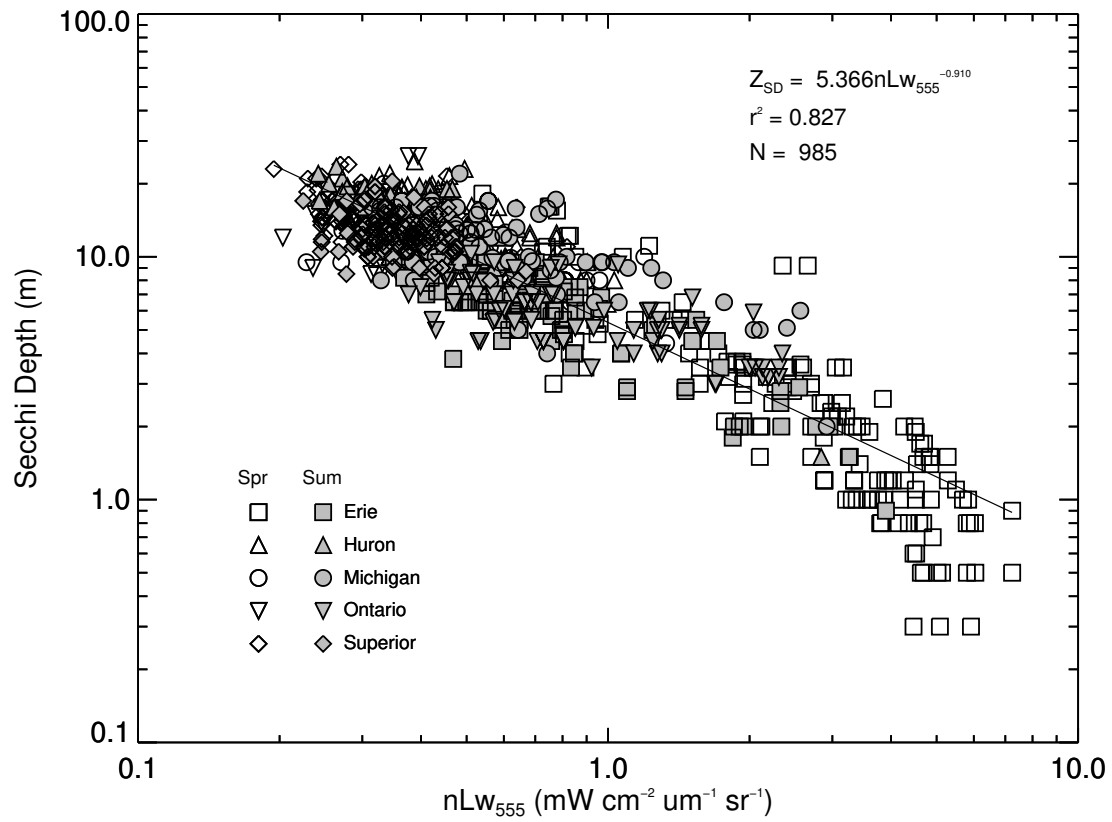


Figure 3

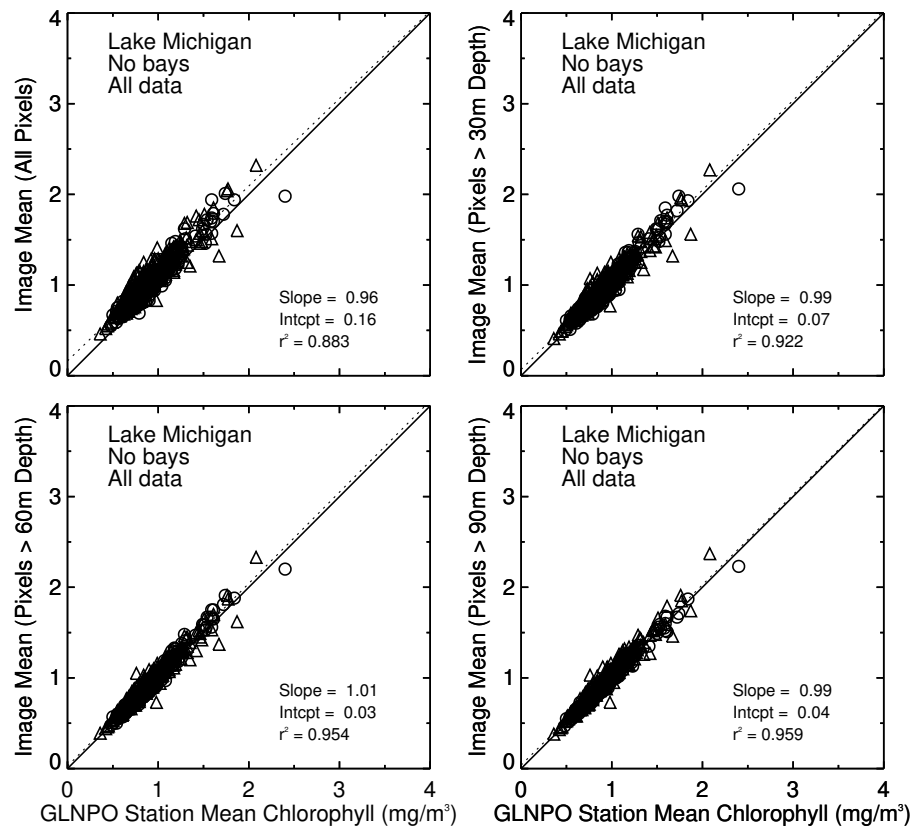


Figure 4

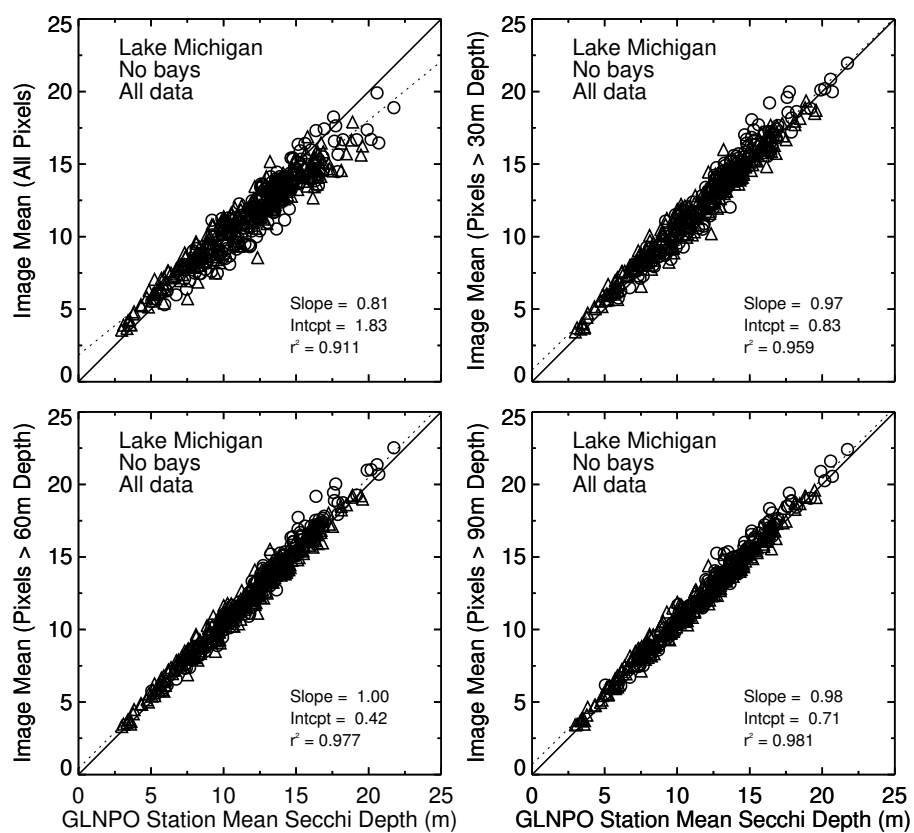


Figure 5

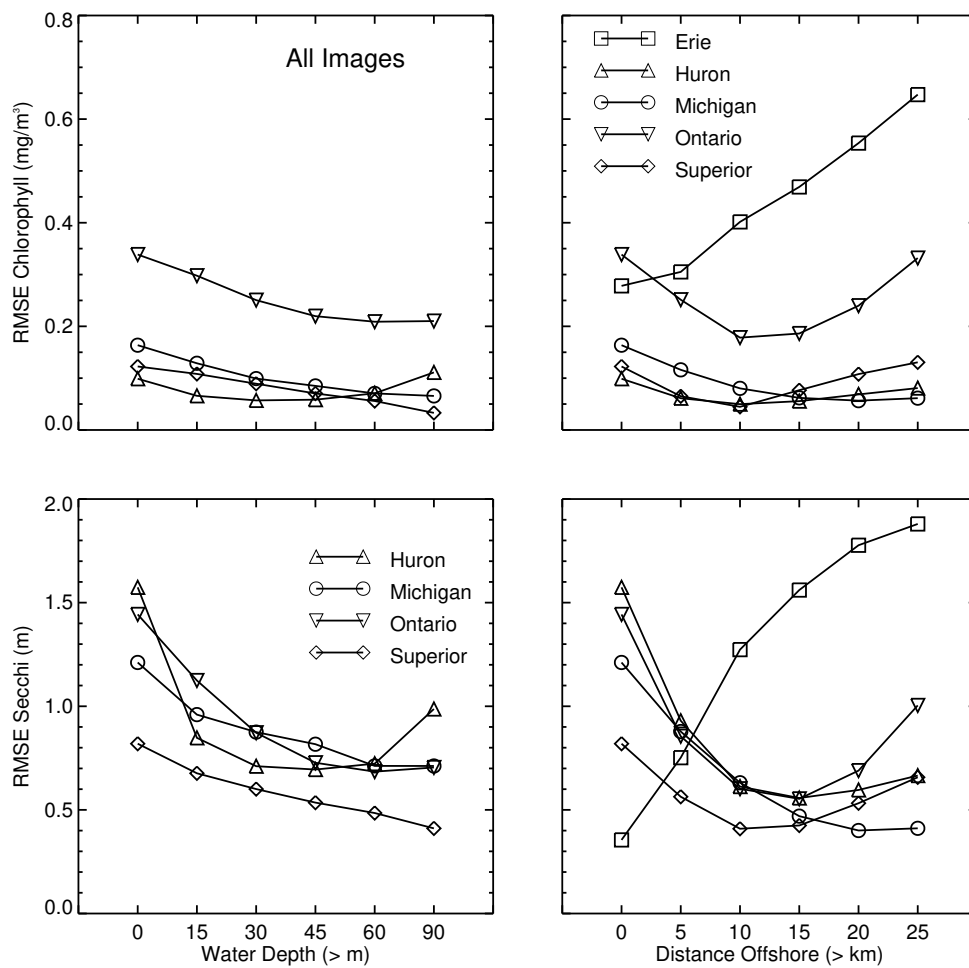


Figure 6

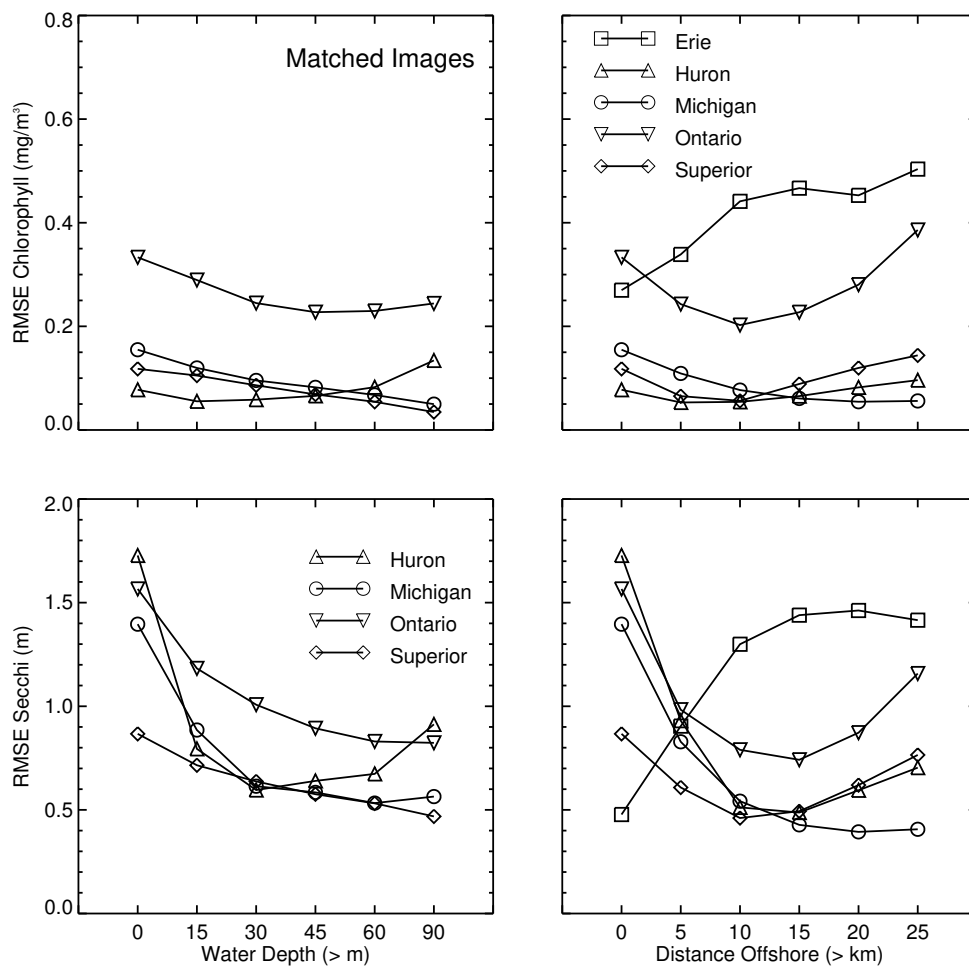


Figure 7

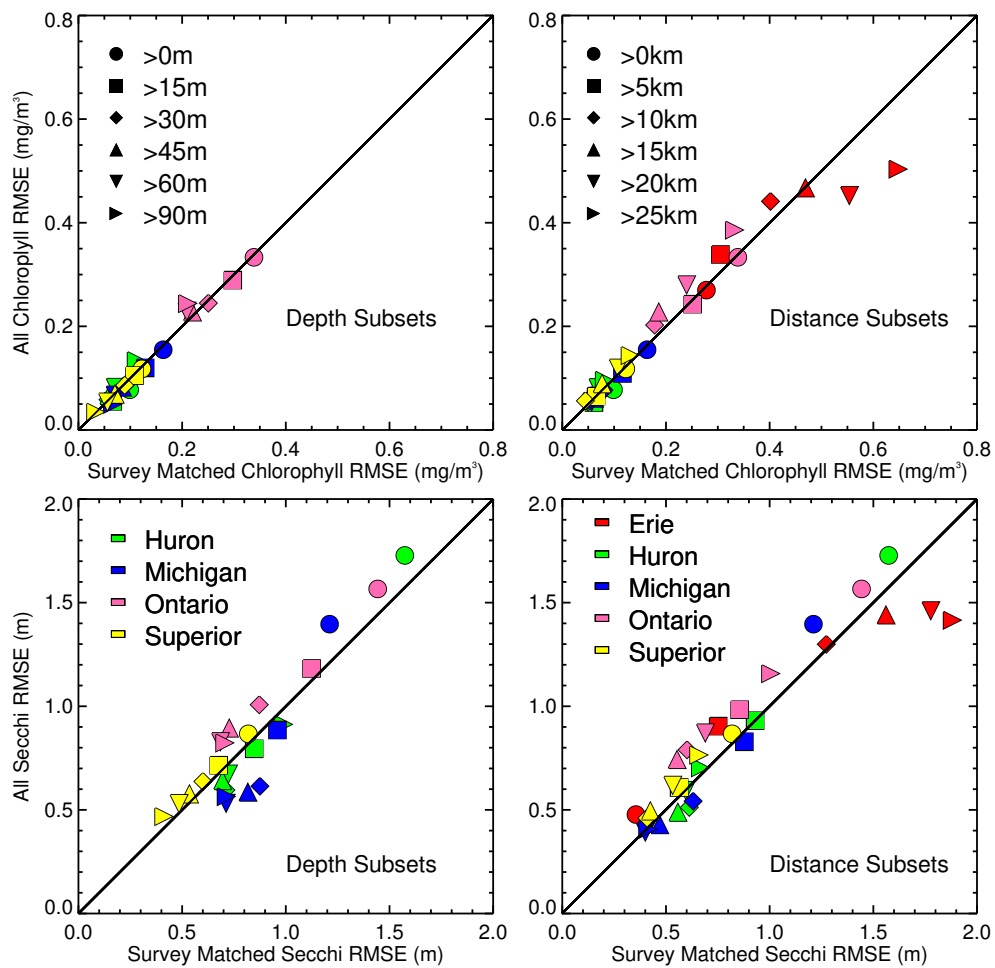


Figure 8

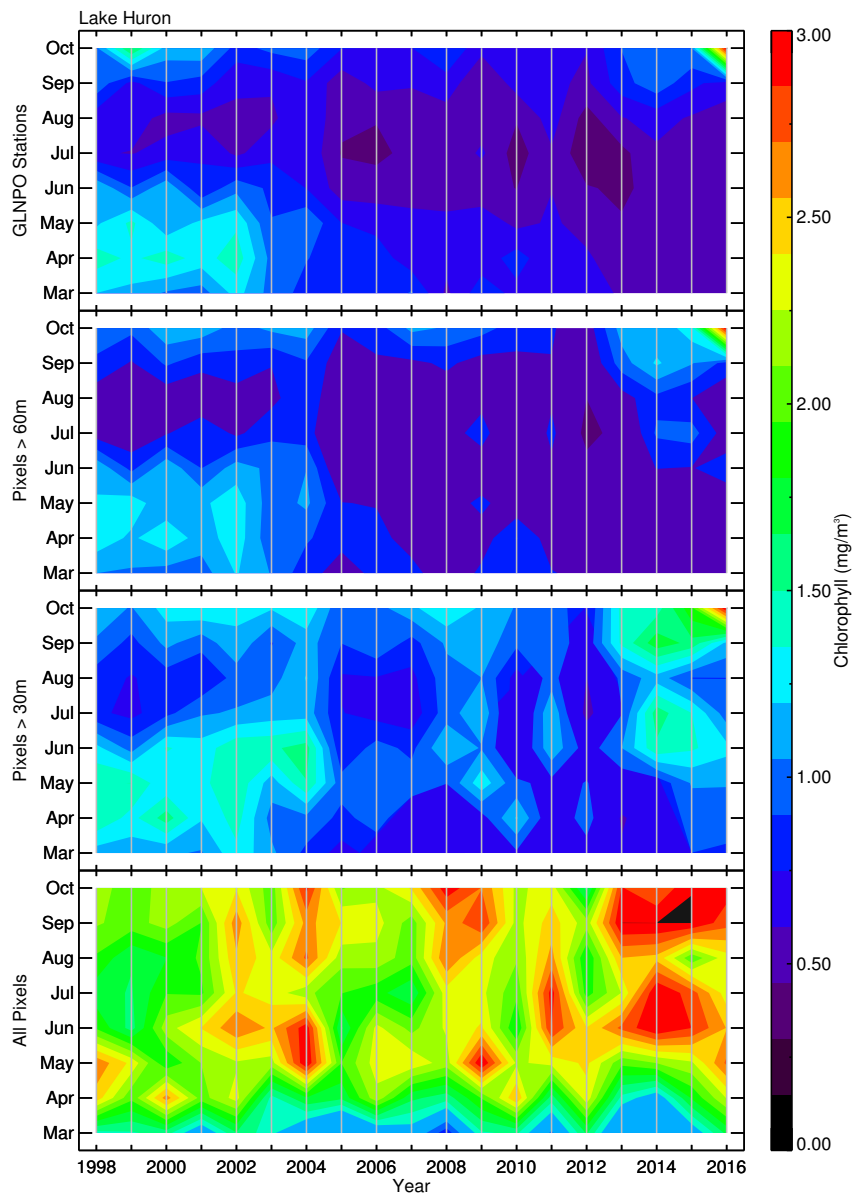


Figure 9

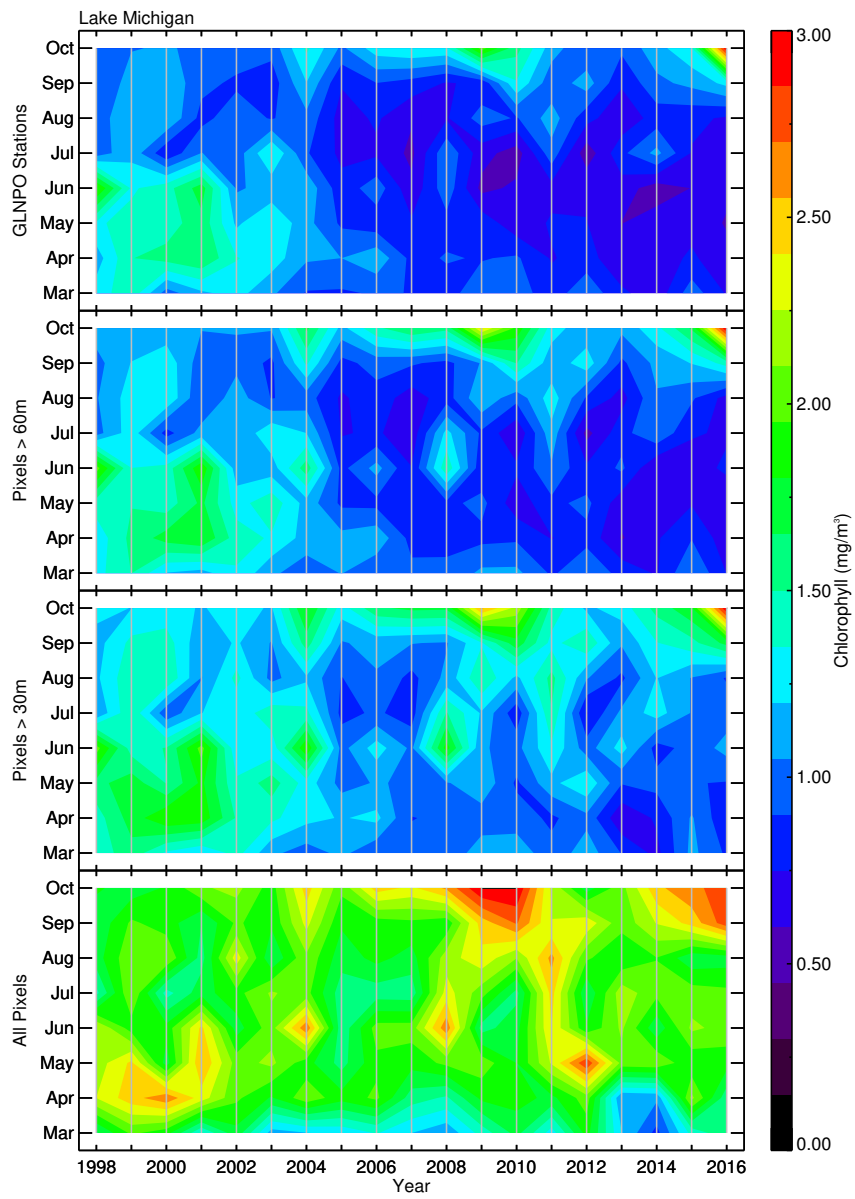


Figure 10