Titel: **OPTICAL DEPTH of “FINE” and “COARSE” AEROSOLS, TOTAL AEROSOL OPTICAL DEPTH, OPTICAL DEPTH of THIN CIRRUS and WATER LEAVING REFLECTANCE**

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Issue	Revision	Date	Changes
1			initial issue
2			**The new (second) version is a modification of the first version of the ATBD in practically every chapter except in the basic inversion equations (chapter 3.1.2.1). This basic chapter was transferred without any change, because up to now there were no reason found o change the basic inversion procedure. But there were done some modifications in the basic aerosol parameterisation model (Appendix A) to specify the suggested model parameters and to define more clearly the range of applicability of the model. These modifications led to revise practically all chapters, thereby specifying estimated figures on errors and of the numbers of figures to be saved in LOOK UP TABLES .**

MERIS/MAPP

Algorithm Theoretical Basis Document

OPTICAL DEPTH of "FINE" and "COARSE" AEROSOLS, TOTAL AEROSOL OPTICAL DEPTH, OPTICAL DEPTH of THIN CIRRUS and WATER LEAVING REFLECTANCE

VERSION: 2

Submitted by:

Bernd Piesik
German Aerospace Center
Institute of Space Sensor Technology
D-12489 Berlin-Adlershof
Rudower Chaussee 5

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1.Introduction

1.1. Algorithm Identification

The following output products will be found by the algorithms:

1. Optical Depth of "FINE" Aerosols	Identification number 1
2. Optical Depth of "COARSE" Aerosols	Identification number 2
3. Total Aerosol Optical Depth	Identification number 3
4. Optical Depth of Thin Cirrus	Identification number 4
5. Water Leaving Reflectance	Identification number 5

2. Algorithm Overview

2.1 Experimental objectives

There are two main objectives of the suggested algorithms for MERIS data use:
First is to present a new concept and algorithm to estimate Aerosol parameters from MERIS data. The algorithm is applicable over water off coast as well as near coasts . But increased errors are expected only , if one applies the algorithm in situations where the "normal" global aerosol production mechanisms are regionally strongly disturbed . Candidates for such seldom but possible "events" are "desert dust storms", "regional forest fires" and "volcanic activity".
This algorithm allows to estimate three new products, the "Optical Depth of "FINE" Aerosols", the "Optical Depth of "COARSE" Aerosols" and the " Optical Depth of Thin Cirrus " from MERIS data. The suggested method allows to take into account regional Aerosol features and to use ancillary data to improve the accuracy for all data products.
The second main objective is to reach higher accuracy in the standard products „ Total Aerosol Optical Depth" as well as in the product „Water Leaving Reflectance". The key to this higher accuracy in these products are the splitting of atmospheric scattering into it's main contributions and to combine the data measured by MERIS with suitable ancillary data from other sources to improve the accuracy.
There are two main experimental goals in the accompanying scientific MERIS validation program: First is to use one typical area ("Baltic Sea") to validate the new concept and all products for typical situations as well as for more complicated situations at high and low levels of all variable parameters involved. The second experimental objective is to use combined satellite and ground measurements to investigate at least two of the basic involved Aerosol assumptions : the key role of Relative Humidity on Aerosol growing and a possible existing systematic error in Aerosol Optical Depth estimations from satellite attributable to deviations from MIE-theory of scattering due to particle asymmetry.

2.2 Historical perspective

The estimation of the „Total Aerosol Optical Depth " will be done permanently from satellite data of AVHRR /1/. Since the Reflectance of the system Ocean/Atmosphere is measured in only one channel , there are a lot of error sources for this product from AVHRR (compare for example the discussion in appendix A). The MERIS data in their combination with ECMWF ancillary data will allow a much higher accuracy in the estimation of the "Total Atmospheric Optical Depth" due to the information content of these data with regard to characteristic Aerosol type parameters . And due to the improved Aerosol parameter

estimation (compare for example the discussion in appendix A) the atmospheric correction accuracy will also increase . As a consequence the resulting product after atmospheric correction , the „Water Leaving Reflectance“, will have increased accuracy too.
Up to now there was no complete access to the final algorithms for the standard MERIS product „Total Aerosol Optical Depth “ from MERIS data . The comparison with the suggested method was therefore at present not possible in detail. A comparison to other algorithms for the products „ Optical Depth of “FINE” Aerosols“, Optical depth of “COARSE” Aerosols” and “ Optical Depth of Thin Cirrus ” is not possible because these products are new products, not suggested before.
For the also suggested product „Water Leaving Reflectance“ there were published the basic steps of the standard MERIS algorithm / 2/. The method in /2/ and the method suggested here are different in some of the underlying assumptions as well as in the data inversion method. The main differences seem to be that the here suggested method should result in higher accuracy compared to the MERIS standard method due to expected higher accuracy in describing the atmospheric scattering situation as well as due to the inclusion of regional features in the algorithms.
The main differences with regard to the inversion procedure itself is, that the approach suggested here will practically work without iteration opposite to the standard MERIS algorithm. It is therefore expected, that the suggested inversion procedure can be made faster than the standard inversion procedure.

3. Algorithm Description

3.1 Theoretical Description

3.1.1 Physics of the problem

3.1.1.1 TOA-basic Reflectance model

Basic to estimate Aerosol parameters from reflected sunlight over oceans is, that under somewhat idealized conditions like “cloud free atmosphere” and negligible ocean reflectance, the registered light at satellite level will be light reflected by permanent atmospheric gases and light reflected at all the other particles one may find along the line of sight between satellite and surface. All these (nonpermanent) but rather different particles in the atmosphere are summarized by the term „Aerosols“. In this way one may write the reflected light as the sum of two major fractions of particles: $L^{TOA}(l)\ °\ L^{R}(l) + L^{A}(l)$,
with L^R – Light reflected at permanent atmospheric gases by Rayleigh-scattering and
L^A - Light reflected at Aerosols.
For convenience we will discuss these reflected light in a normalized way as „Reflectances“ by the definition

(1) $$R^{TOA}(l) \equiv \frac{p \cdot L^{TOA}(l)}{E_o(l) \cdot \cos(q_s)}$$

($E_o(l)$ = Extraterrestrical Irrandiance, q_S = solar-zenith-distance, TOA stands for measurement at “**T**op **O**f **A**tmosphere” level)

In this normalized way the reflected light can be written as a sum of two Reflectance contributions:

(2) $$R^{TOA}(l)\ °\ R^{R}(l) + R^{A}(l)$$

Since $R^R(l)$ can be calculated very accurate, from measurements of $R^{TOA}(l)$ one can find the Aerosol part $R^A(l)$. As suitable channels to measure $R^A(l)$ by MERIS mainly the channels 705 nm, 754 nm, 775 nm, 865 nm, 890 nm (in the following referred to as MERIS NIR channels, those below 705nm as VIS channels) can be used, because these channels are nearly independent of the influence of atmospheric absorption from gases and for most parts of the sea (type 1 water) there is no need to take into account remarkable contribution of radiance reflected in water back to satellite /3/.

These measurable 5 numbers $(R^A(705), \ldots\ldots R^A(890))$ contain, of course, information on Aerosols. To extract suitable Aerosol parameters from $R^A(l_i)$, $i = 1 \ldots 5$ one needs a model, that connects measurable $R^A(l_i)$ to suitable Aerosol parameters . The discussion on suitable Aerosol parameters is found in appendix A. The main results are:

- A 4-parameter-aerosol model is suggested for modeling satellite multispectral reflectance $R^A(l_i)$ for application in nearly all cloud free maritime situations. Enhanced errors in this model are only expected, when the model is also used in situations which represent strong perturbations of the “normal” aerosol production mechanisms as nearby “desert dust storms”, “regional forest fires” or “strong volcanic eruptions”. For our main region of interest– the marine north European coast and the Baltic Sea – this will practically not restrict the application of this model.

- $R^A(l_i)$ should be parameterized as function of the 4 variable parameters:

  - t_A (Total Aerosol Optical Depth)
  - a_1 (Optical Depth rate of “FINE” Aerosols)
  - RH (Relative Humidity)
  - a_{11} (Optical depth rate of the minor part of “FINE” Aerosols)

- The variance $R^A(l_i)$ is typically dominated by the variance of the first two parameters t_A and a_1 . The Total Aerosol optical Depth (t_A) can be written as a sum of two parts, named “FINE” Optical Depth (t_{A1}) and “COARSE” Optical Depth (t_{A2}) . Instead of the two variable parameters t_A and a_1 one can also use the two alternative parameters t_{A1} and t_{A2} to model the multispectral Aerosol reflectance $R^A(l_i)$.
- Both Aerosol parameters (t_A and a_1 or alternatively t_{A1} and t_{A2}) can be estimated from measured $R^A(l_i)$, $i = 1 \ldots 5$. The accuracy of estimation of these parameters from MERIS data is connected with the accuracy by which the other two variables (RH and a_{11}) itself can be estimated .
- An estimation of the parameter Relative Humidity (RH) cannot be found from $R^A(l_i)$, $i = 1 \ldots 5$. This parameter must be estimated from other data sources (ancillary data). The use of ECMWF data seems to be favored for this goal.
- The estimation of the best “fine” Aerosol model (parameter a_{11}) must also be done by using ancillary data. The most simple model will be to neglect this variance and use one fixed candidate model in any case of Aerosol analysis from measured $R^A(l_i)$. The next better is to use air mass circulation data to interpolate between two suitable candidate models, corresponding to low and high level of parameter a_{11} (compare appendix A).

It is therefore necessary at first to model the Reflectance $R^A\ (l_i),\ i = 1\ ...5$ as function of the four above "aerosol" parameters $t_a,\ a_1,\ RH\ ,a_{11}$, (or alternatively of the four parameters t_{A1} , t_{A2} , $RH,\ a_{11}$).
This modeling itself can be done by suitable radiance transfer simulations , including the corresponding marine and continental Aerosol models to give $R^{A(mod)}(l_i;\ t_A,\ a_1,\ ,RH,\ a_{11}\ )$ (λ_i: MERIS-Channels) for all relevant values of these parameters.

3.1.1.2 Basic inversion procedure

With modeled $R^{A(mod)}$ (λ_i;τ_A, a_1, R_H , a_{11}) the estimation of τ_A and a_1 (or t_{A1} and t_{A2}) requires just two steps:

1.Step: estimate the two model parameters ($a_{11} = \hat{a}_{11}(n)$ and $RH = \hat{RH}(n)$) for the scene at pixel n from ancillary data (along the lines given in appendix A).

2.Step: Estimate $\hat{t}_A$ and $\hat{a}_1$ for all pixels (n) by comparison of "measured" $R^{A(meas)}\ (l_i;\ n)$ with modeled $R^{A(mod)}\ (l_i\ ;\ t_{A,}\ a_1\ ,\ \hat{a}_{11}(n)\ \ ,\hat{RH}(n))$ by

$$(3) \qquad \sum_{i=1}^{N_i}\left(R^{A(meas)}(l_i;n) - R^{A(\mathrm{mod})}(l_i;t_A,a_1,\hat{a}_{11}(\mathrm{n}),\hat{RH}(n))\right)\cdot g_i \Rightarrow Min\ !$$

(g_i suitable weighting factors)

3.1.1.3 TOA-Total Reflectance model

3.1.1.3.1 Quasi-Linear Reflectance model

The simple model (1) is at most for very low atmospheric aerosol loading an acceptable approximation for MERIS-Data application. For coastal areas and over inland seas one is typically faced with stronger Aerosol loading than over marine places far off coast. In this case (1) should be extended at least by a term, in publications mostly named "interaction" or "coupling" term /4/:

$$(4) \qquad R^{TOA}(l_i)\ ^o\ R^R\ (l_i) + R^A\ (l_i) + R^{RA}\ (l_i)$$

This term $R^{RA}(l_i)$ is mainly the contribution of those photons scattered at least at both particle types in the atmosphere (aerosols and permanent atmospheric gases) before hitting on the sensor. The term $R^{RA}\ (l_i)$ itself can be found by radiance transfer calculation methods including multiple scattering effects applied to 3 cases:

$R^R\ (l_i)$ – Reflectance calculation with permanent air gases (Rayleigh-scattering-particles) but no Aerosols in the atmosphere.

$R^A\ (l_i)$ – Reflectance calculation with no permanent gases but Aerosols in the atmosphere.

$R^{TOA}\ (l_i)$ – Reflectance calculation with both particles in the atmosphere.

According to definition equation (4) $R^{RA}(l_i)$ is then simply the difference $R^{TOA}(l_i) - R^{R}(l_i) - R^{A}(l_i)$.
In this way all terms on the right side of (4) can be calculated in dependence of the relevant variable aerosol parameters t_A , a_1 , RH , a_{11} (compare Appendix A).

If one analyses the term $R^{RA}(l_i)$ one finds:

- R^{RA} can be neglected for low t_A situations (typical for some off coast marine areas on the southern hemisphere), but R^{RA} is typical not to be neglected over coastal areas or over inland seas with typically strong continental Aerosol part.
- R^{RA} is a complicated function of the Aerosol parameters, viewing and sun geometry parameters (solar zenith distance (θ_S), Viewing zenith distance (θ_V) and azimuth difference of sunr and viewing directions(φ_{SV})) and wavelength.
- Due to the complicated way the term R^{RA} depends on the involved parameters (four Aerosol parameters (t_A ,a_1 , RH , a_{11}) and three geometry-parameters (θ_S, θ_V , φ_{SV}) it seems to be complicated to find simple analytical approximations for R^{RA} and all the other terms in the simplest equation (4) and in the final equation (8) .

To invert equation (4), that is to estimate the two parameters t_A and a_1 (compare Appendix A) from measured reflectance $R^{TOA}(l_i)$ we suggest a “quasi linear” inversion procedure in the following way:

Instead of the two Aerosol parameters t_A and a_1 one can use the two alternative variables t_{A1} and t_{A2} (compare also appendix A) defined according to:

$x_1\ ^o\ t_{A1} = a_1{}^{x}\ t_A$ (x_1 - optical depth of “Fine” Aerosols)

$x_2\ ^o\ t_{A2} = (1-a_1)\cdot t_A$ (x_2 - optical depth of “COARSE” Aerosols)

This will allow to model the measurable reflectance (R^{TOA}) as a sum of the reflectance’s of the three involved scattering particle types:
- molecular (index R stands for Rayleigh scattering law for permanent atmospheric gases)
- fine (x_1)
- coarse (x_2)

by the analog to equation (4) one gets on the right side:

$$(5) \qquad R^{TOA}(l_i)\ ^o\ R^{R}(l_i) + R^{x1}(l_i) + R^{X2}(l_i) + R^{RX}(l_i)$$

As in the case of equation (4): The “interaction term” R^{RX} is only a small part – dominating are the first three parts, representing the scattering at molecules, x_1-Aerosols and x_2-Aerosols.
With this definition the main effect on R^{TOA} due to changing x_1 is a change in the term R^{X1} (and due to changing x_2 the main effect is a change in the term R^{X2}).
And one expects (this will be proven later): If one doubles the number of scattering particles x_1 in the atmosphere one will nearly double the reflected photons, that is one will nearly double the term R^{X1}. In other words: R^{X1} is nearly linear to x_1 . And analog: R^{X2} is nearly linear in x_2 .

This in total suggests to use the alternative formulation of equation (5):

(6) $$R_i^{TOA} \equiv \sum_{1}^{2} K_{ij}\; x_j + R_i^{RC}$$

with

$R_j^{RC} = R^R + R^{RX}$ and $K_{ij} = R^{Xj} / x_j$

(R_i^{TOA} *stands for* $R_{(li)}^{TOA}$), *i = 1 ... N_i* , (N_i= Number of involved channels)

The “nearly linear” dependence of R^{X1} from x_1 (and R^{X2} from x_2) means, that the coefficients K_{ij} in (6) will be “nearly independent” of x_1 and x_2 . That this weak dependence of K_{ij} on x_1 and x_2 is correct can be proven by suitable radiance transfer calculation. Some results are shown in Fig. (1).

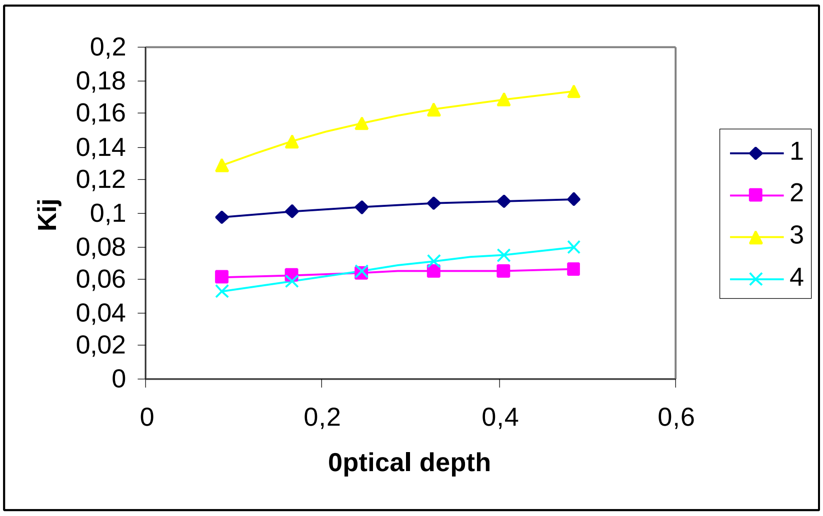

Fig. 1: The change of K_{ij} due to x_1 and x_2 for growing t_A . i: channel 754 nm, Relative Humidity = 80 %, θ_s = 48.78 grad,
K_{i1}: (1) nadir viewing, (3) viewing at edge
K_{i2}: (2) nadir viewing, (4) viewing at edge

Due to the formulation (6) one gets therefore a “quasi linear” connection between measurable data (R_i^{TOA} *(i = 1 ... N_i)* and wanted unknowns *(x_1, x_2)*.
This “Quasi linearity” means: The coefficients *Kij* and R_j^{RC} in (5) are in lowest order independent of the wanted unknowns x_1 and x_2.
Equations (6) are therefore in lowest order a linear equation system for the unknowns .
Owing to this weak dependence of the coefficients K_{ij} and R_i^{RC} on x_1 and x_2 one needs only a rough estimation of the wanted unknowns for the pixel under investigation to calculate these coefficients for use in equation (6) with acceptable accuracy (compare Fig.1).

And this needed estimation of x_1 and x_2 at the pixel under investigation can simply be taken from the inversion results found for the neighboring pixel analyzed one step before . This corresponds to the a priori knowledge, that both unknowns are not changing abruptly from pixel to pixel.
Therefore: Only for the starting pixel one may have no acceptable accurate estimations of x_1 and x_2 for the calculation of the coefficients K_{ij} and R_i^{RC} (R_i^{RGFCS} in the final equation (14)) and it may be necessary to repeat the inversion of (5) by iteration for this starting pixel. But this will typically not be necessary for the vast number of following pixels.
In other words: The suggested inversion procedure is formally an iterative inversion , but practically it is not iterative.
Due to this “quasi linearity” the inversion of (6) itself is possible in a rather simple way. The inversion equations taking into account different noise levels of the measuring system for different channels are given in the following chapter.

To calculate the coefficients K_{ij} and R_i^R in dependence of all involved parameters (3 geometry parameters , 4 Aerosol relevant parameters in this first version) one can use the equations (6) and (5) in the sense of an identity :
Both equations (6) and (5) represent the same term (R_i^{TOA}) but in different formulations. Each reflectance part in equation (5) can be pre-calculated by using suitable radiance transfer calculations analog to those, defined in discussing equation (4). In this way all terms defined on the right sight of equation (5) can be pre-calculated. And using the identity formulation (6) also the needed coefficients K_{ij} and R^{RC} in (6) can be pre-calculated.
In this way the dependencies of all involved coefficients from all involved parameters can be pre-calculated by suitable radiance transfer calculations involving multiple scattering effects. The coefficients K_{ij} and R_i^R itself can than be stored in corresponding LOOK UP TABLES.

Necessary for successful estimation of the 2 unknown reflectance contributions x_1 and x_2 by inversion of equation (6) is, that x_1 and x_2 influence the wavelength dependence of multispectral aerosol reflectance in a different way. According to (6): K_{i1}, K_{i2} represent the “optical reflection response” at channel i to adding particles x_1 or x_2 to the reflecting system. These wavelength depend “optical reflectance responses are” shown for typical remote sensing geometry in Fig. 2.
It demonstrates the necessary different wavelength response for parameter x_1 and x_2 (curves 1 and 2 for nadir viewing, curves 3 and 4 for viewing at MERIS edge). The response of particles x_1 grow to shorter wavelength and particles x_2 show a rather wavelength independent response This difference in the responses for x_1 and x_2 at different wavelength allows the estimation of both parameters from measured R_i^{TOA} in principle already from measurements at two wavelength.

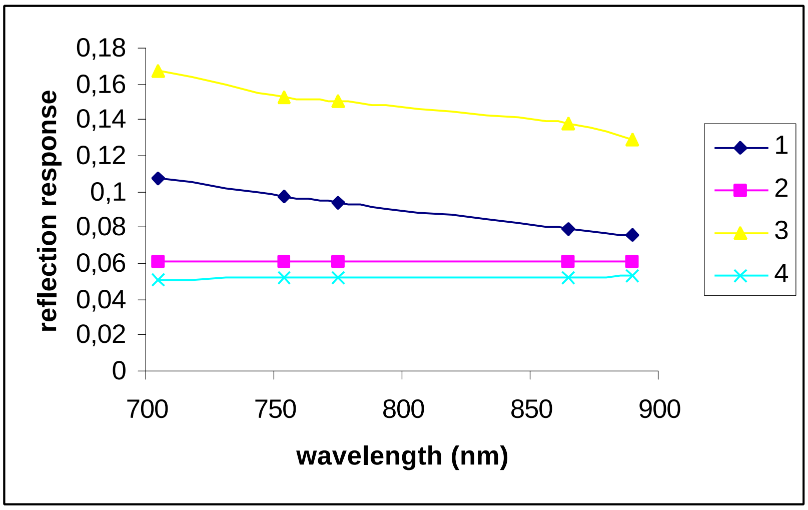

Fig. 2 Optical reflection response K_{ij} versus wavelength i. Relative Humidity = 80 %, θ_s = 48.78 grad,

K_{i1}: (1) nadir viewing, (3) viewing at edge
K_{i2}: (2) nadir viewing, (4) viewing at edge

Up to now it was assumed, that the variance of the reflectance at top of atmosphere(R_i^{TOA}) changes only due to changing the optical depth of particles x_1 and x_2 .
But in reality there are some more important contributions to measured reflectance at satellite level (R_i^{TOA}) which must betaken into account on the right side of (5) and (6):

3.1.1.3.2: Effects of suspended matter in water.

For open ocean water, usually referred to as “case 1 water”, this part can typically be neglected in the NIR part of the spectrum due to low level of suspended matter /5/. This typically no longer holds for Coastal waters and inland seas usually referred to as case 2 waters /5/) . But since coastal water, especially the Baltic Sea , are the main areas of application of the algorithm one should take into account this typically higher level of suspended matter.
In Fig. 3 the wavelength dependence of “Water Leaving Reflectance” R_i^{BOA} was calculated for different amounts of suspended matter for the interesting MERIS channels.

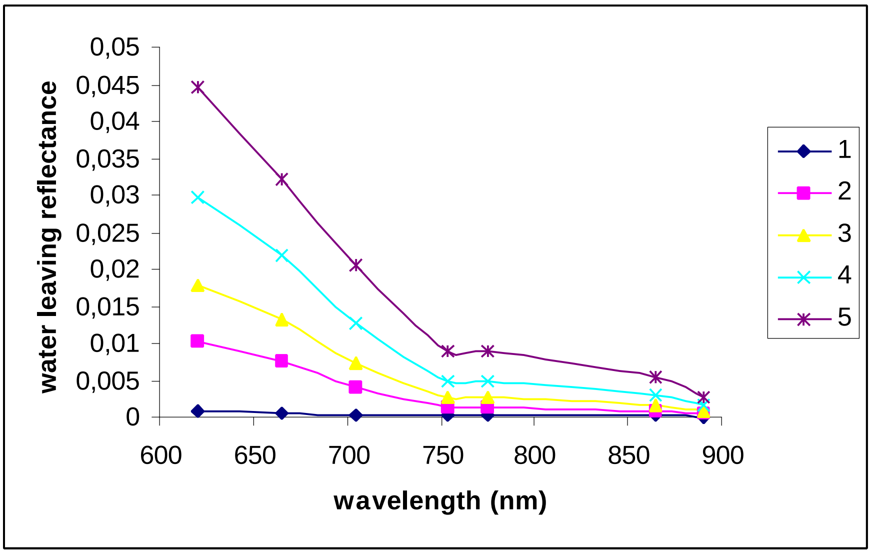

Fig. 3 Water Leaving Reflectance R_i^{BOA} versus wavelength for different amount of suspended matter: Curves (1) to (5) correspond 0.08, 8, 16, 24 and 48 mg/liter

Fig.3 shows, that R_i^{BOA} grows with growing amount of suspended matter. Since the atmospheric transmission only slightly diminishes reflected R_i^{BOA} on the way up to satellite sensor one will have a strong contribution to R_i^{TOA} due to radiance, reflected at suspended material in the ocean water.

The nearly linear connection between R_i^{TOA} and the amount of suspended matter in these channels is seen from Fig.3. This allows to include this additional variance due to sediments in water again by a “quasi linear model” of the kind

(7) $R_i^{BOA} = R_i^{BOA}(0) + K_{i3} * x_3$

In equation (7) x_3 is the concentration of suspended material in the water. $R_i^{BOA}(0)$ is the water reflectance for no suspended material in water.

The reflectance in (7) is the reflectance below the atmosphere. On satellite level this reflectance is seen by a sensor at a little “reduced “ level due to atmospheric extinction between satellite and earth surface. Formally one can therefore describe this contribution to R_i^{TOA} by adding a term

(8) $R_i^{x3} = R_i^{BOA} * T_i^D$

to equation (5).

Modeling shows, that the “extinction” factor T_i^D in (8) is typically below but near to 1 and that T_i^D is slowly decreasing with increasing x_1 and x_2 and very slowly increasing with increasing x_3 .

By using (7) the additional contribution of (8) can be integrated by writing the analog to (6):

$$(9) \qquad R_i^{TOA} \equiv \sum_{1}^{3} K_{ij}\; x_j + R_i^{RCS}$$

with

$$(10) \qquad R_i^{RCS} \;=\; R_i^{RC} + \; R_i^{BOA}\,(0) *T_i^{D}$$

As in case (6): The coefficients in (9) are still only weakly depending on the unknowns (x_1 , x_2 , x_3) . And the wavelength dependence of the new unknown part x_3 is so different to the wavelength dependencies of the parts x_1 and x_2 (compare fig. 2 and fig. 3) that one can separate these three unknowns from measurements of R_i^{TOA} in (at least) three suitable NIR channels.
For MERIS the best channel choice seem to be the channels 705 nm, 775nm, 865 nm . But one should also test the inclusion of channels like 754nm and 890 nm at least to reduce sensor noise effects or to be prepared for alternatives if there are some problems with one of the optimal channels during MERIS flight. The inversion procedure itself (compare section 3.1.2.1) allows to take into account the in the final algorithm measurements in 3 or more channels .
In this way for any water pixel one finds in (practical) 1 step estimations of atmospheric Aerosol optical depth's (x_1 , x_2) as well as suspended material in water (x_3).

There might be another important and in the discussion up to now neglected contribution to R_i^{TOA} under cloud free conditions:

1.1.1.3.3. Effects of rough ocean surface and foam

There may be a strong additional contribution to reflectance at satellite level (R_i^{TOA}).
It comes from light reflected diffuse by foam and from sun light reflected to viewing direction by those facets of rough sea surface which are suitable inclined to act as mirror for light coming from the sun . The last part is typically referred to as glitter. Both contributions can be included in the model by adding a corresponding contribution R_I^{GF} to (5) (as well as to model (6) or (9)):

$$(11) \qquad R_I^{GF} = R_i^{GBOA} * T_i^{DIR} \times (1 - f_f) + f_F *A_i^{F} * T_i^{D}$$

In equation (11) and later Index G and F stand for "**G**litter and **F**oam . Index BOA stands for "**B**ottom **O**f **A**tmosphere ". The first part $R_i^{GBOA} * T_i^{DIR}$ in (11) models the effect of reflected sun light (glitter) at rough ocean surface (R_i^{GBOA}), two times going straight through the atmosphere thereby diminishing by atmospheric transmission loss ($T_i^{DIR} < 1.$). The second part in (11) models the reflection due to foam covering the fraction f_F at the ocean surface. Both parts R_i^{GBOA} and f_F can be related to wind speed, as the driving force of ruffling the sea surface and producing foam (For Some more details sea Appendix B). In this chapter of importance is only, that this part can not be included as a 4. unknown into (9) as this was possible for the discussed parts representing x_1, x_2, x_3.
The reason is, that this ocean surface reflection part R_i^{GF} has a wavelength dependence in the NIR- MERIS-channels, which is rather near to that of x_2. And this, as discussed before, will not allow to separate this contribution from the contribution x_2 . On the other hand: If there is no good estimation of this ocean surface reflectance part from other sources the

error in the estimation of x_2 can drastically increase. It is therefore important for Aerosol parameter measurement from satellite to estimate this reflectance contribution by using suitable data of other sources.
Since parallel to the MERIS-NIR-measurements the wind speed at ocean surface will be given from ECMWF data, one can use the models, given in the Appendix (B), to estimate the glitter part (R_i^{GBOA}) and the foam fraction (f_F) from these ECMWF data.

Formally in the equation analog to (9) the glitter/foam contribution R_i^{GF} will therefore not be included as a further variable unknown but as an additive known part to the additive coefficient R_i^{RCS} :

(12) $$R_i^{RGFCS} = R_i^{RCS} + R_i^{GF}$$

That is: Analog to (9) one now has

(13) $$R_i^{TOA} \equiv \sum_{i=1}^{3} K_{ij} \cdot x_j + R_i^{RGFCS} \quad , \quad i = 1 \,..\, N_i$$

(The superior indices are chosen as said before as a reminder for the terms included in the model: R-Rayleigh-scattering; G-glitter; F-foam, C-Coupling, S-suspended matter, TOA-Top of atmosphere, BOA-bottom of atmosphere).

Since the additive coefficient R_i^{RGFCS} in equation (13) depends only weak on the unknowns x_j the inversion of (13) can run as discussed with regard to equation (6). But the needed additive coefficient R_i^{RGFCS} in equation (13) is now according to (12) and (11) a little more complicated to calculate:
All coefficients in (13) can be calculated in dependence of all involved parameters as discussed with regard to equations (5) and (6) by suitable repeated application of radiance transfer calculation methods. In this way all involved terms and coefficients can be taken from pre-calculated LOOK UP TABLES.
The surface wind speed dependent terms (R_i^{GBOA} and f_f) must be calculated as discussed by integrating the wind speed from other sources - in the MERIS case from included ECMWF data.

1.1.1.3.4 Effects of Thin Cirrus in the upper troposphere:

Not in any case but very often at least in some regions of the scene under investigation there will be found thin cirrus at an optical depth level much beyond the level that cloud classification algorithms can find it. The scenes might therefore be classified “cloudfree” but really contain Thin cirrus at an optical depth level comparable to aerosol optical dept level.

This unknown contribution can be included in principle again as an additional unknown x_4 to (13). But this can only be successful, when the MERIS channel at 760nm will be included in the inversion equations (12). The reason is, that the “optical reflection responses” of x_4 in the channels 705 nm, 754 nm, 775 nm, 865 nm, 890 nm is quite near to that of x_2 and can therefore not be separated from the variable x_2 by using only these channels.
But the “optical reflection response” of x_2 and x_4 are rather different in the channel 760 nm . The reason is, that the contribution x_2 is from scattering particles near the bottom in the atmosphere, but x_4 from particles in a thin layer in the upper troposphere. This difference in

height of both particles means, that there is much more absorbing oxygen in the air above near ground residing x_2-particles than over high in the atmosphere residing x_4 -particles . But oxygen is strongly absorbing in the channel 760nm. Consequently the light absorption in this channel is much stronger for x_2 –particles than for x_4 –particles . For the MERIS channel at 760 nm the extinction due to oxygen above high laying x_4–particles is estimated typical of order 0.6, the extinction due to oxygen above deep laying x_2 –particles is much stronger (order 0.3) . And this will diminish the “optical reflection response” of x_2 –particles much more than for x_4 – particles- that is: x4 – particles contribute therefore much stronger than x_2 – particles to the measured signal in this oxygen absorption channel 760 nm. But in the nearby channels (e.g. 754 nm) both particles contribute practically equally to the signal. This different action of x_2 and x_4 in absorbing channel 760 nm will allow to separate also this Thin Cirrus contribution.

Formally the reflection of this up to now neglected x_4 –particles can be included in the same way as the other x-contributions defined before in the “quasi linear “ formulation:

$$R_i^{TOA} = \sum_{I=1}^{4} K_{ij} x_j + R_i^{RGFCS} \tag{14}$$

$$i = 1 \ldots N_i$$

Now there are 4 unknowns and the inversion procedure demands additionally the measurements of R_i^{TOA} also in the channel at 760 nm .

1.1.1.3.4. Effects of Stratospheric Aerosols

Up to now there where only included scattering by Tropospheric Aerosols, scattering in water, at water surface and at Thin Cirrus clouds. But there are also Aerosols in the stratosphere. Typically Stratospheric background Aerosols are of order 0.005 (in Optical Depth units) / 6/ and are therefore much smaller than dominating Tropospheric Aerosols . But for some time after volcanic eruption there may be a drastically increased regional Optical Depth, which will than spread over the globe . But only for a limited time after eruption one can expect Optical Depth of Stratospheric Aerosols comparable to the Optical Depth from Tropospheric Aerosols . The largest eruption of this century (Mount Pinatubo, June 1991) led within weeks to an Aerosol band around equator (up to 25 degrees north) of optical dept level 0.1 with a rather sharp edge to higher latitudes , where there was only an low increase above the background level. The spreading of Aerosols then proceeded to northern latitudes within a year , gradually decreasing the level to order 0.02 in the European region one year later /6/:

Therefore: In our area of main interest (North European coast and Baltic Sea) one can normally assume a Stratospheric background Aerosol at an optical depth level , characteristic for this area and time (about 0.005....0.02), slowly decreasing in time, if there was no additional strong volcanic eruption in the last month before MERIS data interpretation .

If there was a strong eruption some month before MERIS data application, one should at first check at what time the corresponding “ volcanic cloud “ will reach the region of interest. Depending on the found level of this volcanic contribution one will have to change more or less the MERIS interpretation concept:

If the additional Stratospheric level due to the eruption is of order 0.05 one can find an estimation of the additional “Stratospheric Optical Depth level” by a special version of the MERIS data inversion algorithm: In cases, that there is proven “no Cirrus Optical Depth”, the high in the atmosphere lying volcanic cloud can be separated from the low lying Tropospheric Aerosols in the same way as discussed before for high lying “Thin Cirrus ” by integration of the 760 nm channel as discussed for equation (14).
One must only make sure, that in this case the other possible high lying scattering layer (Thin Cirrus) really does not exist. And this typically will happen in more than about 50 percent of all application cases. One has therefore to look for a region in the scene, which can be qualified as “free of Thin Cirrus ” . In this region the channel 760 nm can now be used to separate the “additional Volcanic Aerosol Optical Depth” instead of “Thin Cirrus Optical Depth” from Tropospheric Optical Depth by using Equation (14), but now with an alternative high layer stratospheric volcanic Aerosol model instead of the “Cirrus layer” model.
If there are more “ Cirrus free” regions in the scene one can interpolate the “ Volcanic Aerosol Optical Depth” between these regions for a corresponding estimated “ Volcanic Optical Depth map”. If there is a situation where there is no region classified “Free of Thin Cirrus “ one can use in this case the last estimated “additional Volcanic Optical Depth map” as input for the MERIS algorithm model (14) after Volcanic activity.

Formally one has the same equations of type (14) for the two cases:

Case A : (MERIS standard case) :Variable Thin Cirrus may be present, but Optical Depth of Stratospheric Aerosols is at fixed background level:
The unknown x_4 in (14) in this case is the Optical Depth of Thin Cirrus (and in the calculation of the coefficients in (14) it was implicitly assumed, that the Stratospheric Aerosols are background Aerosols of a fixed regional optical depth level).

Case B: Variable “Additional Volcanic Aerosol “ may be present, but Optical Depth of Thin Cirrus is at fixed level 0:
The unknown x_4 in (14) in this case is now the Optical Depth of “additional Volcanic Aerosols” (and in the calculation of the coefficients in (14) it was implicitly assumed, that there is no Thin Cirrus present and the stratospheric Aerosols are background Aerosols of a fixed regional optical depth level).
Formally this means: Case A and case B use the same inversion method but only different LOOK UP TABLES.

Since the algorithms of case B are probably not necessary for standard MERIS data use (probably no strong enough volcanic eruption in the month before MERIS analysis at our main region of interest) , this algorithm (case B) will be left out from the MERIS standard procedure (case A).
But this algorithm will be developed parallel to test the implicit assumption of MERIS case A (“ fixed regional optical depth level of stratospheric background Aerosols”): It might be , that there are strong Volcanic eruptions some month before the start of MERIS data use or during MERIS campaign. Case B algorithm shall than be used in situations classified as “free of Thin Cirrus” to verify that the implicit assumption for MERIS standard case A (“ Optical Depth of Volcanic Aerosols” = region background level) is still fulfilled.
If it is not fulfilled, case B algorithm will be used to estimate the “ Optical Depth map of Volcanic Aerosols” as discussed above .This map can than be used for the next time as input for standard case A algorithm instead of the former used assumption “ Volcanic Optical Depth =region background level”.

In this way the standard case A algorithm (14) can be extended to the situation some month after a strong Volcanic eruption, if the additional Volcanic Aerosol level is much about the Stratospheric background level of the region and time.

3.1.1.4 Ancillary data

As already discussed , the coefficients K_{ij} and R^{RGFCS} in the final equation (14) depend on some variable parameters – that is, these parameters are important for the accuracy of determining the wanted unknowns x_1 ..x_4 from inversion of (14). These parameters can not be found from MERIS radiance data but from other data sources:

1. RELATIVE HUMIDITY, *RH*. It characterizes the atmospheric Relative Humidity averaged over the marine boundary layer. Its value is of great importance for the accuracy of Aerosol parameter estimation from MERIS. There seem to be some ways to estimate the RELATIVE HUMIDITY for the air mass under Aerosol analysis. The most accurate way seems to be to use ECMWF Tropospheric temperature and moisture profile data. Up to now it is open, if it is possible, to integrate this special source for estimating the ancillary data map “Relative Humidity”.
2. SURFACE WIND SPEED, w. It’s absolute value dominates the variance of foam cover at ocean surface and the sea surface roughness effect on Reflectance. It’s value is given parallel from MERIS/ADS.
3. ATMOSPHERIC PRESSURE , p_0 . It’s actual value modify the dominating Reflectance contribution (Rayleigh term). It’s value is given parallel from MERIS/ADS.
4. TOTAL OZONE CONTENT , t_{oz} . It’s actual value improves accuracy in the “atmospheric correction” algorithm. It’s value is given parallel from MERIS/ADS.
5. OPTICAL DEPTH of STRATOSPHERIC BACKGROUND AEROSOL, t_{SB} . A value should be chosen for the whole scene, in lowest order according to extrapolation of this value from previous given values for the area of interest.
6. OPTICAL DEPTH OF ADDITIONAL VOLCANIC AEROSOL, t_{vol} . In the standard case A (compare 3.1.1.3.5) this optical depth map will be set zero. In case of recent volcanic activity (case B) a corresponding optical depth map t_{vol} for the scene is needed. The estimation for this map could be found for example by extrapolation from special sites in the scene or from previous scenes (compare 3.1.1.3.5).
7. AIR MASS CIRCULATION DIRECTION , f_{am} . The necessary estimate of the variable parameter a_{11} (Optical Depth MIXING RATE in FINE aerosol part) can be related to the circulation direction for the area of interest (compare appendix A) , that is formally $a_{11}=f(f_{am})$. This direction f_{am} can be estimated from ECMWF data (compare appendix A). (For rather homogenous continental environment this variance can be neglected –a_{11} can be fixed to it’s average value for the region and time of application. In this case the estimation of f_{am} is not necessary).

3.1.1.5 WATER LEAVING REFLECTANCE calculation (ATMOSPHERIC CORRECTION)

It is helpful, to write the analog to (14) under use of the terms defined before in the way:

(15) $R_i^{TOA} = R_i^{A} + R_i^{RI} + R_i^{WBOA} \cdot T_i^{D} + R_i^{RGF}$

This equation, up to now used only for NIR channels is also governing Reflectance in the VIS channels.
The main difference to the NIR channels is, that in the visible part of the spectrum the water reflectance term R_i^{WBOA} in (15) is now highly variable additionally due to variances in other substances in water like chlorophyll and yellow substances /7/ .
But the other terms on the right side of (15) can be calculated very accurate. The only unknown on the right side of (15) is therefore in the VIS channels the reflection R_i^{WBOA} , which characterizes the reflection of sun light at molecules and other material in the water (“water leaving reflectance”).
This “water leaving reflectance” can be found from (15) by measuring of the term R_i^{TOA} and calculation of the other right hand terms ($R_i^{A} + R_i^{RI} + R_i^{RGF}$) and T_i^{D} .
These terms can be calculated with good accuracy, because they are depending on the same parameters (geometry, wind and Optical Depth’s of Aerosols and Thin Cirrus) which are already known from ancillary data or were estimated by inversion of (14) in the NIR channels (Optical Depth’s of Aerosols and Thin Cirrus).
One can therefore calculate the wanted unknown R_i^{WBOA} in the visible part of the spectrum from measured R_i^{TOA} and from pre-calculated LOOK UP TABLES for the terms T_i^{D} and (R_i^{A} + $R_i^{RI} + R_i^{RGF}$) by simply calculating

(16) $$R_i^{WBOA} = \frac{R_i^{TOA(measured)} - R^{RGFAI(calculated)}}{T_i^{D\,(calculated)}}$$

with

$$R_i^{RGFAI(calculated)} = (R_i^{A} + R_i^{RI} + R_i^{RGF})^{(calculated)}$$

This concept is usually called “atmospheric correction” , because the wanted part in the visible channels (R_i^{WBOA}) can only be separated from the measured signal (R_i^{TOA}) when there exist good estimations of basic atmospheric parameters , especially those to characterize atmospheric scattering by Aerosols. This information on Aerosols and other important parameters must than be used to calculate the unknown terms (($R_i^{A} + R_i^{RI} + R_i^{RGF}$) and T_i^{D}) in the equation (16) with high accuracy. This “atmospheric correction” will therefore give good results only , when all actual parameters, influencing the scattering terms ($R_i^{A} + R_i^{RI} + R_i^{RGF}$) and T_i^{D} , are found in a preceding step with good accuracy. This preceding step is the inversion of equation (14), which gives the most influencing Aerosol optical depth’s with best possible accuracy.
There is one more atmospheric variability effect in some of the VIS channels not quantified in the steps before (because of no remarkable effect in NIR channels): The measured Reflectance in some VIS channels varies small but not neglectfully due to the variance of atmospheric ozone content. It is therefore recommendable for higher accuracy of “atmospheric correction” to have estimations of the atmospheric ozone content and to use this information in the calculation of the correction terms in (16).
Modeling shows, that with increasing atmospheric ozone content the previously defined Reflectance and Transmission terms (pre-calculated in corresponding LOOK UP TABLES)

decrease gradually. If one calculates these LOOK UP TABLES for two ozone situations (for expected minimum ozone content and for expected maximum ozone content) one can chose the suitable coefficients by interpolation in these tables according to given ozone content field . This will be done in the algorithm. The “total ozone content” field itself is delivered from ECMWF /CLIMATOLOGY in the MERIS annotation data set.

3.1.2 Mathematical Description

3.1.2.1 Inversion equation

As already discussed in 3.1.1 the result of the modeling is a “quasi linear” connection between measurable quantities (R_i^{TOA}) and wanted unknowns (x_j) for every pixel:

$$R_i^{TOA} = \sum_{j=1}^{Nx} K_{ij} x_j + R_i^{RGFCS} \quad , \qquad i = 1 \ldots N_i \tag{17}$$

(N_i – Number of channels, N_x – number of unknowns).

The coefficients K_{ij} and R_i^{RGFCS} depend as discussed only weak on wanted unknowns. This weak dependence means, that one needs just a rough first guess of x_i for the pixel (n) under investigation. And as already discussed, this first guess of x_i for pixel n will be delivered by the final x_j at the previous pixel n-1.

The inversion for pixel (n) means than: Calculate K_{ij} and R_i by linear interpolation according to the assumed first guess for x_j in the corresponding LOOK UP TABLES . And than estimate x_J at pixel n by looking for the minimum of the function:

$$\sum_{i=1}^{N_i} \left(R_i^{TOA(measured)} - (\sum_{j=1}^{N_x} K_{ij} \cdot x_j + R_i^{RGFCS}) \right)^2 \cdot g_i \Rightarrow Min. \tag{18}$$

g_i are suitable weighting factors, depending on the noise error level of radiance measurements in each of the MERIS channels $i=1 \ldots N_i$.

The resulting equations for x_i are found from mathematics. The final inversion equation will be:

$$x_j = \sum_{s=1}^{N_x} K_{js}^{inv} \cdot \left(\tilde{R}_s^{meas} - \tilde{R}_S^{RGFCS} \right) \qquad j = 1 \ldots N_x \tag{19}$$

- N_x (Number of unknowns:), $N_x = 4$ with Cirrus (and with taking into account channel 760 nm), $N_x = 3$ without Cirrus (and without taking into account MERIS channel 760 nm).

- $K^{inv.}$ is a 4 x 4 matrix (in case $N_x = 3$ it is a 3 x 3 matrix), found from

$$K^{inv} = D^{-1} \quad with$$

(20) $$D_{sj} = \sum_{i=1}^{N_i} g_i \cdot k_{is} \cdot k_{ij}$$

(21) $$- \overset{\sim\, meas}{R_s} \equiv \sum_{i=1}^{N_i} g_i \cdot K_{is} \cdot R_i^{TOA\,(meas)}$$

(22) $$- \overset{\sim RGFCS}{R}{}_s \equiv \sum_{i=1}^{N_i} g_i \cdot K_{is} \cdot R_i^{RGFCS}$$

It is seen , that all the terms on right side of (19) are known since they are calculated from known data in LOOK UP TABLES:

- the weighting factors g_I are found from MERIS channel Noise
- the coefficients K_{js}^{inv} will be found from (20)
- the coefficients $\overset{\sim RGFCS}{R_s}$ will be found from (22)
- the measured Reflectance’s R_i^{TOA} determine the term $\overset{\sim meas}{R_s}$ according to (21).

As discussed before, any necessary coefficient (K_{ij}, R_i^{RGFCS},....) can be calculated by linear interpolation in corresponding pre-calculated LOOK UP TABLES (compare section 3.1.3).

3.1.2.2 Total inversion procedure

For any pixel (n) the measured Reflectance’s R_i^{TOA} , $i = 1 \ldots N_i$ are inverted to the wanted unknowns $x_j(n)$ by using equation (19).
This equation uses coefficients , which are all tabulated in corresponding LOK UP TABLES.
To pick up the correct values in the tables for the pixel (n) under investigation, one needs to know the following parameters:

1. 3 geometry parameters: θ_S (Solar zenith distance) , θ_V (Viewing zenith distance) and φ_{SV} (azimuth difference of sun and viewing directions)
   These parameters itself are found from the ADS-data

2. Rough estimations of the 4 unknowns $x_1 \ldots x_4$ for the pixel under investigation (n)
   These are given from values found for x in the pixel before (n-1)

3. Estimations of ancillary parameters:
- w (WIND SPEED),
- p (ATMOSPHERIC PRESSURE)

- t_{oz} (TOTAL OZONE CONTENT)
- RH (RELATIVE HUMIDITY)
- t_{SB} (OPTICAL DEPTH of STRATOSPHERIC BACKGROUND AEROSOL)

4. Only if necessary one must include also the chose of 2 more parameters:

In case of fresh Volcanic Stratospheric loading (Case B, compare 3.1.1.3.5):
- t_{vol} (OPTICAL DEPTH OF ADDITIONAL VOLCANIC AEROSOL)

In case of strong regional "Fine" continental Aerosol model variance (compare appendix A) :
- f_{am} (AIR MASS CIRCULATION DIRECTION)

In the first version of this MERIS algorithm it is assumed, that for our region of interest one can use only one continental model candidate for each atmospheric circulation direction f_{am} . This corresponds to the assumption , that the variance due to parameter a_{11} within the continental Aerosol models for this region can be neglected. But If new data approve stronger variance than up to now published models /26/, / /27/, /28/ suggest, this will be taken into account according to the algorithm ,suggested in appendix A.
The first version will also refer to the case of negligible fresh volcanic aerosol (t_{vol} =0.), compare 3.1.1.3.5)
If there will be a strong volcanic eruption shortly before MERIS launch or during MERIS flight one has to check, whether the assumption (t_{vol} =0.) will still hold. If it no longer holds the estimation of t_{vol} must be included in the algorithm (case B, compare 3.1.1.3.5).

All above listed parameters are known at pixel n, therefore all needed coefficients in the final inversion equation (19) can be calculated :
The three geometry parameter data are known from MERIS/ADS. The Ancillary parameter data are known as discussed from the corresponding sources of this data and the needed first estimations for the unknowns $x_1 ... x_4$ at pixel n are given from the results of inversion at the previous pixel (n-1).
After one inversion of (19) for pixel n one than finds $x_1 ... x_4$, which are typically accurate enough to be the final values of the wanted unknowns for pixel n . If it is not good enough one has to recalculate the coefficients with the new estimated $x_1 ... x_4$ and to repeat the inversion of equation (19).
This procedure will be repeated for any pixel n to give the wanted unknowns $x_1 ... x_4$ and finishes MERIS atmospheric Aerosol parameter estimation. This finishes the estimation of atmospheric Optical Depth's form MERIS NIR channels.

The next steps will than give the last wanted product, the multispectral WATER LEAVING REFLECTANCE R_i^{BOA} in the VIS channels:
As a result from the preceding steps the values $x_1 ... x_4$ are now known parameters for any pixel n. All needed model parameters (including already given geometry parameters and ancillary parameters) are therefore given for any pixel n. The needed coefficients for the right side of the final inversion equation (16) can than be found by the same interpolation concept from corresponding LOOK UP TABLES for the VIS channels at any pixel n.
From measured R_i^{TOA} at pixel n one can than calculate the wanted WATER LEAVING REFLECTANCE R_i^{BOA} for any pixel n from (16).

3.1.2.3 Flowchart of MERIS data inversion

The flowchart of MERIS DATA inversion is appending.
Here are added some comments to the steps, shown there:

The input for the inversion are MERIS-level1b-data:
TOA radiance's and ancillary data (the source of "Relative Humidity" is still not finally decided).The other basic input is from LOOK UP TABLES (LUT) which contain all data to calculate the needed inversion coefficients for all terms in all needed channels.
The necessary step to interpolate the ancillary data , given at larger grid points to MERIS grid points is already included in the flowchart, but not in the first version of prototype algorithm.
The flow chart is already written for the case of four unknowns , but in the first version of algorithm the LOOK UP TABLES for channel 760 nm and for the VIS channels are lacking.
The corresponding first algorithmic version is therefore at present just for the 3-dimensional case without estimation of " Optical Depth of Thin Cirrus " and without the atmospheric correction step to estimate the "Water Leaving Reflectance".
At present we know from inversion tests, that one should set some flags for special situations (compare section 3.2.3 and 3.2.4) where increased errors in one ore more of the output products is to be expected. The cases for setting corresponding flags can only be given, when the complete error analysis for all products and situations is done.

To check this algorithm one example of simulated maps of "FINE" (x_1) and "COARSE" (x_2) and "sediment" (x_3) fields was chosen , MERIS reflectance fields were simulated for this case, noise was added to the simulated reflectance's and these data were inverted according to (19) . Simulated and inverted fields are appending.

3.1.3 Practical Considerations

The suggested method is a new concept of MERIS data use for atmospheric application.
Up to now there were only estimates of the Total Atmospheric Optical Depth. The suggested concept allows an estimation of the optical depth of the dominating parts of atmospheric Aerosols as well as Thin Cirrus in a way that seems to be rather flexible:
Any model improvement in one or the other model part will typically not change the inversion procedure as a whole, because only the values in the corresponding LOOK UP TABLE must be changed. Especially as long as there are so many not fully validated models included in this or any other algorithm to invert satellite data to Aerosol characteristics, this seems to be of great practical advantage of the algorithm suggested here.
The same is true with regard to the extension of the algorithm if there are sensors with more measurements as in the rather short wavelength range from 705 nm to 890 nm.
These extended data , also polarization measurements, can be included in the given algorithm by the same "quasi linear concept ", suggested here.
The interpolation concept itself has the advantage, that one must not look for special approximations of the effect of each unknown parameter on Reflectance's and transmissions. It is expected that any try of analytical approximations for these terms seems to be extremely difficult, because so many influencing parameters are involved . The

suggested interpolation concept avoids this difficulty. But this interpolation concept has the disadvantage, that the number of figures to be saved and to accessed quickly is rather large . In the case of 3 unknowns (corresponds to neglecting Thin Cirrus effects) the number of figures in the LOOK UP TABLES is of order 100 MB. The extension of the algorithm to 4 unknowns (estimation of optical depth of Thin Cirrus is included) will drastically increase the number of needed data in the Tables . It is estimated that about 1 GB real numbers will be necessary in LOOK UP TABLES for the final algorithm. But this level of data does not seem to be a real problem for modern computers.

3.2. Numerical computation considerations

As already discussed, the formulation of the Aerosol estimation problem from MERIS as a “quasi linear equation” is rather simply to invert. The main numerical problem might be, that each new involved parameter and unknown requires the calculation of any table (of course only those depending from this new included parameter) at least for 2 values of the included parameter (parameter minimum value and parameter maximum value). As an example: Minimum and Maximum Optical Depth of ozone content. This will typically result in doubling the number of figures in the corresponding LOOK UP TABLES . From accuracy reasons one should even make calculations at some more points between the extreme values . In principle one can reach extreme high approximation accuracy if one uses very near discrete calculations for each included parameter. But this will result only in extra ordinary large LOOK UP TABLES without really increasing the accuracy in the output products, since there are some unavoidable error sources : Errors in the fixed model parameter of any involved scattering process, errors in the ancillary data as well as errors in measured MERIS radiance’s.

From first experiences with the algorithm we have just a rough understanding of the number of discretisation points one should use for each of the involved parameters (parameters listed in 3.1.2.2). This will lead to the estimation of about 1 GB figures in the LOOK UP TABLES to save . Since most steps of the inversion algorithm is interpolation in the tables , the quick access of the table data as well as the quick multidimensional linear interpolation in the tables is of great importance for fast inversion.

The here suggested unknowns are opposite to other used parametrisations like those, using the “Angstroem exponent” /8/ nearly linearly connected to measurable reflectance data. This allows to invert measured data to unknowns practically in 1 step without iteration. This basic inversion step should allow a fast inversion procedure by use of a corresponding special processor.

The other basic step of the algorithm, the calculation of the involved coefficients will be done by simple multidimensional linear interpolation in LOOK UP TABLES. It should also be possible to do this second part of the algorithm by special processors to make the calculation of the appropriate coefficients fast.

3.2.1 Interpolation Concept

Any of the coefficients (Kij, R^{RGFCS} ...) needed in the final inversion scheme (compare equations 16 and 19) are found as discussed by interpolation in corresponding LOOK UP TABLES.

The dimension of each of the tables is given by the number of parameters, which characterizes the total model. These variable parameters can be arranged to form a

corresponding multidimensional vector parameter. A list of all included parameters is given in chapter 3.1.2.2.
Each table value represents therefore the value of the corresponding term at a fixed multi-dimensional parameter point. For each step at each pixel all parameters have given characteristic values and fix therefore an multidimensional parameter point laying between the multidimensional parameter points where the tables have been pre-calculated. By multidimensional linear interpolation one can than find the wanted coefficients at the given multidimensional parameter point.
Up to now we did not tried to reduce the number of data necessary in the LOOK UP TABLES to an acceptable minimum , because the up to now done tests showed, that the total number of the data needed in all of the tables will be of order 1 GB real numbers – a quantity which should not result in numeric problems.
By using different numbers of discretisation points for each parameter in different LOOK UP TABLES the number of Figures in LOOK UP TABLES can be drastically reduced without having a real effect on accuracy . But this will complicate the interpolation procedure and may therefore increase the time for the calculation of all needed coefficients. This work should therefore be done only, if there is a real need to reduce the number of allowed data in all needed LOOK UP TABLES.

3.2.2 Calibration and Validation

It is well known that sensors analyzing the ocean/atmosphere Reflectance in the VIS/NIR region need extreme high calibration accuracy's for radiance measurements /9/, /10/.
The wanted accuracy's are typically not reachable by standard calibration methods in the laboratory. Alternatively one performs additionally calibration experiments, by adjusting the calibration in each channel to give best agreement for Aerosol parameters and Water Leaving Reflectance's estimated from sensor data to those estimated from ground based data. This method is typically referred to as "vicarious calibration" / 35/. We should be prepared to perform our own "vicarious calibration" experiments by combining MERIS data with suitable complex ground based experiments.
The validation of all suggested products will be done by comparing MERIS derived output products with simultaneous ground based measurements of the same products by a series of corresponding experiments. The products " Total Optical Depth" and "Water Leaving Reflectance's" are measurable with own ground based systems. " To validate the optical dept of "FINE" and "COARSE" Aerosols one should estimate the same parameters also from ground based aerosol measurements, especially from measured multispectral aerosol optical depth.
The product " Optical Depth of Thin Cirrus " is also not simply be found from ground based measurements. LIDAR measurements seem to be necessary. A corresponding cooperation must be established.

3.2.3 Quality Control and Diagnostic

The algorithms for the output products are based on "typical" model assumptions. That is: As long as there are typical values of the output products, one can assume "typical" errors for

each output product according to the algorithm suggested here. This “typical” error for each output product will be given for the user of the output products . Extended tests of the final algorithms are necessary to estimate these “typical” errors.
But there may be some “abnormal” situations, where the given “typical” errors are expected to increase more ore less drastically. These situations correspond to situations where the involved parameters tend to it’s minimum or maximum value or for situations where the normal aerosol production mechanism is strongly disturbed . Some of these special cases are already given in appendix a, some more cases of strong regional anomaly might be found during application of the algorithm on real MERIS data. All these situations must be flagged and the extended error level for these situations must be given at first from the theoretical point of view.
After launch the estimated error levels in these different situations have to be checked by comparison with ground truth experiments and corrected if necessary.

3.2.4 Exception Handling

Deviations from the standard algorithms will be necessary when some input parameters are lacking. Not all of the input data are of the same importance for the accuracy of the final products. For example, the actual atmospheric pressure p is of low effect for the Aerosol products, but of importance for the product Water Leaving Reflectance. Very important to the error level of all products is the Relative Humidity RH and (depending on the real continental environment) the estimation of the parameter a_{11} which chose the best “fine” continental Aerosol model . The best way of exception handling in situations where one of the ancillary data is lacking, seems to be to use typical values of the missing parameter . Since the missing of actual data will increase the errors in the products, a corresponding flag for „missing ancillary data RH “ or p_0 or .... should be set .
This setting of flags should also be done, when one of the basic TOA radiance’s is missing. But at least three of the 5 suitable MERIS NIR channels (705nm, 754nm, 775nm, 865nm, 890nm) and the radiance at channel 760nm are necessary information . Since the missing of the radiance in one of the channels will also reduce the accuracy of the products, these situations should also be flagged with information on the missing channel.
If the radiance at channel 760 nm is expected to be lacking for a longer time period of MERIS use, one can go to the simplified model $x_4 \equiv 0$ (no Thin Cirrus assumed)” by just a small change in the algorithm. In this case the wanted unknowns are x_1 ,x_2 ,x_3 ,($x_4 \equiv 0$) and one has the standard algorithm for MERIS NIR data use without channel 760 nm (compare 3.1.1.3).
In pixels with “Thin Cirrus present” this will result in higher errors in the Aerosol Optical Depth’s, but in pixels with “no Thin Cirrus present” there really will be no additional error due to the lacking channel 760nm. Since many situations are without “Thin Cirrus present” one will have good results in many cases.
Deviations from the standard procedure may also be necessary, if one of the estimated parameters (x_1 ...x_4 , R_i^{BOA}) will be negative. There are some reasons, that the results of inversion may lay outside the physical like calibration errors, strong deviations in some implicit model assumptions, real errors in the ancillary data. These situations of “results out of physical allowed range ” should also be flagged .
A detailed analysis of these flagged cases must help to find the reasons and correct it at least for the following period of MERIS data use.

3.2.5 Output Products

The output products are :

- Optical Depth of “FINE” Aerosols
- Optical Depth of “Coarse Aerosols”
- Total Aerosol Optical Depth
- Optical Depth of Thin Cirrus
- Water Leaving Reflectance (multispectral)

To compare these results with the “Total Aerosol Optical Depth” , estimated from other sensors or algorithms this product can simply be found by adding the 2 products (Optical Depth of “Fine” and “Coarse” Aerosols) as well as the used stratospheric background Aerosol Optical Depth in Standard case A (compare section 3.1.1.3.5). In case B the “additional Volcanic Aerosol Optical Depth” t_{vol} has also to be added (in standard case A this contribution is set to zero) .
In the algorithms the Optical Depth’s are to be understood as “ Optical Depth at a fixed reference wavelength $?_0$. In the prototyp algorithm the reference wavelength 754 nm was chosen to calculate the LOOK UP TABLES.
To make the found “ Optical Depth’s fields” easy comparable to other sensor output of the same parameter but calculated for a different wavelength there will be developed a special conversion program .This program will be transferred to any user on request.

Some further remarks to the products should be helpful:

The definition of the two products “Optical depth of “FINE” and “COARSE” Aerosols” was given in Appendix A. There are two more points of interest to point to:
-The sum of the two products, named “Optical Depth of “Fine” and “Coarse “Aerosols” are also an estimation of the “Tropospheric Aerosol Optical Depth” .
-The two tropospheric contributions (“FINE”) and (“COARSE”) are representing practically the efficiency of rather different aerosol producing mechanisms (compare the discussions in /25/, /12/). This difference in mechanism should make both optical depth fields interesting to optimize aerosol effects in climate models like ECHAM /33/.

The Water Leaving Reflectance (R_i^{WBOA}) is the radiance leaving the water from below the surface , but found just above the surface and normalized to Irradiance and sun position according to the Reflectance definition in equation (1).

The “Suspended Matter” is a „by-product“ of the inversion of measured data (unknown x_3). It gives good estimations for suspended matter only for high suspended material in water. Since there are expected more accurate estimations of this parameter for a larger range of Suspended Matter variance from other MERIS algorithms, the delivery of this (possible) product is not foreseen at present. If there are requests at least to compare this with other estimations it can also be included in the list of output products.

4.Error budget estimates

Up to now there was not enough capacity to calculate the overlapping error effects of all the thinkable error sources which might be involved in every assumption necessary to every layer in the total ocean/atmospheric system to quantify the errors in each of the products for all relevant geometry’s and in all interesting application cases.

At present we can give only a first estimation of the supposed main error sources for the defined products as well as an first estimation of the expected error level for the products under typical application conditions. The test of all supposed relevant error sources on all different output products for all relevant situations and cases must be done with the final algorithm. But at present the focus of the work is on finishing the development of all programs necessary to calculate each figure in each needed LOOK UP TABLE for each MERIS channel. Extended error budged estimations can be made only after filling each LOOK UP TABLE. The results of these estimations will be given later.

Product „Total Aerosol Optical Depth “

Up to now published methods to estimate “Total Aerosol Optical Depth” from satellite /1 /, /14/ are modeling the basic Aerosol Reflectance by using MIE scattering theory for spherical particles.
At present there is great activity to establish methods to calculate Aerosol Reflectance for different non spherical shaped particles . The main change due to deviations from spherical shape seems to be an enhancement of scattering at medium scattering angles /15/ , but there might also be some effect on the backward scattering direction /16/, /24/ , typically important in passive satellite remote sensing.
It is expected, that this enhanced scattering effect will be important for Thin Cirrus and for dust Aerosol components . For Aerosols , interacting strongly with atmospheric water vapor (dominating components „Water Soluble“ and „Sea Salt“) the degree of enhancement might typically be neglectfully, but this is not validated up to now. Since the application of the algorithm will be in situations with dominating Aerosol components of type „Water Soluble“ and „Sea Salt“, the modeling of all Reflectance’s is at present done by spherical MIE theory . Only if the accompanying MERIS validation program shows an systematic underestimation of Optical Depth the scattering functions used will have to be corrected correspondingly. The remaining non spherical error level on Optical Depth might be not much beyond some percent, but this is highly speculative and may fail, if the marine air is near extreme dry levels.
If one neglects this “non spherical” error effect, than the most important error source for “Total Aerosol Optical Depth” estimation seems to be the error due to erroneous estimation of Relative Humidity from the ancillary data source. This error may result of up to 30 percent error in Total Optical Depth, if there are no estimations of the actual Relative Humidity and one uses therefore a fixed “most probable” standard level of about 75 % but actually the Relative Humidity is 95 %.
All other error sources seem to be much smaller for the product “Total Optical Depth”. The method to deliver this ancillary parameter “Relative Humidity” from other sources is therefore of basic importance for the accuracy of the product “Total Optical Depth”. If one will be able to estimate Relative Humidity with accuracy of about 12 % the “Total Optical Depth” is expected to increase accuracy to a level of up to 10 percent.
This high accuracy seems to be endangered mainly due to sea surface effects:
In special situations much higher errors are possible due to errors in the estimation of the additive term R^{RGFCS} in equation (14). This term contains a more or less part of specular reflected sunlight (“glitter”). The error in the estimation of the glitter part is connected with the error in the estimation of the surface wind speed from ECMWF data and the suitability of the COX-MUNK –MODEL /17 / of sea surface inclination facets statistics. These error sources result in corresponding “glitter” Reflectance errors, which are strongly dependent on sun elevation and viewing directions . It’s effect to the error of “Total Aerosol Optical Depth” can reach from neglectfully to dominating , even in one MERIS scene. Not only for Aerosol application but also for chlorophyll application it is therefore necessary to cut the scene into

two regions, in a region dominated by glitter effects and corresponding "glitter" errors (not recommended for MERIS algorithm application) and a second region, not dominated by glitter and recommended for all MERIS ocean applications. There is no sharp error jump from the "recommended region" to the " not recommended region" and the error quantification for pixels near the border in the "recommended region" should be done with care to define the optimal border of the "recommended region" for different wind levels and geometry's.
For high winds another error source in the additive term R^{RGFCS} is due to estimated foam Reflectance at sea surface. There are some error sources in this part, concerning the models for foam fraction versus wind speed /18/, /19 / and foam albedo /20 /. At least for winds above about 12 m/sec the error level for the output product will increase due to this error.

Product „ Optical Depth of "FINE" Aerosols

Since this part is typically the dominating part of "Total atmospheric Optical Depth" in coastal regions all above given error sources are typically dominating also the error level of this product. But there are some more error sources, mainly acting on this output product: At first this are errors due to sensor noise and sensor calibration which might dominate the errors in this product at least for low Aerosol loading . To estimate the consequences one needs information of real sensor calibration accuracy in the used channels and more important on the accuracy and stability of radiance difference measurements for neighboring channels. At present we are lacking those "intercalibration"n data for MERIS channels to discuss this error consequences. Information on radiance noise level in MERIS channels was taken from /21/. The assumed noise level results in much higher fluctuations in this output product than for the "Total Aerosol Optical Depth". One will have to integrate about 4*4 pixels to reach about the same level of fluctuation in both products. But this is still an acceptable geometric resolution to use the "Aerosol Optical Depth of "FINE" Aerosols" in Aerosol applications.

Product „ Optical Depth of "COARSE" Aerosols

As in the case of estimation of the "FINE" aerosols, the noise and intercalibration errors are additionally to errors in Relative humidity of great influence on the error for this product. Two more uncertainties will effect mainly the error of this product:
-There will be an error in the estimation of the Sea surface reflectance contribution ("glitter" and "foam") . Errors in this part lead typically mainly to errors in the Optical dept of the "COARSE" aerosol part. An underestimation of the Sea surface reflectance contribution results in an overestimation of this "COARSE" part and vice versa.
-The continental environment of the marine region of interest may lead to an hardly predictable rate of "dust like" aerosols mixed in the "COARSE" aerosols. It will depend on the region and on wind level, which rate really can be found. The level of this rate will accordingly effect the error and the optimal chosen rate in the final algorithm for the region of interest.

Product " Optical Depth of Thin Cirrus "

As already mentioned , the simulation of the corresponding LOOK UP TABLES is just in the beginning. One of the main error sources for this product seems to be the model for oxygen transmission /3/. But this might possibly be corrected (compare following section) . Next to these errors, the errors due to variances in the vertical distribution of all tropospheric aerosol components and stratospheric aerosols as well as the height of the Thin cirrus layer iare expected to dominate the Thin Cirrus separation. But real figures for these expected error levels can only be given after finishing the corresponding LOOK UP TABLES..

Product “Water Leaving Reflectance”

Since there is a comparable product from MERIS standard algorithms, originally it was not planned to deliver the “Water Leaving Reflectance” . But there are some hints, that it makes sense to offer also this product. The main reason is, that the suggested algorithm for estimation of Aerosol parameters and Thin Cirrus should allow a more accurate estimation of the real scattering situation in the atmosphere and on sea surface than standard MERIS methods. This will allow the atmospheric correction (compare section 3.1.1.5) principally with higher accuracy.
Up to now we did not start the calculation of the corresponding “LOOK UP TABLES”. After Finishing the LOOK UP TABLES the error tests shall be done and the results will also be given in the following version of ATBD.

5.Assumptions and limitations

There are a lot of models necessary to describe the effect of variances from water, water surface, troposphere, stratosphere and Thin Cirrus on measured reflectance over oceans. The main assumption with regard to the tropospheric aerosols is, that particle number distribution over marine places is typically dominated by mainly “Fine” continental origin particles and mainly ”COARSE” marine originated particles.
The aerosol size distribution is therefore to be described (at least) as a sum of two parts , populating the number size distribution in two size ranges (Bimodal size distribution). Size distribution measurements suggest the use of a log-normal size distribution around the corresponding two size mode maximums for both two size ranges.
Since the aerosol reflectance is mainly changing due to the range the aerosol particles are concentrated in, one will get good results also if the actual particle size distribution is rather far from this “bimodal” log-normal shape as long as the real particles are dominating in the size range spanned by the two mode size maximums. At present there seems to be no size distribution measured which tends to concentrate the particle size much below the used “FINE” range maximum, but situations with particle size concentrations much above the used “COARSE” range can happen since there are aerosol production mechanisms which tend to produce a lot of large particles. The best known case seem to be the situation when atmospheric circulation pushes desert dust storm aerosols out of the water. In this case the algorithm should not be used. There are at least two other special cases where the “normal” marine and continental aerosol production mechanisms are strongly disturbed: “Regional forest fires” and “strong volcanic activity” . The algorithm should at least be modified in the used components to cover also these situations.
Therefore : At least for nearly all of the real situations one may expect good results in the estimation of the optical depth’s of aerosols in these two ranges “FINE” and “COARSE”. But the errors may increase, when the model will be used for the above mentioned special “events” or if there are other up to now unknown reasons for a change in basic aerosol parameters of the used aerosol component models.
To find out the highest level of allowed “perturbations”, one should also simulate multispectral signals at satellite height for aerosol situations typically found for these special “event” situations and apply the inversion algorithm on these cases. These special tests should be made in algorithm tests.

Another basic assumption is the assumption, that the aerosol scattering function can be calculated by using MIE scattering theory for spherical particles. There are hints, that the scattering function calculated this way are underestimating the real scattering function in some cases. In section 4 this effect was already discussed including an idea to use real MERIS data to avoid this problem after some time of MERIS data use.
It is also assumed, that the dust part of Aerosols is only a minor continental Aerosol part. As already discussed in appendix A this is suggested by the published continental Aerosol data measured /25 / and modeled /26/. This assumption might be true in our main application region (north European coastal areas and Baltic sea. But some risks may exist for high wind situations. This should also be tested in a systematic application of MERIS at our preferred test area (Baltic Sea).
The published continental models suggest only a small variation (small in the effect on reflectance but not necessary in the real deviation from bimodal number size distribution) within the continental Aerosol models if the region of interest is far away from large bare soil areas like deserts as well as from industrial areas. These models are therefore expected to be good continental candidates for Aerosols in air masses rushing in to north European coast and to the Baltic Sea region from different directions. But this is not validated up to now and should also by tested by systematic comparison of Aerosol results from MERIS for different directions of air masses rushing in.
In cases of Thin Cirrus present, there are some special assumptions made which should also be tested and reported in the next version of ATBD. Own measurements of oxygen atmospheric transmission in the necessary MERIS channel at 760 nm confirmed model calculations of oxygen atmospheric transmission with errors typically up to about 10 percent . But modeling suggests, that the variances in oxygen transmission due to atmospheric variances are expected much smaller. That is : There may be some systematic errors in oxygen transmission calculation, probably due to line shape and strength uncertainties. If this is true, corresponding systematic errors should be found in the separation of Thin Cirrus Optical Depth from Total Optical Depth. These systematic deviations can than be corrected experimentally by some special kind of “vicarious calibration” /35/,/36/ to adjust the used oxygen transmission model .

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Appendix A

Parametrisation of multispectral Aerosol Reflectance

The quantitative interpretation of light reflected by Aerosols in the line of sight between earth surface and satellite sensor needs a model, that connects measurable quantities like the multispectral Aerosol Reflectance $R^A(l_i)$, $i = 1 .... N_i$ to interesting Aerosol parameters.
In this appendix the variance in $R^A(l_i)$ is analysed to define a model that connects this variance in $R^A(l_i)$ to the variance of suitable aerosol parameters.

Except from situations shortly after strong volcanic activity most of the Aerosols are found in the tropospheric part of the atmosphere near the earth surface. These Tropospheric Aerosols are related to the nearby earth surface type:
Each part of earth surface can be regarded as an Aerosol source due to its ability to add characteristic Aerosols and gases to the air above it. Different types of surfaces produce different Aerosols and gases. The injected material will than be transported by circulation (thereby changing some of the injected gases to Aerosols by chemical and physical reactions) to the place, where the Aerosol analysis from measured $R^A(l_i)$, $i = 1 .... N_i$ will take place.
In this way the measurable Aerosol Reflectance represents more or less the Aerosol emission sources on earth surface, the air mass has passed in the latest hours and days before measured multispectral $R^A(l_i)$, $i = 1 .... N_i$ is be analysed.
To model the optical response of the N real aerosols in the path across the atmosphere the “external mixing” principle was formulated in / / : The N real aerosols behave in applications as if they are made of a mix of only a few different aerosol components $N=N_1 + N_2 +...$ Each of these aerosol components is represented by a characteristic substance, particle size distribution , complex index of refraction and based on these data also of optically parameters like extinction coefficient, single scattering albedo and scattering function.
In our application case the model should be used for aerosols over marine areas. There has been a lot of experimental work to analyse tropospheric aerosols and it’s variance over marine places (see for example / 31/, /12/,/13 /). Common to all experiments is, that particle number size distribution measurements and chemical analysis of aerosol particles suggest that tropospheric aerosols should be composed of at least two components: The number size distribution of the first component has it’s maximum value at a diameter of about 0.06 µm and is dominated by continental origin particles, the second component is centred at much larger dimensions (factor of order 10 times larger) and is dominated by particles produced by wind action on water surface.
This suggests to model tropospheric aerosols over marine places to be made of two components. In the basic maritime models of Shettle and Fenn /34 /, /11/ and the radiation commission /37 / the first aerosol component (diameter of about 0.06 µm / 26/.) was assumed to be chosen according to the properties of the aerosol component “water-soluble” , the second aerosol component (diameter about 0.6 µm) according to the properties of the aerosol component “oceanic” /37 /. The experimental data suggest, that the numbers N_{A1} and N_{A2} , which characterise the numbers of both parts are highly variable figures over marine places /12 /.
Since in lowest order Aerosol Reflectance will grow with growing Aerosol numbers, the variability of aerosol reflectance at satellite will strongly be connected to the variability of these two numbers. That is: In the simplest model (neglecting any other reason for aerosol reflectance variability) the aerosol reflectance at satellite ($R^A(l_i)$, $i = 1 .... N_i$) will depend only on the two numbers N_{A1} and N_{A2} , which characterise the “amount” , the two aerosol

components will be found along a vertical path in the troposphere. Formally, the multispectral aerosol reflectance ($R^A(l_i)$, $i = 1 .... N_i$) should be modelled in this simplest model quantitatively as a function of the two variables N_{A1} and N_{A2}.
Instead of the variables N_{A1} and N_{A2} one can use also other parameters to characterise the “amount” of the two components like the volumes V_{A1} and V_{A2} or the optical depth at a fixed reference wavelength (τ_{A1} and τ_{A2}). The last choice has the practical advantage, that both figures over marine places are typically of the same order of magnitude. To discuss the variance effect of these two parameters on the multispectral aerosol reflectance $R^A(l_i)$ one can alternatively use the 2 variables

(1) $\tau_A = \tau_{A1} + \tau_{A2}$
and
(2) $a_1 = \tau_{A1}/\tau_A$

τ_A in (1) represents the Total Aerosol Optical Depth and a_1 in (2) the rate, at which the optical depth of the smaller is mixed in the Total Aerosol Optical Depth. In the following the two parts are named “fine and “coarse” according to the classification in /25 /.
Using these two variables one can simply see the strong variance one should expect in the total optical depth (τ_A) as well as in the rate (a_1) these two components are mixed in the troposphere above a maritime place near north European coasts: The rate $a_1 = \tau_{A1}/\tau_A$ is expected to vary between nearly negligible ($a_1 \sim 0.$) for air masses rushing in from the Atlantic to nearly dominating ($a_1 \sim 1.$) for airmasses rushing in from the European continent.
There is another strong reason for variances in the aerosol optical properties:
From the work of Haenel / 22/ one expects, that atmospheric water vapour can strongly interact with atmospheric aerosols. With growing Relative Humidity aerosol particles tend to bind more atmospheric water which therefore results in a change of particle diameter distribution to bigger particles as well as in a change of the refractive index of the aerosol components .
The effect of Relative Humidity (parameter RH) variance as well as of Optical Depth Ratio (parameter a_1) variance on aerosol reflectance variance s shown in Fig. A1 :

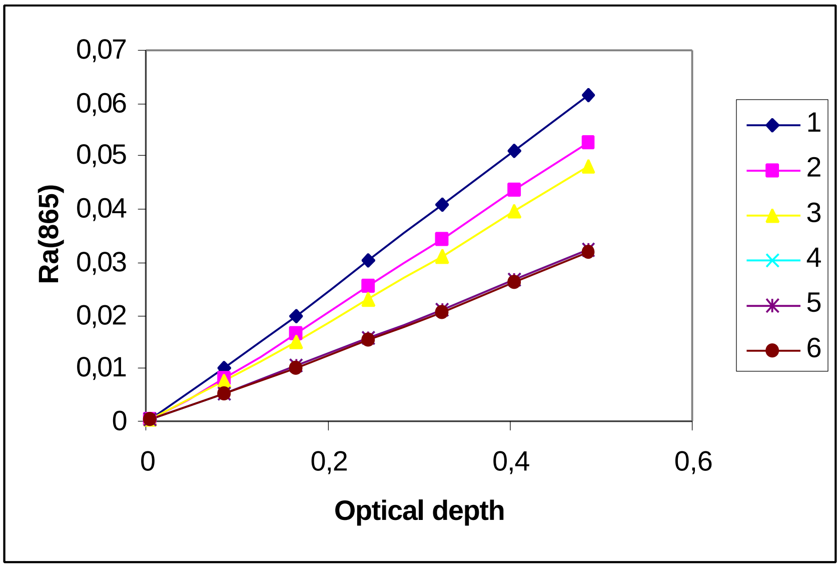

Fig. A1: The change of Aerosol Reflectance $R^A(l_i)$ (at reference channel 865 nm) with Total Aerosol Optical Depth t_A for different values of parameters a_1 and RH . Solar zenith distance $\theta_s = 48.78°$, Nadir viewing direction.
(curves 1-3) : $a_1 = 1$ (dominating fine continental Aerosol particles)
with RH = 50 % (curve 1), 70 % (curve 2) , 90 % (curve 3)
(curves 4-6): $a_1 = 0$ (dominating marine Aerosol particles)
with RH = 50 % (curve 4), 70 % (curve 5) , 90 % (curve 6)

Fig.A1 demonstrates, that the measured level of Reflectance $R^A(l_i)$ at a fixed wavelength (here was chosen the wavelength 865nm according to a corresponding MERIS channel) changes nearly linear with Total Aerosol Optical Depth t_A . From measured R^A (865 nm) one can therefore estimate the Total Aerosol Optical Depth.
But the relation between measurable R^A (865 nm) and Total Aerosol Optical Depth t_A is strongly depending on the two other parameters a_1 and RH . The effect due to parameter a_1 variance is especially near coasts expected to be much stronger than due to variance of parameter RH .
From Fig A1 it can also be seen, that the accuracy of Total Aerosol Optical Depth estimation from measured R^A (865 nm) can have errors up to order 30 %, if there are no reliable actual estimations of the parameters a_1 and RH . To reduce the error in the Total Aerosol Optical Depth estimation the accurate estimation of parameter a_1 is more important than the accurate estimation of parameter RH .

The parameter a_1 dominates the wavelength dependence of measurable multispectral Aerosol Reflectance $R^A(l_i)$, $i = 1 \ldots N_i$. . This is demonstrated in Fig A2 where the wavelength dependence , normalised to it's value at 865 nm is shown.

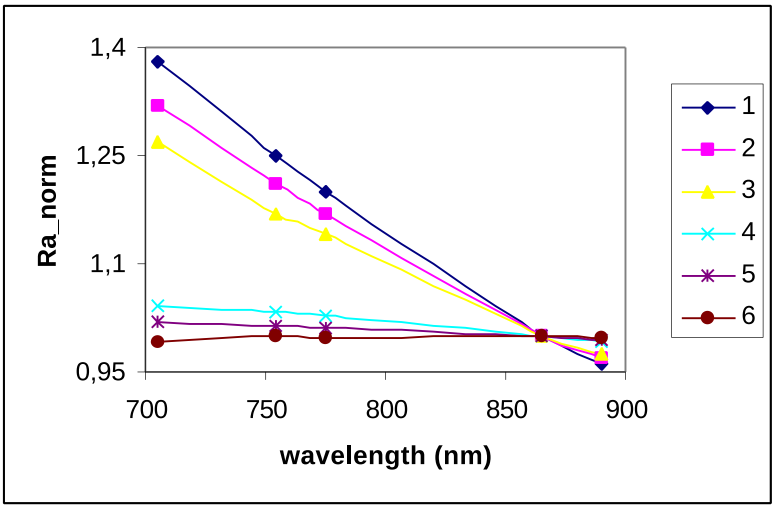

Fig. A2: $R^A(l_i)$, normalised to $R^A(865)$ for the NIR-Channels 705 nm, 754 nm, 775 nm, 865 nm, 890 nm are shown for different values of a_1 and RH (50, 7, 90 %), "averaged continental" Aerosol model, Solar zenith distance $\theta_s = 48,78°$,nadir viewing direction.
(curves 1-3) : $a_1 = 1$ (dominating fine continental Aerosol particles)
with RH = 50 % (curve 1), 70 % (curve 2) , 90 % (curve 3)
(curves 4-6): $a_1 = 0$ (dominating wind driven marine Aerosol particles)

with RH = 50 % (curve 4), 70 % (curve 5) , 90 % (curve 6)

Fig.A2 shows, that the inclination of the normalised reflectance Ra_norm to shorter wavelength is much less depending on the variance of parameter RH than on the variance of parameter a_1 .
The measured normalised wavelength dependence Ra _norm =(R^A (λ_i)/R^A (865)) can therefore be used to estimate the parameter a_1 .
On first sight it may be expected, that also the other unknown parameter RH can be estimable from measured wavelength dependence. But one can show, that there are some more in the discussion up to now neglected uncertainties in the modelling which prevent an estimate of both two unknown parameters (a_1 and RH) from the rather short wavelength range (some NIR channels) , the Aerosol reflectance R^A (l_i) can really be measured from satellite with acceptable high accuracy .
Fig. A2 shows also, that the accuracy of estimation of parameter a_1 from measured R_A (λ_i) will also depend on the accuracy of estimation of the parameter RH . As discussed, the parameter RH itself can not be estimated from measured R_A (λ_i) , but because it's effect on multispectral reflectance R_A (λ_i) is only of lower importance compared to the effects of τ_A and a_1 one needs just a rough estimation of the parameter RH. And there seem to exist some possibilities to reach this rough estimation of parameter Relative Humidity RH by the use of suitable ancillary data. At present the most promising way seems to be to use data nowadays available from atmospheric circulation models like those of the EUROPEAN CENTRE for MEDIUM RANGE WEATHER FORECASTS (ECMWF).

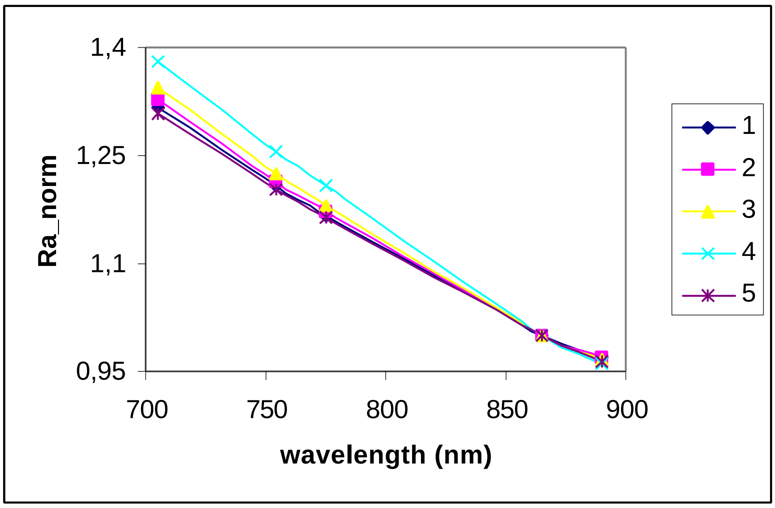

Fig. A3: R^A (l_i), normalised to R^A (865) for the NIR-Channels 705 nm, 754 nm, 775 nm, 865 nm, 890 nm are shown for dominating continental part (a_1 =1.), nadir viewing, solar zenith distance = 48,78° ,
curve (1): number ratio “soot/water soluble” = 12:10, Rh=70 %
curve (2): number ratio “soot/water soluble” = 24:10, Rh=70 %
curve (3): number ratio “soot/water soluble” = 48:10, Rh=70 %
curve (4): number ratio “soot/water soluble” = 12:10, Rh=40 %
curve (5): number ratio “soot/water soluble” = 12:10, Rh=70 %, number ratio “dust like/water soluble”=1: 35 000

It will depend on the marine region of interest, if additional to the above defined main variance origins (variances due to $t_{\mathbf{A}}$, $\mathbf{a_1}$ and **RH**) there might be further variance reasons with non negligible effect on multispectral reflectance $R^A(l)$.

In our application case (aerosols over north west European coast and Baltic Sea) there might possibly one more reason for non negligible variances:

The nearby continent seems not to be "homogenous" enough to neglect continental aerosol variances at least in the "fine" aerosol component:

Particle size distribution measurements over continental areas as summarized by Whitby /25 / suggest a bimodal structure in this "fine" particle size range . Corresponding to this published continental Aerosol models try to describe this "fine" particle range as composed of two Aerosol components, in most cases using the aerosol components named "water soluble" and "soot" / 27 /. The dominating mode (in optical depth units but not in number units) is the "water soluble" mode. It is expected, that the ratio , the two components "soot" and "water soluble" are mixed are not constant over the continent. The published models suggest the number ratio for "polluted" (or "urban") regions to be of order 4:6 / 27 / or 7:3 / 26) and of order 1:16 / 27 / or 5:9 / 26 /) for "average" continental regions.

It is expected, that the OPAC data / 26 / are the most reliable data available at present with regard to this rate. In Fig. A3 the variances effect due to this "soot" to "water soluble" ratio variance on normalised reflectance is shown , using the OPAC data.

The change in the "soot/water soluble" number ratio from "average" to "polluted" levels (curves (1) to (2)) is much smaller than the change from average values in Relative Humidity to low values (curve (1) to (4)). This seems to suggest, that this variance reason is also negligible compared to the three up to now discussed variance effects (variances due to $t_{\mathbf{A}}$, $\mathbf{a_1}$ and **RH**) . But actually at present there seem to be strong uncertainties in the "soot" to "water soluble" ratio one may really find over or near the continental region, the air mass is coming from . This uncertainties for example are demonstrated in the differences of this ratio in the two published models / 26/, /27/. If one assumes the rate "soot" to "water soluble" is up to now underestimated by a factor of 2 and one therefore doubles the soot part for the "polluted" continental region, one gets curve (3) instead of (2) in fig.A3. Now the reflectance change from "average" to "polluted" continental (curves (1) to (3) in Fig.A3) reaches already about half of the change level one would find if the Relative Humidity changes from "average " to "dry" conditions (curve (1) to (5)).

In this case one should therefore try to have at least an estimate of the ratio "soot" to" water soluble" for the continental region surrounding the marine region , the Aerosol interpretation from measured Aerosol reflectance $R^A(l_i)$ is to be done. There is another aspect which supports the need to estimate this ratio for aerosol interpretation: As discussed it needs a rather high soot level to have a remarkable change in the wavelength dependence in the reflectance within NIR channels. But the soot effect on aerosol reflectance as well as due to the strong absorbing character of soot on aerosol transmission grows with smaller wavelength . Errors in the soot rate estimation are therefore of greater effect in the application known as "atmospheric correction" which uses reflectance and transmission calculations especially in the visible part of the spectrum.

Formally: The first ("fine") component (numbers N_{A1}) is made up of two sub-components $N_{A1} = N_{A11} + N_{A12}$.

At present the two sub-components are probably best modelled by the model components "soot" (N_{A11}) and "water soluble" (N_{A12}). In complete analogy to the discussion which led to equations (1) and (2) one can change from numbers (N_{A11} , N_{A12}) to optical depth (τ_{A11} , τ_{A12}) of the two sub-components which represent the "fine" aerosols:

$$\tau_{A1} = \tau_{A11} + \tau_{A12} \tag{3}$$

and

(4) $a_{11} = \tau_{A11}/\tau_{A1}$

The parameter a_{11} in (4) describes the rate, the optical depth of the minor component is mixed in the “fine” (index 1) aerosol part which is according to (3) made of two sub-components (at present probably best modelled by the “soot“ (index 11) and “water soluble” (index 12) component).
For our main area of interest (northern European coast , especially the Baltic Sea) one might expect to find rather different values of the parameter a_{11} if the air mass rushes in from sparse populated Scandinavia (expected rather low “soot” to “water soluble” ratios in this case correspond to rather low levels of parameter a_{11}) or if the air masses rushes in from industrialised dense populated middle European continent (probably much higher values in parameter a_{11}).
The simplest way to take into account this regional variance in the modelling of the Aerosol reflectance seems to be:
One expects the ratio “soot” to “water soluble” to change between a minimum value (probably for airmasses rushing in to the Baltic sea from Scandinavia) and a maximum value (probably for airmasses rushing in to the Baltic sea from the middle European continent) . If f_{am} describes the direction of the airmass circulation the parameter a_{11} will vary between it’s minimum value for airmasses rushing in from direction 1 (f_{am1}) and maximum value for direction 2 (f_{am2}) . If the airmasses rush in for other directions (f_{am}) one can estimate the parameter a_{11} by interpolation according to the circulation angle. Formally : $a_{11}=f(f_{am})$ .The needed angle f_{am} to estimate a_{11} can itself be estimated from available circulation data like ECMWF.
The parameter a_{11} allows therefore to take into account the experimental known regional aerosol variance within the “fine” aerosol part by relating this parameter to data estimable also from available circulation data.

The discussion up to now corresponds to assume, that the variance in the optical properties of aerosols is due to the variance of the 4 parameters t_A , $\mathbf{a_1}$, **RH ,** $\mathbf{a_{11}}$ (or according to definitions (1) and (2) alternatively by the 4 parameters t_{A1} , t_{A2} , **RH ,** $\mathbf{a_{11}}$ **.)**

There are reported also reasons for variances within the “coarse” component. The data of Gathmann / 12 / suggest that the wind action on ocean surface produces also a bimodal structure in the “coarse” component , that is this second component is also made from two parts: $N_{A2} = N_{A21} + N_{A22}$ in complete analogy to the first “fine” component treatment. Formally one could proceed the same way as in the case of the variance within the “fine” mode: One can define a corresponding parameter a_{22} that describes the variance of the rates of the two sub-components within the “coarse” mode. But opposite to the parameter a_{11} which describes the variance within the “fine” mode the variance effect of parameter a_{22} on aerosol optical properties is much below the effect of a_{11} . Therefore this variance reason , described by to a_{22} , can be neglected in the aerosol parametrisation model. Formally this corresponds to setting the parameter a_{22} to it’s fixed expectation value for all application cases of the model.
There is another “independent” reason for variance within the “coarse” model. According to the models in /27 /, /26 / air masses over the continent contain a small amount of dust particles which have dimensions typical for the “coarse” range. If this continental air mass approaches the coast it will be mixed with maritim origin air masses due to local circulation and turbulence. Then this mixed air mass will be pushed out above the sea by global

circulation. At least right near to the coast the air mass will therefore contain a residual of this continental dust particles. The variance effect due to this dust part is also of negligible effect on aerosol optical properties if one assumes the rates, these dust particles might have according to published continental models /27 /, /26 /. That is: This variance effect is therefore not strong enough that one should introduce a corresponding fifth variable model parameter in the aerosol parametrisation model .

The 4- parameter- aerosol model (parameters t_A , $\mathbf{a}_1$, **RH ,** $\mathbf{a}_{11}$ or alternatively t_{A1} , t_{A2} , **RH ,** $\mathbf{a}_{11}$) is therefore suggested for modelling satellite multispectral aerosol reflectance $R^A(\lambda_i)$, i = 1 .... N_i for application in nearly all cloud free situations.
The term “nearly all” is to be understood as a remainder, that occasionally one should be confronted with situations, where the “ normal” aerosol production process of the marine region of interest is strongly disturbed . Candidates for such “abnormal” aerosol production situations are “desert dust storms” , “regional forest fires” or “volcanic activity”. If one uses the above model without changing the basic assumption with regard to particle distribution and refractive index of the components also for these “events” one will expect increased errors in the estimation of aerosol parameters from multispectral reflectance measurements. But to adopt the aerosol parametrisation model to these “special” cases is out of the scope of this algorithm. This will practically not be an application restriction for the marine north European coast and the Baltic Sea. But the use of the model for air masses residing above the Mediterranean Sea should be restricted to air mass circulation situations avoiding high level of desert dust from the African continent.

Up to now only variances were discussed, which refer to aerosols in the troposphere, because the variability of these aerosols “normally” dominate the effect of aerosols in the stratosphere. In this “normal” case the stratospheric aerosol can be assumed to be of type “stratospheric backgound” with optical depth t_{SB} fixed at a value typically for the area and time of application of this algorithm (compare 3.1.1.3.5)
But for a certain time interval after strong volcanic activity there may be a strong increase of fresh volcanic aerosols in the stratosphere accompanied by strong variances in space and time /15 /. In this special case one should take into account a further variable aerosol optical depth part . A method to estimate this “fresh volcanic” part by using MERIS data in this special case (case B) is discussed in chapter 3.1.1.3.5.

Appendix B

Rough surface reflection modelling

The ocean surface contribution to satellite Reflectance is changing mainly due to wind effects:
The wind stress roughens the ocean surface. Each oblique surface part reflects the incoming light according to Fresnel law from a direction depending of the normal of that oblique surface part. The distant sensor integrates over all these tiny different mirrors on the surface. The distribution of the normal direction of these tiny mirrors was investigated by Cox and Munk /17/ . It depends on the wind speed as the driving force. Radiance transfer modelling shows, that the variance of wind may change the satellite signal not only in the so called „glitter directions” (many tiny mirrors at surface reflect mostly the direct sunbeam) , but a rest of reflected sun beam is found also outside these „glitter directions“ . If this part is not taken into account, this will lead to an overestimation of Aerosol Optical Depth.

When the wind is strong enough, the interaction with the surface will also produce foam. This process starts at about 7 m/sec wind speed and the fraction of surface ,filled with foam growth rapidly with growing wind speed /18 /. There are a lot of investigations to quantify this fraction growing with wind speed /19/. In this process of growing also temperature differences air/water play a role. Typical results are shown in /18/.
The „ Reflectance of foam itself was studied by different authors. The values given by Koepke /20/ seem to be best to represent foam „albedo“.

In total these effects can be taken into account by the equation

$$R_I^{GF} = R_i^{GBOA} \times T_i^{DIR} \times (1 - f_f) + f_F \times A_i^F \times T_i^D$$

The first part $R_i^{GBOA} \times T_i^{DIR}$ in (11) models the effect of specular reflected light at rough ocean surface, two times going through the atmosphere (glitter contribution). The second part $f_F \times A_i^F \times T_i^D$ in (11) models the reflection due to foam covering the fraction f_F at the ocean surface. Both parts R_i^{GBOA} and f_F are related to wind speed.
The change of the foam fraction due to wind speed is chosen here according to /18/.
The change of = R_i^{GBOA} due to wind speed can be calculated by using the equations in /30/.

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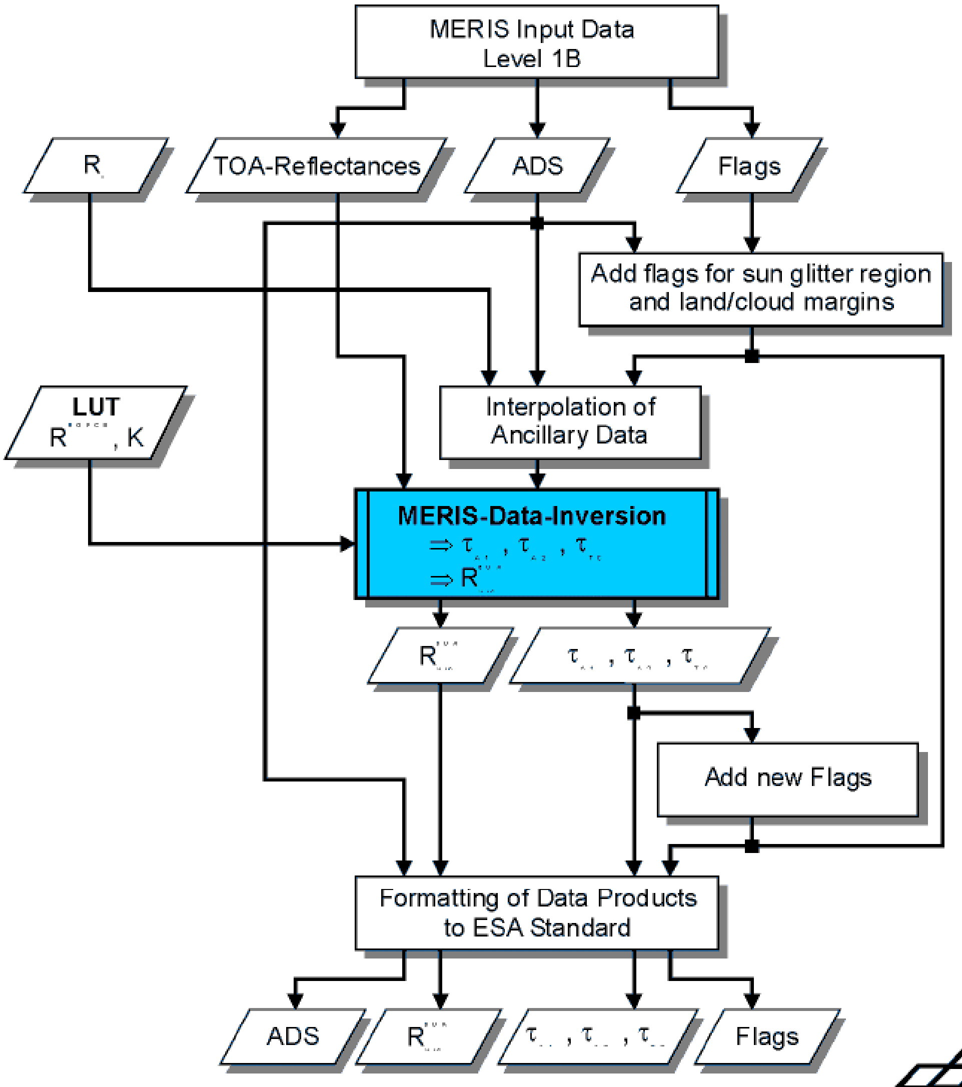
Flowchart of complete inversion



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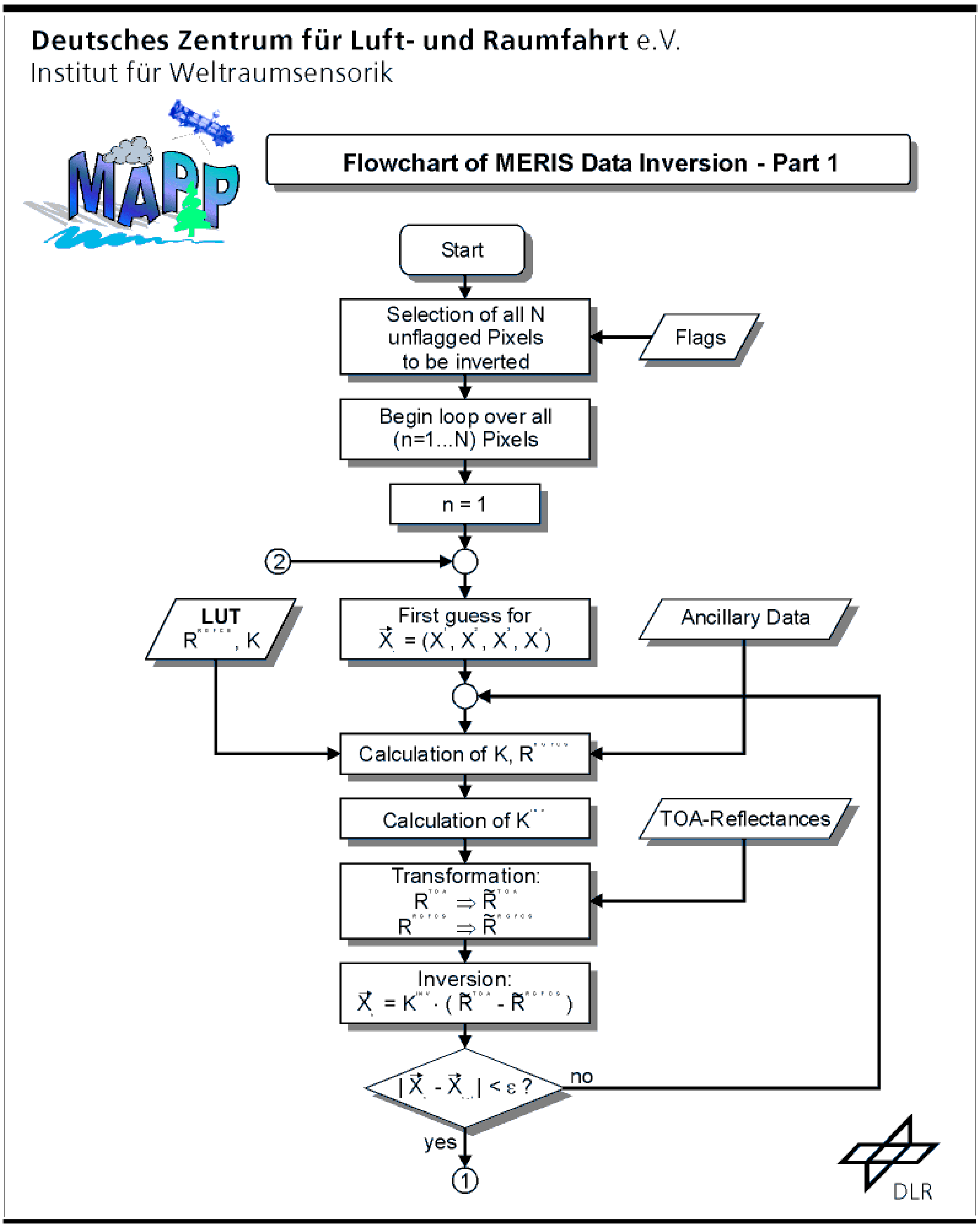

FC_MINV1_0199.CDR

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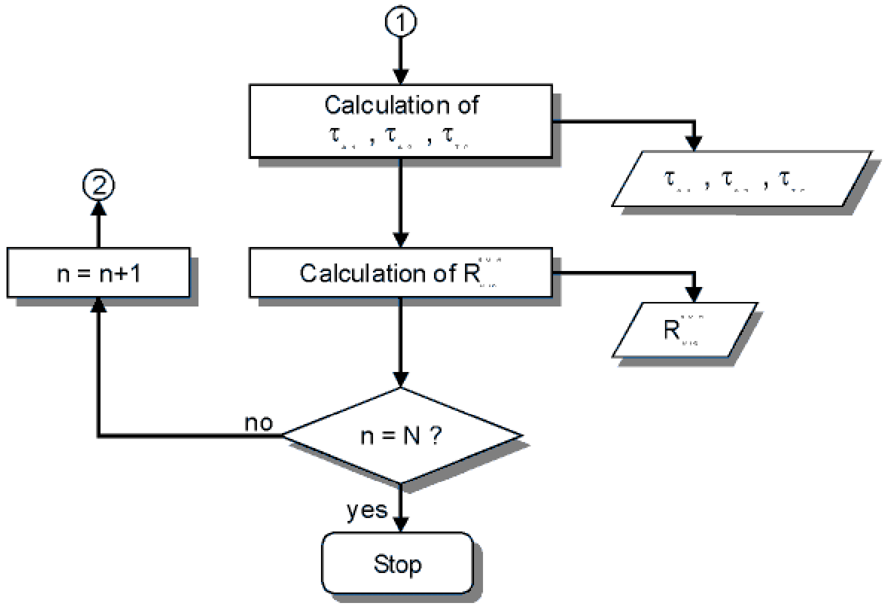
Flowchart of MERIS Data Inversion - Part 2



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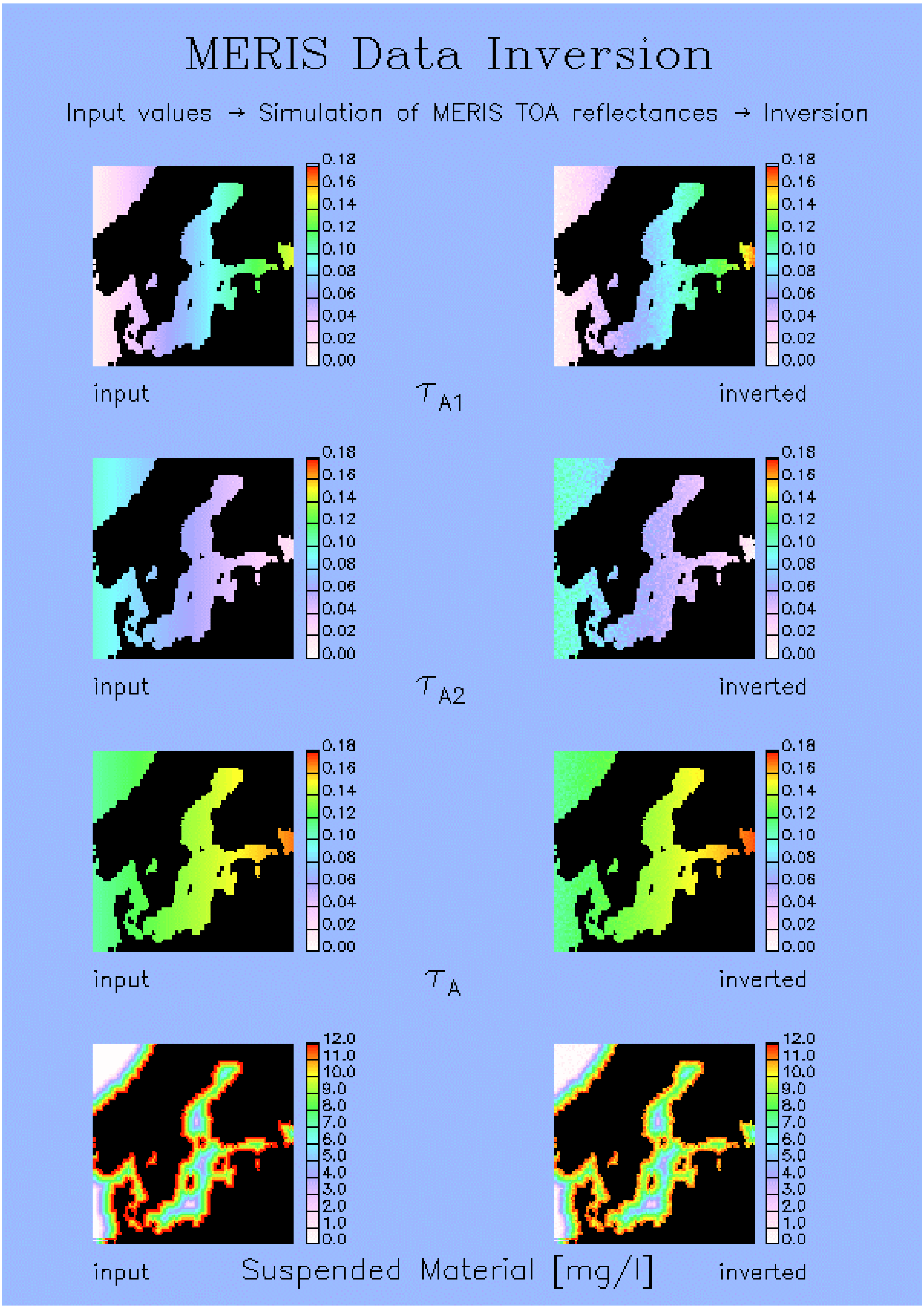
MERIS Data Inversion
Input values → Simulation of MERIS TOA reflectances → Inversion
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
input
τ_{A1}
inverted
input
τ_{A2}
inverted
input
τ_A
inverted
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
input
Suspended Material [mg/l]
inverted