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Water Resources Research

RESEARCH ARTICLE

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Key Points:

- MYD09 (R_Land) products were evaluated using in situ data and reflectance derived using ocean color based NIR and SWIR atmospheric corrections
- R_Land(645) and R_Land(645/555) demonstrated high accuracy in terms of daily spatial distributions, seasonality, and long-term trends
- Improved data quality in R_Land(645/555) was found when data are binned by 7×7 pixels in space and 32 days in time

Supporting Information:

- Figure S1

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Can MODIS Land Reflectance Products be Used for Estuarine and Inland Waters?

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Abstract Although designed for land surfaces, MODIS Aqua surface reflectance data products (MYD09, termed as R_Land in this work) have also been used for water applications. Yet to date their uncertainties and general suitability in such applications have rarely been documented. In this study, R_Land products of two regions (Chesapeake Bay and Taihu Lake) between July 2002 and December 2015 are evaluated against in situ measurements and against reflectance products derived by the MODIS Ocean Team using atmospheric correction schemes specifically designed for water applications, namely the default atmospheric correction method based on the near-infrared (NIR) bands (denoted as R_NIR, data products available from NASA) and alternative atmospheric correction method based on the shortwave-infrared (SWIR) bands (denoted as R_SWIR, data products not available from NASA but require customized processing by the user), respectively. Results suggest high accuracy in R_Land(645) and R_Land(645/555) for both Chesapeake Bay and Taihu Lake in terms of daily spatial distributions, seasonality, and long-term trends. A sensitivity test also shows improved data quality in R_Land(645/555) when data are binned by 7×7 pixels in space and 32 days in time. Improved data quality can also be obtained for R_Land(645) when data are only binned in time to minimize the patchiness noise in R_Land daily images. Given the fact that most users do not have the capacity to process low-level data to obtain R_SWIR and the standard NASA R_NIR products often lack coverage over inland waters because they are optimized for global oceans instead of inland waters, this study provides a general guide on the applicability of the widely available R_Land products in inland and estuarine water applications in the absence of customized R_NIR or R_SWIR data products for local regions.

1. Introduction

Despite significant progress in the past two decades in algorithm and product development, assessment and monitoring of water quality of estuarine and inland waters using satellite measurements still face significant challenges (Mouw et al., 2015). One such challenge is the lack of accurate surface reflectance data to be used as inputs of the various inversion models to estimate water quality parameters such as turbidity, water clarity (Secchi Disk Depth), total suspended sediment concentration (TSS), chlorophyll-a concentration, among others. There are mainly two reasons leading to this challenge.

One is due to fundamental difficulties in atmospheric correction over these optically complex waters. This is true even for a perfectly calibrated satellite sensor after vicarious calibration (Franz et al., 2007; Wang, 2005), as the assumptions behind the atmospheric correction approaches often do not hold, not to mention other factors contributing to this problem (e.g., land adjacency effect, Feng & Hu, 2017). While the details of the atmospheric correction approaches for water applications can be found in the literature, for completeness they are briefly introduced here. The classical atmospheric correction over global oceans is based on the assumption that ocean is dark in the near-infrared (NIR) wavelengths (i.e., black-pixel) due to strong water absorption and much weaker scattering of water (Gordon, 1997; Gordon & Wang, 1994). This assumption is known to fail in turbid waters due to enhanced particle scattering (and therefore reflectance) in the NIR wavelengths; therefore several approaches have been proposed to overcome this difficulty, with various assumptions in either the spatial homogeneity of the atmosphere (Hu et al., 2000), aerosol scattering spectral shapes (Ruddick et al., 2000), the relationship between chlorophyll concentration and NIR reflectance (Siegel et al., 2000), or the relationship between water's optical properties in the red and NIR bands (Bailey et al., 2010; Stumpf et al., 2003) (see review by Jamet et al., 2011; Wang, 2010). Currently, this latter approach

has been used by the U.S. NASA as the operational algorithm to produce the standard (or default) surface reflectance data products for global waters (termed as R_{NIR} in this study). However, it is well known that the assumed optical relationship between the red and NIR bands depends on particle size distributions that may vary from region to region; therefore their applications in estuarine and inland waters often require regional validations (this alone may not be a big problem for a user, but the biggest problem is lack of data coverage—see below). To overcome the problem of varying optical relationship between the red and NIR bands, the same “black-pixel” atmospheric correction approach but with the atmospheric correction bands shifted from the NIR to the shortwave-infrared (SWIR) bands has been proposed for turbid waters (Novoa et al., 2017; Vanhellemont & Ruddick, 2015; Wang & Shi, 2007), as water is essentially black even for extremely turbid waters due to much stronger water absorption in the SWIR than in the NIR. In this study, surface reflectance products derived from the SWIR atmospheric correction are termed as R_{SWIR} . In principle, as long as the atmosphere is not dominated by strongly absorbing aerosols (Chander et al., 2009), SWIR-based atmospheric correction should work once the SWIR bands have sufficient signal-to-noise ratios and are vicariously calibrated. The SWIR-based atmospheric correction is available in the NASA software package SeaDAS as an alternative approach to process coastal and inland waters.

Two is due to practical reasons, and this is perhaps the most limiting factor for the general users instead of algorithm developers. Specifically, for many inland and estuarine waters, usable R_{NIR} or R_{SWIR} data products are simply not available to a general user who has no capacity for customized data processing. First, although the R_{NIR} data products are available, they are generally not ready for applications over inland and estuarine waters because

1. The highest-resolution R_{NIR} data products are at 1 km, and they are only available as daily snapshots without map projection. In order to establish time series to examine spatial and temporal patterns, a user needs to perform quality control of every pixel using the “l2_flags” data field, and bin the quality controlled data to georeferenced maps at user specified spatial and temporal resolutions. This is often impractical for a user.
2. The R_{NIR} data products are generated using globally optimized parameterization during data processing, for example, with a Rayleigh-corrected reflectance (R_{rc}) of 0.027 at ~ 869 nm (after sun-glitter correction) being used to screen clouds (Wang & Shi, 2006). For maritime aerosols, this corresponds to about 0.3 in aerosol optical thickness at 869 nm. Above these threshold values, no R_{NIR} data is generated for the pixel. For many coastal and inland waters, this can present a significant problem on R_{NIR} availability (e.g., Qi et al., 2014 for Taihu Lake). To overcome this difficulty, some customized data processing can be used to increase the threshold, for example to 0.04 for Tampa Bay (Le et al., 2013b), but this requires data processing at low-level. Likewise, although SWIR bands are proposed for cloudscreening over turbid waters (Wang & Shi, 2006), that approach also requires customized data processing at low-level, which is often not readily available for a user.
3. While the above two problems exist for all ocean-color sensors, for the Moderate Resolution Imaging Spectroradiometer (MODIS) there is an addition problem of data saturation, which prevents generation of R_{NIR} data products. MODIS ocean bands were designed to be more sensitive than land bands; therefore easier to saturate (Hu et al., 2012). The standard SeaDAS processing optimized for global oceans; if one of the ocean bands saturates over the pixel then R_{NIR} is not generated for all bands over the pixel.
4. Although globally binned R_{NIR} data products at daily, 8 day, monthly, or longer temporal intervals, they suffer from problems #2 and #3 for inland and estuarine waters, and the resolution of these binned data products is often not enough (e.g., 4 km or coarser).

As a result, the R_{NIR} data products, readily available for the community to use, are often not applicable for inland and estuarine waters. In many case, they simply show no coverage in those waters. This is simply because that these data products were not designed for inland and estuarine waters.

Second, for MODIS measurements, high-quality R_{SWIR} products require significant effort in recalibrating and denoising the SWIR bands as well as in software modification and data processing (e.g., Li et al., 2017). This is in addition to the data binning requirements after R_{SWIR} products are generated from daily snapshots. Similarly, although Rayleigh-corrected reflectance (R_{rc} , dimensionless) can also be used for turbid water applications (Duan et al., 2014; Feng et al., 2014b; Markham et al., 2008; Zhang et al., 2016), these data products also require customized data processing and they are not available to the general user.

The general lack of readily usable surface reflectance data products for inland and estuarine waters leaves no choice for a general user but to use the MODIS land surface reflectance products (MYD09 for Aqua and MOD09 for Terra), derived for land applications (Kaufman et al., 1997; Vermote & Vermeulen, 1999) and distributed by the MODIS Land Team (https://lpdaac.usgs.gov/data_access). The atmospheric correction method used to generate such products used the blue and red bands to estimate aerosol contributions after assuming certain relationship between surface reflectance in these bands, and then interpolated to other bands (Kaufman et al., 1997). Although named as “land surface reflectance,” the data products (denoted as “R_Land” in this study) do have global coverage including estuarine and inland waters; therefore have been used to study water quality in estuaries and inland waters (Chen et al., 2015; Constantin et al., 2016; Doxaran et al., 2009; Hou et al., 2017; Olmanson et al., 2011; Park & Latrubesse, 2015; Pavelsky & Smith, 2009; Petus et al., 2010, 2014; Song et al., 2017; Tarrant et al., 2010; Wang et al., 2015; Wu et al., 2007). Indeed, although designed for land studies, compared with the MODIS ocean bands, MODIS land bands have higher spatial resolutions (250–500 m) and larger dynamic ranges (Hu et al., 2012), making them particularly useful for relatively small water bodies (Binding et al., 2012; Chen et al., 2007; Feng et al., 2014a; Hu et al., 2004; Kahru et al., 2004; Kutser et al., 2007; Lahet & Stramski, 2010; Markham et al., 2008; Saldías et al., 2012). It appears that the typical problem of no data in the ocean-color oriented data products might be overcome by these widely distributed R_Land data products, as any user can download and make direct use of these products for studies of estuarine and inland waters.

However, the uncertainties and general applicability of R_Land for water applications are generally unknown, making it difficult to assess (in the absence of direct ground validation) the fidelity of water properties derived from R_Land. Because of the much higher dynamic range, MODIS R_Land data are known to contain higher uncertainties than those specifically derived for water applications using the ocean bands. For example, for typical clear oceanic waters with a reflectance of 0.04 (dimensionless) at 443 nm (Hu et al., 2013), the theoretical uncertainty for R_Land is ~ 0.007 ($0.005 + 5\% \times 0.04$) (Vermote et al., 1997), accounting for 14% of the ocean reflectance, which is ~ 3 times of uncertainties required for ocean applications (5%). In addition, the uncertainty estimates (i.e., $0.005 + 5\% \times R$) of R_Land were mainly based on AERONET data collected over land surfaces (<https://landval.gsfc.nasa.gov/ProductStatus.php?ProductID=MOD09>), while little is known about their uncertainties over water bodies. Previous applications of R_Land products for water applications were mainly restricted to turbidity estimates for highly turbid waters due to their strong reflectance in the red (Doxaran et al., 2009), but for general water applications the uncertainties of R_Land data products still need to be quantified, and in particular compared with those from other approaches.

Therefore, the overall goal of this study is to provide recommendations for the use of R_Land for estuarine and inland water applications, with the following specific objectives:

1. Compare and evaluate R_Land, standard ocean-color reflectance product (R_NIR), and alternative product (R_SWIR) from MODIS Aqua measurements for a large estuary (Chesapeake Bay) and a moderate lake (Taihu Lake) at various spatial and temporal scales.
2. Determine the most appropriate spectral band(s) of R_Land that are feasible for water quality assessment and monitoring of estuaries and inland waters, and make recommendations on temporal and spatial bins to minimize potential bias or artifacts.

The selection of Chesapeake Bay and Taihu Lake as two test regions is because they represent typical estuarine and inland waters, respectively. Specifically, Chesapeake Bay is a moderately turbid estuary, where Chl-a concentration ranges from ~ 1 to $\sim 50 \text{ mg m}^{-3}$ (Le et al., 2013a). On the other hand, Taihu Lake is characterized by large turbidity, where concentrations of total suspended sediments (TSS) change from < 10 to $> 300 \text{ mg L}^{-1}$ (Shi et al., 2015) and Chl-a ranges between < 10 and $> 400 \text{ mg m}^{-3}$ (Zhang et al., 2009).

2. Data Sets and Methods

2.1. Remote Sensing Data

All available MODIS Aqua daily R_Land (i.e., MYD09, dimensionless reflectance) for 4 bands (469 nm (blue), 555 nm (green), 645 nm (red), and 859 nm (NIR)) covering Chesapeake Bay (6,186 granules) and Taihu Lake (5,155 granules) were obtained in this study (see locations in Figure 1). The data between July 2002 and December 2015 were downloaded from the U.S. NASA Land Processes Distribution Active Archive Center (LP DAAC) (data accessed in December 2016, Collection 6) (<http://doi.org/10.5067/MODIS/MYD09.NRT.006>)

Figure 1. (a) Locations of satellite-to-in situ matching pairs (green circles) in Chesapeake Bay of the U.S. and (b) Taihu Lake of China. In situ data of Chesapeake Bay were collected from a cruise in July 2011 and data archived in NASA's Sea-BASS archive, and data of Taihu Lake were collected from 12 cruises between 2005 and 2014 spanning four seasons (Li et al., 2017). The background images are the MODIS RGB composites on (a) 12 April 2003 and (b) 29 October 2012, respectively.

and were projected into a cylindrical equidistance (rectangular) projection using the MODIS Reprojection Tool (https://lpdaac.usgs.gov/tools/modis_reprojection_tool). The 645 and 859 nm bands have a spatial resolution of 250 m, and 469 and 555 nm bands have a spatial resolution of 500 m. To facilitate comparison and to compose Red-Green-Blue (RGB) true color images, the 500 m bands were resampled to 250 m. Therefore, all MODIS data used in this study have the same 250 m pixel resolution.

The performances of R_{Land} for four MODIS bands (469, 555, 645, 859 nm) were examined in this study. In addition to single-band images, band ratios (645/555, 859/645, and 469/555) were also explored, as they have been widely used in ocean-color applications. For example, band ratios of 645/555 and/or 859/645 have been used to map TSS concentrations (Doxaran et al., 2002; Feng et al., 2014a; Hou et al., 2017), band ratio of 469/555 can be used as the input of a two-band (OC2) algorithm to estimate Chl-a (O'Reilly et al., 2000).

For each MYD09 file, the corresponding Level-1A data were downloaded from the NASA Goddard Space Flight Center (GSFC, <https://oceancolor.gsfc.nasa.gov/>) (data accessed in December 2016). These MODIS data were then processed with the l2gen module of SeaDAS (version 7.3) using the SWIR-based AC method to derive remote sensing reflectance (R_{rs} , sr^{-1}) (Wang & Shi, 2007), and then converted to reflectance (R_{SWIR} , dimensionless) by multiplying π to match R_{Land} . Before applying the AC, the radiance data in the two SWIR bands (1,240 and 2,130 nm) were smoothed through a noise reduction scheme to remove noise and improve SNR (Li et al., 2017). No vicarious calibration was applied to these AC bands, and their default vicarious gains (1.0) specified in SeaDAS were used. In the l2gen processing, data quality flags (l2_flags) for each pixel were also generated and recorded, which were used to discard low-quality data during the subsequent product evaluation. Note that these products (R_{SWIR}) are not distributed by NASA or other agencies, so a user must download the low-level data and process them to obtain R_{SWIR} on the user end. While such R_{SWIR} generation procedures require considerable efforts from users, especially for long-term data processing.

In contrast to the above R_{SWIR} data products, standard Level-2 R_{rs} data products are available and distributed at NASA GSFC, where a user can download and make direct use of these reflectance products. These have been derived using the default AC method embedded in SeaDAS (i.e., NIR iteration). Corresponding to each downloaded MYD09 granule, the Level-2 R_{rs} data products were downloaded from NASA GSFC (data

accessed in December 2016, reprocessing 2014.0), and then multiplied by π to convert to reflectance R_{NIR} (dimensionless). Because there is nearly no coverage by these products over Taihu Lake (Qi et al., 2014) due to saturation of the sensitive MODIS ocean bands (Hu et al., 2012), these data products were obtained for only Chesapeake Bay.

Finally, to test how aerosols could influence R_{Land} and to examine whether reflectance without removing aerosol effects could be used for water applications, a partial atmospheric correction was applied to Level-1 data to derive R_{rc} (Hu, 2009):

$$R_{\text{rc}} = \pi L_t^* / (F_0 \times \cos \theta_0) - R_r \quad (1)$$

where F_0 is the extraterrestrial solar irradiance, θ_0 is the solar zenith angle, L_t^* is the calibrated at-sensor radiance after correction for gaseous absorption, and R_r is the reflectance due to Rayleigh (molecular) scattering estimated using the 6S radiative transfer code (Vermote et al., 1997). Note that during this processing the water surface Fresnel reflectance (Querry, 1969) was regarded as part of the surface reflectance and therefore included in R_{rc} (in contrast, if R_{rc} were to be derived using SeaDAS code, the Fresnel reflectance would *not* be included in R_{rc}). The retention of Fresnel reflectance in R_{rc} is to match R_{Land} , where the effects of Fresnel reflection is not corrected.

All four reflectance products (R_{Land} , R_{NIR} , R_{SWIR} , R_{rc}) are dimensionless, and they were georeferenced into the same rectangular projection and resampled to the same 250 m pixel resolution. All MODIS data used in this study have the same 250 m pixel resolution from either the original bands or resampled data. The resampling of coarse resolutions (1 km or 500 m) to finer resolution of 250 m is to have coregistered spectral bands, while the resampling will not impact either validation or final products because a spatial homogeneity test was used to select the matching pairs (satellite and field measurements) and the final products were examined through spatial and temporal binning. Three band ratios of 645/555, 859/645, and 469/555 for each product were also estimated. Because R_{SWIR} at 859 nm generally showed negative values in Chesapeake Bay (see results below), the ratio of 859/645 was not calculated for this region.

2.2. Product Comparison

Daily snapshot images or band-ratio images were gridded into monthly composites. The 32-bit $I2_flags$ generated concurrently with R_{SWIR} were checked for all the reflectance products when composing monthly data. If a water pixel was flagged as “cloud” or “high-glint”, it was considered as invalid and discarded. The remaining pixels were used to calculate monthly mean values. These two flags were selected instead of a complete list of flags (e.g., straylight, negative water-leaving radiance, etc.) used by the NASA OBPG for generating global Level-3 composites (<https://oceancolor.gsfc.nasa.gov/atbd/ocl2flags/>) was because: (1) such a complete list of flags is not available for R_{Land} data products that are available to every user, and even if we demonstrate high performance on fully masked R_{Land} , common users may not benefit from our efforts because no complete $I2_flags$ are available; and (2) clouds and severe sun-glint contaminations can be masked using other methods (Ackerman et al., 2010) or through manual work on the R_{Land} images.

In addition to monthly mean products, climatological monthly mean products were also generated for the 12 calendar months. Then, monthly anomalies, derived as the monthly deviations to the monthly climatologies, were calculated for each month between July 2002 and December 2015. The correlations between monthly mean values of different reflectance products represent the similarities of temporal patterns, while the relationships and relative differences between time series of monthly anomalies indicate the consistencies of the long-term trends.

2.3. Determination of Optimal Spatial and Temporal Bins

Daily R_{Land} images often contain unrealistic spatial patchiness (see results below), leading to sharp artificial gradients. To reduce the impact of these errors, daily images at 250 m pixel resolution can be binned to coarser spatial and/or temporal resolutions. This is because that although the advantages of 250 m data on daily snapshot is obvious when used to study spatial patterns (Franz et al., 2006), for assessment of water quality changes, especially in the context of long-term trends, data products at a single location are rarely used. Instead, when tracking the water quality dynamics over a long period for a lake or estuary, previous studies tended to focus on the monthly, seasonal or annual mean conditions of the entire region (Binding

et al., 2007; Gallegos et al., 2011; Wang et al., 2011, among many others). More importantly, the determination of optimal spatial bin size could also help to recognize the applicability of R_Land. For example, if the required spatial bin size (to observed consistent patterns) exceeds the size of an estuary or lake, R_Land would not be applicable for the study region.

The optimal spatial and temporal bin sizes for R_Land were determined through correlation (i.e., consistency) of R_Land and R_SWIR time series. This is because that (1) no such patchy features were found in the R_SWIR images and (2) global and regional validations demonstrated satisfactory performance of R_SWIR (Wang & Shi, 2007), and thus the agreements of R_Land and R_SWIR could also be used to justify the validity of R_Land. For each variation in the spatial/temporal bin size, R^2 between the two time series was calculated. The steps are as follows:

1. Daily R_Land and R_SWIR data were binned into multiday composites (4, 8, 12, . . . , 32 day), where pixels of clouds and sun-glint were excluded. Then, the temporally binned products were spatially binned to different grid sizes (3×3 , 5×5 , . . . , 15×15 pixels). For each bin size, mean values within the corresponding time interval and/or spatial grid were calculated, and the resulting data with different temporal (i , $i = 4, 8, 12, \dots, 32$) and spatial (j , $j = 1, 3, 5, \dots, 15$) bins were denoted as $R_SWIR_{t=i, s=j}$ and $R_Land_{t=i, s=j}$ for R_SWIR and R_Land, respectively.
2. For any combination of temporal and spatial bins, >100 random points were generated within the study region (Taihu Lake or Chesapeake Bay) from the long-term $R_SWIR_{t=i, s=j}$ and $R_Land_{t=i, s=j}$ data between 2002 and 2015. Then, the correlation between $R_SWIR_{t=i, s=j}$ and $R_Land_{t=i, s=j}$ was calculated from each of these random points using the 14 year time series, and the mean R^2 of all the random points was used to represent the agreement (or disagreement) between R_Land and R_SWIR for that bin combination.

2.4. In Situ Data

Field measurements of spectral reflectance were conducted in July 2011 Chesapeake Bay (Le et al., 2013a). Additional reflectance data for this region were also available and downloaded from the NASA SeaBASS

Figure 2. MODIS images of R_Land (a), R_SWIR (b) and R_NIR (c) for Chesapeake Bay on 12 April 2003, where their corresponding RGB composite image is shown in Figure 1a. The patchy features in the R_Land images are clearly shown in the enlarged rectangles in Figure 2a.

archive (<https://seabass.gsfc.nasa.gov/>) (Werdell & Bailey, 2005). Normalized water-leaving radiance (nL_w , in $mW\ cm^{-2}\ sr^{-1}\ \mu m^{-1}$) collected by the AERONET ocean-color (AERONET-OC) site (Zibordi et al., 2004) located at the Chesapeake Bay (site name: COVE_SEAPRISM, location: $36.9^\circ N$, $75.71^\circ W$) were also used to validate the reflectance products, and the nL_w data were normalized to the extraterrestrial solar irradiance to convert into R_{rs} . For Taihu Lake, spectral reflectance data were also collected through 12 field surveys between 2005 and 2014 spanning all four seasons (Li et al., 2017). The in situ measurements from the two regions were obtained across different seasons, representing seasonality of the water and aerosol properties. R_{rs} data of 416 stations were acquired with an Analytical Spectral Device (ASD) portable field spectrometer FieldSpec[®] Pro FR (350–2,500 nm) or FieldSpec[®] Pro VNIR (350–1,000 nm). These data have been used extensively in other studies to examine the bio-optical properties and water quality of Taihu Lake (Sun et al., 2013; Zhang et al., 2008, 2015). Rigorous above-water Ocean Optics protocol (Mueller et al., 2003) was followed for both data collection and data reduction. Similar to converting MODIS-derived R_{rs} to dimensionless R , these in situ R_{rs} were also multiplied by π to convert to dimensionless surface reflectance (i.e., R).

Several quality-control criteria were applied when selecting satellite-to-in situ matching pairs. First, the time difference between satellite and in situ measurement was restricted to <3 h (Bailey & Werdell, 2006). Second, to

account for the spatial disparities between MODIS ($250 \times 250\ m^2$ pixel size) and in situ (a single point) data, a homogeneity test was applied. Only when the coefficient of variation (CV, standard deviation/mean) of 3×3 MODIS pixels centered at the in situ station was <0.4 was MODIS data selected for evaluation (Harding et al., 2005). Third, R_{Land} pixels with spatial patches (see images below, possibly caused by erroneous aerosol correction) were excluded through visual inspection. Such excluded pixels were also excluded in R_{NIR} and R_{SWIR} . The resulting number of matching pairs was 102 for Taihu Lake and 77 for Chesapeake Bay, respectively (see locations in Figure 1).

3. Results

3.1. Comparison of Daily Reflectance Products

R_{Land} and R_{SWIR} daily images for four bands are illustrated in Figure 2 for MODIS data collected on 12 April 2003 over Chesapeake Bay. The general spatial patterns are similar between R_{Land} and R_{SWIR} , with higher values in nearshore waters than in offshore waters. For most waters, however, R_{Land} is generally higher than R_{SWIR} , and $R_{SWIR}(859)$ generally shows negative values in Chesapeake Bay. While R_{SWIR} images appear to contain noise due to the low-SNR SWIR bands used in the atmospheric correction, noticeable patchiness is found in R_{Land} images in the central region of Chesapeake Bay, which is associated with the use of a 10×10 pixels (1 km resolution) moving window to conduct the AC process (Kaufman et al., 1997). The corresponding band-ratio images (645/555 and 469/555) for R_{Land} and R_{SWIR} are presented in Figures 3a and 3b. Unlike single-band images, the band-ratio images show similar magnitudes between R_{Land} and R_{SWIR} , particularly for 645/555 for its spatial patterns and magnitudes except for some near shore water (circled in red). However, the spatial patterns of 469/555 appear very different between R_{Land} and R_{SWIR} .

Similar to Figures 2 and 3, Figure 4 shows comparisons between R_{Land} and R_{SWIR} as well as their band ratios for Taihu Lake. Similar to the findings for Chesapeake Bay, R_{Land} appears higher than R_{SWIR} for all four bands. Yet, $R_{SWIR}(645/555)$ is higher than $R_{Land}(645/555)$, while comparable magnitudes were found for the other two ratios (859/645 and 469/555) between R_{SWIR} and

Figure 3. (top plots of a–c) MODIS band-ratio images of 645/555 and (bottom plots of d–f) 469/555 for R_{Land} , R_{SWIR} , and R_{NIR} , derived from the images shown in Figure 2. The region outlined in white appears to be affected by land adjacency effects.

Figure 4. (a–g) MODIS single-band and (h–m) band-ratio images of R_Land and R_SWIR for Taihu Lake on 29 October 2012, where their corresponding RGB composite image is shown in Figure 1b.

R_Land. Although spatial patchiness is not obvious in the daily R_Land images on this particulate date (29 October 2012), such artifacts were found to be more apparent in many other days (see example in supporting information Figure S1).

For comparison, the R_NIR images of Chesapeake Bay on the same day are also presented in Figure 2c and Figures 3c and 3f), where the reflectance values appear to be closer to R_SWIR than to R_Land. Although the three types (R_NIR, R_SWIR, and R_Land) of reflectance products demonstrated similar spatial patterns in terms of both single-band reflectance and band ratios (except for 469/555), the images of R_NIR showed much smoother patterns than those of R_Land and R_SWIR, attributing primarily to the high SNR of the NIR ocean bands used in the AC for the former products (Hu et al., 2012). Unfortunately, the R_NIR for Taihu Lake was simply not available due to saturation of certain ocean bands, prohibiting the comparison of R_NIR with R_SWIR and R_Land for this turbid lake.

3.2. Comparison of Long-Term Monthly Data

Monthly mean time series of single-band data between July 2002 and December 2015 for all pixels of Chesapeake Bay are shown in Figure 5, where the agreements between all three reflectance products can be observed for the 555 and 645 nm bands in their seasonality (low in summer and higher in winter) and monthly fluctuations. Long-term monthly data of these two bands are significantly correlated among all three reflectance products ($R^2 > 0.67$, $p < 0.05$ for R_Land versus R_SWIR and R_Land versus R_NIR). In

Figure 5. Monthly mean reflectance of single bands for Chesapeake Bay between July 2002 and 2015. The comparison is made between R_{Land} , R_{SWIR} , and R_{NIR} , where coefficients of determination (i.e., R^2) between R_{Land} and the other two products are annotated.

contrast, the agreement for the 469 and 859 nm bands is much worse between R_{Land} and R_{SWIR} , with $R^2 = 0.02$ and 0.27 , respectively, which may due to the problematic AC process for either of the two products in this region. Similar to the findings from the daily images, R_{Land} showed much higher values than R_{NIR} and R_{SWIR} for nearly every month.

Monthly mean band ratios (645/555 and 469/555) corresponding to Figure 5 are plotted in Figure 6. Similar to those shown in the daily images, the three products shared comparable magnitudes and temporal patterns for 645/555, with R^2 being 0.68 between R_{Land} and R_{SWIR} and 0.76 between R_{Land} and R_{NIR} . In contrast, no significant correlation can be found in the 469/555 ratios from the three products.

Similar to Figures 5 and 6, for Taihu Lake the monthly R_{Land} and R_{SWIR} data between July 2002 and December 2015 are shown in Figures 7 and 8 for single bands and band ratios, respectively. High consistency was observed for the 645 and 859 nm bands between R_{Land} and R_{SWIR} , with R^2 of 0.69 and 0.56 , respectively. On the contrary, the agreements of R_{Land} and R_{SWIR} were very poor for the 469- and 555-nm bands with insignificant relationships ($R^2 < 0.03$) found between the two products. For band ratios, the agreement between R_{Land} and R_{SWIR} is excellent for 645/555 in terms of their temporal patterns (not magnitude), with R^2 reaching 0.90 ($p < 0.05$). The 859/645 band ratio also showed significant correlation ($R^2 = 0.56$, $p < 0.05$). On the other hand, the dynamic ranges in both the 645/555 and 859/645 ratios are much smaller from R_{Land} than from R_{SWIR} .

Figure 6. Monthly mean reflectance ratios for Chesapeake Bay between July 2002 and 2015. The comparison is made between R_Land, R_SWIR, and R_NIR, where coefficients of determination between R_Land and the other two products are annotated.

Figure 7. Monthly mean reflectance of single bands for Taihu Lake between July 2002 and 2015. The comparison is made between R_Land, R_SWIR, and R_NIR, where coefficients of determination between R_Land and the other two products are annotated.

Figure 8. Monthly mean reflectance ratios for Taihu Lake between July 2002 and 2015. The comparison is made between R_{Land} , R_{SWIR} , and R_{NIR} , where coefficients of determination between R_{Land} and the other two products are annotated.

The agreements between R_{Land} and R_{SWIR} for certain bands and band ratios were observed not only in the monthly data, but also in the long-term monthly anomalies (Table 1). In general, whenever monthly mean data (either single-band or band-ratio) showed significant correlations between R_{Land} and R_{SWIR} , the corresponding monthly anomalies also exhibited strong correlations and smaller differences. As such, when they were used to examine water quality patterns, similar relative changes could be expected with R_{Land} and R_{SWIR} .

Table 1

Coefficients of Determination (i.e., R^2) Between R_{Land} and R_{SWIR} for Various Bands and Band Ratios

	Band	Monthly	Monthly anomaly (MRD ^a)	Monthly climatology
Chesapeake Bay	469	0.02	0.03 (137.9%)	0.03
	555	0.67	0.39 (154.0%)	0.84
	645	0.73	0.65 (95.3%)	0.93
	859	0.27	0.00 (286.3%)	0.63
	469/555	0.05	0.16 (137.9%)	0.54
	645/555	0.68	0.66 (62.5%)	0.70
	859/645	0.00	0.04 (95.3%)	0.01
	469	0.03	0.18 (93.3%)	0.05
Taihu Lake	555	0.10	0.32 (84.1%)	0.02
	645	0.69	0.76 (66.4%)	0.89
	859	0.56	0.11 (87.5%)	0.76
	469/555	0.03	0.05 (286.3%)	0.18
	645/555	0.90	0.91 (81.3%)	0.94
	859/645	0.56	0.29 (87.5%)	0.69

^aMean relative differences between monthly anomalies of R_{Land} and R_{SWIR} .

3.3. In Situ Validations

All reflectance data (including band ratios) were further validated using satellite in situ matching pairs for both Chesapeake Bay and Taihu Lake, with results presented in Figures 9 and 10, respectively. Statistical uncertainty measures, including R^2 , Root-Mean-Square Errors or RMSE, Mean Relative Errors or MER, mean and median ratios, were all listed in Table 2.

The standard R_{NIR} products showed the lowest uncertainties for Chesapeake Bay (Figure 9 and Table 2), in terms of both single-band and band-ratio comparisons. For Taihu Lake where R_{NIR} products are not available, R_{SWIR} showed better performance than R_{Land} for the 859 nm band (Figure 12d and Table 2), but the opposite was found for the other three bands.

The most striking finding is that, the band ratio of 645/555 showed the highest accuracy from R_{Land} than from R_{NIR} or R_{SWIR} , and satisfactory $R_{Land}(645/555)$ data were obtained in both study regions. This is particularly true for Taihu Lake, where the data points aligned tightly on the 1:1 line (Figure 10e). Statistical measures also showed high fidelity in $R_{Land}(645/555)$, with RMSE = 8.9%,

Figure 9. Comparisons between in situ measured and MODIS-derived reflectance and reflectance ratios for Chesapeake Bay. The comparison is made on R_Land, R_SWIR, and R_NIR, where the coefficients of determination and RMSE between in situ data and MODIS products are annotated. Note that R_Land includes the surface Fresnel reflection but R_SWIR and R_NIR do not.

$R^2 = 0.69$, and mean ratio = 1.01 for Taihu lake ($n = 102$) and $RMSE = 59.9\%$, $R^2 = 0.66$, and mean ratio = 0.84 for Chesapeake Bay ($n = 71$) (Table 2). As water properties of the two study regions represent most of the estuarine and lacustrine conditions, R_Land products appear to be able to observe 645/555 reflectance ratios with high fidelity.

4. Discussion

4.1. Reasons for the Disparities Between the Three Reflectance Products

As shown above, R_Land was nearly always higher than R_SWIR and R_NIR for all four MODIS bands. One reason may be due to the difference in their reflectance definitions. While the former includes water surface Fresnel reflectance, the latter two do not. Additionally, the assumptions and procedures for aerosol estimations varied significantly between land based and ocean-based AC algorithms. Specifically, the land based algorithms first estimated aerosol contributions using blue and red bands and then interpolated to other bands. In contrast, the ocean-based algorithms derived aerosol information from either the NIR or the SWIR bands and then extrapolated to the visible bands (Gordon & Wang, 1994; Wang & Shi, 2007). Such an extrapolation led to generally more accurate products for wavelengths closer to the AC bands than for other wavelengths (e.g., Table 2). Indeed, the different aerosol correction schemes in R_Land and R_SWIR are believed to be the major reasons leading to higher R_Land. Such an effect can also be clearly demonstrated through comparison between R_Land and R_{LC} , with the latter not corrected for aerosol at all (see below).

The R_SWIR products often showed noises due to the low SNRs of the SWIR bands used in the AC algorithm. Indeed, even after some additional effort was used to smooth the two SWIR bands, residual noises were still evident, especially for moderately turbid waters in Chesapeake Bay (Figures 2 and 3). Additionally, substantial amount of negative R_SWIR values were observed in all spectral bands in this area. This is possibly due to lack of vicarious calibration of the SWIR bands. In contrast, the operational R_NIR products showed higher-quality images (Figures 2 and 3) and more accurate reflectance values (Table 2) than R_SWIR. These results were also consistent with those of Werdell et al. (2010), who showed increased number of negative water-leaving radiance and flatter frequency distributions in the R_SWIR products than in the R_NIR products. Furthermore, SWIR bands are more prone to land adjacency effects than other bands (Feng & Hu, 2017), leading to additional artifacts in some nearshore waters (outlined in white in Figure 3). Unfortunately, the standard R_NIR products often have no coverage over highly turbid lakes or highly turbid atmosphere

Figure 10. Comparisons between in situ measured and MODIS-derived reflectance and reflectance ratios for Taihu Lake. The comparison is made on R_Land and R_SWIR, where the coefficients of determination and RMSE between in situ data and MODIS products are annotated. Note that R_Land includes the surface Fresnel reflection but R_SWIR and R_NIR do not.

due to saturation of certain ocean bands, making them nearly useless for these regions. On the other hand, in this work the SWIR bands were not vicariously calibrated (i.e., default gain = 1.0 was used). When local data are used to adjust the vicarious gains of the SWIR band data, R_SWIR could be derived with much higher accuracy than shown here. However, as stated earlier, the goal of this paper was not to demonstrate how to improve atmospheric correction through local tuning, but to perform a trade study to show which existing reflectance products can be used for water applications, and at what levels of effort.

Table 2

Statistical Measures of Satellite-to-In Situ Reflectance Comparisons for Different Reflectance Products for Chesapeake Bay and Taihu Lake

	Products ^a	Band	RMSE (%)	MRE (%)	Mean ratio	Median ratio	R ²
C. Bay N=71	R_Land	469	484.5	273.0	3.13	2.29	0.00
		555	169.1	89.2	1.76	1.37	0.12
		645	181.6	106.5	1.59	1.25	0.28
		645/555	59.9	33.1	0.84	0.91	0.66
		469/555	297.5	121.8	1.04	1.57	0.07
	R_SWIR	469	193.3	126.3	1.12	1.06	0.12
		555	68.4	41.7	0.97	0.88	0.21
		645	157.8	97.7	0.70	0.67	0.26
		645/555	654.8	167.5	−0.36	0.80	0.16
		469/555	196.8	130.3	0.80	1.38	0.32
	R_NIR	469	104.8	74.3	1.00	0.95	0.42
		555	55.1	26.3	0.94	0.84	0.50
		645	70.2	44.5	0.94	0.79	0.52
		645/555	44.8	27.3	0.97	0.98	0.89
Taihu Lake N=102	R_Land	469	86.3	65.6	1.57	1.46	0.62
		555	78.9	64.8	1.28	1.36	0.16
		645	42.9	35.1	1.14	1.20	0.02
		859	43.3	36.1	1.15	1.21	0.12
		859	184.4	135.7	2.08	1.79	0.01
	R_SWIR	645/555	8.9	5.0	1.01	1.00	0.69
		859/645	166.5	88.6	1.68	1.42	0.00
		469/555	56.9	36.1	0.95	1.13	0.18
		469	112.7	66.3	0.77	0.66	0.31
		555	73.1	48.9	1.05	0.82	0.12
		645	71.5	41.2	1.10	0.86	0.05
		859	34.1	54.6	0.63	0.93	0.71
		645/555	21.2	15.2	1.11	1.03	0.68
		859/645	83.7	36.5	0.93	1.04	0.32
		469/555	65.0	44.7	0.60	0.70	0.06

Note. The data products sources are also listed.

^aR_Land products were obtained from https://lpdaac.usgs.gov/data_access; R_NIR products were obtained from <https://oceancolor.gsfc.nasa.gov/>; R_SWIR products were generated using the I2gen module of SeaDAS (version 7.3) using the SWIR-based atmospheric correction method, with MODIS Level-1A data obtained from <https://oceancolor.gsfc.nasa.gov/as> the I2gen inputs. In the SWIR-based atmospheric correction, vicarious calibration of the SWIR bands was not applied.

In terms of data availability, the most available reflectance products for all estuaries and inland waters are the R_Land products. A user can download and make direct use of these products without additional AC effort. Unfortunately, spatial patchiness can often be found in R_Land products, likely due to the use of 10×10 pixels (1 km pixel resolution) as a moving window to apply the AC algorithm. When large aerosol gradient occurs between two adjacent boxes or when aerosol retrieval fails in one box, patchiness tends to occur (Kaufman et al., 1997) (in contrast, the ocean-based AC treats each pixel independently, thus not suffering from such patchiness problems). This suggests that although R_Land is widely available for all water bodies, it is difficult to use the daily snapshot images.

4.2. Recommendations for R_Land Products for Water Applications

The above results showed that R_Land products are at least consistent with R_SWIR for both reflectance at 645 nm and for reflectance ratio of 645/555, in terms of their spatial and temporal patterns (not magnitude). The consistency was found on both daily and monthly scales for both highly turbid Taihu Lake and moderately turbid Chesapeake Bay. Further validations with in situ data also demonstrated acceptable accuracy in R_Land(645/555). Indeed, high correlations were observed not only on long-term monthly mean time series, but also on the associated monthly anomalies between R_Land and R_SWIR for both R_Land (645) and R_Land(645/555). Given the wide data availability, R_Land (645) and R_Land(645/555) appear to be applicable for water applications, for example, through estimating water turbidity or TSS.

For highly turbid waters such as those in Taihu Lake, R_Land(859) and R_Land(859/645) are also significantly correlated with R_SWIR(859) and R_SWIR(859/645), respectively. Additionally, R_Land(555)

Figure 11. R^2 between R_{Land} and R_{SWIR} for (a) 645 and (b) 645/555 when the data are gridded through different combinations of spatial and temporal bins.

and $R_{\text{SWIR}}(555)$ also agreed well for Chesapeake Bay. Thus, these R_{Land} products (i.e., 555, 859, and 859/645) may also be useful for water applications. However, without similar analysis and comparison with R_{SWIR} , it is hard to conclude for waters with unknown optical properties or water constituents.

To reduce the effect of random noise such as patchiness in the R_{Land} data products, spatial and/or temporal bins may be used in converting daily images at 250 m resolution to weekly or monthly means at coarser resolution. As shown in Figure 11, the coefficient of determination (i.e., R^2) as a function of temporal bin size and spatial bin size is plotted along the y axis. Each point represents the mean conditions of >100 randomly selected pixels in Taihu Lake. For brevity, the results for Taihu Lake are illustrated here, but results for Chesapeake Bay are very similar. Generally, daily R_{Land} data (both 645 and 645/555) showed much lower correlations with R_{SWIR} than temporally binned products, where their correlations increased monotonically with longer temporal bin size. For example, with a 15×15 pixel spatial bin, R^2 between $R_{\text{Land}}(645/555)$ and $R_{\text{SWIR}}(645/555)$ increased dramatically from <0.1 for daily data to 0.8 for 32 day bin.

Unlike temporal binning, the consistency between R_{Land} and R_{SWIR} for 645 and 645/555 appeared to be less sensitive to spatial bin size after a certain value. For example, for a temporal bin size of 20 days, R^2 between $R_{\text{Land}}(645/555)$ and $R_{\text{SWIR}}(645/555)$ appeared plateaued after the spatial bin size of 7×7 . The same can be said for a temporal bin size of 32 days. Thus, a combination of spatial (7×7 or 9×9) and temporal ($\sim$ monthly) bins is recommended for applying R_{Land} (645/555) to study turbidity changes. On the other hand, the consistency between $R_{\text{Land}}(645)$ and $R_{\text{SWIR}}(645)$ appeared to be independent to spatial bins. Thus, when $R_{\text{Land}}(645)$ data are to be

used to study water turbidity changes, only temporal binning is required. Interestingly, the requirement of spatial bin size of 7×7 pixels for $R_{\text{Land}}(645/555)$ provides a lower bound for estuarine or lake size assuming adjacency effect is negligible, which is about $250 \times 250 \times 7 \times 7 = 3.0625 \text{ km}^2$.

4.3. Relationships Between R_{Land} and R_{rc}

Although the effect of spatial patchiness in R_{Land} can be minimized through temporal/spatial data binning, such a binning will smear all short-term and small-scale features. Then, are there any reflectance products that can retain the fidelity of spatially/temporally binned R_{Land} products without patchiness and without losing the original temporal and spatial details in daily products?

Such reflectance products appear to be R_{rc} . It is obvious that the patchiness in the R_{Land} products was caused by residual errors in aerosol corrections, thus a product without aerosol correction at all (i.e., R_{rc}) should be able to avoid this problem. Indeed, this argument is confirmed by comparing R_{Land} (Figure 2) and R_{rc} (Figure 12) images from the same MODIS granule, as the only difference between the two products is the aerosol correction in R_{Land} . R_{rc} images not only demonstrated similar spatial patterns in both single-band and band-ratio products (except for 469/555), but also showed lower noisy without any patchiness, as compared with those of R_{Land} and R_{SWIR} . The relatively large aerosol contributions in the blue bands may have led to the noticeable difference in the band-ratio image of 469/555 between these products. Similar observations have been made for Taihu Lake, where R_{rc} images showed similar spatial patterns as in R_{Land} image but with much reduced noise and patchiness (see supporting information Figure S1).

The consistency between R_{rc} and R_{Land} can also be verified through x-y density plots. Figure 13 shows an example for MODIS data collected on 12 April 2012 over Chesapeake Bay, where the two data sets were highly correlated ($R^2 > 0.94$, $n = 100,905$). Likewise, similar correlations were also observed in other MODIS images for Chesapeake Bay and for Taihu Lake (see supporting information Figure S2), indicating that R_{rc} products are as

Figure 12. MODIS R_{rc} images on 12 April 2012 for Chesapeake Bay. Their corresponding R_{Land} , R_{SWIR} , and R_{NIR} data are shown in Figures 2 and 3, respectively.

effective as R_{Land} products for water applications. More importantly, no spatial or temporal binning is required for R_{rc} to avoid the patchiness noise in daily R_{Land} products. Indeed, R_{rc} data have been used successfully for water quality monitoring applications in many inland and coastal waters (Duan et al., 2014; Feng et al., 2014b; Markham et al., 2008; Zhang et al., 2016). However, unlike R_{Land} products (MYD09) that are available to all users from the NASA data center, R_{rc} products are generally not available and they require trained skills in low-level data processing, posing difficulties to general users. Notably, SeaDAS could also output a surface reflectance product (ρ_{rs}), where the values are very close to the 6S generated R_{rc} ; therefore, it is possible to derive R_{rc} using SeaDAS ρ_{rs} as a surrogate.

5. Summary and Conclusions

Given the various surface reflectance products that can be generated from MODIS measurements over estuaries and inland waters, a general user often faces the question of which products to use and at which level of effort. The uncertainties in these products may differ, and the effort required to obtain or generate them may also differ. To date, there has been a lack of comparison of these products in terms of their accuracy, consistency, and ease of use in the user's perspective. This study is meant to be the first step towards filling this knowledge gap to provide a general guide on the applicability of the various reflectance products in estuarine and inland water applications.

While R_{NIR} is designed for water applications and, when available, it is also shown to be more accurate than other products, it often suffers from signal saturation or false cloudmasking over highly turbid waters or atmospheres. Therefore, even if R_{NIR} products are readily available to all users for global oceans, they are generally not applicable for applications of estuarine and inland waters. This problem can be overcome by customized data processing from low-level MODIS data using the SWIR bands for atmospheric correction, leading to R_{SWIR} products. Yet the level of effort required in such a process is often beyond a user's capacity, making it impractical for most users. Likewise, R_{rc} data products are also useful for estuarine and inland water applications, but generating R_{rc} data products also requires significant amount of effort on the user end, as these products are generally not available.

In contrast, MODIS Aqua land surface reflectance products (MYD09 or R_{Land}) generated by the MODIS Land Team are readily available to all users, but the remaining question is whether they are applicable for water applications. Using a moderately turbid estuary (Chesapeake Bay) and highly turbid lake (Taihu Lake) as test cases, this study performed a thorough evaluation of R_{Land} in reference against R_{NIR} , R_{SWIR} , and R_{rc} at various spatial and temporal scales. R_{Land} products generally showed higher reflectance values than R_{SWIR} and R_{NIR} due to their different treatment of surface Fresnel reflectance and aerosol effects. Despite the difference in magnitude, spatial and temporal patterns derived from $R_{Land}(645)$ and $R_{Land}(645/555)$ agreed well with those from the R_{SWIR} and R_{NIR} (when available) products in both study regions. Limited field data also confirmed the fidelity of $R_{Land}(645)$ and $R_{Land}(645/555)$, and these two products appear applicable in water color applications.

In order to minimize the effect of patchiness in daily R_{Land} images, a sensitivity test was conducted through spatial and temporal binning with different bin sizes. It was found that a combination of spatial (7×7 pixels) and temporal (32 day) binning may provide gridded $R_{Land}(645/555)$ products with the highest fidelity, while only a 20 day temporal bin size was sufficient for the $R_{Land}(645)$ products without the need for spatial binning. Another important finding in this study is that R_{Land} was found to be highly consistent

Figure 13. Scatter plot between R_{rc} and R_{Land} for each MODIS land band using MODIS data collected from Chesapeake Bay on 12 April 2012. Color indicates density of matchups.

with R_{rc} indicating that R_{rc} products (either 645 or 654/555) can be used as effectively as R_{Land} products, with additional benefits of minimized image patchiness and noise. Unfortunately, similar to R_{SWIR} , R_{rc} products are also not available to most users, making R_{Land} products a first choice for most users.

It is noted that the study is focused on two regions only, and extending the findings to other regions may require caution unless other regions are similar in water's optical properties and atmospheric properties to those studied here. Furthermore, the SWIR bands used in the atmospheric correction were not vicariously calibrated, otherwise the accuracy of the R_{SWIR} products may be improved. Nevertheless, it is believed that the findings that $R_{Land}(645)$ and $R_{Land}(645/555)$ can be applied to study estuarine/inland waters have significant implications on global-wide water quality assessment and monitoring, especially for small inland water bodies. On the other hand, the study here does not devalue any effort to improve atmospheric correction over estuarine and inland waters, as most "standard" reflectance products still contain high uncertainties in the blue bands. Finally, freely available surface reflectance products from other satellite instruments (e.g., MODIS Terra, Sunomi NPP-VIIRS, and Landsat series sensors) are also directly accessible, and the methods of this study may be extendable to those data sets to examine their potential strengths and weakness in water applications.

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Erratum

In the originally published version of this article, author Lian Feng's second affiliation was listed without the "Now at." This has since been corrected to include "Now at" the School of Environmental Science and Engineering, Southern University of Science and Technology, Shenzhen, Guangdong, China. This version may be considered the authoritative version of record.