

MAPPING WATER CONSTITUENTS IN LAKE CONSTANCE USING CHRIS/PROBA

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ABSTRACT

CHRIS-PROBA data were acquired at 3 days in 2003 and one day in 2004 at the Eastern part of Lake Constance. Field campaigns were organised at these days in order to measure optical parameters of the water and the atmosphere and concentrations of water constituents from ship for validation. Five deep water sampling stations were chosen. The modular inversion program (MIP) developed by Heege, Miksa and Kisselev was used for the coupled retrieval of water constituents and aerosol concentrations, for atmospheric and water surface corrections and for optical closure and sensor calibration tests. Different viewing angles of CHRIS images of 2003 were used to test the atmospheric correction algorithm. Spectra were calculated and adjusted to the measured ones by fitting the concentrations of 3 aerosol types (rural, maritime, urban) and 3 water constituents (suspended matter, chlorophyll, Gelbstoff). The resulting mean relative error for suspended matter is 17%, for chlorophyll it is 28% which is within the error margin of the measurements. Maps of chlorophyll, suspended matter and Gelbstoff were generated for all viewing angles of CHRIS/PROBA where sunglint contamination is absent. By comparing these maps the accuracies of the resulting water constituents are determined. Looking at one pixel from different angles, the water constituent concentration is supposed to be the same. The mean relative error for each sampling station is 37% for chlorophyll and 24% for suspended matter. A more detailed statistical analysis is in preparation.

1. INTRODUCTION

The development of remote sensing algorithms for inland waters has a long tradition at Lake Constance. Due to the good research infrastructure and the well-studied biological, physical and optical properties, the lake is a nearly perfect site for algorithm improvements and validation activities.

Actually, the main problem of remote sensing of inland lakes is the atmosphere. There exists no operational software for sensors on satellite and aircraft which corrects automatically and reliably the atmospheric influence. Such a program is actually being developed at DLR and TUM in cooperation with the Russian Academy of Sciences. Basis is a software which has been developed for analysis of data from the airborne sensor DAEDALUS [1, 2]. It was re-designed as a generic, sensor-independent program, which is now in the testing and optimisation stage. The paper presents first results for CHRIS, obtained with the actual version of this Modular Inversion Program (MIP). Particularly, the potential of CHRIS is investigated for determining the concentrations of the water constituents chlorophyll, suspended matter, and Gelbstoff.

2. MATERIALS AND METHODS

2.1 Optical in-situ data

In water. Three TriOS RAMSES submersible radiometers (www.trios.de) were used for optical measurements in the water: one for measuring upwelling radiance spectra (L_u), one for upwelling irradiance (E_u), and one for downwelling irradiance (E_d). Each sensor has 190 useable channels from 320–950 nm, i.e. the spectral sampling interval is 3.3 nm. The three instruments are mounted on a frame such that their optical axes are aligned parallel to each other and the three entrance optics are on the same level. Also a pressure and a tilt sensor are attached to the frame in order to measure depth and inclination. All devices are connected to a control unit which ensures that all measurements are made simultaneously. The measurements were performed in 0.5 m depth at a distance of 3–4 m from the ship's bow which was oriented into the direction of the sun.

Atmosphere. The optical density (OD) of the atmosphere was measured using two Microtops II

instruments (www.solar.com). A Sunphotometer was used to measure OD at 380, 440, 500, 675, and 870 nm, and a Ozonometer to determine OD at 305, 312, 320, 936, and 1020 nm. The aerosol optical thickness (AOT) at 380, 440, 500, 675 and 870 nm was calculated by correcting for ozone and water vapour, whose concentrations were derived from the Ozonometer data, and for Rayleigh scattering.

2.2 Biochemical in-situ data

The water samples were collected from ship using a Ruttner bottle of 1 m length in 0.5 m and 2.5 m depth, i.e. the average concentrations of the depth ranges 0-1 m and 2-3 m were obtained. The analysis was done by two independent laboratories at the University of Konstanz (KN) and the Biologiebüro Weyhmüller (BBW).

CHL. Pigment concentration CHL was measured photometrically as the sum of chlorophyll-a and pheophytin-a after the method of Nusch [5]. Depending on the concentration of particulate matter, a defined volume of water (0.5 to 3.0 l) was filtered directly after sampling through a glass fibre filter, which retains particles larger than ca. 1 μm . The KN laboratory uses as filter Schleicher & Schuell No. 6 VG, BBW uses Whatman GF/F. The pigment-loaded filters were stored in cooling boxes for few hours until the end of the campaign. Then, in the laboratory, they were either immediately analysed, or further stored in a refrigerator at -18°C . The samples were always kept in darkness from the beginning of the filtration process on. The analysis started with pigment extraction in hot ethanol (90 %). The BBW laboratory treated the samples with ultrasonic in order to enhance the yield and performed a centrifugation of the solution in order to separate particulate matter; these steps were not made at the KN laboratory. The transmission of the solution was measured in a 10 cm cuvette at 665 and 750 nm using a photometer. After treating the solution with hydrochloric acid (2 mol/l HCl), which converts chlorophyll-a into pheophytin-a, the transmission was measured again at the same wavelengths. From the transmission measurements and the filtration volume the concentrations of chlorophyll-a and pheophytin-a were calculated using the equations in [5].

TSM. For measuring total suspended matter, a defined volume of water (0.5 to 3.0 l) was filtered directly after sampling through a pre-weighed glass fibre filter, which retains particles larger than ca. 1 μm . The KN laboratory used as filter Schleicher & Schuell No. 6 VG (preheated), BBW uses Whatman GF/F (not preheated). The filters were transported in a cooling box to the laboratory and stored at about -18°C for some hours to few days. Then they were dried in an oven for 2 hours at 105°C and weighed. The difference between this weight and the pre-weighed filter gives the TSM

mass. Normalisation with the water volume yields TSM concentration. The inorganic fraction of TSM was determined by combusting the dried filter for 4 hours at 550°C and weighing the filter once more.

YS. Concentration Y and spectral shape S of Gelbstoff (also termed dissolved organic matter (DOM), dissolved organic carbon (DOC), yellow substance, or gilvin) was measured as follows. The water samples were filtered using pre-rinsed membrane filters of 0.2 μm pore size (Sartorius Type 11307). The filtered water was stored in glass bottles in darkness in a cooling box for some hours. Then, spectral measurements were made using a Perkin-Elmer Lambda-2 dual-beam spectrophotometer and two quartz cuvettes of 5 and 10 cm pathlength. At both pathlengths the transmission of each sample was measured from 190 to 1100 nm at a sampling interval of 1 nm. The ratio of the two transmission spectra was converted into absorption of water plus Gelbstoff using the Lambert-Beer law. The Gelbstoff absorption spectrum $a_Y(\lambda)$ was calculated by subtracting the absorption spectrum of pure water. Two parameters were derived from this spectrum: absorption at 440 nm (Y) as a measure of concentration, and spectral slope S as an indicator of the wavelength-dependency. Both parameters were calculated by linear regression of $\ln a_Y(\lambda)$ from 420 to 460 nm; the logarithm accounts for the nearly exponential wavelength dependency of $a_Y(\lambda)$.

2.3 CHRIS-PROBA data

PROBA is a small ESA satellite launched on 22 October 2001. The instrument payload includes the Compact High Resolution Imaging Spectrometer CHRIS, which is both a hyperspectral and multi-angle sensor. It has a ground sampling distance of 17 m at nadir and covers the spectral range from 400 to 1050 nm with a spectral sampling interval between 1.25 and 11 nm. CHRIS is operated in different modes. Our data were acquired in mode 2 ("water mode"), which provides images of 766 x 748 pixels at full geometric resolution and 18 spectral channels, whose gains are adjusted individually such that the dynamic range is suited for water targets. The center wavelengths (nominally at 410.5, 442.4, 490.2, 509.6, 529.6, 561.2, 569.8, 590.4, 622.0, 650.7, 671.7, 679.9, 685.6, 706.3, 755.3, 780.8, 872.1, 1019.0 nm) of different overpasses may differ by a few nanometers due to temperature effects of the sensor. For each overpass we received 5 images at along track angles of 0° , $\pm 36^\circ$ and $\pm 55^\circ$. More information about CHRIS is available at <http://www.rsac1.co.uk/chris/>.

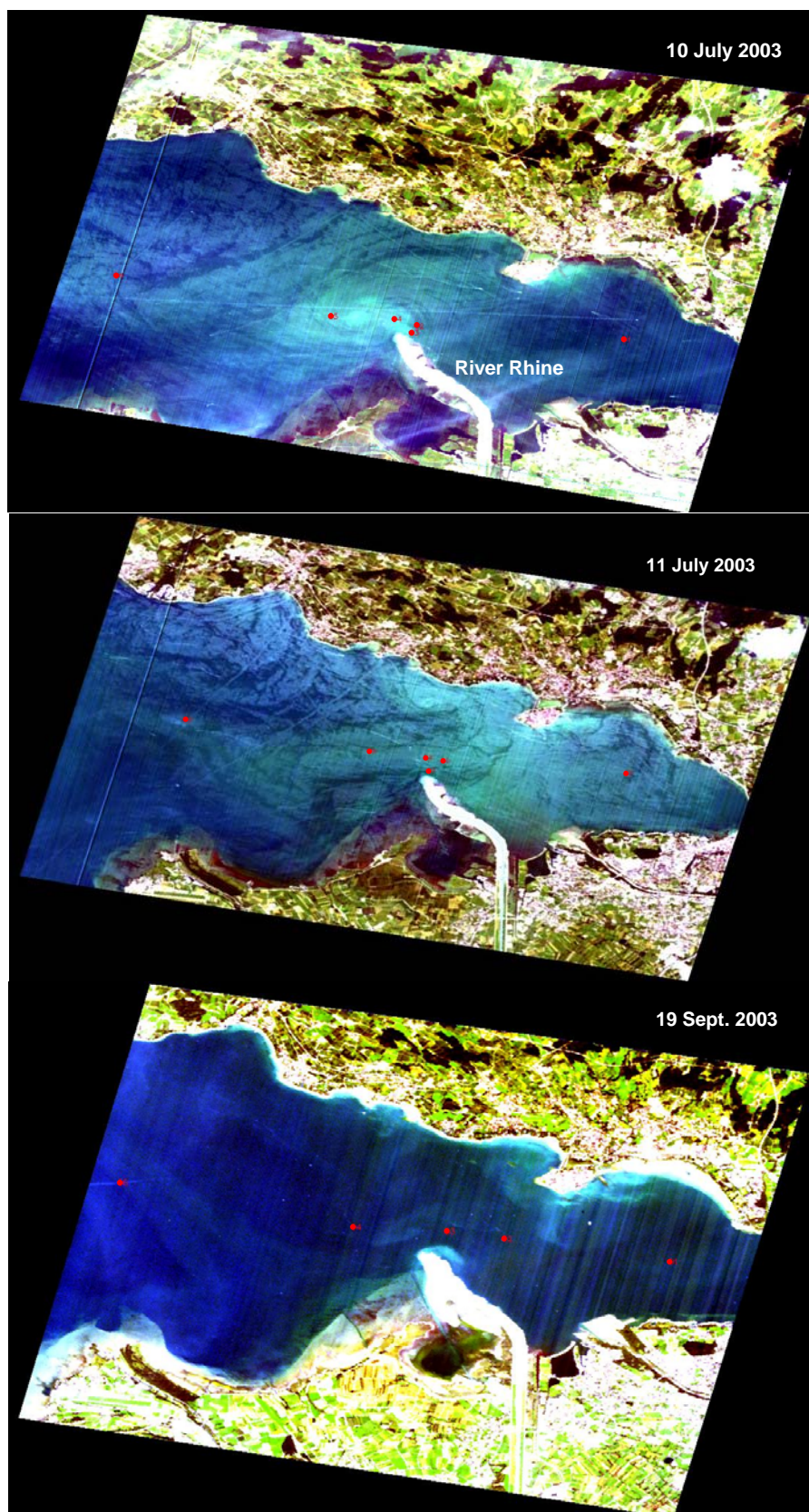


Fig. 1: CHRIS images from Lake Constance and sampling positions (red circles).

3. DATA SET

3.1 Test site

Lake Constance (Bodensee) is a pre-Alpine lake, which is shared between Germany, Switzerland, and Austria. It serves as drinking water reservoir for about 4 million people and as important recreation area. After water quality had decreased towards the eutrophic state at the end of the 1970ies, the lake is now on its way to re-oligotrophication after sewage diversion and waste water treatment in the catchment area. With an area of 571 km² it is the third largest lake in Central Europe. The length is 63 km, the maximum width 14 km, the maximum depth 254 m. The river Rhine, which passes the lake, is the main inflow and outflow. It imports significant amount of mineral particles.

3.2 Available data

Three CHRIS data sets à 5 look angles are available for 2003 and four data sets for 2004. Each image was destriped by J. Settle (ESSC) and

were performed at 6 to 8 stations. Water samples were taken in 2 depths at each station (at 0.5 and 2.5 m). A duplicate determination of the concentrations of pigment (CHL = sum of chlorophyll-a and phaeophytin), total suspended matter (TSM), and Gelbstoff (YS) was performed on 10, 11 and 19 July 2003 by two independent laboratories.

3.3 Situation at the CHRIS overflight days

The atmospheric conditions were quite different for the three days in 2003, while the concentrations of water constituents were similar. The variability of each constituent was low at each day, i.e. less than a factor of 2.

Although there was no large variability in water constituents, all three CHRIS images of Fig. 1 show distinct patterns in the lake which can be attributed clearly to the water body, e.g. on 10 July the two gyres near the mouth of the river Rhine, or on 11 July the greenish coloured regions. This indicates that CHRIS is suited to monitor concentration values typical for Lake Constance and small concentration differences.

Table 1. Data set collected in 2003 and 2004. X = used in this study, x = additional data, – = not measured.

Parameter	Sensor	July 10 2003	July 11 2003	Sept. 19 2003	April 22 2004	June 17 2004
L _u (TOA)	CHRIS-PROBA	x	X	X	x	X
Ship coordinates	GPS	X	X	X	X	X
L _u ⁺ , E _d ⁺	ZEISS MCS	x	x	x	-	-
L _u ⁻ , E _u ⁻ , E _d ⁻	TriOS RAMSES	x	x	X	-	-
OD Atmosphere	MICROTOS	X	X	X	X	X
CHL	Photometer	2X	2X	X	-	-
TSM org., inorg.	Balance	2X	2X	X	-	-
YS absorption spectrum	Dual-beam spectrophotometer	X, x	X, x	X	-	-
Detritus absorption	Integrating sphere	x	x	x	-	-
a*(λ) Phytoplankton	Integrating sphere	x	x	x	-	-
Secchi depth	Secchi disk	X	X	X	-	-
CTD	Multisonde	–	–	x	-	-
Photo	Digital camera	x	x	x	x	X

geometrically corrected using ground control points. Validation campaigns were performed on five of these days. On July 14 2004 too many cirrus clouds were present to deliver exact validation. On the other two dates in 2004 only atmospheric properties were validated. Optical and biochemical in-situ data were measured from ship at all days in 2003. Table 1 gives an overview on the collected data. Only a part of the data is used and described in this paper (marked as "X" in Table 1); the other data are mentioned for completeness, but no description is given here.

The research vessel "Robert Lauterborn" of the University of Constance and the RV "Thienemann" of the Institute for Lake Research in Langenargen were used for the campaigns. Ship measurements

4. MODULAR INVERSION PROGRAM

The Modular Inversion Program (MIP) is a processing and development tool designed for the recovery of hydro-biological parameters from multi- and hyperspectral remote sensing data [2,3]. A flow chart is shown in Fig. 2. The architecture of the program consists of general and transferable algorithms based on physical inversion schemes that derive bio-physical parameters from the measured radiance signal at the sensor. Inverted parameters include e.g. the variable constituents of the atmosphere, the concentration of water constituents and the reflectance characteristics of substrates in shallow waters.

Table 2. Conditions at CHRIS overpasses.

Parameter	10 July 2003	11 July 2003	19 Sept. 2003
Overflight time of CHRIS (local time)	12:40	12:52	12:48
Sun zenith / azimuth angle (°)	28 / 149	28 / 149	47 / 163
CHRIS zenith / azimuth angle (°)	5 angles	5 angles	5 angles
Aerosol optical thickness at 870 nm	0.155	0.064	0.082
Aerosol Angström exponent	0.82	1.63	1.52
Number of stations in CHRIS	6	6	5
Secchi depth (m)	2.9 – 3.5	2.9 – 4.5	3.1 – 3.9
CHL (µg/l)	1.8 – 3.3	1.4 – 2.6	2.6 – 4.4
TSM (mg/l)	1.5 – 2.6	1.1 – 2.0	1.4 – 1.8
Y (m ⁻¹ at 440 nm)	0.13 – 0.20	0.15 – 0.23	0.23 – 0.30
S (nm ⁻¹ at 440 nm)	0.013 – 0.019	0.011 – 0.014	0.009 – 0.012

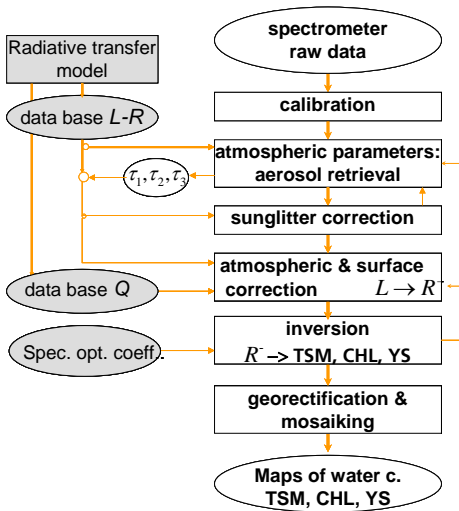


Fig. 2: Flow chart of the Modular Inversion Program MIP.

Various program modules are implemented for the inversion and processing of remote sensing data. These modules are partly iteratively coupled. The internal structure of MIP is also modular, so that a separate treatment of different functions is possible. The most important internal modules are libraries of algorithms and optimisation methods, functions

for the interaction of different databases, and program-user-dialog functions.

Different program modules exist for the retrieval of aerosols, atmosphere and water surface corrections, the retrieval of water constituents [1,2] in optically deep waters or bottom coverages in shallow water areas [3,4].

In present applications, two radiative transfer databases are used for the aerosol retrieval: the atmospheric correction and the bi-directionality correction of the underwater light field. The databases are generated by a radiative transfer model. Radiative transfer is simulated in a coupled, plane-parallel atmosphere-ocean system, currently by use of the FEM-method [6]. The model calculates radiances in a vertically inhomogeneous (multilayer) atmosphere-ocean system with respect to all angle dependencies of the sun and observer geometry.

Both databases were calculated with optical parameters for a mid-latitude summer standard atmosphere. The first database was generated for an atmosphere-ocean system with a Lambert reflector of defined reflection R_L at 1 cm depth. Therefore, for the first database the underwater radiance was assumed to be isotropic. The water surface was

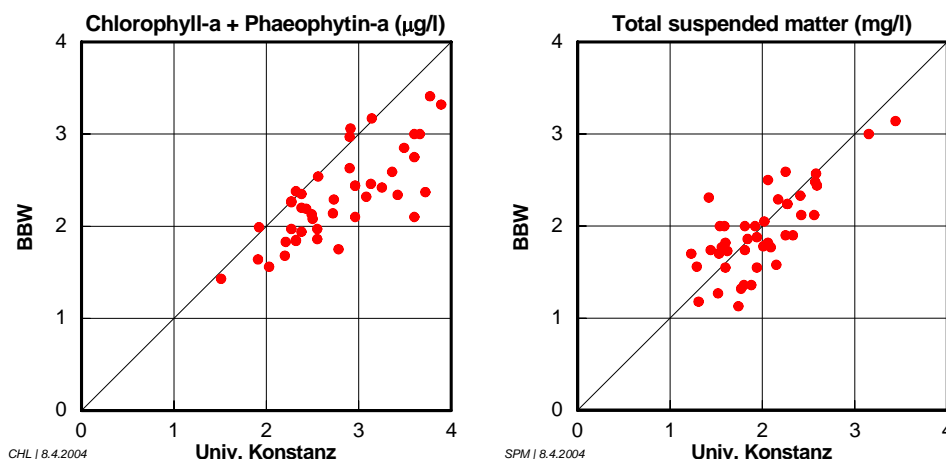


Fig. 3: Comparison of CHL and TSM values obtained by two independent laboratories.

modeled as flat, so that no sun glitter contributed to the upwelling radiances. The free parameters of the database are three types of aerosols τ_1 , τ_2 , τ_3 (continental, maritime, urban), each with 4 optical depths between 0.01 and 0.5 (at 550 nm), 7 reflection values for $R^-_L(\lambda)$ between 0 and 0.6, 17 observer altitudes h , 17 azimuth differences $\Delta\phi$ between sun and observer, 8 sun zenith θ_{sun} and 8 observer zenith angles θ . The main data base contains 3 wavelength regions with different resolutions. The second database is needed to correct the artificial Lambert reflectance values R^-_L for the bi-directionality of the underwater light field to $R^- = E_{up}/E_{down}$ by $R^- = R^-_L \pi/Q$. Values of $Q = E^-_{up}/L^-_{up}(\theta, \phi)$ were calculated with a standard atmosphere as described above, but with a fixed medium aerosol concentration and an expanded water body. Q is calculated as function of $\lambda, h, \Delta\phi, \theta, \theta_{sun}$ and the water constituent concentrations.

5. RESULTS AND DISCUSSION

5.1 Accuracy of in-situ data

In order to estimate the accuracy of the concentrations of water constituents, a duplicate determination of CHL and TSM was performed for 44 samples from 10, 11 and 19 July 2003 by two independent laboratories (KN, BBW). Water samples were taken in two depths (0.5 m, 2.5 m) at 6-8 stations each day. The comparison of the obtained concentration values is shown in Fig. 3.

CHL. The CHL values obtained at KN are on average 19 % higher than those measured at BBW. If this systematic effect is corrected by dividing all KN values by 1.19, the relative differences $|KN-BBW| / 0.5 |KN+BBW|$ range from 0 to 36 % at an average of 11 %. If, alternately, the mean of the KN and BBW values is taken as correct value, the relative differences range from 0 to 52 % at an average of 19 %. Thus, the in-situ CHL values of an individual laboratory may have a systematic error in the order of 20 %; the statistical error is also ~20 %.

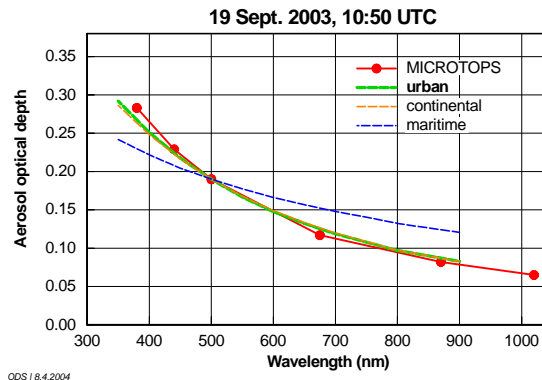


Fig. 4: Aerosol selection for forward calculation.

TSM. No significant systematic difference exists between the two laboratories. The relative differences range from 0 to 48 % at an average of 15 %. Thus, the statistical error of TSM is in the same order as that of CHL

5.2 Forward calculation

The initial step of using MIP, irrespective of making forward calculations or inverse modelling, is to reduce the two data bases to smaller mission data bases. This is accomplished by using the geometric and flight information given of the recorded scene.

The main parameters which have to be taken into account are flight heading, pitch angle and the position of the sun. Regarding the pitch angles, some difficulties have arisen as the calculation of the angles under which CHRIS had recorded the images proved to be difficult. Therefore, an error for the length of path through the atmosphere cannot be excluded.

Forward calculations in MIP require six input parameters. The water body is parameterised by the concentrations of pigment (CHL), total suspended matter (TSM), and Gelbstoff (Y). The atmosphere is parameterised by aerosol optical depths τ_a of maritime, rural and urban aerosol.

- First step is the calculation of the subsurface irradiance reflectance, R^- , which utilises the analytical equation of Albert [7] for optically deep waters with based on the inherent optical properties absorption, a , and backscattering, b_b . Both are additive, i.e. the contributions from pure water and all optical active water constituents have to be added. MIP includes a data set of consistent inherent optical properties from Lake Constance [1,2]. The second step is conversion of R^- to remote sensing reflectance $R^-_L = R^- Q(\lambda, \Delta\phi, \theta, \theta_{sun}, CHL, TSM, Y)/\pi$ by accounting for sun and viewing geometries using the Q data base.
- The third step is conversion to radiance at sensor altitude, L , using the L-R database.

Forward calculations were performed for 19 Sept. 2003 for the five stations within the CHRIS image and the five viewing angles of CHRIS. For calculating R^- and R^-_L , the in-situ data of CHL, TSM, Y from the five stations were taken. For calculating the atmospheric influence, the aerosol type was determined by analysing the OD measurement of the Microtops sun photometer at the time of the CHRIS-PROBA overflight. Fig. 4 shows the comparison between this measurement and the normalised OD spectra of the three aerosol types included in MIP. It can be seen that the

measurement reveals a slightly steeper increase from long to short wavelengths than any of the three aerosol types. The closest agreement yields urban aerosol, hence this aerosol type was used for forward calculation. Its optical thickness was set to the value of the measurement, $\tau_a(870) = 0.082$

5.3 Inversion

Inverse modelling is accomplished by calculating a theoretical spectrum using a set of initial values for

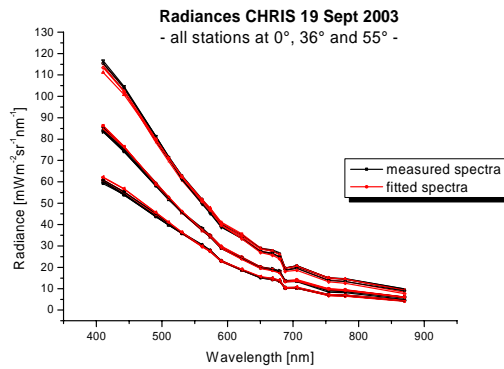


Fig. 5: Comparison of measured and fitted TOA radiances

the required six parameters. Assumed water constituent concentrations are converted into subsurface irradiance reflectance R^- . A bi-directional correction for the underwater light field is applied to calculate R^-_L using the Q database. Using assumed aerosol optical thicknesses of the three aerosol types urban, rural and maritime, radiances at sensor altitude, L , are calculated and compared to the measured spectra. The retrieval is divided into three parts. The first part retrieves aerosol concentrations and suspended matter concentration in the wavelength region above 750 nm. Then this approximation of atmospheric parameters is used to retrieve water constituents in the region below 750 nm. The last step is to use the whole wavelength region and all parameters to check the retrieved values.

The set of parameters is changed until the difference between measured and modelled spectra is minimal. Since there exist an extreme large number of possible parameter combinations, an effective algorithm of the iteration process has to be used to select a new set of parameter values from the previous set. MIP uses the downhill Simplex method [9, 10]. As the success of the minimisation method depends on the initial values, it is important to achieve reasonable first approximations of water constituent concentrations and aerosol optical thickness. If water constituent concentrations and aerosol optical thickness from previous optimisations of surrounding image pixels exist, their mean value is taken as initial value.

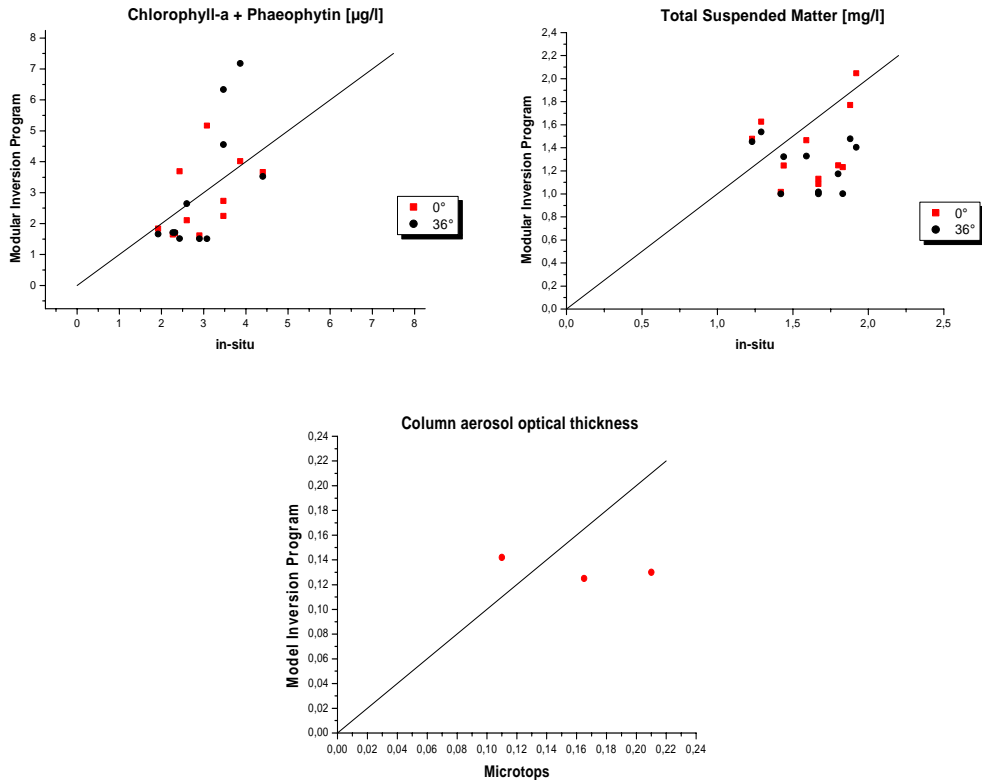


Fig. 6: Comparison of fitted parameters with in-situ values.

Otherwise, a routine for the search of start values is initialised. In the 6-dimensional parameter space of the database some combinations are statistically chosen and the inversion is started from all these grid points. The region with the majority of points is taken as the region where the absolute minimum is searched. The borders of this region are determined and a set of parameters inside this region is chosen as start values.

For testing inversion, the CHRIS image of 19 Sept. 2003 and 11 July 2003 were selected as no cirrus clouds were visible on this day. CHRIS spectra were extracted at all five stations by averaging 3 x 3 surrounding pixels. These served as input spectra for the inversion algorithm. The first two channels were ignored due to the results of forward calculation which indicated large differences between simulated and measured radiances (see section 5.2). Fig. 5 shows the comparison of top of atmosphere radiances between fitted and CHRIS spectra.

There is an overall reasonable agreement of magnitude and curve form. However, it is striking that the fitted spectra of the five stations differ much more than the CHRIS spectra. This points to a numerical problem of inversion, which is underpinned by Fig. 6. In this Figure all inversion results are plotted against the in-situ measurements of chlorophyll, suspended matter, Gelbstoff and aerosol optical thickness. All nadir scenes available for Lake Constance were used and all stations are accounted for. While TSM and Y values scatter around the 1:1 line, almost half of the fitted CHL values are outliers which drop to a concentration of 0.5 $\mu\text{g/l}$.

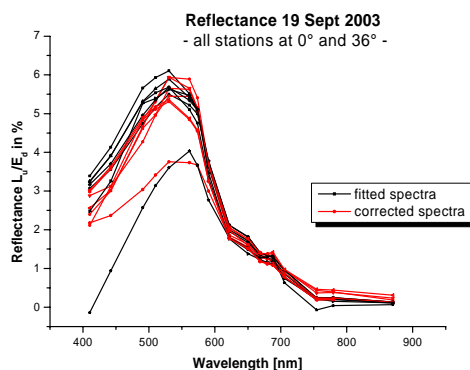


Fig. 7: Comparison of reflectance spectra

Fig. 6 shows that total suspended matter is retrieved in an acceptable way with a mean relative difference of 24 %, which is within the error margin of in-situ data. Improvements are necessary for chlorophyll; the mean relative difference is 33 %. Gelbstoff had to be kept constant. No conclusion can be drawn for aerosol optical thickness since the 3 data points are not enough for doing statistics.

A further test of inversion results is shown in Fig. 7. Calculated remote sensing reflectance spectra R_L (blue) are compared with atmospheric corrected spectra. The comparison is done for all five stations of 19 Sept. 2003 and 11 July 2003 and two images of CHRIS (nadir and 36°). A very good agreement is observed for wavelengths above 500 nm. A problem has arisen while correcting the spectra

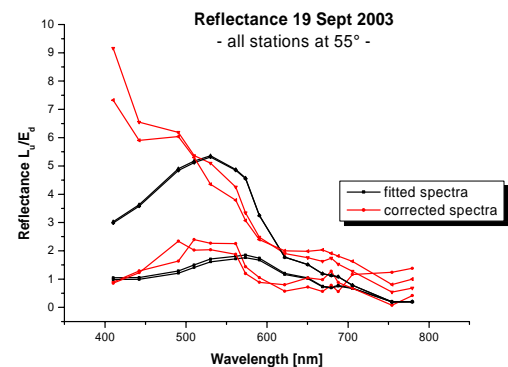


Fig. 8: Reflectance spectra of atmospheric corrected spectra and fitted spectra at 55° angle

from the steepest viewing angle of CHRIS (Fig.8). The atmospheric corrected CHRIS spectra are too variable for the algorithm to fit the reflectance spectra. This may be a hint that the volume scattering functions of our aerosol models are not sufficient for such great viewing angles.

5.4 Maps of chlorophyll and suspended matter

The resulting maps were retrieved using a constant atmosphere (Fig. 9-12). Gelbstoff wasn't retrieved but the in-situ values were applied. Land was masked but not the shallow water areas. 19 September 2003 the water was very homogenous whereas in 17 June 2004 structures were visible in the water. The intensities on the multi-angle images of one day are very similar. This is a very good sign that the atmospheric correction is correct. A more detailed statistical analysis is in progress.

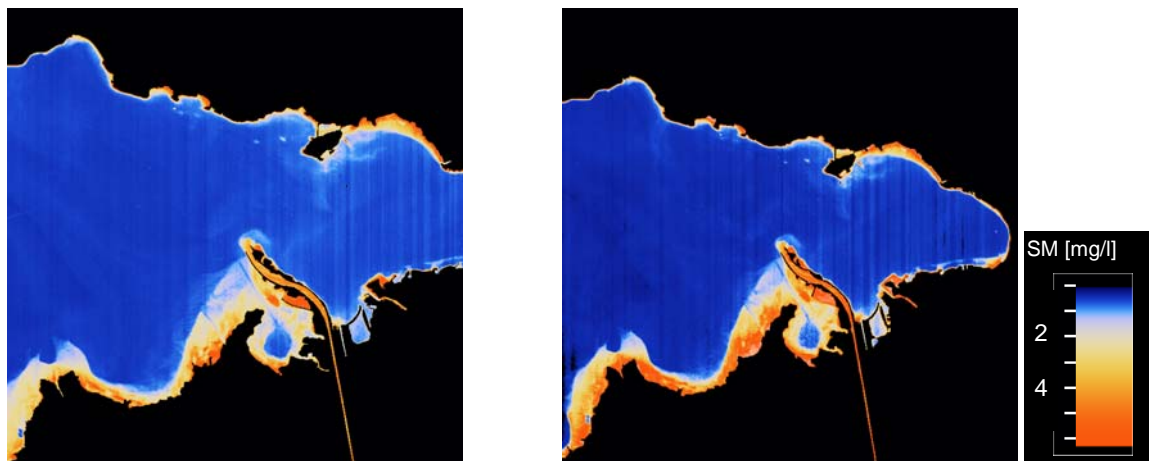


Fig. 9: Maps of suspended matter (SM) on 19 September 2003, land is masked, shallow water areas not masked

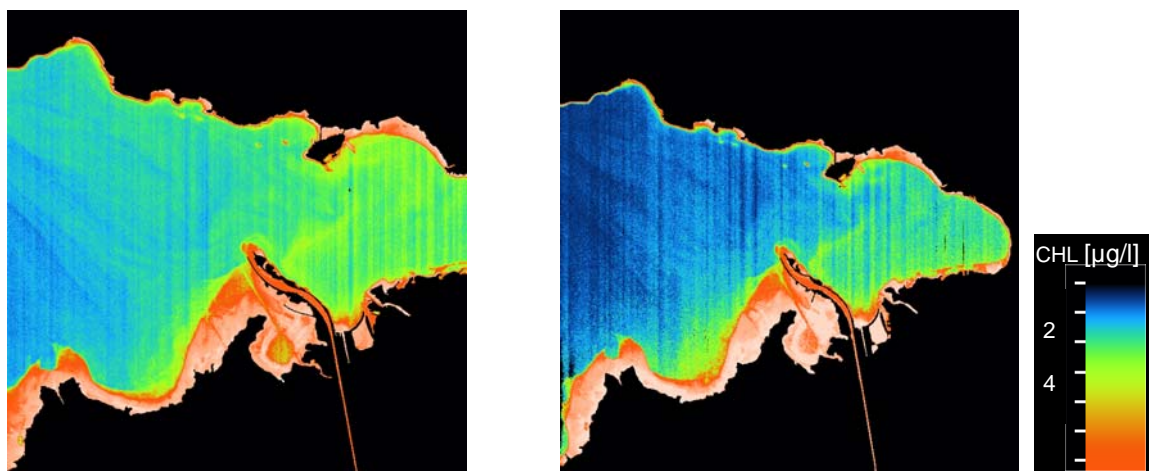


Fig. 10: Maps of chlorophyll on 19 September 2003, land is masked, shallow water areas not masked

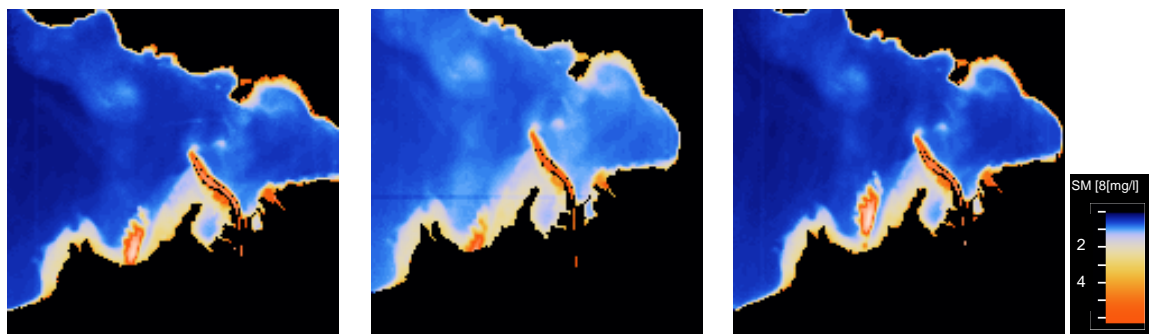


Fig. 11: Maps of suspended matter on 17 June 2004, land is masked, shallow water areas not masked

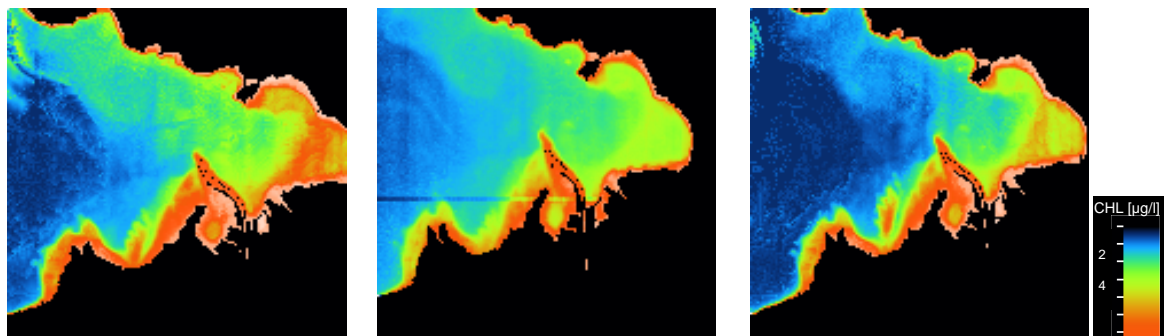


Fig. 12: Maps of chlorophyll on 17 June 2004, land is masked, shallow water areas not masked

6. SUMMARY AND OUTLOOK

Although CHRIS was not designed for ocean colour applications, its spectral coverage, radiometric resolution, and calibration accuracy are sufficient to derive quantitatively the concentrations of the water constituents total suspended matter and Chlorophyll or Gelbstoff from mode 2 data. The results for chlorophyll were not satisfactory, i.e. almost half of the retrieved concentration values were significant outliers at an unrealistically low concentration of 0.5 µg/l. However, we expect that also chlorophyll can be retrieved accurately if some improvements in calibration and modelling are made.

We will work on improving atmosphere correction. When this is done, we will repeat the presented analysis with focussing on chlorophyll retrieval. By comparing the results from different viewing angles, the accuracies can be determined and error sources can be identified.

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