Remote estimation of chlorophyll-a in turbid inland waters: Three-band model versus GA-PLS model

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Accurate remote retrieval of chlorophyll-a (Chl-a) concentrations for inland and coastal turbid waters is a challenging task due to their optical complexity. An adaptive model was developed based on the merits of coupling a genetic algorithm to select spectral variables and partial least squares (GA-PLS) for regression. The objectives of this paper are: (1) to evaluate the GA-PLS model performance using datasets collected from 1140 stations encompassing a wide range of Chl-a and suspended sediment from nine water bodies across Central Indiana (CIN), USA, South Australia (SA), Taihu Lake (THL) in East China and Shitoukoumen Reservoir (STKR) in Northeast China with comparison to a widely accepted three-band model, and (2) to evaluate the GA-PLS spatial transferability with simulated ESA/Sentinel3/OLCI and Hyperion spectra. The GA-PLS and the three-band model yield accurate calibrations (Cal) for the SA dataset with R² above 0.98, and the corresponding validation (Val) shows relative root mean squared error (rRMSE) of less than 6.2% with narrow-band spectra. Both the GA-PLS and three-band model show stable performance for the CIN dataset (Cal: R² = 0.91 and 0.77; Val: rRMSE = 20.1% and 33.4%), THL dataset (Cal: R² = 0.91 and 0.88; Val: rRMSE = 30.1% and 33.7%), and STKR dataset (R² = 0.84 and 0.82; rRMSE = 29.1% and 33.2%). The results also reveal that simulated OLCI datasets degrade both the GA-PLS performance, and particularly the performance of the three-band model due to the coarser and discontinuous spectral configuration. Contrastingly, both the GA-PLS and the three-band model show improved results with the simulated Hyperion datasets. Our observation indicates that the GA-PLS model outperforms the three-band model in terms of spatial transferability; however, the three-band model has its own merits, considering its simplicity. Further analyses indicate that spectral measurement protocols, instrumentations, and inorganic suspended matter affect the GA-PLS and three-band model performances.

1. Introduction

Algal blooms are one of the most important issues concerning environmental agencies, water management authorities and public health organizations (Backer, 2002; Li et al., 2010; Wang et al., 2004). Particularly cyanobacterial blooms in surface water systems pose a health concern for humans, livestock, and native wildlife across the globe (Codd et al., 2005; Hunter et al., 2010). Despite increasing concern about algal blooms in lakes and reservoirs, water resource managers lack a reliable monitoring tool capable of providing information about the spatial distribution and composition of blooms (Duan et al., 2009; Simis et al., 2005; Vincent et al., 2004). Monitoring algal blooms in situ water sampling is time and labor intensive, and often limited to infrequent collections at a small number of stations within a lake or reservoir. Remote sensing has increasingly been used in water quality monitoring and management as a tool to supplement traditional field-based sampling methods (Gons, 1999; Gons et al., 2008; Li et al., 2010; Schaeffer et al., 2012; Vincent et al., 2004). This monitoring is commonly achieved through spectral quantification of chlorophyll-a (Chl-a) concentration, an indicator of the trophic condition of a freshwater body (Song et al., 2012a; Trevisan & Forsberg, 2007).

Morel and Gordon (1988) identified three different approaches to quantifying water quality parameters from remotely sensed data. The empirical (first) and semi-empirical (second) approaches are based on relationships between measured spectral quantities and water quality parameters (Gitelson, 1992; Gurlin et al., 2011). In the former approach, the relationships are established primarily through statistical regression without necessity of a clear bio-optical basis, while in the latter approach, the relationships are determined based on
spectral characteristics that are reasonably well understood (Gons, 1999; Simis et al., 2005). The third approach is the bio-optical approach based on the inherent optical properties (IOPs) and apparent optical properties (AOPs) of water constituents (Binding et al., 2008; Brando & Dekker, 2003; Gordon et al., 1975; Lee & Carder, 2004). Water constituents are expressed in their mass specific absorption and backscattering coefficients and related to the bulk IOPs (Kirk, 2003; Morel, 2001). Although bio-optical models are thought to be more stable and universal, the prerequisite of IOPs parameters hinders their wide application in water quality studies. The empirical or semi-empirical models are still widely utilized (Gitelson et al., 2008; Morel, 2001; Moses et al., 2012a; Simis et al., 2005) for estimating Chl-α.

Both empirical and semi-empirical models involve association of single bands, band combinations or band ratios with water quality constituents (Gitelson et al., 1993; Han & Rundquist, 1997; Odermatt et al., 2012). These models require that in-situ water quality data be taken concurrently with remote sensing data acquisition. Regression relationships in empirical and semi-empirical models can be linear, exponential or polynomial according to the concentration of various optically active constituents (OACs) (Gilerson et al., 2010; Yang et al., 2011). Linear semi-empirical models have been used to relate variables such as phytoplankton pigment concentration to field, airborne or satellite spectra (Kutser et al., 1998; Millie et al., 1992; Simis et al., 2005; Vincent et al., 2004; Zima & Gitelson, 2006). A few studies have used exponential or polynomial models to explain the relationship between water constituents and spectral reflectance (Mittenzwey et al., 1992; Odermatt et al., 2012; Schalles & Yacobi, 2000). Another technique used to increase the success of an empirical or semi-empirical model is to transform the data when the model is developed, like the log transformations of water constituents and spectral variables (Fraser, 1998; Kallio et al., 2001; Rundquist et al., 1996). Currently derivative and band ratio are the most commonly used spectral variables in empirical and semi-empirical models (Chen et al., 1992; Han, 2005; Han & Rundquist, 1997).

Quibell (1991) investigated the additive effect of sediments on the upwelling radiance of pure algal cultures and found that the addition of particulates increased reflectance at wavelengths longer than 550 nm. However, Chen et al. (1992) suggested that the first derivative could be used to reduce the water–sediment–chlorophyll composite signal, and suspended-sediment effects can be removed by a second-order derivative analysis. This conclusion is supported by later investigations by Goodin et al. (1993) and Han (2005). Han and Rundquist (1997) also conducted a study to examine the spectral response of algal chlorophyll with varying suspended sediment concentrations in a controlled experiment, and found that the additive effects of suspended sediment on reflectance between 400 and 900 nm causes uncertainty on estimated Chl-α concentration (Gitelson et al., 2008; Yang et al., 2011). Further work indicated that the commonly used NIR/red ratio performed best for relatively low Chl-α concentration, and the first derivative of reflectance at around 690 nm was best for relatively high Chl-α concentration (Rundquist et al., 1996).

A variety of band ratio algorithms have been developed for retrieval of algal pigments in turbid waters. All are based on the properties of the reflectance peak near 700 nm (Gitelson, 1992; Gitelson et al., 2008; Han & Rundquist, 1997; Odermatt et al., 2012), or the ratio of that reflectance peak to the reflectance at or near 670 nm, the red Chl-α absorption band (Han & Rundquist, 1997). Gons et al. (2008) used the ratio of reflectance at 704 nm and 672 nm and the absorption and backscattering coefficient at these wavelengths to assess a wide range of Chl-α concentration. More recently, a three-band tuning model has been developed by Dall’Olmo et al. (2003) and Dall’Olmo and Gitelson (2005) with in situ collected remote sensing reflectance just below the water surface. This model has been validated with datasets collected from various turbid productive inland waters showing relatively good stability and transferability (Gitelson et al., 2007, 2008, 2009; Moses et al., 2012a). The developed algorithm was also tested with data collected over Lake Taihu (Sun et al., 2009) and Shitoukoumen Reservoir located in Northeast China (Song et al., 2012b; Xu et al., 2009). However, these tests demonstrated varied performances of the three-band model, implying a large and comprehensive dataset is needed to further validate the effectiveness of the three-band model (TBM).

As an attempt to overcome the limitation of empirical algorithms based on band ratios or derivative analysis for the non-linearity between Chl-α and water leaving radiance, different investigators applied neural networks (NN), genetic algorithms (GA) or support vector machines (SVM) to develop water quality algorithms for pigment concentration retrieval (Gross et al., 2000; Keiner & Yan, 1998; Sun et al., 2009; Zhan et al., 2003; Zhang et al., 2002). These heuristic algorithms can partially overcome some nonlinear relationships among various OACs, and can be divided into two categories according to their optimization features. The first is local optimization methods (Zhang et al., 2002), and the second is global optimization methods. The genetic algorithm (GA) is a global optimization method for solving variable subset selection problems (Gouveinec et al., 2004). Partial least square (PLS) regression is a standard multivariate regression method developed by Herman Wold (1966). The combination of GA and PLS has proven to be an effective approach for the estimation of vegetation biochemical constituents and soil properties (Farifeth et al., 2007; Li et al., 2007), and the potential application for water quality quantification has been tested (Song et al., 2012a, 2012b).

The model spatial transferability is a challenge for the remote sensing community though many efforts have been taken to solve this problem (D’Alimonte et al., 2003; Gitelson et al., 2008; Vincent et al., 2004). Since the TBM has been shown to be more stable and effective in turbid productive inland waters (Gitelson et al., 2008, 2009; Sun et al., 2009; Xu et al., 2009), the spatial transferability of the GA-PLS model will be compared with the TBM using various datasets. This is achieved by investigating the performance of the GA-PLS and the TBM for estimating Chl-α from remote sensing reflectance (Rrs) measured for optically complex and productive case-II waters located in the Midwest of USA, South Australia, and East and Northeast China. Additionally, remote sensing reflectance data used in this study include in situ spectra of inland water bodies measured in different seasons and with three different procedures. This provides an opportunity for testing the transferability of the GA-PLS and the TBM, and examining the influence of remote sensing reflectance data collection procedure on model accuracy.

2. Materials

2.1. Study area and datasets

Four independent datasets from nine water bodies were used to calibrate and validate the GA-PLS and TBM. The first dataset containing 713 samples was collected in 43 field surveys from 2005 to 2010 in four water supply reservoirs in Central Indiana, USA (CIN). Detailed information on the four reservoirs, i.e., Eagle Creek Reservoir (ECR), Morse Reservoir (MR) and Geist Reservoir (GR), Monroe Reservoir (MOR) can be found in Randolph et al. (2008) and Song et al. (2012a). The second dataset was collected in three water supply sources for Adelaide in South Australia (SA), i.e., the Myponga Reservoir (MPR: 35°24′S 139°27′E), the Murray River at Mannum (MMR: 34°44′55.11″S, 139°19′33.22″E) and at Wellington (MRW: 35°23′27.21″S, 139°27′33.11″E), respectively. Sixty samples were collected during six field trips from February to March 2009 (Table 1). The third dataset was collected in Taihu Lake (THL: 120°10′27.21″E, 31°10′45.24″N), which is the largest freshwater lake in East China with an average storage capacity of 4.76 × 1010 m³. From this water body 105 samples were collected during two field
surveys conducted in 2008 and 2010. The optical properties and water quality characteristics for THL can be found in Ma et al. (2006) and Le et al. (2009). The selection of the optimal number of PLS components is a key step to obtaining a model with good predictive capability. Leave-one-out cross validation was applied in this study to determine numbers of PLS components and a PLS model was built using N−1 samples, and the abundance of the sample left out was then predicted. The prediction error sum of squares (PRESS, see Eq. 1) was used to derive the root-mean-square error of cross-validation (RMSECV, see Eq. 2), a measure for determining the optimal number of PLS components.

\[
PRESS = \sum_{i=1}^{N} (y'_i - y_i)^2
\]

(1)

\[
RMSECV = \sqrt{\frac{PRESS}{N}}
\]

(2)

where \(y'_i\) is the predicted value for the sample \(i\), \(y_i\) is measured concentration of the sample \(i\), and \(n\) is the number of components used in a PLS model.

3. Retrieval algorithms

3.1. GA-PLS model

3.1.1. GA-PLS description

The genetic algorithm (GA) applied in this study includes five components: encoding, population initialization, individual selection, crossover, and mutation (Li et al., 2007). Input spectral variables were encoded into binary data: zeros and ones as chromosomes (see Fig. 1 in Song et al., 2012b). A detailed description on GA applied in this study can be found in Li et al. (2007) and Song et al. (2012b). A subset of bands sensitive to Chl-a concentration were determined and further processed by PLS for regression.

A simple PLS model consists of two outer relations and one inner relation (see Fig. 1 in Song et al., 2012b). Let \(X [n \times m]\) represent an explanatory matrix, the first outer relation is derived by applying principal component analysis (PCA) to \(X\), resulting in the score matrix \(T [n \times a]\) and the loading matrix \(P [a \times m]\), and an error matrix \(E [n \times m]\), i.e., \(X = TP + E\), where \(a\) is the number of latent variables accounting for a response variable matrix can be derived by decomposing \(Y\) into the score matrix \(U [n \times a]\), the loading matrix \(Q [a \times p]\), and the error term \(F [n \times p]\), i.e., \(Y = UQ + F\). The inner relation \(U = BT\) is a multiple linear regression between the score matrix \(U\) and \(T\), in which \(B\) is an \(n \times n\) regression coefficient matrix determined via least square minimization (Geladi & Kowalski, 1986). The goal of the PLS model is to minimize the norm of \(F\) while maximizing the covariance between \(X\) and \(Y\) by the inner relation. In this study, both GA and PLS were combined to optimize the spectral variables and cross-validate the model output (Song et al., 2012b).

The selection of the optimal number of PLS components is a key step to obtaining a model with good predictive capability. Leave-one-out cross validation was applied in this study to determine numbers of PLS components and a PLS model was built using \(N−1\) samples, and the abundance of the sample left out was then predicted. The prediction error sum of squares (PRESS, see Eq. 1) was used to derive the root-mean-square error of cross-validation (RMSECV, see Eq. 2), a measure for determining the optimal number of PLS components.

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\]

(1)

\[
RMSECV = \sqrt{\frac{PRESS}{N}}
\]

(2)

where \(y'_i\) is the predicted value for the sample \(i\), \(y_i\) is measured concentration of the sample \(i\), and \(N\) is the number of components used in a PLS model.

3.2. Laboratory measurements

For the CIN samples, Chl-a was extracted in 90% buffered acetone and its concentration determined fluorometrically with a TD-700 Fluorometer (Turner Designs, Inc., Sunnyvale, CA) following EPA Method 445.0 (EPA, 1997). All steps in the Chl-a extraction processes were performed under subdued light conditions, and details can be found in Randolph et al. (2008). Total suspended matter (TSM), organic and inorganic suspended matters were determined gravimetrically (Song et al., 2012a). The samples from another three datasets were extracted for Chl-a using 90% acetone and measured with a Shimadzu UV2401 spectrophotometer (Shimadzu, Inc., Tokyo, Japan). The procedure was detailed in Song et al. (2012b).

2.2. In situ data collection

2.2.1. Water quality data

Coordinates for water sample stations were recorded using a global positional system (GPS); water clarity was measured as Secchi disk depth (SDD); turbidity was determined using YSI 600XLM-SV multi-parameter probes (YSI, Yellow Springs, Ohio, USA) positioned 25 cm below the water surface. Surface water grab samples were collected at each location at approximately 0.5 m below the water surface. Simultaneously, spectra were collected in the way that will be detailed in the next section.

2.2.2. Spectral measurement

Two instruments and four spectral measurement protocols were applied for various field surveys. The spectral datasets for SA and CIN 2007, 2008 and 2010 were collected using two inter-calibrated Ocean Optics USB4000 spectrometers, following the above and below water spectral measurement procedures introduced by Gitelson et al. (2008). Details on the spectral measurement procedure can be found in Song et al. (2012a). Reflectance spectral datasets are labeled as OO-AW for the spectra measured using the above water procedure, and as OO-BW for the spectra measured using the below water procedure.

In situ spectral datasets for CIN 2005 and 2006 were collected using an ASD FieldSpec visible and near-infrared (VNIR) (ASD, Inc., Boulder, CO) recording continuous radiance from 348 nm to 1074 nm with 1 nm increment, following an above water surface spectral measurement procedure. Details on spectral measurement and instrumentation can be found in Randolph et al. (2008) and Li et al. (2010). We refer to the spectra measured under this procedure as ASD-AW.

The spectral datasets for STKR in Northeast China and THL in East China were collected with an ASD spectrometer following the procedure described in Mobley (1999), which has been suggested by International Ocean Color Coordinate Group (IOCCG). The detailed information on spectral measurement and instrumentation for STKR can be found in both Xu et al. (2009) and Song et al. (2012a), and for THL in Ma et al. (2006). We refer to reflectance spectra measured under this standard procedure as ASD-ST.

Table 1

<table>
<thead>
<tr>
<th>Regions</th>
<th>Year</th>
<th>Waters</th>
<th>Spectra</th>
<th>Chl-a</th>
<th>TSM</th>
<th>ISM</th>
<th>SDD</th>
<th>Surveys (N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SA</td>
<td>2009</td>
<td>MPR</td>
<td>24</td>
<td>24</td>
<td>24</td>
<td>2</td>
<td>24</td>
<td>2</td>
</tr>
<tr>
<td>EC</td>
<td>2008, 2010</td>
<td>THL</td>
<td>105</td>
<td>105</td>
<td>105</td>
<td>105</td>
<td>2</td>
<td>2</td>
</tr>
<tr>
<td>NEC</td>
<td>2006–2009</td>
<td>STKR</td>
<td>262</td>
<td>262</td>
<td>262</td>
<td>262</td>
<td>14</td>
<td>14</td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td>1140</td>
<td>1140</td>
<td>1029</td>
<td>730</td>
<td>1139</td>
<td>67</td>
</tr>
</tbody>
</table>

Notes: CIN, four reservoirs (MR, Mores Reservoir; GR, Geist Reservoir; EC, Eagle Creek Reservoir; MOR, Monroe Reservoir); MRW, Murray River at Wellington Point; MRM, Murray River at Mannum; SA, three water supply sources (MPR, Myponga Reservoir; MRW, Murray River at Wellington Point; MRM, Murray River at Mannum); THL, Taihu Lake in East China (EC), and STKR, Shitoukoumen Reservoir in Northeast China (NEC).
3.1.2. GA-PLS implementation

Correlation coefficients between Chl-α concentration and original spectral data, band ratios, and reflectance derivative were calculated to select the diagnostic spectral variables. In this study, 100 spectral variables, including 50 band ratios, 30 derivatives and 20 narrowband reflectance values highly correlated with Chl-α concentration were processed by GA for PLS modeling. The major risk of using PLS is over fitting because of too many latent variables (i.e., spectral variables). To minimize this risk, three criteria were applied in the program, which are detailed in Li et al. (2007). A moving average (window size 3) was applied to the frequency of selection for the variables to take into account of high spectral correlation and to assure that the highly correlated spectral bands are selected together. The fitness function with which the individuals are subjected to evaluation is the percentage of predicted variance of a constituent abundance, defined as:

$$100 - \left\{ \frac{1}{n} \sum_{i=1}^{n} \left( \frac{y_i - \bar{y}^i}{\sigma_y} \right)^2 / \left[ \frac{1}{n} \sum_{i=1}^{n} \left( \frac{y_i - \bar{y}}{\sigma_y} \right)^2 / \sigma_y \right] \right\} \times 100$$ (3)

where $n$ is the number of samples to be considered, $k = n - 1$ in the case of cross-validation. The result of GA-PLS modeling is evaluated based on the root mean square error in the dataset (RMSE), which is written as:

$$\text{RMSE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (y_i - \hat{y}_i)^2}$$ (4)

where $N$, where $y_i$ and $\hat{y}_i$ have the same notation as detailed above.

3.2. Three-band model

Based on the bio-optical model (Gordon et al., 1975) and Chl-α absorption feature in the red and NIR region, the TBM using NIR and red spectral bands, was developed by Dall’Olmo and Gitelson (2005) and Gitelson et al. (2008) for retrieval of Chl-α in turbid, productive waters. The NIR-red three-band algorithm is formulated as (Gitelson et al., 2008):

$$\text{Chl-α} \times 100 = R(\lambda_1) - R(\lambda_2)$$ (5)

The effectiveness of the TBM has been proven for a variety of waters using in situ collected spectra (Gilersen et al., 2010; Gitelson et al., 2008; Sun et al., 2009; Xu et al., 2009), and MERIS or MODIS image data (Moses et al., 2012a; Yang et al., 2011). The selection of an optimal band has been detailed in several papers (Dall’Olmo & Gitelson, 2005; Gitelson et al., 2008; Xu et al., 2009).

3.3. Data processing

3.3.1. Spectra preprocessing

The pre-determined 100 spectral variables for GA-PLS are normalized to the $[-1, 1]$ range to obtain similar numerical weights for data with various magnitudes through the following equation:

$$x_{i,j} = \left[ x_{i,j} - \bar{x}_{i,j} \right] / \sigma_j$$ (6)

where $x_{i,j}$ and $\sigma_j$ are the mean and standard deviation of $x_{i,j}$ values, respectively, for the $j$th dimension. To further evaluate the model performances, reflectance spectra in accordance to space-borne ESA/Sentinel3/OLCI and EO-1/Hyperion spectral band configurations were also simulated from the in situ spectral datasets. Spectra simulation was implemented in ENVI 4.7 (ITT, Inc., Boulder, CO) using the in situ spectral datasets. All the spectral data were imported into ENVI for building a spectral library, and then the Spectral Resampling Parameters module was applied to resample spectra into OLCI and Hyperion spectral configuration through predefined spectral central band positions.

3.3.2. Datasets grouping methods

In this study, one half of the samples from a grouped datasets were used for calibrating the GA-PLS model and the other half for validating, which was accomplished by selecting every other sample. In accordance with research objectives, two sample grouping methods were applied to test performance stability of various models. (1) PRIMARY analysis: various datasets were divided into two groups, furthermore the influence of in situ spectral data collection procedures was tested in this section; (2) spatial transferability analysis: for an in-depth comparison, three datasets were used for the GA-PLS and TBM calibration, and the remaining dataset was used for model validations.

3.4. Model evaluation

Root mean square error (RMSE), relative RMSE (rRMSE), and mean absolute errors (MAE) were selected as indices for the evaluation of model accuracy. The rRMSE and MAE are written as:

$$r\text{RMSE} = 100 \times \frac{\text{RMSE}}{\bar{y}}$$ (7)

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^{N} |y_i - \hat{y}_i|$$ (8)

where $N$ is the number of samples in the dataset, and $\bar{y}$ denote the mean of the measured value. The coefficient of determination ($R^2$) and the ratio of prediction to deviation (RPD) were also used for the evaluation of model performances (Miehle et al., 2006). The detailed definition and description of these two parameters can be found in Cacuci (2003). As $R^2$ is a very commonly used parameter, its mathematical expression will not be repeated here, and the formula for RPD is written as:

$$\text{RPD} = \frac{\text{SDP}}{\left( \frac{1}{N} \sum (y_i - \bar{y})^2 - \frac{1}{N} \left( \left[ \frac{\left( \bar{y} - y \right)^2}{N} \right] / (N-1) \right) \right)^{1/2}}$$ (9a)

where $\text{SDP}$ is determined by the follow equation:

$$\text{SDP} = \left[ \frac{\sum y_i^2 - \left( \bar{y}^2 / N \right) / (N-1) \right]^{1/2}$$ (9b)

The percent difference between predicted and measured Chl-α was also calculated:

$$\text{RE} = \frac{|\hat{y}_i - y_i|}{y_i} \times 100$$ (10)

where $\text{RE}$ denotes the relative error for estimating Chl-α concentration. According to Williams (2001), a model is accurate if $R^2$ and RPD values are higher than 0.91 and 2.5; and can be regarded as good when $R^2$ ranges 0.82–0.9 with an RPD higher than 2. If the $R^2$ lies between 0.66 and 0.81 with RPD higher than 1.5, the model is considered to be an approximate prediction, while it is generally regarded as a poor prediction when the $R^2$ ranges from 0.5 to 0.65.
4. Results

4.1. Water quality characteristics

The dataset includes a large diversity of inland waters with varying OACs. The four reservoirs in CIN exhibit high Chl-a concentrations (range: 2.8 to 285.5 μg/L; average: 59.42 μg/L). The same is observed in THL from East China (range: 0.46 to 97.2 μg/L; average: 28.2 μg/L). Both exhibit waters with a greenish color due to high algae concentrations suspended in the water column. In contrast, the STKR has low Chl-a concentration (average: 13.8 μg/L), while waters in SA have medium Chl-a concentrations (19.1 μg/L), in which MRM and MRW, respectively, show average Chl-a of 26.7, 19.1 μg/L; while MPR exhibits lower averaged Chl-a concentration of 8.32 μg/L (see Table 2).

The suspended sediment in four reservoirs from CIN and THL from East China are relatively low and dominated by phytoplankton, TSM concentration ranges from 1.6 mg/L to 81.4 mg/L with an average of 21.8 mg/L. The water in the MPR from SA is more transparent with low suspended sediment. The sampling stations from Murray River, East China are relatively low and dominated by phytoplankton, TSM concentration ranges from 1.6 mg/L to 81.4 mg/L with an average of 21.8 mg/L. The water in the MPR from SA is more transparent with low suspended sediment. The sampling stations from Murray River, i.e., MRM and MRW, have a grayish yellow color with higher suspended sediment compared to MPR. The water is highly turbid due to the relatively low total suspended matter (Fig. 2 and Table 2).

Table 2

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Parameter</th>
<th>Mean</th>
<th>Median</th>
<th>Min</th>
<th>Max</th>
<th>SD</th>
<th>CV</th>
<th>N</th>
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</thead>
<tbody>
<tr>
<td>CIN</td>
<td>SDD (cm)</td>
<td>63.2</td>
<td>60</td>
<td>24</td>
<td>150</td>
<td>24</td>
<td>0.39</td>
<td>302</td>
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<td>05-06</td>
<td>TSM (μg/L)</td>
<td>17.2</td>
<td>15.6</td>
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<td>54.4</td>
<td>8.8</td>
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<tr>
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<td>56.0</td>
<td>2.2</td>
<td>182.6</td>
<td>28.5</td>
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<td>07-08-10</td>
<td>SDD (cm)</td>
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<td>51.7</td>
<td>31</td>
<td>124</td>
<td>21.3</td>
<td>0.36</td>
<td>408</td>
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<tr>
<td>CIN</td>
<td>TSM (μg/L)</td>
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<td>17.7</td>
<td>3.4</td>
<td>81.4</td>
<td>7.8</td>
<td>0.43</td>
<td>408</td>
</tr>
<tr>
<td>CIN</td>
<td>ISM (μg/L)</td>
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<td>14.6</td>
<td>2.2</td>
<td>71.3</td>
<td>6.4</td>
<td>0.42</td>
<td>303</td>
</tr>
<tr>
<td>CIN</td>
<td>Chl-a (μg/L)</td>
<td>57.6</td>
<td>43.8</td>
<td>0.2</td>
<td>285.5</td>
<td>45.2</td>
<td>0.78</td>
<td>408</td>
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<tr>
<td>CIN</td>
<td>ISM: Chl-a</td>
<td>0.47</td>
<td>0.37</td>
<td>0.27</td>
<td>2.65</td>
<td>0.88</td>
<td>1.37</td>
<td>303</td>
</tr>
<tr>
<td>SA</td>
<td>SDD (cm)</td>
<td>89.6</td>
<td>83</td>
<td>20</td>
<td>271</td>
<td>76.8</td>
<td>0.87</td>
<td>60</td>
</tr>
<tr>
<td>CIN</td>
<td>TSM (μg/L)</td>
<td>17.6</td>
<td>16.4</td>
<td>2.0</td>
<td>94.1</td>
<td>17.4</td>
<td>0.99</td>
<td>60</td>
</tr>
<tr>
<td>CIN</td>
<td>ISM (μg/L)</td>
<td>14.1</td>
<td>13.7</td>
<td>1.6</td>
<td>78.3</td>
<td>17.4</td>
<td>1.23</td>
<td>60</td>
</tr>
<tr>
<td>CIN</td>
<td>Chl-a (μg/L)</td>
<td>19.1</td>
<td>17.2</td>
<td>6.3</td>
<td>75.3</td>
<td>13.5</td>
<td>0.71</td>
<td>60</td>
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<tr>
<td>CIN</td>
<td>ISM: Chl-a</td>
<td>1.21</td>
<td>1.41</td>
<td>0.52</td>
<td>4.21</td>
<td>1.62</td>
<td>1.35</td>
<td>60</td>
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<tr>
<td>THL</td>
<td>SDD (cm)</td>
<td>52</td>
<td>45</td>
<td>12</td>
<td>180</td>
<td>32</td>
<td>0.62</td>
<td>105</td>
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<tr>
<td>CIN</td>
<td>TSM (μg/L)</td>
<td>28.4</td>
<td>25.1</td>
<td>1.6</td>
<td>68.1</td>
<td>23.7</td>
<td>0.83</td>
<td>105</td>
</tr>
<tr>
<td>CIN</td>
<td>ISM (μg/L)</td>
<td>17.3</td>
<td>16.1</td>
<td>0.5</td>
<td>51.1</td>
<td>14.5</td>
<td>0.84</td>
<td>105</td>
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<tr>
<td>CIN</td>
<td>Chl-a (μg/L)</td>
<td>28.8</td>
<td>27.9</td>
<td>0.5</td>
<td>97.2</td>
<td>27.9</td>
<td>0.97</td>
<td>105</td>
</tr>
<tr>
<td>CIN</td>
<td>ISM: Chl-a</td>
<td>0.99</td>
<td>1.61</td>
<td>0.37</td>
<td>3.41</td>
<td>1.13</td>
<td>1.14</td>
<td>105</td>
</tr>
<tr>
<td>STKR</td>
<td>SDD (cm)</td>
<td>38</td>
<td>23.7</td>
<td>5</td>
<td>120</td>
<td>61.3</td>
<td>1.61</td>
<td>262</td>
</tr>
<tr>
<td>CIN</td>
<td>TSM (μg/L)</td>
<td>58.8</td>
<td>54.7</td>
<td>3.7</td>
<td>225.2</td>
<td>54.7</td>
<td>0.93</td>
<td>262</td>
</tr>
<tr>
<td>CIN</td>
<td>ISM (μg/L)</td>
<td>47.3</td>
<td>42.6</td>
<td>2.1</td>
<td>187.7</td>
<td>44.6</td>
<td>0.94</td>
<td>262</td>
</tr>
<tr>
<td>CIN</td>
<td>Chl-a (μg/L)</td>
<td>13.8</td>
<td>10.6</td>
<td>0.5</td>
<td>47.5</td>
<td>10.6</td>
<td>0.77</td>
<td>262</td>
</tr>
<tr>
<td>CIN</td>
<td>ISM: Chl-a</td>
<td>4.31</td>
<td>2.91</td>
<td>3.21</td>
<td>7.14</td>
<td>2.13</td>
<td>0.49</td>
<td>262</td>
</tr>
</tbody>
</table>

4.2. Remote sensing reflectance

All the reflectance spectra of four datasets and their corresponding coefficient of variation (CV) are shown in Fig. 2. Reflectance spectra show an absorption trough and reflective peak in the red spectral region (600–700 nm), which provide essential information for algal pigment monitoring in turbid inland waters. All the water bodies except STKR show a trough at 625 nm caused by strong phycocyanin absorption (Dekker et al., 1991; Li et al., 2010; Simis et al., 2005), demonstrating the existence of cyanobacteria in these inland waters. The second absorption trough at about 675 nm is related to strong Chl-a absorption in the red band (Han & Rundquist, 1997). In contrast, the reflectance trough for STKR is not pronounced for most of samples. A strong reflective peak around 690–700 nm is related to the interaction of algal-cell scattering and a combined effect of pigment and water absorption (Gitelson, 1992; Gitelson et al., 2008; Han & Rundquist, 1997; Rundquist et al., 1996; Yang et al., 2011). The magnitude of the peak varied widely, but with various patterns due to the concentration of Chl-a and tripton (Fig. 2a-c vs. Fig. 2d), which illustrates that backscattering by non-algal suspended matter exerts a critical role and predominantly controls the reflectance pattern in this spectral region.

All the reflectance spectra drop quickly from 700 nm to 740 nm, and flatten out between 740–790 nm. In the spectral region 700–790 nm, the reflectance is mostly controlled by the scattering from all particulate matter (Glierson et al., 2010; Gitelson et al., 2008; Yacobi et al., 2011). Large variation in the NIR spectra suggests significant variability of TSM in the water bodies as confirmed by the data presented in Table 2 and Fig. 2d. Spectral features beyond 800 nm are not discussed in detail due to their limited spectral information for estimating Chl-a. Our investigation indicates that reflectance magnitude is low for water bodies from CIN, the MPR from SA, and THL from East China due to the relatively low total suspended matter (Fig. 2 and Table 2). Furthermore, the above-water Rs spectra are noisier than the below-water measurements, particularly at wavelengths beyond 700 nm (see the supplementary Fig. s1), and smoother spectra were obtained through ASD spectrometer than that from Ocean Optics USB 4000 spectrometer (see supplementary Fig. s1a and c), indicating that ASD spectrometer might perform slightly better than Ocean Optics spectrometer.

4.3. All band ratio analysis

2-D correlograms were generated by sequential regression of all possible reflectance ratios (250,000) in the spectral range of 400–900 nm against Chl-a concentration (Fig. 4). Several “hot spots” indicate relatively broad regions of high correlation coefficient (R) between band ratio and Chl-a concentration. Apparently, the R values vary across different datasets, ranging from 0.85 (CIN) to 0.99 (SA). It can be seen that the best performing band combinations are located in the red and NIR spectral domain (range of 650–720 nm) for Chl-a, which is consistent with the band ratio analysis for empirical models (Dall’Olmo & Gitelson, 2005; Gitelson, 1992; Han & Rundquist, 1997; Yacobi et al., 2011). The relatively low R value for CIN is mainly due to the large variation of dataset collection conditions: 45 surveys in five years, two instruments and procedures for spectra measurement. Also, it is worth noting that the STKR dataset shows a narrow window with higher R values (Fig. 3d), implying only very limited spectral windows are effective for estimating Chl-a based on band ratio. These sensitive band ratios are also determined for GA-PLS modeling as detailed above.

4.4. Model performance with original spectra

4.4.1. Three-band model calibration

The TBM (Eq. 5) tuning resulted in three bands: λ1 = 665 nm, λ2 = 704 nm, and λ3 = 793 nm for the CIN dataset and a strong
linear relationship ($R^2 = 0.77$) for Chl-a estimates (Fig. 4a). The same optimization for the SA dataset gave rise to three bands $\lambda_1 = 677$ nm, $\lambda_2 = 698$ nm, and $\lambda_3 = 721$ nm (Fig. 4b) and yielded a nearly perfect linear relationship ($R^2 = 0.99$). For the THL dataset, the final three bands are respectively $\lambda_1 = 667$ nm, $\lambda_2 = 696$ nm, and $\lambda_3 = 721$ nm, with $R^2 = 0.88$ (Fig. 4c). In spite of high TSM concentration, the final three-band index for STKR (respectively $\lambda_1 = 672$ nm, $\lambda_2 = 689$ nm, and $\lambda_3 = 716$ nm) shows a strong linear relationship ($R^2 = 0.82$) with Chl-a concentration (Fig. 4d). Note that the first band, $\lambda_1$, for the water bodies CIN and THL is quite close; the coefficients for calibration models also show close values (see Fig. 4a and c). Similarly, band positions for SA and STKR are close due to the similar occurrence of high suspended matter, and much lower slope value for the regression models (see Fig. 4b and d). The final three-band positions for the aggregated dataset are shown in Table 3, and the corresponding TBM yielded a calibration result with $R^2 = 0.79$, which is considered to be acceptable given the large dataset measured with various instruments and procedures across different water bodies bearing varying OACs.
Fig. 3. Correlation analysis between all band ratios vs. Chl-a concentration for each study region, (a) the CIN dataset; (b) the SA dataset; (c) the THL dataset; and (d) the STKR dataset.

Fig. 4. Three-band algorithms calibration with the four datasets, (a) CIN dataset; (b) SA dataset; (c) THL dataset; and (d) STKR dataset.
4.4.2. Three-band model validation

The results for TBM validation with each dataset are illustrated in Fig. 5(a–d). It can be seen from Fig. 5a that the TBM with the CIN dataset yielded low RMSE (19.14 μg/L) and MAE (13.7 μg/L) considerably larger concentration range in the dataset (0.3–285.5 μg/L), but obviously underestimated Chl-a concentration as indicated by the slope 0.77 and the larger intercept value 14.3. As expected, the model performed well for the SA dataset with a low RMSE (1.21 μg/L) and MAE (0.91 μg/L), and validated samples are evenly distributed along 1:1 line. The TBM with both the THL and STKR datasets achieved low RMSE and MAE values (Fig. 5c–d) with slope values close to unity (0.93 and 0.89, respectively). The TBM is considered to show comparable performances with the CIN, THL and STKR datasets with respect to the resultant rRMSE values (33.4°, 33.7° and 33.2° μg/L, respectively).

As mentioned above, the CIN datasets for 2005 and 2006 were collected utilizing the ASD-AW procedure, while the dataset for 2007, 2008, and 2010 was collected utilizing the OO-BW procedure, which may impact model accuracy. The TBM calibration results for these two datasets are shown in Table 3, and indicate some variation in both three-band indices and regression coefficients. The TBM calibration and validation for the CIN05-06 dataset are shown Fig. 5e. Compared with Fig. 5a, the calibrated and validated samples are more evenly distributed along 1:1 line. Further, no obvious underestimation is observed for the TBM with the aggregated CIN05-06 dataset. Similarly, the TBM performed even better for the aggregated CIN07-08-10 dataset (Fig. 5f), which is most likely due to the fact that the OO-BW spectral measurement procedure effectively avoids the effects of water-air interface interaction and the wind speed on the reflected spectral signal (Morel & Gentili, 1993).

4.4.3. GA-PLS calibration and validation

The results from GA-PLS calibration with the various datasets are summarized in Table 4. It can be seen that the GA-PLS model performed marginally better as indicated by the R² and RPD values (Table 4). Compared with the TBM for the CIN dataset, GA-PLS yielded lower RMSE (12.01 vs. 19.1 μg/L), MAE (7.6 vs. 13.7 μg/L), and rRMSE (20.13 vs. 33.4%). It is also worth noting that GA-PLS shows no obvious underestimation for Chl-a concentration with a slope value close to unity and intercept value close to zero. As shown in Fig. 6b, both the GA-PLS and TBM models reveal comparable prediction for the SA dataset based on their RMSE (1.17 μg/L vs. 1.21 μg/L), MAE (0.90 μg/L vs. 0.91 μg/L) and rRMSE values (5.9 μg/L vs. 6.1%). According to William’s criteria (2001), both models achieved accurate performance (Fig. 5b vs Fig. 6b). According to Eqs. (9a) and (9b), a very small denominator for Eq. (9a) was achieved for the SA data set, thus a high RPD value was obtained. It can be observed that GA-PLS with the THL and STKR datasets marginally outperformed TBM with the former showing smaller RMSE, MAE and rRMSE values than the latter. The slope and intercept values for THL and STKR also support this conclusion (Figs. 5c-d and 6c-d).

4.5. Model performance with simulated spectra

4.5.1. TBM calibration

The simulated OLCI spectral band 7 (665 nm), band 9 (708 nm) and band 10 (753 nm) were plugged into Eq. (5), resulting in regression equations and the coefficients of determination for various datasets (Fig. 7a–d, Table 3). Compared with the results for the TBM using the original spectra (Fig. 4), the calibration accuracy was more or less degraded for each dataset; the model accuracy for STKR was significantly decreased, but shows no obvious degradation for the SA dataset. It can be observed that the band positions and equations for the simulated OLCI (Fig. 7a–d) and original spectral datasets (Fig. 4a–d) show some similarity to the equation form and R² for the CIN dataset, but with large discrepancy for the other datasets. It is also worth noting that better performance for TBM with reflectance spectra from OO-BW was confirmed by the simulated OLCI spectra for both CIN05-06 and CIN07-08-10 datasets (see supplementary Fig. s2).

Similarly, the simulated Hyperion spectral bands 28 (671 nm), 30 (711 nm) and 34 (752 nm) for the CIN (Fig. 7e), SA (Fig. 7f) and THL (Fig. 7g) datasets were used to generate TBM spectral parameters tied to Chl-a concentration. The TBM with the simulated Hyperion bands (Fig. 7e–h) shows higher calibration accuracy than those for the simulated OLCI spectra (Fig. 7a–d). Particularly, the tuned TBM with optimal bands for STKR achieved better calibration results with the simulated Hyperion spectra (Fig. 7h) with comparable R² (0.75) to that (0.82) for the original spectra (Fig. 4d). The TBM calibration results for both the aggregated OLCI and Hyperion datasets are shown in Table 3, and the models with the simulated Hyperion dataset show better performance than that with the simulated OLCI spectra due to the finer spectral resolution for the Hyperion sensor; optimal bands can be determined through the tuning process.

4.5.2. TBM validation

The TBM validation results for the simulated OLCI and Hyperion spectra are shown in Fig. 8. It can be seen that the TBM using simulated Hyperion bands yields marginally better results than that from the simulated OLCI spectra (see Fig. 8b and a), implying that the TBM applied to finer spectral resolution data gives rise to a better performance for phytoplankton monitoring. It is also worth noting that the TBM with the simulated OLCI and Hyperion spectra tends to underestimate Chl-a concentration.

4.5.3. GA-PLS performance

The measured and predicted Chl-a concentrations via GA-PLS modeling of the simulated OLCI and Hyperion spectra for calibration samples are shown in Fig. 9a–b. It can be seen that GA-PLS is more effective for estimation of Chl-a concentration, showing high coefficients of determination (OLCI: R² = 0.89; Hyperion: R² = 0.91). Given the spatiotemporal variation of OACs, the sun-target-sensor geometry, spectral measurement procedures and instrumentation, GA-PLS is a robust modelling approach for Chl-a estimation with the simulated OLCI spectra. As expected, the GA-PLS model with the simulated Hyperion spectra outperforms that with the simulated OLCI spectra for the validation datasets (Fig. 9c–d). It is worth noting that the GA-PLS model using the simulated OLCI spectra tends to underestimate Chl-a of the validation samples (Fig. 9c), while no obvious underestimation trend can be observed for the simulated Hyperion dataset (Fig. 9d).

4.6. Spatial transferability

4.6.1. TBM performance

In this section, we use three of the four datasets to calibrate TBM, and the remaining dataset to validate the model independently. The
above analyses indicate that TBM with the narrow-band spectra or the simulated Hyperion spectra outperforms those with the simulated OLCI spectra. We used the simulated OLCI spectra to test the TBM spatial transferability assuming that better results would be achieved with hyperspectral remote sensing data. For the simulated OLCI spectra, $\lambda_1 = $ band 7, $\lambda_2 = $ band 9, and $\lambda_3 = $ band 10 were applied to model calibration and validation datasets. The TBM calibration results with samples from various datasets except CIN are presented in Fig. 10a, showing relatively low accuracy ($R^2 = 0.62$). A significant underestimation is observed for model validation with the CIN dataset (Fig. 10b), which is further suggested by a slope value far from unity (0.44) and high $rRMSE$ (49.5%). The TBM calibrated with the NON-SA dataset and non-THL dataset has similar accuracy and regression parameters (Fig. 10c and e). The TBM validated on the SA and THL datasets also performed well (Fig. 10d and f). Although the TBM calibration for NON-STKR is similar to NON-SA and NON-THL (Fig. 10g), the validation result for STKR is quite

![Fig. 5. Scatter plot of three-band model predicted and measured Chl-a concentration for various validation datasets: (a) CIN dataset, (b) SA dataset, (c) THL dataset, (d) STKR dataset, (e) CIN ASD-dataset, and (f) CIN OO-dataset. All RMSE, $rRMSE$, MAE are based on validation samples only.](image)

Table 4
The GA-PLS model performances for calibration of each dataset.

<table>
<thead>
<tr>
<th>Datasets</th>
<th>Model calibration</th>
<th>RMSE</th>
<th>$R^2$%</th>
<th>MAE</th>
<th>RPD</th>
<th>$R^2$</th>
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<tr>
<td>CIN</td>
<td></td>
<td>11.29</td>
<td>19.37</td>
<td>7.24</td>
<td>4.73</td>
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<td>1.06</td>
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<td>0.87</td>
<td>22.52</td>
<td>0.99</td>
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<td>31.85</td>
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<td>3.60</td>
<td>0.89</td>
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<tr>
<td>STKR</td>
<td></td>
<td>3.87</td>
<td>27.36</td>
<td>3.01</td>
<td>4.10</td>
<td>0.84</td>
</tr>
<tr>
<td>Narrow band aggregated</td>
<td></td>
<td>12.31</td>
<td>28.73</td>
<td>7.9</td>
<td>4.43</td>
<td>0.91</td>
</tr>
</tbody>
</table>
Fig. 6. Scatter plot of measured Chl-a vs. predicted Chl-a using the GA-PLS modeling for various datasets, (a) CIN dataset; (b) SA dataset; (c) THL dataset, and (d) STKR dataset. The validation results (RMSE, rRMSE, MAE) for GA-PLS with each dataset are presented in subplots.

Fig. 7. Three-band model calibration using Sentinel-3/OLCI and Hyperion simulated spectra. The first row is the results from simulated OLCI spectra, (a) CIN dataset, (b) SA dataset, (c) THL dataset, and (d) STKR dataset; (e)-(h) in the second row are the result from corresponding simulated Hyperion spectra.
different from the others (Fig. 10h), of which the samples are scattered with higher rRMSE (77.3%).

4.6.2. GA-PLS performance

The test for the GA-PLS spatial transferability was conducted with various datasets and the results are shown in Fig. 11. Comparison of Fig. 11a-b with Fig. 10a-b shows that GA-PLS with the NON-CIN dataset achieved a better performance ($R^2 = 0.85$). The GA-PLS validation with the CIN dataset also yielded a higher performance with respect to the TBM ($rRMSE = 40.1\%$ vs. $49.5\%$, and slope $0.71$ vs. $0.44$). Compared with the TBM calibration, the same conclusion holds true for the GA-PLS calibrations with the NON-SA and NON-THL datasets (Fig. 11c vs. Fig. 10c and Fig. 11e vs. Fig. 10e), implying similar model calibrations. Furthermore, the GA-PLS also achieved stable validations with the SA and THL datasets (Fig. 11d and f). The GA-PLS models resulted in lower $rRMSE$ values ($17.1\%$ and $40.82\%$) compared with that from the TBM ($19.8\%$ and $47.2\%$). It can be seen from Fig. 11g that GA-PLS with the NON-STKR dataset yielded marginally better calibration ($R^2 = 0.78$) than the TBM with same dataset, with slightly better performance achieved for the validation with the STKR dataset (see Fig. 11h vs Fig. 10h). In general, it can be observed that GA-PLS has higher spatial transferability than TBM considering the results derived from the current study.

**Fig. 8.** Three-band model validation results for (a) simulated OLCI and (b) Hyperion spectra.

**Fig. 9.** The GA-PLS model calibration results for (a) simulated OLCI and (b) Hyperion spectra, and validation results for (c) simulated OLCI and (d) Hyperion spectra.
5. Discussion

5.1. GA-PLS vs. TBM

Through the above analyses, it has been shown that the GA-PLS model outperformed TBM with the CIN datasets, and marginally better than TBM with the THL and STKR datasets. As shown in Table 5 (all numbers in Table 5 represent spectral band positions), the spectral variables accommodated by the GA-PLS model for each dataset reveal some common trends, where
band ratio and first derivative reflectance (RDR) are the major input spectral variables. Particularly for the CIN dataset, three derivative spectral variables explain most of the better performance for GA-PLS with respect to the TBM. Further, these ratios are generally determined for empirical models using band ratios (Gitelson et al., 2007, 2008; Han, 2005; Han & Rundquist, 1997; Song et al., 2012b). Incorporating more spectral variables, particularly derivative spectral variables, may explain why GA-PLS performed better than the TBM in most cases. Chen et al. (1992) and Han and Rundquist (1997) pointed out that derivative analysis is an effective approach for random noise reduction and removing the effects of suspended matter on Chl-a concentration estimation.

It should be pointed out that the TBM has turned out to be one of the most effective modeling approaches for estimating Chl-a in turbid inland waters (Gitelson et al., 2007, 2008, 2009; Song et al., 2012a; Xu et al., 2009; Yang et al., 2011; Zhang et al., 2011). Our test with a large dataset measured with various portable spectrometers and different protocols (OO-BW, ASD-AW, ASD-ST), and thus containing uncertainties in addition to those due to various OACs for nine waters across three countries, confirms that the TBM is stable with various water bodies. The TBM consistently shows robust performances with acceptable to good results for narrow-band spectra, simulated OLCI and Hyperion spectra as well (Williams, 2001). It should be emphasized that the major merit of TBM is its simplicity of implementation and application to image data.

Our results also indicate that both GA-PLS and TBM generate better calibration and validation with narrow-band spectra (including simulated Hyperion spectra) than with the simulated OLCI spectra. This is particularly true for the GA-PLS model, which is likely due to the fact that more spectral variables are involved in the modeling. In this case derivative spectral variables were identified as important spectral variables. More spectral variables used by the GA-PLS model also explain why no obvious over- or under-estimation occurred compared with the TBM results for highly eutrophic water bodies. The TBM consistently shows robust performances across three countries, containing uncer-


ties of ISM concentration is more likely affected by ISM concentration in the water column (Randolph et al., 2008). Similar findings are reported for remote estimation of Chl-a concentration using TBM (Gitelson et al., 2008, 2009; Le et al., 2009). Further analysis for the GA-PLS model revealed a similar pattern (results not presented here) due to the fact that this approach is mainly based on sensitive band ratios or derivatives, particularly band ratios which bear a similar trend with the TBM results.

5.3. Error versus spectral measurements

Remote sensing models for estimating Chl-a with in situ remote sensing reflectance are generally measured with various procedures and instruments (Gitelson et al., 2008; Gons, 1999; Randolph et al., 2008; Simis et al., 2005; Song et al., 2012a). Modeling errors introduced by data collection rather than algorithms may exist. As detailed above, remote sensing reflectance spectra in the current study were measured with three procedures and two portable spectrometers. Although the water was placid, the potential error caused by skylight reflection, water-air interface refraction, and water surface undulation could affect spectral reflectance shape and magnitude (Mobley, 1999; Morel & Gentili, 1993), which ultimately exert an influence on model accuracy (see Fig. 5e and f).

In 2010, remote sensing reflectance spectra from 117 stations were collected by following three procedures, e.g., ASD-AW, OO-AW and OO-BW, respectively during 7 field surveys over Eagle Creek, Morse and Geist reservoirs in central Indiana, US. The TBM was optimized for the first two bands, and the third bands were fixed to 753 nm (i.e., OLCI band 10 central wavelength) with spectra from three measurement protocols (Fig. 13). It can be seen that the first band positions (λ1) are close for the above-water datasets (Fig. 13a, c). The second band position (λ2) for the ASD dataset (Fig. 13c) shows differences from that for the OO datasets (Fig. 13a-b), which is probably due to the potential differences in the radiometric characteristics between the ASD and Ocean Optics spectrometer as suggested by Moses et al. (2012b). The coefficients of determination indicate that the TBM with the OO-BW dataset performed the best in three models. The TBM performances with the simulated OLCI bands were summarized in Table 6. It is more comparable through fixed bands for the three datasets collected with different protocols and instruments. As shown in Table 6, the TBM with the OO-BW dataset still performed better than with OO-AW and ASD-AW, indicating that below-water measurements are effective to diminish noises. Furthermore, it can be seen that ASD portable spectrometer is more stable for high quality remote sensing reflectance collection by showing high determination of coefficient (R2 = 0.89) with ASD-AW dataset than that from OO-AW dataset (R2 = 0.84).

The TBM evaluations indicate that the OO-BW dataset yielded lowest rRMSE (17.4%), followed by ASD-AW (20.5%) and OO-AW.

Table 5

Spectral variables determined for the GA-PLS implementation with various narrow-band spectral datasets.

<table>
<thead>
<tr>
<th>Datasets</th>
<th>Spectra variables selected for GA-PLS model</th>
</tr>
</thead>
<tbody>
<tr>
<td>CIN</td>
<td>R702/697, R704/665, R737/696</td>
</tr>
<tr>
<td>SA</td>
<td>R710/676, R714/674, R854/676, R857/687, R754/Rs547, R753/Rs753</td>
</tr>
<tr>
<td>THL</td>
<td>R761/679, R767/672, R760/667</td>
</tr>
<tr>
<td>STKR</td>
<td>R702/694, R706/694, R701/696</td>
</tr>
<tr>
<td>Aggregated</td>
<td>R706/697, R709/665, R723/695</td>
</tr>
</tbody>
</table>

high TSM concentration, which is responsible for poor model spatial transferability for both GA-PLS and TBM (Figs. 10h and 11h).

5.2. RE versus ISM

The influence of ISM on the Chl-a estimation accuracy with the TBM was analyzed because of its stable model performance for various datasets (Gitelson et al., 2008; Song et al., 2012a; Tyler et al., 2006), in addition to the fact that GA-PLS is also partially based on sensitive band ratios (Song et al., 2012b). The relationships between the relative error, RE (Eq. 10), and ISM or ISM:Chl-a ratio for the aggregated dataset are presented in Fig. 12. It is apparent that no correlation between the RE and ISM is observed for the aggregated dataset. However, a significant correlation between the RE and ISM: Chl-a ratio is shown (Fig. 12b) with higher ISM:Chl-a ratios resulting in larger TBM-yielded errors for estimated Chl-a. Thus, the ISM versus Chl-a ratio affects the TBM performance, indicating that lower Chl-a concentration is more likely affected by ISM concentration in the water column (Randolph et al., 2008).
A better performance was achieved through the GA-PLS modeling with the same datasets by showing lower rRMSE values (Fig. 13d). It indicates that different data collection procedures and instrumentations cause differences for the same Chl-\(a\) concentration. Although the TBM employing band ratio likely reduces the error resulting from the sun-target-sensor geometry, the result indicated that the difference introduced by instrumentations and spectral measurement procedures cannot be ignored for modeling accuracy analyses (Moses et al., 2012b, also see the supplementary Fig. 1s). Note that laboratory analysis is another uncertainty source for model accuracy as indicated in Fig. 1b, implying that at least about 8% uncertainty may be introduced into the modeling results.

6. Conclusions

This study shows that the GA-PLS model can be effective tools for estimating Chl-\(a\) using \textit{in situ} measured spectra bearing differing OACs. The GA selected spectral variables are generally determinant of Chl-\(a\) diagnostic spectral variables caused by the optical properties of the pigments as reported in the literature. The GA-PLS outperforms
TBM for estimating Chl-a due to more sensitive spectral variables being integrated by the hybrid modeling, and accommodation of other OAC influences. The current observation has further proven that the TBM, which developed from bio-optical modeling, is a robust modeling approach for estimating Chl-a in a variety of inland waters. Both the GA-PLS and TBM result in acceptable to accurate modeling performance with the simulated OLCI and Hyperion spectra (Williams, 2001). Furthermore, both models perform better with the narrow-band spectra than the simulated OLCI spectra.

Our study results indicate that GA-PLS demonstrates better spatial transferability. Differences in suspended mineral particles and phytoplankton community structure among reservoirs could explain the low model performance (e.g., STKR), and generally, the closer the OACs among water bodies, the better the algorithm spatial transferability (e.g., THL). Our results also indicate that developing a robust algorithm for estimating Chl-a requires a larger dataset encompassing a larger range of Chl-a concentration. Similarly, both GA-PLS and TBM trained with a large dataset measured in different water bodies of different seasons may be used to predict Chl-a concentration. However, GA-PLS shows a marginally better spatial transferability because more sensitive diagnostic spectral information is accommodated in the modeling process, which likely reduces influences from other OACs more effectively.

Future studies will be focused on: (1) testing GA-PLS and TBM with samples from inland waters of different regions with varied OACs; (2) scaling up the use of spectrometer platforms to include satellite imagery, e.g., TERRA/MODIS or Sentinel3/OLCI sensors. Investigation on the spectral variable determination based upon the IOPs of water quality parameters is also desirable. Such robustness for the GA-PLS model has been tested with the in situ datasets collected by using hand-held sensors (e.g., ASD and Ocean Optics USB4000 spectrometers), and will be further tested with airborne and satellite image data for estimating Chl-a.

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Appendix A. Supplementary data

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References


