Developing water quality retrieval models with \textit{in situ} hyperspectral data in Poyang Lake, China

Fangyuan Chen\textsuperscript{a}, Di Xiao\textsuperscript{a} and Zhuochao Li\textsuperscript{b}

\textsuperscript{a}School of Resource and Environmental Sciences, Wuhan University, Wuhan, China; \textsuperscript{b}State-owned Assets Supervision and Administration Commission of Caidian District, Wuhan, China

\section*{ABSTRACT}
Applying remote sensing techniques to develop the retrieval models and further to obtain the spatiotemporal information of water quality parameters is necessary for understanding, managing, and protecting lake ecosystems. This study aimed to calibrate and validate the retrieval models for estimating the concentrations of chlorophyll a ($C_{\text{CHL}}$), suspended particulate matter ($C_{\text{SPM}}$), and dissolved organic carbon ($C_{\text{DOC}}$) with the \textit{in situ} hyperspectral measurements in Poyang Lake, China in 2010 and 2011. The model calibration and validation results indicated that: (1) for $C_{\text{CHL}}$ retrieval, significantly strong and moderate correlations existed between the measured and estimated values ($\rho=0.92$ and $\rho=0.76$) using the exponential model and the three-band model, respectively, with biased estimation observed for the exponential model; (2) for retrieving $C_{\text{SPM}}$, there was a strong correlation between the measured and estimated values ($\rho=0.95$) using the exponential model; and (3) no significant correlation between measured and estimated $C_{\text{DOC}}$ values was found with our developed models. More work is needed to allow the water quality of Poyang Lake to be accurately and steadily estimated, especially for $C_{\text{CHL}}$ and $C_{\text{DOC}}$.

\section*{1. Introduction}
Lakes provide multiple benefits to society through commerce, esthetics, tourism, recreation, and biodiversity conservation (Jorgensen, Loffler, and Rast 2005; O’Sullivan and Reynolds 2005), and these provisions are greatly influenced by water quality. Therefore, applying remote sensing techniques to develop the retrieval models and further to obtain the spatiotemporal information of water quality parameters is necessary for understanding, managing, and protecting lake ecosystems. To date, several important water quality parameters can be estimated through remote sensing techniques, including: (1) phytoplankton, the biomass of which is generally derived from chlorophyll a ($\text{CHL}$) concentration; (2) suspended particulate matter (SPM), including suspended particulate inorganic matter (SPIM) and suspended particulate organic matter (SPOM); and (3) dissolved organic carbon (DOC), in which yellow substance (also known as color/chromophoric dissolved organic matter) is a dominant component (Ma et al. 2010).

Several types of multispectral (several spectral bands) or superspectral (tens of spectral bands) remote sensing data, such as Landsat (Allan et al. 2011; Brezonik, Menken, and Bauer 2005; Carpenter and Carpenter 1983), advanced spaceborne thermal emission and reflection radiometer (Kishino, Tanaka, and Ishizaka 2005; Nas et al. 2009; Volpe, Silvestri, and Marani 2011), moderate resolution imaging spectroradiometer (MODIS) (Giardino et al. 2010; Kilham and Roberts 2011; Song and ke 2015; Zhang et al. 2010), and medium-resolution imaging spectrometer (MERIS) (Doerffer and Schiller 2007; Odermatt, Giardino, and Heege 2010; Tang et al. 2009), have been employed to retrieve the aforementioned water quality parameters. These images generally perform well in retrieving water quality parameters; however, they also have several limitations. One limitation is their low spatial resolutions (more than several hundred meters) or long repeating cycles (more than ten days), and another very important one is their wide bandwidths (more than 10 nm) or small numbers of wavebands (several or tens of), which cannot accurately capture the spectral characteristics of water quality parameters (Dekker et al. 1992).

Hyperspectral (hundreds of spectral bands) remote sensing techniques can acquire near-continuous spectral information of the Earth’s surface, with a very narrow bandwidth (less than 10 nm) and a large number of wavebands (typically 200 or more) throughout the visible and infrared regions of electromagnetic spectrum (Govender, Chetty, and Bulcock 2007). Many studies
have explored their potentials on water quality retrievals with different data sources, including in situ hyperspectral measurements (Sun, Li, and Wang 2009; Yacobi et al. 2011), and airborne (Kallio et al. 2001; Thiemann and Kaufmann 2002) or satellite hyperspectral images (Chen et al. 2011; Giardino et al. 2007). These studies indicated that hyperspectral remote sensing might overcome some limitations of multispectral and hyperspectral remote sensing techniques and have potentials for improving water quality estimations. However, the applications of airborne and satellite hyperspectral images were very limited due to data availability and/or affordability, and thus the in situ hyperspectral measurements were employed frequently.

Based on the data sources mentioned above, three kinds of models are employed for retrieving water quality parameters (Giardino et al. 2007; Ma et al. 2010): empirical, semi-empirical, and semi-analytical model. Semi-analytical models might be more suitable for different water bodies compared with empirical and semi-empirical ones due to their strict theories (Giardino et al. 2007; Ma et al. 2010). However, their applications are limited because of the difficulties or inaccuracies in obtaining model-driving parameters (Ma et al. 2010). Empirical and semi-empirical models are frequently applied currently. However, they do not have strict theoretical foundations, and their styles or coefficients are often region- and time-dependent due to the different optical properties at different water bodies or time periods. Therefore, empirical and semi-empirical models generally need to be calibrated or validated for a specific water body.

Poyang Lake is the currently largest freshwater lake in China, and some studies have been conducted to retrieve its water quality parameters during recent years, such as Chen et al. (2007) employed in situ hyperspectral measurement to simulate TM and MERIS data and developed SPM retrieval models. Feng et al. (2012) used MODIS data to observe long-term turbidity changes in this lake, and Wu et al. (2013) compared different MODIS-based models for retrieving SPM. However, no unified model exists for SPM retrieval in Poyang Lake; when referring to chlorophyll, very few studies were focused on CHL retrieval, the empirical model developed by Feng et al. (2015) could not be used in highly turbid area in northern Poyang Lake. Huang, Gao, and Zhang (2015) combined artificial neural network and clustering techniques to predict CHL separately, as no simple and common model has yet been achieved. Since the results from these studies are limited to exploring remote sensing-based methods for retrieving the water quality parameters of this huge and dynamic lake system, this study aims to calibrate and validate the retrieval models for estimating the concentrations of CHL ($C_{CHL}$), SPM ($C_{SPM}$), and DOC ($C_{DOC}$) with the in situ hyperspectral measurements in Poyang Lake, which may lay foundations for retrieval models selection in the airborne or satellite hyperspectral image-based water quality parameter estimations.

2. Materials and methods

2.1. Study area

Poyang Lake (115°47′–116°45′E, 28°22′–29°45′N) is located on the southern bank of the middle Yangtze River (Figure 1). It is a seasonal lake with the fluctuation of water level, and its size fluctuates from less than 1000 km² in dry season to about 4000 km² in rainy season. The lake receives water from five rivers (Raohe River, Xinjiang River, Fuhe River, Ganjiang River, and Xiushui River) and drains into the Yangtze River through a channel in the north.

With the increasing population and intensive economic activities within Poyang Basin during recent decades, the water quality of Poyang Lake shows a clear downwards trend due to agricultural chemical inputs as well as industrial and waste discharges (Deng et al. 2011; Zhen et al. 2011). Although the average $C_{CHL}$ is low in general for the whole lake, eutrophication was found in some regions (Wan and Yan 2007; Wang et al. 2007). Suspended sediment (or SPIIM) is one of dominant factors affecting the water quality of Poyang Lake (Jin, Liu, and Tu 1990), and its concentration fluctuates largely due to the sand discharges from the five rivers, the water backflows from the Yangtze River, and the dredging activities (Cui, Wu, and Liu 2009; Cui, Zhai, and Wu 2013; Wu et al. 2007). Such water quality degradation greatly and negatively impacts this lake ecosystem.

2.2. Fieldwork

Fieldwork was carried out on 16–18 October 2010 and 8–10 August 2011, and 85 sampling sites (47 in 2010 and 38 in 2011) were distributed along main channel due to low water levels (Figure 1). At each sampling site, the wind velocity and direction were measured using a wind velocity indicator, the geographical coordinate was recorded using a global positioning system receiver (Garmin Ltd.), the spectra were measured with a portable ASD FieldSpec Pro Dual VNIR spectrometer (ASD Inc.), and about 1500 ml of surface water was collected from around 0–50-cm water depth and was kept in a refrigerator for less than 10 h before the measurements of $C_{CHL}$, $C_{SPM}$ and $C_{DOC}$ were made in the laboratory.

2.3. Spectral measurement

The ASD FieldSpec Pro Dual VNIR spectrometer used in this study has a spectral range of 350–1050 nm with a spectral sample interval of 1.4 nm. Prior to the field campaign, the absolute radiance calibrations of two spectrometer detectors were performed. At each sampling
site, the measurements were carried out following the NASA protocol (Mueller, Fargion, and McClain 2003) and the steps described by Ma, Tang, and Dai (2006) and Ma et al. (2010): (1) the radiance from a 25 × 25 cm gray diffuse reflectance standard with 25% reflectivity was measured; (2) the radiances from the water and sky were measured synchronously using two detectors; (3) the above-mentioned two steps were repeated once; and (4) the radiance from the reflectance standard was measured again.

2.4. Constituent concentration measurement

The concentrations of the main water constituents were measured according to the investigation criteria about the lakes of China (Huang 1999). A spectrophotometric determination method was used to measure the $C_{\text{CHL}}$: (1) each water sample was filtered using a Whatman GF/F glass fiber filter with a 0.45 μm pore size, and acetone was used to extract chlorophyll a from the filtered sample; (2) the sample was read before and after its acidification using a UV2401 spectrophotofluorometer (Shimadzu Corp.); and (3) the $C_{\text{CHL}}$ value of the water sample was calculated by comparing the readings with a known standard (Duan et al. 2010a). The $C_{\text{SPM}}$ was measured gravimetrically: (1) the water sample was filtered using a pre-weighted Whatman GF/F glass fiber filter with a 0.45 μm pore size; (2) the filter was dried for 2 h at 110 °C and reweighed after cooling to room temperature; and (3) the $C_{\text{SPM}}$ was calculated by dividing the difference in weight before and after filtering by the water sample volume (Ma, Tang, and Dai 2006a). A Model 1020 Total Organic Carbon (TOC) Analyzer (O. I. Corp.) was used to measure the $C_{\text{DOC}}$ after the water sample was filtered using a Whatman GF/F glass fiber filter with a 0.45 μm pore size (Ma et al. 2006a).

2.5. Remote sensing reflectance calculation and pre-processing

The abnormal radiance measurements from the gray diffuse reflectance standard, water, and sky were removed considering their spectral characteristics. The remote sensing reflectance at each sampling site was then calculated using the remaining measurements with the following equation (Ma et al. 2006a; Ma et al. 2010):
where \( R_n \) (sr\(^{-1}\)) is the remote sensing reflectance of water body; \( L_w \), \( L_{sky} \), and \( L_p \) (W m\(^{-2}\) sr\(^{-1}\)) are the mean measured radiances from water, sky, and gray diffuse reflectance standard; \( \rho_w \) indicates the water–air interface reflectance rate, and its value is 0.022, 0.025, and 0.028 for a wind velocity of 0, 5, and 10 m/s, respectively; \( \rho_p \) is the reflectance rate of gra diffuse reflectance standard, and its value is 0.25; and \( \pi \) (sr) is the solid angle.

The first-order derivative of \( R_n \) \( (R'_n) \) might improve water quality retrieval (Ma et al. 2010), and it was derived with the following equation:

\[
R'_n(i) = \frac{R_n(i + 1) - R_n(i)}{\lambda(i + 1) - \lambda(i)}
\]

where \( R'_n(i) \) (sr\(^{-1}\)/nm), \( \lambda(i) \) and \( R_n(i) \) are the first-order derivative, \( \lambda \) and wavelength at band \( i \), respectively.

Only the \( R_n \) and \( R'_n \) at the wavelengths of 400–900 nm were employed for model calibration and validation. The samples with incorrect spectrum (non-typical Case-II water spectrum) or water constituent concentration measurement (negative value) were removed from the following statistics and analysis.

### 2.6. Model calibration

The data-set in 2010 was employed for model calibrations. The \( C_{CHL}, C_{SPM} \) and \( C_{DOC} \) values of remaining water samples were statistically described, and the correlations among them were analyzed. The spectra of \( R_n \) and \( R'_n \) were visualized and analyzed. The correlation analysis of \( R_n \) and \( R'_n \) against \( C_{CHL}, C_{SPM} \) and \( C_{DOC} \) was then implemented, respectively, in order to find the potential bands for model calibrations. Finally, in order to find the best-fitting model for retrieving water quality parameters, the widely used simple linear \((y = a + bx)\), quadratic \((y = a + bx + cx^2)\), power \((y = ax^b)\), and exponential \((y = a e^{bx})\) models of \( C_{CHL}, C_{SPM} \) and \( C_{DOC} \) against a single potential band (including \( R_n \) and \( R'_n \)) or band combinations were calibrated with the least squares technique; while two- (Equation (3)) and three-band (Equation (4)) models (Chen et al. 2011; Duan et al. 2010b; Gilerson et al. 2010; Gitelson et al. 2009; Gurlin, Gitelson, and Moses 2011) were especially calibrated for \( C_{CHL} \) due to their wide and successful applications in many cases. The determination coefficients \((R^2)\) and estimated standard errors \((SE)\) of all tested regression models were compared to determine the best-fitting one of each water quality parameter.

\[
C_{CHL} \propto R^{-1}_n(\lambda_1)R'_n(\lambda_2)
\]

2.7. Model validation

Two-step model validations were carried out for the best-fitting model of each water quality parameter. The first step was leave-one-out cross-validation (LOOCV) with the data-set in 2010. LOOCV was proposed by Craven and Wahba (1978) and is considered as an almost unbiased estimator of model validation (Cawley and Talbot 2004) with the following process: (1) one sample was selected as a validation datum and removed from total \( n \) samples; (2) the remaining \( n-1 \) samples were employed as training data to fit a regression model with the same form as above-developed best-fitting model, using the least squares technique; (3) the fitted regression model was then used to estimate the water quality parameter value of that excluded sample; (4) the aforementioned steps (1–3) were repeated until each sample was selected once, and, thus, the water quality parameter values of all water samples were estimated; and (5) the correlation coefficient \((r)\) between the measured and estimated values of all water samples was calculated to assess model accuracy, while the null hypotheses that the slope and intercept of the linear regression line between measured and estimated values were equal to 1 and 0, were tested, respectively, to assess estimation bias. The second step was an independent validation. To each water quality parameter, the best-fitting model was applied to the data-set in 2011 to estimate the values of remaining water samples from \( R_n \) or \( R'_n \), and the \( r \) value between the measured and estimated values was calculated to assess model accuracy.

### 3. Results

#### 3.1. Measurement analysis

Thirteen samples in 2010 were removed from the following statistics and analysis, one with a negative \( C_{CHL} \) value and twelve without the typical spectral property of Case-II water. Ten of the removed samples were collected on 16 October 2010, when the waves caused by high wind velocities (>5 m/s) greatly affected the accuracies of spectral measurements. Four samples in 2011 were removed because they missed the typical spectral property of Case-II water.

The statistical results for \( C_{CHL}, C_{SPM} \) and \( C_{DOC} \) of the remaining 34 water samples in 2010 are shown in Table 1. StdDev means standard deviation and CoeVar is coefficient of variation. The results showed that the \( C_{SPM} \) had high values with moderate variation (average
3.2. Retrieval models of water quality parameters

The correlation analysis between $C_{\text{CHL}}$ and $R_{\text{rs}}$ (Figure 4(a)) showed that the correlation coefficient obtained the lowest value ($r = -0.31, p = 0.074$) at the wavelength of 900 nm and was about 0.59–0.60 at the wavelengths over 666–682 nm; while the highest correlation between $C_{\text{CHL}}$ and $R_{\text{rs}}' (r = 0.88, p < 0.001)$ was observed at the wavelengths of 681 and 692 nm (Figure 4(b)).

The exponential model of $R_{\text{rs}}'$ at 681 nm obtained the best fitting of all tested simple models for retrieving $C_{\text{CHL}}$, and it explained 74% of the variation of $C_{\text{CHL}}$ with an SE of 3.399 μg/l (Figure 4(c)). The LOOCV result showed a significantly strong correlation between the measured and estimated $C_{\text{CHL}}$ values ($r = 0.82, p < 0.001$) at a significance level of 0.05 in Figure 4(d), where the solid line is the regression line between the estimated and measured values, and the dashed line is 1:1 line. The null hypotheses tests of the intercept being equal to 0 and the slope being equal to 1 for the regression line between the measured and estimated values indicated that the intercept and slope were not significantly different from 0 ($t = 0.532, df = 32, p = 0.599$) and 1 ($t = -0.902, df = 32, p = 0.374$) at a significance level of 0.05, respectively.

The three-band model using 681, 698, and 750 nm had the best fitting result among all tested two- and three-band models for retrieving $C_{\text{CHL}}$, and it explained 77% of the variation of $C_{\text{CHL}}$ with $C_{\text{SPM}} = 54.20 \text{ mg/l, CoeVar} = 60.54\%$, the $C_{\text{CHL}}$ was low with high variation (average $C_{\text{CHL}} = 9.42 \text{ μg/l, CoeVar} = 70.28\%$), and the $C_{\text{DOC}}$ was low with low variation (average $C_{\text{DOC}} = 3.00 \text{ mg/l, CoeVar} = 18.33\%$). The correlation analysis (Figure 2) indicated a significantly weak and negative relation between $C_{\text{SPM}}$ and $C_{\text{CHL}}$ and a non-significant correlation between $C_{\text{DOC}}$ and $C_{\text{CHL}}$ as well as between $C_{\text{DOC}}$ and $C_{\text{SPM}}$ at a significance level of 0.05.

The $R_{\text{rs}}$ spectra in 2010 (Figure 3(a)) showed a typical spectral characteristic of Case-II water: the $R_{\text{rs}}$ increased with increasing wavelength over 400–550 nm, and it was much higher than 0 in the near-infrared region; while there were two SPM reflectance peaks at around 580 and 810 nm as well as an absorption peak and a reflectance peak of CHL at about 672 and 700 nm. The $R_{\text{rs}}'$ (Figure 3(b)) generally ranged from −0.001 to 0.001 sr−1/nm, but it had values with large fluctuation at the wavelengths around 760 nm.

![Figure 2](image-url)  
**Figure 2.** Correlations between the concentrations of different water quality parameters of 34 water samples in 2010. (a) $C_{\text{CHL}}$ and $C_{\text{SPM}}$; (b) $C_{\text{CHL}}$ and $C_{\text{DOC}}$; (c) $C_{\text{SPM}}$ and $C_{\text{DOC}}$.

![Figure 3](image-url)  
**Figure 3.** Spectra of remote sensing reflectance ($R_{\text{rs}}$) (a) and its first-order derivative ($R_{\text{rs}}'$) (b) over 400–900 nm at the 34 sampling sites in 2010.
showed that the intercept and slope were not significantly different from 0 (\(t = 0.504, \text{df} = 32, p = 0.618\)) and 1 (\(t = -0.881, \text{df} = 32, p = 0.385\)), respectively. Compared with the exponential model of \(R'_{\text{rs}}\) at an \(SE\) of 3.237 \(\mu\text{g/l}\) (Figure 4(e)). Its LOOCV result indicated a significantly strong correlation between the measured and estimated \(C_{\text{CHL}}\) values (\(r = 0.88, p < 0.001\)) (Figure 4(f)). The null hypotheses tests showed that the intercept and slope were not significantly different from 0 (\(t = 0.504, \text{df} = 32, p = 0.618\)) and 1 (\(t = -0.881, \text{df} = 32, p = 0.385\)), respectively. Compared with the exponential model of \(R'_{\text{rs}}\) at

![Figure 4](image-url). Model calibration results for estimating \(C_{\text{CHL}}\) with 2010 data-set (\(n = 34\)). (a) correlation coefficient between \(C_{\text{CHL}}\) and \(R'_{\text{rs}}\); (b) correlation coefficient between \(C_{\text{CHL}}\) and \(R'_{\text{rs}}\); (c) model of \(C_{\text{CHL}}\) against \(R'_{\text{rs}}\); (d) LOOCV result of (c); (e) the best-fitting three-band model for \(C_{\text{CHL}}\); (f) LOOCV result of (e).
681 nm, the three-band model obtained a better result for estimating \( C_{\text{CHL}} \).

There existed significantly positive correlations between \( C_{\text{SPM}} \) and \( R'_{\text{a}} \) \((r > 0.6)\) over the wavelengths of 400–900 nm, and the strong correlations \((r \geq 0.85)\) were observed between 714 and 900 nm \((\text{Figure 5(a)})\). The greatest positive and negative correlations between \( C_{\text{SPM}} \) and \( R'_{\text{a}} \) were found at 775 nm \((r = 0.87, p < 0.001)\) and 880 nm \((r = -0.91, p < 0.001)\), respectively \((\text{Figure 5(b)})\).

The exponential model of \( R'_{\text{a}} \) at 775 nm best explained the variation of \( C_{\text{SPM}} \) \((R^2 = 0.93, SE = 9.074 \text{ mg/l}, p < 0.001)\) \((\text{Figure 5(c)})\). The LOOCV result showed a significantly strong correlation between the measured and estimated \( C_{\text{SPM}} \) values \((r = 0.95, p < 0.001)\) \((\text{Figure 5(d)})\). The results of the null hypothesis tests showed that the intercept and slope were not significantly different from 0 \((t = 0.771, df = 32, p = 0.482)\) and 1 \((t = -1.151, df = 32, p = 0.258)\), respectively.

The correlation between \( C_{\text{DOC}} \) and \( R'_{\text{a}} \) was very low over 400–900 nm, and the highest one was found at 616 nm but not significant at a significance level of 0.05 \((r = -0.26, p = 0.131)\) \((\text{Figure 6(a)})\). The highest significantly positive and negative correlations between \( C_{\text{DOC}} \) and \( R'_{\text{a}} \) were observed at the wavelengths of 745 nm \((r = 0.44, p = 0.010)\) and 791 nm \((r = -0.37, p = 0.031)\), respectively \((\text{Figure 6(b)})\). The exponential model of \( R'_{\text{a}} \) at the wavelength of 745 nm had the best fitting of all tested simple models for retrieving \( C_{\text{DOC}} \); however, it could only explain 20% of the variation of \( C_{\text{DOC}} \) with an SE of 0.501 mg/l \((\text{Figure 6(c)})\). The LOOCV result indicated a non-significant correlation \((r = 0.33, p = 0.057)\) between the measured and estimated values \((\text{Figure 6(d)})\).

### 3.3. Estimation of water constituent concentration

The best-fitting simple models were applied to the remaining 34 water samples in 2011 to estimate the \( C_{\text{CHL}}, C_{\text{SPM}}, \) and \( C_{\text{DOC}} \) values, respectively. A significantly strong correlation was observed between the measured and estimated values for \( C_{\text{CHL}} \) \((r = 0.92, p < 0.001)\) \((\text{Figure 7(a)})\) and \( C_{\text{SPM}} \) \((r = 0.95, p < 0.001)\) \((\text{Figure 7(b)})\); however, a clear biased estimation was observed for \( C_{\text{CHL}} \); no significant correlation was found between the measured and estimated \( C_{\text{DOC}} \) values \((r = 0.30, p = 0.0853)\) \((\text{Figure 7(c)})\). The validation result of three-band model of 681, 698, and 750 nm showed a significantly moderate correlation between the measured and estimated \( C_{\text{CHL}} \) values \((r = 0.76, p < 0.001)\), and the estimation was unbiased \((a = -0.001, b = 1.000)\) \((\text{Figure 7(d)})\).

### 4. Discussion

#### 4.1. Water constituent concentration in Poyang Lake

In this study, we found that the \( C_{\text{SPM}} \) \((\text{average } C_{\text{SPM}} = 54.20 \text{ mg/l})\) was much higher when compared with \( C_{\text{CHL}} \) \((\text{average } C_{\text{CHL}} = 9.42 \mu g/l)\) and \( C_{\text{DOC}} \) \((\text{average } C_{\text{DOC}} = 3.00 \text{ mg/l})\); meanwhile, the measured \( C_{\text{CHL}} \) values (average \( C_{\text{CHL}} = 9.42 \mu g/l, \text{maximum } C_{\text{CHL}} = 24.65 \mu g/l)\) indicated that the lake was close to a eutrophic status as a whole. Several studies \((\text{Wan and Yan 2007; Wang et al. 2007})\) showed that eutrophication occurred at some regions of Poyang Lake, where the flow velocities were slow. These results together indicated that Poyang Lake would possibly face the same eutrophication problem as many other lakes in the world.

We observed that there was a significantly negative but weak correlation between the \( C_{\text{SPM}} \) and \( C_{\text{CHL}} \) values \((r = -0.42, p = 0.01)\) at a significance level of 0.05. Such relation indicated that SPM in Poyang Lake was not dominated by the degradation production of phytoplankton but from land-based sources or sediment resuspension. No significant correlation between \( C_{\text{DOC}} \) and \( C_{\text{CHL}} \) \((r = 0.30, p = 0.09)\) revealed that DOC was also not dominated by the degradation production of phytoplankton and possibly came from agricultural chemical inputs or industrial and waste discharges \((\text{Deng et al. 2011; Zhen et al. 2011})\).

#### 4.2. Characteristics of water quality parameters in Poyang Lake

Generally, two CHL absorption peaks exist around the spectral ranges over 430–450 nm and 650–700 nm for the Case-II waters \((\text{Ma et al. 2006b})\); such characteristic was confirmed by the case of Poyang Lake, in which one inconspicuous and one clear CHL absorption peaks were observed at the wavelengths of 439 and 678 nm, respectively \((\text{Wu et al. 2011})\). This absorption characteristic of CHL could explain why most of the potential bands for retrieving \( C_{\text{CHL}} \) were found at 666–682 nm \((R'_{\text{a}})\) and 681–692 nm \((R'_{\text{a}})\) in this study. Such a result is coincident with that found in Taihu Lake and Chaohu Lake \((\text{Ma et al. 2010; Yunlin Zhang et al. 2009})\) and the Pearl River Estuary \((\text{Xing et al. 2008})\) in China, as well as the Geist and Morse Reservoirs in Indiana \((\text{Randolph et al. 2008})\). However, it is different from the result obtained by Wang et al. \((2007)\), who found that the potential bands for \( C_{\text{CHL}} \) estimation appeared at 652 and 774 nm in Poyang Lake. We could not compare such difference, because they only employed nine samples and the model estimation accuracy are much lower \((R^2 = 0.42–0.43)\), while the model is not applicable to another date.

We found that the correlation between \( C_{\text{CHL}} \) and \( R'_{\text{a}} \) was weak \((\text{absolute value of } r \leq 0.6)\) in this study, which confirms that a single original reflectance band has limitation and is not suitable for \( C_{\text{CHL}} \) estimation \((\text{Ma et al. 2010})\). In this study, we found that the exponential model of \( R'_{\text{a}} \) at 681 nm explained 74% of the variation of \( C_{\text{CHL}} \) which indicated that the spectral derivative method can enhance CHL absorption features \((\text{CLOUTIS 1996})\) and resulted in a better \( C_{\text{CHL}} \) estimation. Such a result is similar to that from a controlled experiment by Rundquist et al. \((1996)\) as well as from Taihu Lake and Chaohu Lake in China \((\text{Ma et al. 2010})\), which together indicated the
Figure 5. Model calibration results for estimating $C_{\text{SPM}}$ with 2010 data-set ($n = 34$). (a) correlation coefficient between $C_{\text{SPM}}$ and $R_{rs}$; (b) correlation coefficient between $C_{\text{SPM}}$ and $R_{rs}/\text{uni}2032$; (c) model of $C_{\text{SPM}}$ against $R_{rs}(775)$; (d) LOOCV result.

Figure 6. Model calibration results for estimating $C_{\text{DOC}}$ with 2010 data-set ($n = 34$). (a) correlation coefficient between $C_{\text{DOC}}$ and $R_{rs}$; (b) correlation coefficient between $C_{\text{SPM}}$ and $R_{rs}/\text{uni}745$; (c) model of $C_{\text{DOC}}$ against $R_{rs}(745)$; (d) LOOCV result.
radiance, which can be captured by a remote sensing sensor and used for retrieving water quality parameters (Kirk 1994; Ma et al. 2006a). The absorption coefficients of CHL, SPM, and DOC are almost 0 at the near-infrared wavelengths, especially for water bodies with low CHL, and, thus, the water-leaving reflectance is dominated by the backscattering coefficient of SPM at these wavelengths in Case-II waters (Doxaran, Cherukuru, and Lavender 2006; Ma et al. 2010). These inherent optical properties of Case-II waters result in the significantly strong correlations between $C_{SPM}$ and $R_{rs}$ over 714–900 nm observed in this study, which confirms that the near-infrared bands have the most potential for retrieving $C_{SPM}$ reported in many studies (Ma et al. 2009; Onderka and Pekárová 2008; Wang and Lu 2010).

Although the near-infrared bands have the most potential for retrieving $C_{SPM}$, existing models have different types, inputting bands or accuracies. For example, Kallio et al. (2001) employed linear models for estimating the $C_{SPM}$ values of 11 lakes in Finland (band = 705–714 nm, $R^2 = 0.82–0.91$), and Ma et al. (2010) developed linear models (band = 828 nm, $R^2 = 0.90$; band = 788 nm, $R^2 = 0.77$) and power models (band = 804 nm, $R^2 = 0.83$; band = 760 nm, $R^2 = 0.57$) for Taihu Lake as well as potential of the $R_{rs}$ at around 690 nm for retrieving $C_{CHL}$ in different types of lakes.

Recently, some studies reported that the three-band model could improve the $C_{CHL}$ estimation in different water bodies, such as Taihu Lake (Li et al. 2012), Chagan Lake (Duan et al. 2010a), and Pearl River Estuary (Chen et al. 2011) in China, the Dnieper River and Taganrog Bay in Russia (Moses et al. 2009a, b) as well as the Fremont State Lakes in USA (Gitelson et al. 2009; Gilerson et al. 2010). In our study, the three-band model explained 77% of the variation of $C_{CHL}$ and performed better than the exponential model of $R_{rs}$, which confirmed the potential of three-band model for retrieving $C_{CHL}$. However, the estimation accuracy of the three-band model calibrated in our study was lower than or similar as that of most of these studies. Such a low estimation accuracy could be caused by the fact that the spectral signal of CHL is masked by that of SPM due to lower $C_{CHL}$ and higher $C_{SPM}$ in Poyang Lake; therefore, the limited three-band model needs to be improved further for accurately retrieving $C_{CHL}$, especially for turbid water bodies such as Poyang Lake.

For Case-II waters, the absorption and backscattering coefficients of CHL, SPM, and DOC affect water-leaving radiance, which can be captured by a remote sensing sensor and used for retrieving water quality parameters (Kirk 1994; Ma et al. 2006a). The absorption coefficients of CHL, SPM, and DOC are almost 0 at the near-infrared wavelengths, especially for water bodies with low $C_{CHL}$, and, thus, the water-leaving reflectance is dominated by the backscattering coefficient of SPM at these wavelengths in Case-II waters (Doxaran, Cherukuru, and Lavender 2006; Ma et al. 2010). These inherent optical properties of Case-II waters result in the significantly strong correlations between $C_{SPM}$ and $R_{rs}$ over 714–900 nm observed in this study, which confirms that the near-infrared bands have the most potential for retrieving $C_{SPM}$ reported in many studies (Ma et al. 2009; Onderka and Pekárová 2008; Wang and Lu 2010).

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an exponential model (band = 722 nm, $R^2 = 0.86$) for Shitoukoumen Reservoir in China. Compared with these models, the best-fitting model for retrieving $C_{SPM}$ calibrated in this study (band = 775 nm, $R^2 = 0.93$) had a higher estimation accuracy. In addition, the differences of model styles or inputting bands could be explained by the different water constituents of different water bodies or different time periods. Therefore, it is important to further evaluate the retrieval model robustness for $C_{SPM}$.

In this study, we also found that the correlation between $C_{DOC}$ and $R'_{\text{rs}}$ was very low over 400–900 nm, while the correlation between $C_{DOC}$ and $R_{\text{rs}}$ was also weak, which indicates that the model with a single band is not suitable for $C_{DOC}$ retrieval. Such a result is similar to that found in Taihu Lake (Ma et al. 2010), in which the $R_{\text{rs}}$ and $R'_{\text{rs}}$ could only explain 39% and 43% of the variation of $C_{DOC}$ respectively. Such a low estimation accuracy could be explained by two factors: one is that DOC has no clear spectral characteristics, while the strong absorption bands for DOC in the blue region of spectrum were also the strong absorption bands for CHL and SPM; and the other is that the absorption of DOC within strong absorption bands is further masked by those of CHL and SPM due to their high concentrations in Case-II waters (Ma et al. 2010). It is a big challenge to retrieve $C_{DOC}$ from very weak water-leaving radiance due to the low concentration and spectral characteristics of DOC.

4.3. Implications and limitations

Our results generally support the past research on in situ hyperspectral data-based $C_{CHL}$, $C_{SPM}$, and $C_{DOC}$ retrievals, and they might be applicable to other water bodies which have similar optical properties as Poyang Lake. Meanwhile, airborne and satellite hyperspectral images have great potentials for estimating some water quality parameters over large areas, and the models developed in this study could be applied to the hyperspectral images and provide methodological foundations for their applications in retrieving water quality parameters.

Since our results were only based on two-time period data collections along the main channel, and they still have spatial and temporal limitations unavoidably. Poyang Lake is a naturally dynamic system with large seasonal or yearly fluctuations in the water level and area; meanwhile, it is also suffering from serious environmental impacts caused by increasing population and intensive economic activities within its watershed. These natural and anthropogenic factors result in a great spatial and temporal heterogeneity of water constituents in this lake. However, most of the water quality retrieval models developed in this and other studies are empirical or semi-empirical, and they are very preliminary and often region- and time-dependent due to the different water constituents at different regions or at different time periods. More studies should be carried out to validate and improve these existing models or to develop new models to allow the water quality of Poyang Lake to be accurately and steadily estimated by remote sensing techniques.

5. Conclusions

The in situ hyperspectral measurement-based retrieval models for $C_{SPM}$, $C_{CHL}$, and $C_{DOC}$ in Poyang Lake were calibrated and validated. The main results are summarized as follows:

1. The three-band model of 681, 698, and 750 nm obtained the best result for retrieving $C_{CHL}$ with a moderate accuracy, showing the potential of this model for $C_{CHL}$ retrieval in turbid water body.

2. $C_{SPM}$ can be well estimated with a high accuracy using an exponential model of $R_{\text{rs}}$ at the infrared band of 775 nm.

3. $C_{DOC}$ can be best explained by the exponential model of $R'_{\text{rs}}$ at 745 nm, but the accuracy was very low.

More work should be carried out in the future to improve the existing models or to develop new models for accurately and steadily estimating the water quality of Poyang Lake, especially for $C_{CHL}$ and $C_{DOC}$.

Funding

This study was supported by the Forestry Non-Profit Industry Scientific Research Special Project “The Research of Ecosystem Service and Evaluation Techniques of Coastal Wetlands, China” [grant number 201404305].

Notes on contributors

Fangyuan Chen is currently a PhD candidate in Wuhan University. His main research interests include remote sensing of environment and GIS applications.

Di Xiao is currently an undergraduate student in Wuhan University. Her research focuses on remote sensing of inland lakes.

Zhuochao Li received his master’s degree from Wuhan University. His current research interest is remote sensing-based chlorophyll monitoring for inland lakes.

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