

DETERMINATION OF COASTAL WATER PROPERTIES USING SATELLITE IMAGING SPECTROMETER DATA

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ABSTRACT

The difficulty of the remote sensing of coastal water is the presence of more than one constituent with high variability ranges, different correlation and spectral behavior. The constituents are superimposing in their influence on the resulting total spectrum. For the improvement of remote sensing of coastal zones it is not only necessary to build a new generation of sensors that offer spectrally higher resolved data, but one has also to develop a new methodology that allows the separation and determination of the water constituents based on the entire spectral signature of the different components of the water body. The imaging spectrometer MOS flying on the Indian remote sensing satellite IRS-P3 provides since March 1996 remote sensing data for the scientific community. In the paper the instrument and mission will be introduced. A new methodological approach was implemented to derive different case II water constituents as well as atmospheric turbidity for the application of MOS-data in coastal regions. A new point of the method is the uniform consideration of atmospheric and water related contribution to the remote sensing signal.

1. INTRODUCTION

If remote sensing of the earth's environment wants to contribute to the actual challenges of ecosystem research it has to move towards quantitative estimation of geophysical parameters of different objects and different scales. For coastal water this means the distinction between different classes of water constituents. Case 2 waters, typically found in coastal zones and river plumes, are characterized by higher chlorophyll concentrations and significant concentrations of inorganic suspended matter (sediments) and dissolved organic matter (gelbstoff). The task of remote sensing now is to use the different optical influences of the water constituents on the light spectrum to investigate and map the different constituents of the water body quantitatively. The advantage of the use of remote sensing technique is to get regularly data from large areas, which would be nearly impossible with in-situ ship measurements. The problem contains two sides. On the one side one must have the necessary measurement technology (e.g. imaging spectrometers with high spectral and radiometric resolution), on the other side an appropriate interpretation technology must be provided. The classical approach (CZCS, SeaWifs) with

atmospheric correction using one near-infrared band and color ratios from two or three bands for estimating chlorophyll concentration is no more possible because of the complex situation in case 2 waters. The paper will introduce both a multispectral imaging spectrometer (the Modular Optical Scanner, MOS) and a new method for interpreting the satellite data for case 2 waters (the Principal Component Inversion, PCI). The PCI is a multivariate regression technique basing on model inversion, which uses principal component analysis as an information extraction tool, for the interpretation of the atmosphere-ocean measurements. A new aspect of the algorithm is that a special atmospheric correction procedure is not more necessary. The consideration of atmospheric influence is implicitly included, equally with the water parameters.

2. THE MOS INSTRUMENT AND MISSION

The sensorics for remote sensing of ecosystems by plane or satellite has been dynamically developed in the last years. For this purposes in the DLR was developed the MOS system [Zimmermann 1996, Neumann 1995]. MOS was especially designed for remote sensing of the ocean-atmosphere system. It will be used on the Indian remote sensing satellite IRS-P3, which was successfully launched on March 21, 1996. In table 1 the main technical parameters of the MOS devices are listed. MOS consists of two spectrometers (MOS-A and MOS-B) and a CCD line camera (MOS-C) with medium spatial resolution and high radiometric precision. The MOS devices A and B are working by the principle of imaging spectrometer. The advantages of remote sensing experiments basing on this principle are:

- the high number of spectral channels
- the high spectral resolution of each channel
- the geometric identity of the spectral images.

The atmospheric spectrometer MOS-A measures in four channels in the oxygen absorption band (O_2 -A) at 760 nm. These measurements allow estimations of the atmospheric turbidity and the proof of stratospheric aerosols. The simultaneous measuring bio-spectrometer MOS-B is working in 13 spectral channels with a bandwidth of 10 nm in the visible (VIS) and in the near infrared (NIR) spectral range from 408 to 1010 nm for the investigation of ocean color. The MOS-C allows an additional investigation of the surface roughness of the ocean and the differentiation of cloud types.

The wavelengths of the spectral channels of MOS-B were chosen in opportunity of the spectral characteristics of the water constituents, to have the possibility to get quantitative definitions of concentrations. Here is the main effort in the development of algorithms for coastal zones, where the large number of spectral channels in the MOS is the assumption for the quantification of parameters concentrations. Otherwise there can be defined vegetation signatures („red edge“) and the atmospheric content of water vapor from absorption-measurements in the NIR.

The mission IRS-P3 is a common Indian-German experimental mission in the field of earth remote sensing. IRS-P3 is an abbreviation of Indian Remote Sensing Satellite, Polar launcher No 3. This satellite was launched on March, the 21, 1996 with the third test launch of an Indian rocket PSLV (Polar Satellite Launch Vehicle). The rocket, the bus and the launch facilities were putted at disposal by the ISRO (Indian Space Research

Organization), the DLR takes part in the scientific payload with the imaging spectrometer MOS. The payload consists of three devices :

- the Wide Field Sensor WiFS from the ISRO
- the Modular Optoelectrical Scanner MOS from the Institute of Space Sensor Technology of the DLR
- an X-Ray-experiment for radioastronomy from the ISRO.

The mission serves scientifically-technological and methodological experiments. Because of the pre-operational character of the mission there does not exist an on-board storage for the data. The receive is only real time possible over interesting areas in the radar view of ground stations. The control of the payload is performed by the control station in Hyderabad. The German Space Operations Center GSOC of the DLR works as a backup station and control center for the European receiving area.

Parameter	MOS-A	MOS-B	MOS-C
Spectral Range [nm]	755 – 768	408 – 1010	SWIR
No. of Channels	4	13	1
Wavelengths [nm]	756.7; 760.6; 763.5; 766.4 O ₂ A-band	408; 443; 485; 520; 570; 615; 650; 685; 750; 870; 1010 815; 945 (H ₂ O-vapor)	1600
Spectral halfwidth [nm]	1.4	10	100
FOV along track x [deg]	0.344	0.094	0.14
Across track [deg]	13.6	14.0	13.4
Swath Width [km]	195	200	192
No. of Pixels	140	384	299
Pixel Size x*y [km ²]	1.57x1.4	0.52x0.52	0.52x0.6 4

table 1 Modular Optical Scanner MOS-IRS

3. THE CASE 2 PROBLEM

In developing case 2 interpretation algorithms the main problem is to formulate the relationship between the spectrum of water leaving radiances and the corresponding concentrations of water constituents using as much spectral bands as available. This is nearly impossible to do on an empirical basis. Radiative transfer modeling is therefore the tool that can be used to solve the problem. This also has the advantage that an analytical approach can be developed. On the other hand the direct inversion of the problem mathematically is very complicated. Therefore indirect solutions and approximations have to be used. One possible way is the inverse modeling technique developed by Doerffer et. al. [Doerffer 1993, 1997]. This inversion technique is very consumptive with respect to computing power and convergence problems may occur. Due to that a simplification and a more straight forward computing strategy is needed, what lead to the neural network approach

A different approach was developed first for the MOS instrument by Krawczyk et. al. [Krawczyk 1993, 1995, Neumann 1995a] and forms the basis for the algorithms considered here. The main question is to systematically determine the weighted contribution of each available spectral band to the estimate of the desired geophysical

parameter, i.e. chlorophyll, gelbstoff and sediments. The idea is to derive a simple to realize relationship between the radiance spectra and the geophysical values based on radiative transfer modeling and information-theory analysis of the signal's multivariate statistics. Signal-to-Noise ratio and radiometric resolution of the measurements are accounted for their influence on the estimation accuracy during algorithm development. The analysis of the spectral and statistical information content of the MERIS data is done by principal component analysis (PCA) of well-defined simulated data sets. Through the applied specific optical model of the water body the inverse algorithm can be tuned or optimized for regional and seasonal specifics. The entire procedure of PCA and deriving the inverse estimation formulas is called Principal Component Inversion (PCI). In the result a computationally fast and robust technique for retrieving water constituents from remotely sensed data under case 2 conditions is available.

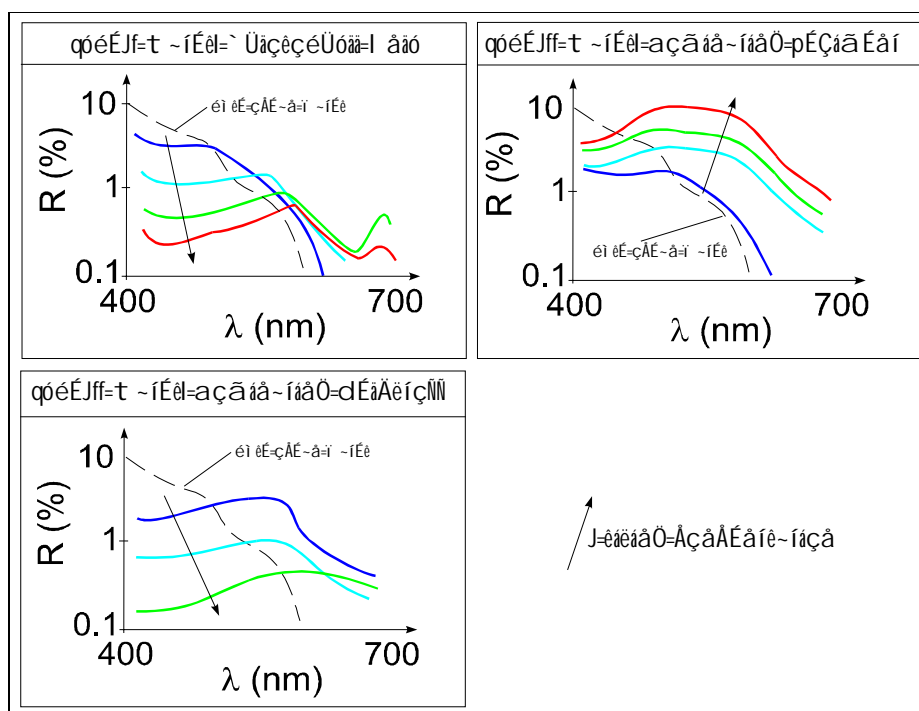


Figure 1: Influence of water constituents on reflectance spectra

The physical background determining the spectral signature of the remitted light from the water body are scattering and absorption processes caused by the water constituents and the water itself. For case 2 waters always two or more components are influencing the spectrum. For the following investigations of the case 2 water problem we are concentrating onto three main classes of constituents: Phytoplankton containing the chlorophyll (scattering and absorption), Gelbstoff or dissolved organic matter DOM (absorption) and suspended inorganic material or sediments (scattering). Figure 1 illustrates quantitatively the influence of these components on the reflectance spectrum. Due to the nearly total absorption of light by the pure water below 400 nm and above 700 nm only this limited range allows to assess water constituents. One clearly sees that no part of the spectrum can be related to the influence of one component only. In practice different mixtures and covariations of the constituents may occur for wide ranges of variability of each component making the inversion even more complicated. Especially in coastal regions and river estuaries high concentrations of suspended matter may mask the

influence of other constituents. This leads to limits for the discriminability and retrievability of different water constituents. However, the decomposition of the components is possible in many of the cases of coastal water if:

- a sufficient number of spectral bands are available in the instrument (number of bands is large compared to the number of parameters to be estimated)
- sufficient spectral coverage (VIS → NIR)
- a specific biooptical model based on inherent optical properties (IOPs) and/or experimental data is available

In a more general sense this described situation for case 2 waters obviously causes limitations for the applicability of the “classical” color ratio algorithms since they are not able to separate the single components and may be heavily influenced by the cross-correlation between them. Thus multiband or even hyperspectral retrieval algorithms are needed. Although, of course, the signals in different spectral band will not be uncorrelated each band contributes information that allows the distinction and quantification of the parameters. To build such kind of algorithm is the attempt to assess not only radiance/reflectance values in the single bands but *the shape of the spectral signature* as an additional information.

4. ALGORITHM DESCRIPTION

Since the more complicated state of case 2 water requires the estimation of more than one water constituents simultaneously each of them influencing the spectral behavior of the investigated water body in a different manner with additional overlaying and masking effects, the major goal was to derive an algorithm that implies the following features:

- estimation of a multiple parameter set p
- discrimination between parameters
- simple to implement
- fast in use for the processing of huge data sets.

As the simplest approach therefore a linear estimation between the measured TOA satellite radiance data L and the parameter p was chosen.

$$\hat{p}_i = \sum_j k_{ij} L_j + C_i \quad (1)$$

where

\hat{p}_i - estimate of the geophysical parameter, e.g. pigment, aerosol-optical thickness etc.

k_{ij} - weighting coefficient of channel j for parameter i

L_j - measured radiance in channel j

C_i - offset value for parameter p_i

j - measurement channel number, from 1 to N , where N - number of spectral channels in the instrument.

It is one of the basic ideas of the proposed algorithm to use directly the TOA radiance values and to account for the atmospheric influence implicitly. The background for this approach is, that the application of an explicit atmospheric correction does not increase the information content regarding water constituents: Although the result of atmospheric scattering is the major effect that one sees in satellite data they contain already all signal variation caused by the water constituents. In other words, what is not resolved in the TOA data cannot be seen also after atmospheric correction. The atmospheric correction only realizes a kind of „dimensionality reduction“ of the data. Thus it should be possible to build an algorithm that reconstructs water constituents directly from top of atmosphere measurements. Of course it is up to discussion whether the used here linear estimates are appropriate to achieve the necessary accuracy. But the general approach could also be modified for more sophisticated estimators. The entire process of deriving the algorithm consists of 6 steps.

4.1 Step 1: Modeling

The analysis process requires a data set as input where top-of-the atmosphere (TOA) radiances in all available spectral channels are combined with the corresponding values of geophysical parameters that shall be retrieved from the spectral measurements. Such data sets can be provided either from a large number of remote and field data or from radiative transfer modeling. For the investigations presented in this document models are used, since there are insufficient high spectral resolution space data and corresponding field measurements available. The modeling gives "measured" TOA radiances dependent on concentrations of different water constituents and atmospheric turbidity. The models were basically taken from the literature [Gordon 1978 ,Sturm 1981, Sathyendranath, 1989] and modified to meet the parameters and capabilities of the MOS instrument [Krawczyk, 1993 1995]. The models used are simplified compared to a complete solution of the radiative transfer equation. This was done to reduce the numerical expense ,to test the potential of the proposed method. Although the models influence the derived estimates, they are not crucial to the general algorithm development. More sophisticated models have to be chosen for advanced studies. For the calculation the variability range for each input parameter and the correlation between parameters must be accounted for. This is done by selecting corresponding spatial patterns (images) of chlorophyll-a, yellow substance, sediments and atmospheric turbidity that are overlaid as inputs for the modeling process. For each simulated pixel the corresponding radiance values in the 13 spectral channels of MOS and the values of input parameters are written to a data file which is then fed into the analysis and inversion process.

4.2 Step 2: Principal Component Analysis

PCA provides a powerful tool for analyzing the information content of high-dimensional data sets such as spectral high resolution imagery [Ingebritsen 1985, Fischer 1985]. However, it is problematical to find a physical interpretation of principal components for remote sensing applications, since the PCA is primarily a mathematical tool. In the following the PCA is used to estimate the information content of experimental or modeled data sets, to rearrange (transform) the data in a manner suitable for analysis and to separate the useful information from noise contained in the data. Principal components are computed from the input data sets using the eigenvectors of the spectral covariance matrix. To account for an interpretation affect through measurement noise, the simulated radiance data are normalized to unity errors. Expected measurement errors (noise) are

known from laboratory analysis for each MOS channel. The transformation builds an orthogonal representation of the original data:

$$PC_k = \sum_{m=1}^N \frac{U_{km}(L_m - \bar{L}_m)}{\Delta L_m} \quad (2)$$

where PC_k - kth principal component, k from 1 to N
 N - number of spectral bands used in the original data set
 U_k - kth eigenvector of the covariance matrix
 L_m - radiance in the mth spectral band
 \bar{L}_m - mean radiance value in the mth spectral band
 ΔL_m - noise-equivalent radiance, measurement error.

By properties of the transformation the principal components are uncorrelated and contain successive degrees of information in the statistical sense, i.e. the higher the order of the component the smaller its total variance, the more noise or "uninterpretable" information it contains. This corresponds to the ordering of eigenvalues: $\lambda_i > \lambda_j$ for $i < j$.

4.3 Step 3: Intrinsic Dimensionality

First the spectral covariance matrix for the entire set of simulated radiance data is computed and then diagonalized. The diagonalization is necessary to perform the principal component analysis. The calculation of covariances is done using error-normalized radiance values: $Cov\{L_j/\Delta L_j\}$ where ΔL_j denotes the noise-equivalent radiance for the jth spectral band. This normalization automatically accounts for the radiometric resolution of the instrument considered in the context of algorithm development. The eigenvalues λ_k and the eigenvectors U_k of the spectral covariance matrix are then computed. Because of the error-normalization of radiances for calculating the covariance matrix the eigenvalues give a direct estimate of the signal-to-noise ratio of the corresponding principal component $\lambda_k = SNR^2(PC_k)$ with λ_k the k-th eigenvalue of the spectral covariance matrix, k from 1 to N, SNR the signal-to-noise ratio and PC_k the k-th principal component.

The SNR of each principal component is a measure of its significance in the statistical sense considering the measurement error. Using the eigenvalues λ_k one can determine the intrinsic dimensionality D of the measurement data which is equal to the number of principal components containing significant information and corresponds to the number of independent parameters that can (at least theoretically) be retrieved from the spectral measurement data set: $D = \max(k)$ with $\sqrt{\lambda_k} \gg 1$. Two groups of principal components are separated:

- a) those representing significant measurement information ($k \leq D$) and
- b) those containing non-interpretable variations such as noise, quantization error etc.

For the further analysis and determination of the coefficients in eq. (1) only the significant principal components are used.

4.4 Step 4: Reverse Correlation

The question is now how the representation of the spectral information in the form of principal components can be used to derive the desired coefficients. The first point to consider is that the principal components contain *the same information* as the original spectral radiance data, except the small noise-like portion of information that is

suppressed by reducing the number of used components to the "significant" ones. That again means that it must be possible to reconstruct not only the radiance values from the principal components which can, in fact be done very easily by the reverse transformation) but also the input parameters of the modeling [Krawczyk 1995, Neumann 1995a]. Because of the linear estimate for the determination of the geophysical parameters defined in eq. (1) a linear estimate is also chosen with the principal components:

$$\hat{p}_i \sim \sum_{m=1}^D C_{im} PC_m \quad (3)$$

where C_{im} - correlation coefficients between the i th parameter and the m th principal component.

Using the principal components and the corresponding geophysical parameters, which can be taken from the simulated TOA radiance data, one can build a regression formula that allows it to determine the required correlation coefficients C_{im} :

$$\frac{\hat{p}_i - \bar{p}_i}{\sigma_i} = \sum_{m=1}^D \frac{C_{im} PC_m}{\sqrt{\lambda_m}} \quad (4)$$

where \hat{p}_i is the estimate of the parameter p , \bar{p}_i is the mean value of the parameter and σ_i is the variance of the parameter. This regression must now be performed for each simulated pixel and each principal component, i.e. for the entire data set. Based on the results in step 3 only the significant principal components are used for the regression analysis. This suppresses noise from the data, especially avoiding noise amplification and significantly reducing the number of computations. It does *not* reduce the accuracy of the algorithm, since all of the usable portion of information contained in the data is applied.

4.5 Step 5: Reverse transformation into radiances

Although one can now determine coefficients to estimate geophysical parameters from the principle components, this is not what is finally needed. Formula (4) cannot be used directly to interpret any measured scene, since the principal components do not carry a clear physical sense. They strongly depend on the inherent statistic of the investigated scene and therefore on the values of the parameters and their correlations. But there is a way out: because principal components and radiances are equivalent to reconstruct the informative part of a scene one can apply transformation (2) to eq (4) and yields a representation of the regression formula based on the TOA radiance values:

$$\frac{\hat{p}_i - \bar{p}_i}{\sigma_i} = C_{i1} \sum_{j=1}^D \frac{U_{1j}(L_j - \bar{L}_1)}{\Delta L_j \sqrt{\lambda_j}} + C_{i2} \sum_{j=1}^D \frac{U_{2j}(L_j - \bar{L}_j)}{\Delta L_j \sqrt{\lambda_j}} + \dots \quad (5)$$

4.6 Step 6: Determination of coefficients for the linear estimator

From equation (5) one now can compute the coefficients k_{ij} and m_i used in the linear estimate for each parameter and each wavelength band.

These six steps have to be performed for different variability ranges of the input parameters, different models with respect to specific optical properties of the water body and the atmosphere and different viewing geometries. Thus a look-up-table (LUT) is generated that contains the coefficients which are used to compute the physical parameters from actual TOA measurements. Fortunately this LUT can be calculated in the forefield of the mission. The resulting coefficients are model depending and

nonadequateness of the model causes systematic misinterpretation errors. The theoretical investigations made in preparation of the MOS mission show the promising potential of the proposed algorithm, especially regarding the discrimination of different water constituents. This is only possible because of the high spectral resolution and the large number of spectral bands provided by the MOS instrument or similar sensors.

5. Algorithm Discussion

The main disadvantage is that the original relation describing the dependence between geophysical parameters and satellite radiances is nonlinear. Therefore the linear approach is always an approximation with good accuracy only for limited ranges. From this follows that it is useful to subdivide the entire value range of geophysical parameters into subranges and to define for each of them a special interpretation coefficient set k and m for equation (1). These coefficient sets are then collected in a look-up-table (LUT). For an interpretation of a concrete data set the appropriate input from the look-up-table must be chosen through a special estimation procedure. The strategy of use of a look-up-table also allows the consideration of different water types in different regions, e.g. the specific bio-optical properties of the water constituents in the Baltic Sea are different from those in the Mediterranean Sea or the open ocean. The expected concentration values and correlation between constituents are also varying. The interpretation accuracy therefore can be improved by generating special LUTs accounting for this. Now another aspect should be mentioned to avoid some disadvantages of the linear approach caused by the original nonlinear parameter dependence on radiances. An improvement can be achieved by the introduction of some auxiliary parameters instead of the original geophysical ones through a semi-logarithmic set-up.

$$q = p + \alpha \ln p \quad (\alpha = 0.1) \quad (6)$$

This is a mixture of the linear approach and a clear logarithmic. It was found from numerical tests that the only logarithmic approach did not significantly improve the interpretation accuracy. Especially for higher concentrations of Chlorophyll and Sediment the linear estimate gave better results, in opposite to this for low concentrations the logarithmic approach was better. The semilogarithmic approach is a compromise: for low values the logarithmic behavior in (6) dominates but for large values the linear part. Another advantage of this set-up is that now the definition range of the retrieved geophysical parameters is always positive. In the clear linear approach results could tend into negative regions, what on one hand is unphysical, but on the other hand is only a sign of insufficient accuracy.

5.1 Accuracy consideration

For a theoretical test of the potential of the proposed algorithm there was simulated a test data set of MOS-radiances varying the following geophysical parameters:

Chlorophyll	C	from 0 to 20 $\mu\text{g/l}$
Sediment	$b_s(550\text{nm})$	from 0 to 10 $1/\text{m}$
Gelbstoff	$a_\gamma(440\text{nm})$	from 0 to 1 $1/\text{m}$
optical thickness	$\tau_A(750\text{nm})$	from 0 to 0.5

in uncorrelated patterns. These parameters then were retrieved with the described algorithm. The retrieval errors (dp/p) are presented in figure 2. One can see the sharp peak around zero and a fast decrease to the both flanks.

For all parameters a large amount of data lies within a 30% error boundary (dotted line). An additional improvement could be achieved subdividing the entire parameter ranges into several subranges and computing different entries into the estimation coefficient look-up-table. Through a special segmentation algorithm the optimal coefficient set was chosen for the interpretation (without use of a-priori simulation knowledge). These results are shown as solid lines in figure 2.

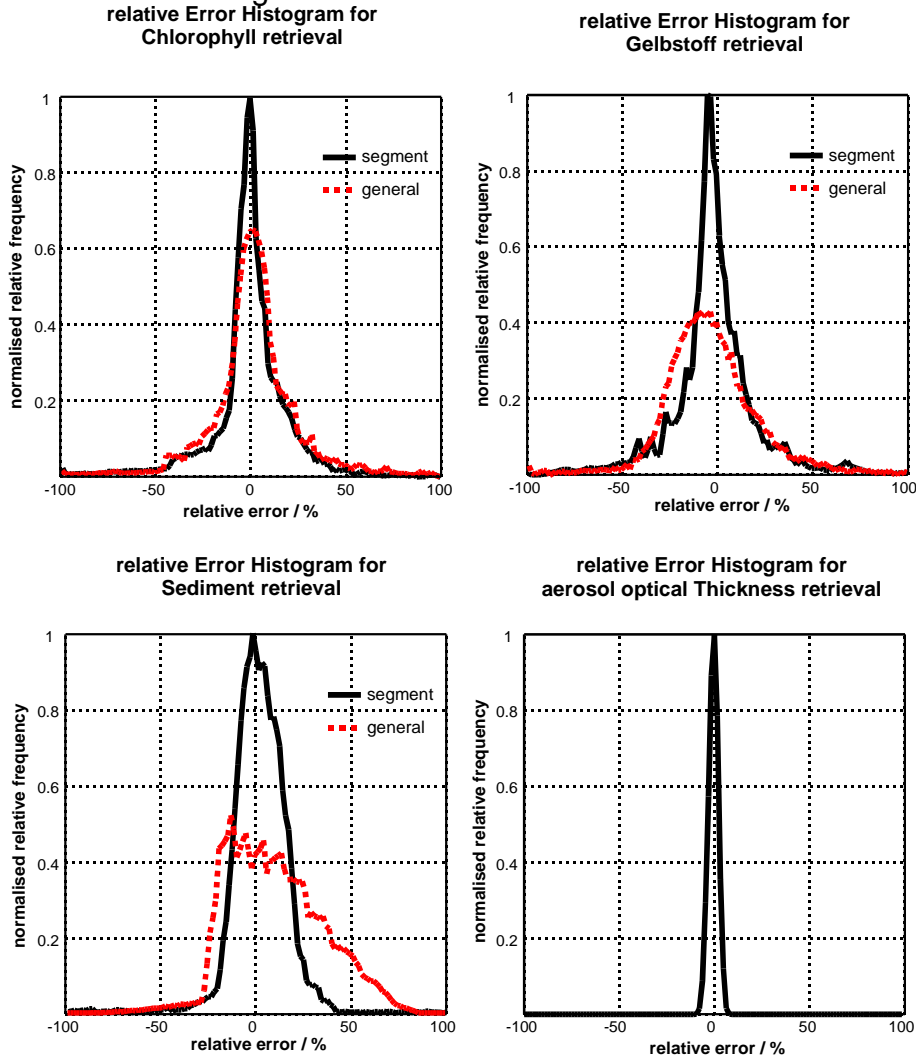


figure 2 relative error histograms for parameter retrieval

6. Application Examples

The introduced algorithm was applied to a number of MOS overflight data representing different situations regarding the water type and atmospheric situation. The following 2 examples show the usability of the algorithm for a European and an American coastal water case.

FIGURE 3: The image shows an overpass over the Street of Gibraltar. It demonstrates impressively how the PCI algorithm applied to TOA radiances is able to discriminate between the atmospheric and in-water features. Although the atmosphere shows high dynamics and structuring, the water constituent maps are not influenced by this pattern.

FIGURE 4: This overpass over the Pacific coast shows a total different type of water than we usually observe along the European coasts. Except in the bays it seems to be almost

case-I water showing only chlorophyll variation. But the derived water constituents show clearly that the used "global case-II" model during generation of coefficients for PCI is also able to handle this situation.

7. Conclusion

The above explanations show that using spectral high resolution data it is possible to derive different water constituents even under complicated case-II conditions in coastal waters. It was also demonstrated that the approach of direct retrieval from top-of-atmosphere radiance data is feasible. However, this is still only a first step demonstrating the methodology and a lot of investigation and work has to be done in implementing more precise models in the process of generating the look up tables of coefficients for the PCI. This is concerning specific water models (regional and seasonal) as well as radiative transfer through the atmosphere.

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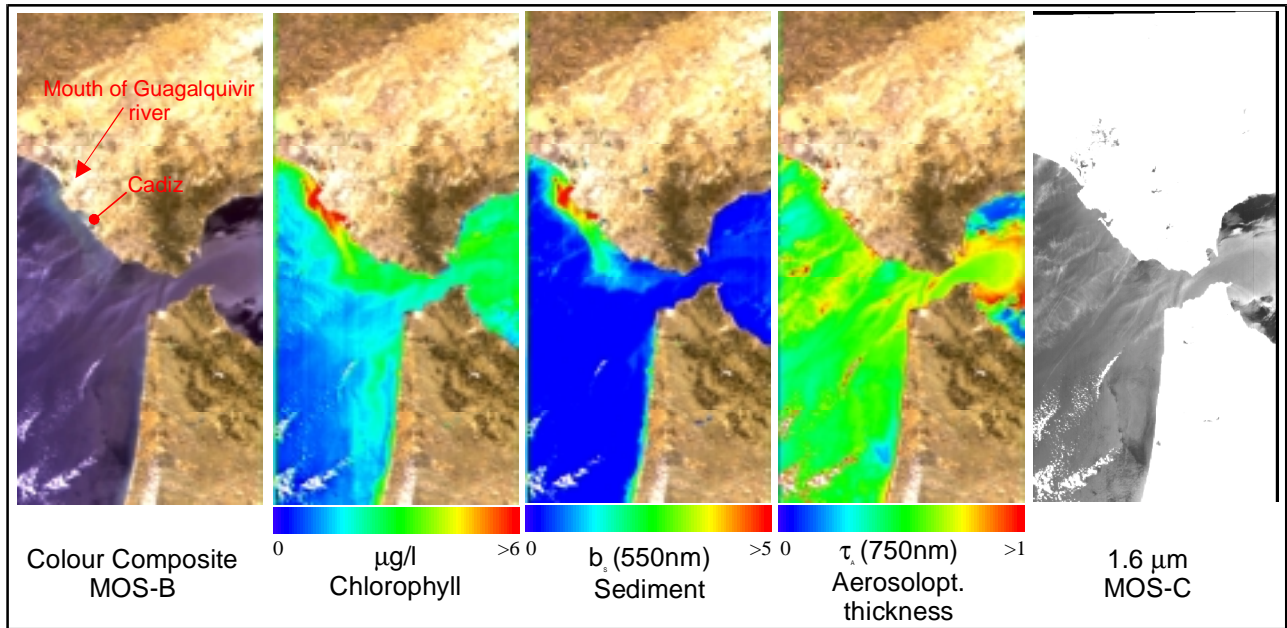


Fig. 3: Street of Gibraltar, May 9, 1997; derived water constituent and atmospheric turbidity by PCI applied to TOA radiances

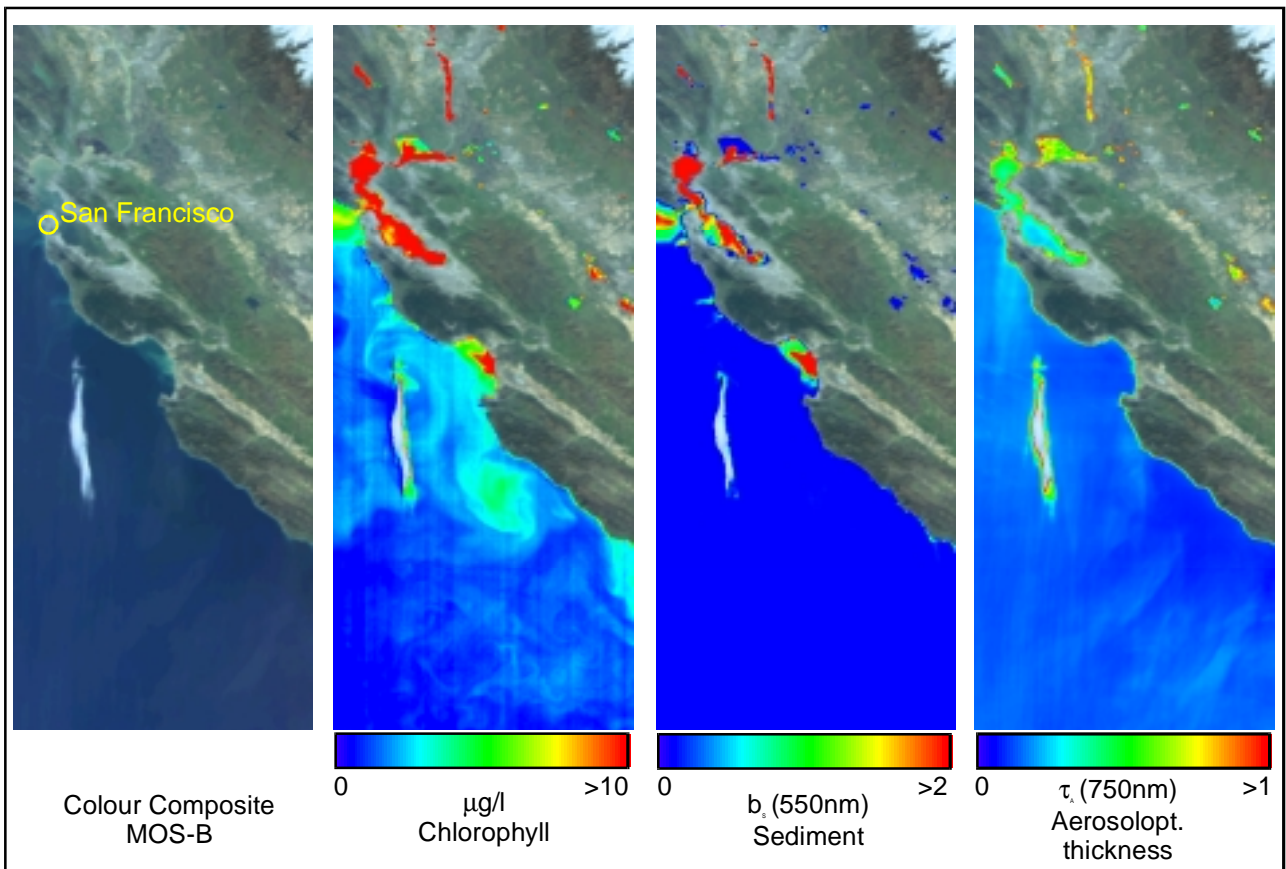


Fig. 4: Pacific coast south of San Francisco, March 10, 1998;