AN INTERCOMPARISON OF ANALYTICAL INVERSION APPROACHES TO RETRIEVE WATER QUALITY FOR TWO DISTINCT INLAND WATERS

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ABSTRACT

An intercomparison of a curve fitting and least squares approach is presented for the estimation of CHL, CDOM and TSM for two inland waters. In the inversion procedures two different bio-optical models were used, i.e. the Gordon model and the model of Albert and Mobley. The intercomparison is based on simulated APEX reflectance data. For these simulations two field campaigns were organised on the Scheldt river and Lake Constance to collect water samples. They were analysed for the optical properties and concentration values of the three optically active constituents. Reflectance data were then simulated using Hydrolight and the models of Gordon and Albert and Mobley. These simulations were used to test several inversion approaches. The curve fitting with the model of Albert and Mobley provided the best results for the Scheldt river. For Lake Constance no single procedure outperformed the others.

1. INTRODUCTION

Inland waters are very diverse and can include lakes, rivers, ponds, streams, springs as well as bogs, marshes and swamps. These inland waters are often valuable ecosystems that offer water supply, energy, transport and recreation. These values are more and more recognized, leading to protection measures and monitoring initiatives. In the Western world the monitoring is often regulated by laws (e.g The EU Water Framework Directive, 2000/60/EC) which ensure that the information is well documented and area covering .

Remote sensing of inland waters is gaining importance since the advent of new sensors with improved spectral and spatial capabilities. Remote sensing can serve as an additional source of information to support water quality monitoring programs. Best results are obtained by combining Remote sensing data with the results of traditional sampling programs.

Data from multispectral satellite sensors such as NASA's Moderate Resolution Imaging Spectroradiometer (MODIS) and Sea-viewing Wide Field-of-view Sensor (SeaWiFS), and the European Space Agency's Medium Resolution Imaging Spectrometer (MERIS) have been used to monitor inland waters. Budd and Warrington [2] for instance developed algorithms to estimate chlorophyll *a* and Total Suspended Matter (TSM) concentrations from SeaWiFS imagery.

Often these satellite sensors lack the required spatial resolution to fulfill the monitoring tasks for inland waters. Airborne data or higher resolution satellite data could be more appropriate. Giardino *et al.* [3] used Hyperion data to test the integration of Remote sensing derived products into the water quality monitoring programs of Lake Garda. In this study the spatial and spectral resolutions of Hyperion were considered highly suitable. Airborne datasets have been used to study various Finnish lakes. According to Kallio [7], Remote sensing can be a valuable tool, particularly in lake-dense regions where the number of lakes and the variation in the lakes is so high that only a small portion of them can be monitored using traditional in-situ methods.

To retrieve water quality parameters for these inland waters different models are available in the literature. They range from simple site-specific empirical algorithms to purely analytical. In the analytical approach the water constituent concentrations are physically related to the measured reflectance spectra using sophisticated radiative transfer models (e.g. Hydrolight). These radiative transfer models are being used for example to generate Look-Up-Tables and train sophisticated neural networks [10] to retrieve concentrations values.

The semi-analytical approach uses simplified bio-optical models which describe the relationship between water reflectance and the concentration of constituents and their Specific Inherent Optical Properties (SIOPS). A well known bio-optical model is the one developed by Gordon [4]. More recently Albert and Mobley [1] derived a new equation for the irradiance reflectance and remote sensing reflectance for deep and shallow water applications. These models are then inverted [5]

using e.g. a least squares or a curve fitting approach [8] to derive concentration values.

In this paper a few approaches based on these bio-optical models are tested to retrieve concentrations of TSM (Total Suspended Matter), CHL (Chlorophyll) and CDOM (Coloured Dissolved Organic Matter). In a first stage the optical properties of 2 different inland waters were studied. Next realistic APEX [6] (Airborne Prism Experiment) Remote sensing reflectances were simulated, which form the basis of the initial algorithm testing. This algorithm testing is part of the MICAS project and is planned to be further elaborated on calibrated APEX imagery, available in the second quarter of 2010.

2. STUDY AREA

To form a solid basis for algorithm testing two inland waters were chosen with clear distinct water properties:

- A river on the edge of its estuary at the port of Antwerp: The Scheldt, Belgium
- An oligotrophic perialpine lake: Lake Constance, Switzerland

The locations of these waters are given in Figure 1 and 2.

Figure 1: Location of the Scheldt study site

Figure 2: Location of the Lake Constance site

3. METHODOLOGY

3.1 Field Campaign

An intensive field campaign was organized on 18/06/2009 and 23/06/2009 on Lake Constance and the river Scheldt respectively. Water was sampled from vessels and pontoons ca. 50cm below the water surface. The water samples were stored in dark bottles and were kept cool using dry ice immediately after sampling. They were used for concentration measurements and to analyse the inherent optical properties in the lab. At discrete points the backscatter meter from Wetlabs was used and recorded backscattering information at three wavelengths: 440 nm, 595 nm and 780 nm.

3.2 Specific inherent optical properties

Water samples, taken during the field campaigns, were analysed in the lab for their component concentrations and optical properties. The specific absorption spectra of particles, non-algae particles and phytoplankton were measured using a LICOR integrating sphere attached to an ASD spectrometer following the methods described by Tassan and Ferrari [11] and REVAMP protocols [12]. To retrieve the CDOM absorption coefficient of the water samples, a beam attenuation of the filtered water was measured with Ocean Optics equipment in a transparent cuvet. As only dissolved matter is present in the filtered water, the attenuation spectra could be assumed to be equal to its absorption. Specific backscattering for the TSM was retrieved from in-situ *BB-3* measurements.

3.3 Simulations

Reflectance data were simulated using Hydrolight, the bio-optical model of Albert and Mobley [1] and the bio-optical model of Gordon [4]. The Hydrolight radiative transfer model calculates radiance distributions and related quantities like irradiance and reflectance for specified water, illumination and viewing conditions [9]. The ranges for the TSM, CDOM and CHL concentrations used in the simulations were chosen to be representative for the day of our field campaign. The selected ranges were:

Lake Constance: CDOM: 0.3 -> 0.45 m-1
CHL: 0 -> 2 µg/l
TSM: 0 -> 3 mg/l

Scheldt: CDOM: 1.1 -> 2.5 m-1
CHL: 0 -> 30 µg/l
TSM: 20 -> 150 mg/l

The same input concentrations were used for the simulations with the Gordon and Albert and Mobley models. The Gordon model is defined as follows:

$$R(0-,\lambda) = f * \frac{b_b(\lambda)}{a(\lambda)+b_b(\lambda)} \quad (1)$$

with $a(\lambda)$ the spectral total absorption coefficient at wavelength λ (m^{-1}), $b_b(\lambda)$ the spectral total backscattering coefficient at wavelength λ (m^{-1}) and f an empirical factor which depends on solar and viewing geometry.

The Albert and Mobley model starts from the Gordon model but adds an expression for the f-factor making this f-factor dependent on the optical properties, the solar zenith angle and the wind speed:

$$R(0-) = p_1(1+p_2x+p_3x^2+p_3x^3)(1+p_5\frac{1}{\cos\theta_s})(1+p_6u)x$$

with

$$x = \frac{b_b}{a+b_b} \quad (2)$$

$$\theta_s = Solar\,Zenith\,angle$$

$$u = wind\,speed$$

p1 = 0.1034
p2 = 3.3586
p3 = -6.5358
p4 = 4.6638
p5 = 2.4121
p6 = -0.0005

For algorithm testing (combination of semi-analytical model - Gordon or Albert and Mobley - and inversion procedure) realistic spectra were simulated with Hydrolight. For interpretation of the inversion
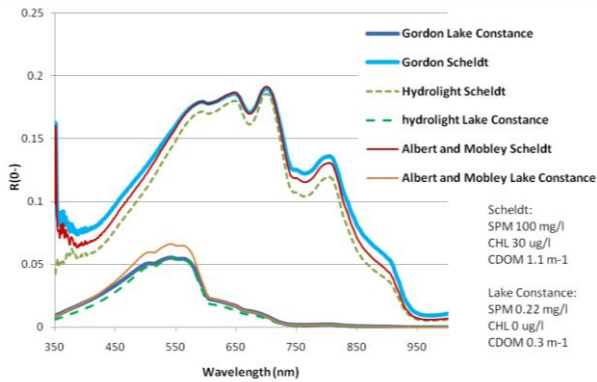

Figure 3: Simulated subsurface irradiance reflectances

procedure itself the semi-analytical models were used for both forward and inverse modeling. Figure 3 shows two sets of simulated subsurface irradiance reflectances (R0-), one for the Scheldt river, one for Lake Constance. Simulations were done with Hydrolight, the Gordon model and the model of Albert and Mobley.
After the simulations the reflectance data were resampled to APEX wavelengths.

3.4 Algorithm selection

A least squares and curve fitting approach was tested on the simulated data.

3.4.1 Linear Least Square Approach

In this approach the model of Gordon [4] was chosen as bio-optical model (1). The factor f was calculated according to Walker [13]:

$$f = \frac{1}{1+\dfrac{\overline{\mu_d(\lambda)}}{\overline{\mu_u(\lambda)}}} \quad (3)$$

μ_d is the average cosine of the downwelling light and μ_u the average cosine of the upwelling light.
The IOP $a(\lambda)$ and $b_b(\lambda)$ are linear functions of the constituents' concentrations and their SIOPS. Equation (3) can therefore be written as (omitting the wavelength dependencies of the factors) :

$$R(0-) =$$

$$f \cdot \frac{b_{bw}+TSM\cdot b_{b,P}^*}{a_w+g440\cdot\tilde{a}_{CDOM}+CHL\cdot a_{ph}^*+NAP\cdot a_{NAP}^*+b_{bw}+TSM\cdot b_{b,P}^*}$$

$$(4)$$

where

a_w the absorption of pure water (m^{-1})

b_{bw} the backscattering of seawater (m^{-1})

$g440$ CDOM absorption at 440 nm (m^{-1})

$\tilde{a}_{CDOM}$ CDOM absorption normalized by the absorption at 440 nm (m^{-1})

CHL the concentration of chlorophyll-a (mg m^{-3})

NAP the concentration of non-algal particles (g m^{-3})

TSM the concentration of suspended matter (g m^{-3})

$b_{b,p}^*$ the specific backscattering coefficient of marine particles (m² g^{-1})

a_{ph}^* the specific absorption coefficient of chlorophyll-a (m² mg^{-1})

a_{NAP}^* the specific absorption coefficient of non-algal particles (m² g^{-1})

For m number of wavelengths equation (4) can be written as a linear system of equations :

$$y = A \cdot x$$

with

$$A = \left[\frac{R(0-,\lambda)}{f} \tilde{a}_{CDOM,\lambda}, \quad \frac{R(0-,\lambda)}{f} a^*_{ph,\lambda}, \right.$$

$$\left. \frac{R(0-,\lambda)}{f} a^*_{NAP,\lambda} - b^*_{b,p,\lambda} \left[1 - \frac{R(0-,\lambda)}{f} \right] \right] \quad (5)$$

And

$$y_\lambda = -a_{w,\lambda} \cdot \frac{R(0-,\lambda)}{f} + b_{b,w,\lambda} \left[1 - \frac{R(0-,\lambda)}{f} \right]$$

with $\lambda = 1,...,m$

and

$$x = \begin{bmatrix} g440 \\ CHL \\ NAP \end{bmatrix}$$

To simultaneously estimate the concentrations of the water constituents a least-square approach was used for solving the system of linear equations.

3.4.2. Curve fitting approach

In the curve fitting approach TSM, CHL and CDOM concentrations ($\hat{c}$) are estimated by minimizing the error between modeled ($\hat{R}$) and measured (R) spectra. In this approach both the model of Albert and Mobley and Gordon was used in the minimization. The measured spectra (R) are replaced by the simulations to have full control over the inputs. The algorithm starts with a set of initial concentrations values for CDOM, TSM and CHL. The optimizer then calculates the RMSE between simulated (R) and modeled ($\hat{R}$) spectra and subsequently adjusts the input concentrations ($\hat{c}$) until a minimum RMSE is obtained.
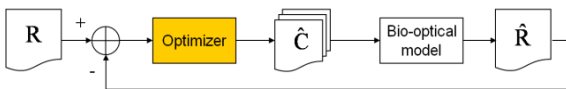

Figure 4: Curve fitting procedure

4. RESULTS AND DISCUSSION

As a first test the curve fitting and least squares approaches were tested using the same model for forward and inverse modeling. This allows us to look into the errors due to the inversion procedure itself. The results for the TSM concentrations for the two study sites are shown in Figures 5 and 6. For both study sites the two approaches perform almost perfect. The results for the CHL and CDOM estimations were similar.
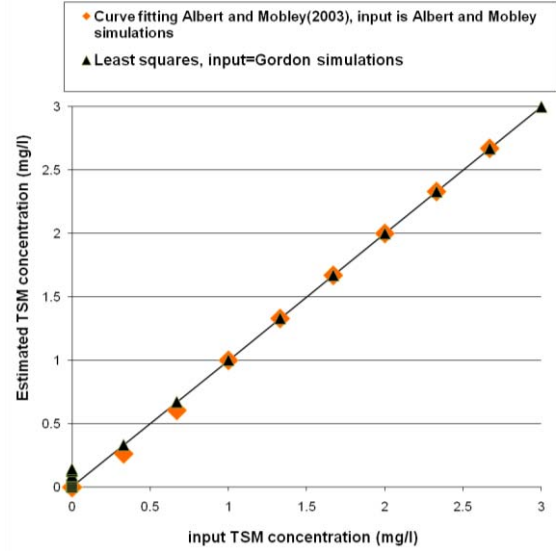

Figure 5: Intercomparison of Least squares and curve fitting approach for Lake Constance using the Gordon and Albert and Mobley bio-optical models for forward simulation and inverse modeling.
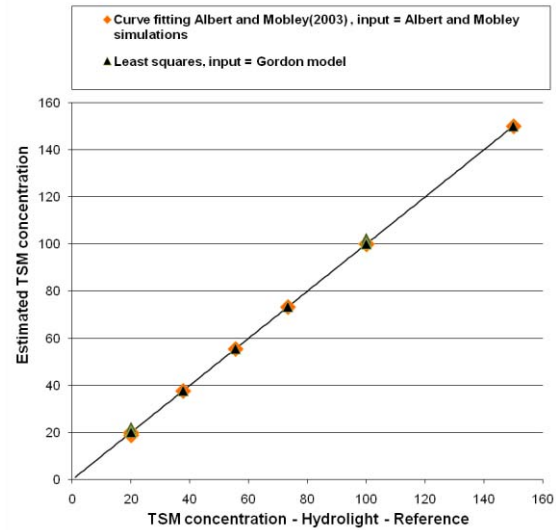

Figure 6: Intercomparison of Least squares and curve fitting approach for the Scheldt using the Gordon and Albert and Mobley bio-optical models for forward simulation and inverse modeling.

In a second step, the Hydrolight simulations were used as input. The results are shown in Figures 7 and 8.
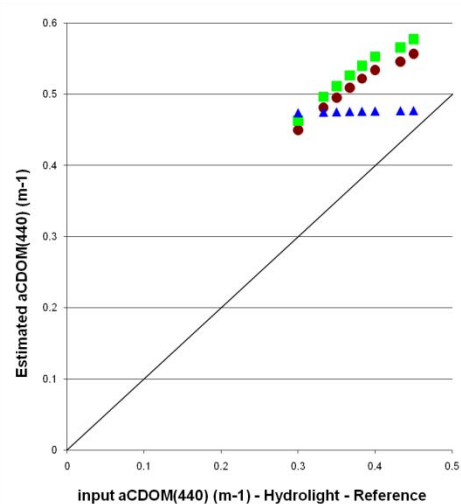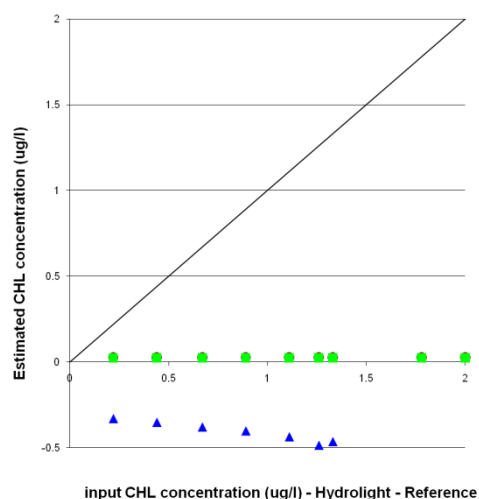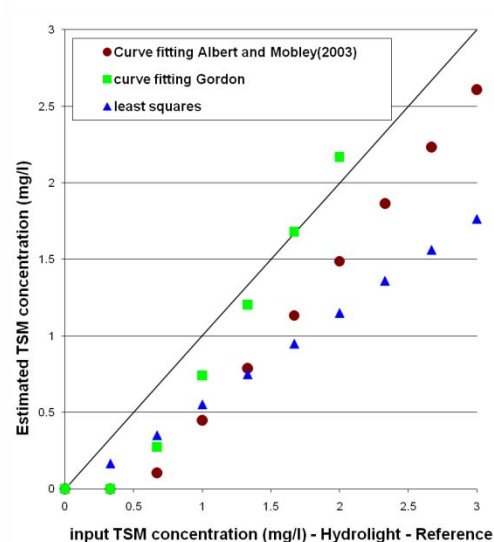
Figure 7: Intercomparison of Least squares and curve fitting approach for Lake Constance using Hydrolight simulations.
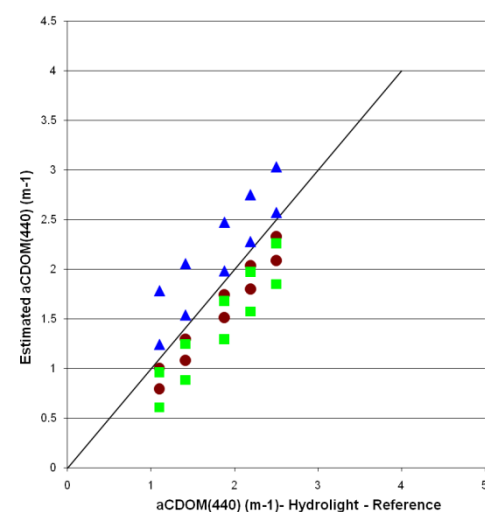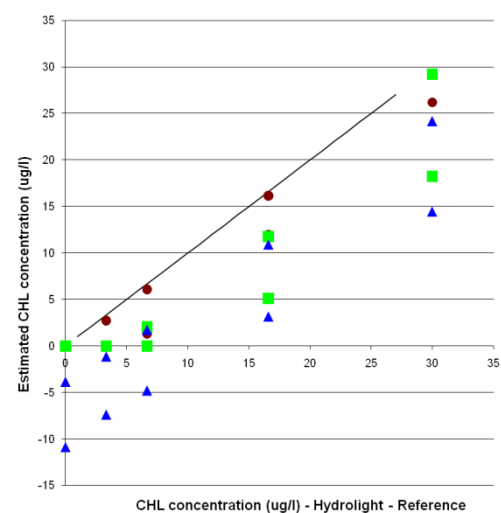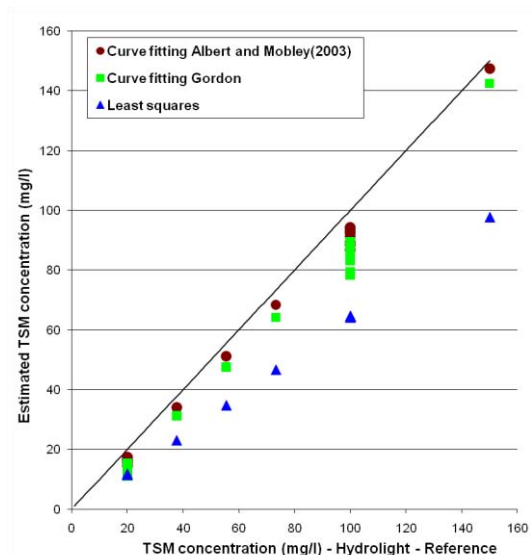

Figure 8: Intercomparison of Least squares and curve fitting approach for the Scheldt using Hydrolight simulations.

For Lake Constance none of the inversion procedures performs better than the others. All procedures are able to estimate the TSM concentration within reasonable error margins. They all fail however to estimate the 0 to 2 µg/l CHL concentration. The Least squares approach even results in negative CHL concentration values. The CDOM concentration is overestimated by all three approaches. For the Scheldt River, the Albert and Mobley curve fitting outperforms the other procedures for all three constituents. For these higher CHL, CDOM and TSM concentrations the Albert and Mobley performs very well. In particular for the CHL estimations, the Gordon model seems to be less suited. For both CHL and CDOM the least squares inversion performs worst and for low CHL concentrations the procedure results in negative CHL estimations.

Overall the least squares approach seems to be least suitable to derive concentration values for CDOM, CHL and TSM. This approach is restricted to linear forward models only, in which case an analytical expression can be found. One of the problems of this approach is the presence of negative concentration values when applying to realistic data. A curve fitting technique, where non-linear models can be used, is therefore preferred. Particular for the Scheldt dataset, with higher CHL, TSM and CDOM concentrations, it is suggested to have an f-factor which is dependent on the SIOPS, wind speed and solar zenith angle as is the case for the Albert and Mobley model.

Further research includes the development of a new minimization criterion for curve fitting. Modeled and simulated spectra will be wavelet transformed. Instead of minimizing the difference between modeled and simulated spectra using a simple RMSE, the RMSE will be combined with specific wavelet features. Several types of errors and noise will be added to the simulated spectra to find robust features.

5. ACKNOWLEDGEMENT

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