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Retrieval of aerosol optical properties using MERIS observations: Algorithm and some first results

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Abstract

The MEdium Resolution Imaging Spectrometer (MERIS) instrument on board ESA Envisat made measurements from 2002 to 2012. Although MERIS was limited in spectral coverage, accurate Aerosol Optical Thickness (AOT) from MERIS data are retrieved by using appropriate additional information. We introduce a new AOT retrieval algorithm for MERIS over land surfaces, referred to as eXtensible Bremen AErosol Retrieval (XBAER). XBAER is similar to the “dark-target” (DT) retrieval algorithm used for Moderate-resolution Imaging Spectroradiometer (MODIS), in that it uses a lookup table (LUT) to match to satellite-observed reflectance and derive the AOT. Instead of a global parameterization of surface spectral reflectance, XBAER uses a set of spectral coefficients to prescribe surface properties. In this manner, XBAER is not limited to dark surfaces (vegetation) and retrieves AOT over bright surface (desert, semiarid, and urban areas). Preliminary validation of the MERIS-derived AOT and the ground-based Aerosol Robotic Network (AERONET) measurements yield good agreement, the resulting regression equation is $y = (0.92 \pm 0.07) + (0.05 \pm 0.01)x$ and Pearson correlation coefficient of $R = 0.78$. Global monthly means of AOT have been compared from XBAER, MODIS and other satellite-derived datasets.

Keywords

AOT; MERIS; Retrieval

1. Introduction

A lack of accurate global knowledge of aerosol scattering and absorption, through its impact directly or indirectly on atmospheric radiative transfer, remains one of the largest uncertainties to assessing the Earth’s changing energy budget (Boucher et al., 2013). To improve our understanding of the direct and indirect radiative effects and to better assess the health impact of fine aerosol particles (van Donkelaar et al., 2010), a better understanding of

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Uncited reference
Kaufman et al., 1997b

the global aerosol properties and knowledge of the amounts and distributions of aerosol are required.

The solar extraterrestrial radiation passing through the atmosphere is modified by absorption, scattering and emissions within the atmosphere by gases, aerosols, clouds and at the earth's surface. The wavelength dependence and magnitude of the absorption and scattering by aerosol particles depends on their size distribution, shape, composition and amount. The spectrum of the electromagnetic radiation measured (by a satellite) at the top of the atmosphere (TOA) contains information about aerosol optical properties and can be used to retrieve them. The contribution of TOA reflectance by aerosol is typically a fraction of the total reflectance and is wavelength dependent. The information content about aerosol optical properties in the TOA reflectance, determined from spectrometers on satellite platforms, is limited by the measurements viewing geometry, spectral coverage and spatial resolution (e.g. Tanre et al., 1996 and references therein). The retrieval of aerosol properties from such satellite observations is often an ill posed inverse problem.

Previously the “information content” provided by multi-spectral, single view satellite observations for retrieving Aerosol Optical Thickness (AOT) has been investigated (e.g. Tanre et al., 1996 and references therein). Due to lack of ‘information content’ regarding to aerosol optical properties observed by satellite instruments, retrieval algorithms require the use of knowledge about i) aerosol properties; ii) surface types (land, ocean, ice or snow); iii) surface spectral reflectance (SSR); iv) molecular scattering and absorption; v) the sky conditions, i.e. cloud amount. Accurate retrieval also requires an accurate assessment of the instrument radiometric and spectral calibration and any changes over the lifetime of the instrument in space. All error sources must be well quantified and these errors must be then propagated into the error attributed to the particular retrieved aerosol product. The need for additional knowledge is larger for data products retrieved from single view instruments (Li et al., 2009; Hsu et al., 2013) such as MERIS as compared to multiple viewing instruments such as Along Track Scanning Radiometer (ATSR), Advanced Along-Track Scanning Radiometer (AATSR) and Multi-angle Imaging SpectroRadiometer (MISR) or the observing multiple polarizations such as Polarization & Anisotropy of Reflectances for Atmospheric Sciences coupled with Observations from a Lidar (PARASOL) (de Leeuw et al., 2015; Holzer-Popp et al., 2013), which have intrinsically at least potentially higher information content. However, provided the added knowledge, physical parameterizations and assumptions are sufficiently accurate, then single viewing multiple spectral measurements provide theoretically good information about aerosol optical properties.

Over the past three decades, a variety of relevant passive remote sounding instruments has been launched on different satellites into earth orbit. Different retrieval algorithms to process the observations and retrieve aerosol information have been developed (e.g. Mei et al., 2014; Kokhanovsky et al., 2015 and references therein). Two of the better-known algorithms were developed for retrieving aerosol properties over land and ocean using data from the Moderate-resolution Imaging Spectroradiometer (MODIS) data. They are commonly known as the “dark-target” (DT; Levy et al., 2013; Remer et al., 2013), and “deep-blue” (DB; Hsu et al., 2013; Sayer et al., 2014) algorithms. The DT algorithm is based on the concepts of Kaufman et al. (1997a), and modified by Levy et al. (2007a, 2007b). The DT algorithm uses

three wavelengths (blue, red and short-wave infrared or SWIR) to constrain both the surface and aerosol contributions. In shortwave infrared (e.g. 2.1 μm), the accumulation mode (fine-sized aerosol) aerosol tends to be nearly transparent, which leads to a clear view of the surface. The observed surface properties in SWIR are extrapolated to shorter (visible) wavelengths, and used to constrain surface contribution to TOA reflectance. The aerosol retrieval is based on the minimization of residual (difference between total and estimated surface reflectance) in two visible bands. For brighter (e.g. desert) surfaces, the surface properties in the visible wavelengths (e.g. blue or red) cannot be accurately estimated from the SWIR, so DT approach is not appropriate. DB algorithm was initially developed for those situations. DB does not use observations from the SWIR channels, but rather surface reflectance climatology at short visible wavelength (e.g. Deep Blue = 0.41 μm). A combination of DT and DB algorithms can be used everywhere except for snow/ice surfaces under cloud-free condition (Levy et al., 2013). In addition to DT and DB algorithms, the multiangle implementation of atmospheric correction (MAIAC) algorithm performs high spatial resolution (1 km) aerosol retrievals and atmospheric correction over both dark vegetation surfaces and bright deserts. This uses time series analysis and image-based processing (Lyapustin et al., 2011a, 2011b). Some other attempt for MODIS operational aerosol retrieval includes Xue et al. (2014).

The Medium Resolution Imaging Spectrometer (MERIS), which flew on ENVISAT, observes earth at high spatial resolution in the visible and near infrared spectral regions. Although MERIS may not be optimal for aerosol research due to lack of a SWIR channel, multi-viewing, and/or polarization characteristics (Mei et al., 2014), there are several compelling reasons to develop an aerosol retrieval algorithm for it. First, a standalone aerosol retrieval algorithm for MERIS can provide information for “atmospheric correction” during the derivation of other MERIS products. The retrieved aerosol products can also help to constrain retrievals from other sensors on ENVISAT, such as trace gas retrievals from SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) (Burrows et al., 1995; Bovensmann et al., 1999). Second, such a retrieval algorithm is suitable for measurements of the Ocean and Land Colour Instrument (OLCI) on ESA Sentinel 3, and thus provides a joint MERIS/OLCI long-term aerosol record. Long term data sets are required for climate change and health impact research (e.g. Yoon et al., 2014).

There have been previous attempts to develop aerosol retrieval algorithms for MERIS, with mixed success. For example, the Bremen AErosol Retrieval (BAER; von Hoyningen-Huene et al., 2003, 2011), which was originally developed for use with data from the Sea-viewing Wide Field-of-view Sensor (SeaWiFS), uses the Normalized Difference Vegetation Index (NDVI) to characterize the surface contribution, and assumes a negligible absorbing aerosol type. Santer et al. (2007) adapted DT algorithm for MERIS. BAER performed well in regions such as Europe (Glantz et al., 2009) and Korea (Lee et al., 2006), where NDVI provides a good description of surface properties in mixed soil/vegetation conditions, and aerosol has typically negligible absorption. Although many improvements were proposed to facilitate retrievals in other regions (e.g. Guanter et al., 2008; Davies and North, 2015), BAER has limited accuracy outside of dark-vegetated surfaces and primarily non-absorbing aerosols (de Leeuw et al., 2015; Holzer-Popp et al., 2013). Another algorithm used for

operational AOT retrieval from MERIS by ESA, tends to overestimate AOT (de Leeuw et al., 2015).

A new AOT retrieval algorithm has been developed for use with the measurements of MERIS instrument. This algorithm, which is generic and can be readily adapted and applied to similar multispectral measurements (e.g. OLCI), is introduced and validated in this manuscript. This algorithm has novel cloud screening, aerosol type selection and spectral surface reflectance (SSR) parameterization and a priori AOT first guess data sets as compared to BAER. This algorithm, henceforth called eXtensible Bremen AErosol Retrieval (XBAER), utilizes knowledge gained from working with BAER and other algorithms, including those applied to data from MODIS. To present logically the XBAER algorithm, this manuscript is organized in the following manner. A general overview of XBAER algorithm is given in Section 2. The MERIS instrument and its observations are presented in Section 3. A short description of relevant aspects of the radiative transfer model-SCIATRAN used for creating lookup-table (LUT) is presented in Section 4. Section 5 describes the new cloud mask for XBAER, and includes a comparison between XBAER and the original BAER cloud masking results. Section 6 describes the aerosol type treatment. It describes the relationship between aerosol microphysical/chemical properties and AOT, as well as aerosol types and creation of the LUT using radiative transfer forward calculations. The derivation of one-parametric approximation of SSR along with the monthly spectral coefficients dataset, which is a key issue impacting on AOT retrieval, in addition to the cloud screening and aerosol type treatment, is presented in Section 7. The AOT retrieval algorithm and a sensitivity study are presented in Sections 8 and 9. The auxiliary data used in the retrieval and validation of XBAER data products are described in Section 10. A preliminary comparison of XBAER retrieval results with other satellite products and a validation using AERONET aerosol data products are presented and discussed in Sections 11 and 12.

2. A synopsis of the XBAER algorithm

The XBAER algorithm has been developed for use with simultaneous multi-wavelength reflectance measurements made at the top of the atmosphere (TOA) by instruments such as MERIS. With a minimum number of constraints, and a LUT that comprises a sufficient and adequate data base for the domain of possible aerosol “scenarios”. XBAER derives both AOT and SSR. XBAER can be considered as a series of steps that operate on pixels or retrieval boxes comprising scenes measured by MERIS. These steps comprise and include:

- The Creation of a LUT that uses accurate radiative transfer model (RTM) to simulate reflectance at the TOA. The RTM (SCIATRAN), used for this purpose, is discussed in Section 4, and the LUT is described in more detail in Section 6.
- The identification of clear sky (non-cloudy) scenes and scenes those are free of ice, snow and inland water. This is achieved by a standalone algorithm, called XBAER-CM, which is briefly described in Section 5 and in more detail in a separate publication in Mei et al. (2016a).
- The definition of the aerosol optical properties expected for a scene. Having selected cloud free land ground scenes, it is necessary to define aerosol type in

the scenes. For this purpose the XBAER algorithm adapts the approach taken from DT aerosol type treatment, where aerosol “type” is prescribed for a given location and season. More information about the aerosol type treatment is found in Section 6 and a detailed description is given by Levy et al. (2010).

- The definition of the surface spectral properties. In XBAER algorithm, the given SSR (y) for a certain wavelength is parameterized as a linear relationship $y = ax + b$, where x is Soil-Adjusted Vegetation Index (SAVI) (Huete, 1998; Qi et al., 1998), the slope (a) and intercept (b) coefficients, which are called “spectral coefficients” throughout this paper, are pre-calculated and are dependent on the location, time and wavelength used in the XBAER spectral coefficients dataset. The preparation of the database is described in Section 7.

Having identified cloud free scenes, the aerosol type and the spectral coefficients, the AOT at 0.55 μm and the effective vegetation index for these scenes are then used in the retrieval. For a given geolocation and satellite observation time, all the auxiliary databases (for both aerosol and surface) together with the AOT and effective vegetation index enable the TOA simulated reflectance to be determined. AOT and the effective vegetation index are retrieved by minimizing the difference between simulated and measured TOA reflectance. Details are provided in Section 8.

The current version of XBAER algorithm focuses on the retrieval of AOT and SSR for land ground scenes. The use of XBAER for aerosol retrieval over water and snow is in development and benefits from the experience of retrieval techniques over water (Levy et al., 2013; von Hoyningen-Huene et al., 2003, 2011), and snow (Istomina et al., 2011; Mei et al., 2013). A global data set for aerosol properties under cloud free condition will be created.

3. MERIS instrument

MERIS flew onboard the European ENVISAT satellite from May 2002–April 2012 in a sun synchronous orbit in a descending node, having an equator crossing time of 10:00 am local time. MERIS had 2D array detectors measuring the wavelength range from 380 to 1040 nm, and downlinked fifteen selectable wavelengths with programmable bandwidths between 2.5 nm and 30 nm (see Table 1). To further optimize the data rate, MERIS measurements were provided at two different spatial resolutions, either 300 m $\times$ 300 m or 1 km $\times$ 1 km. A full swath width was 1150 km. As a result MERIS provided global coverage at the equator in $\sim$ 2.5 days but more rapidly at higher latitudes. A successor to ENVISAT’s MERIS is the OLCI instrument on Sentinel-3, which was launched successfully on 16 Feb. 2016. It has twenty-one spectral bands and a swath width of 1270 km achieving global coverage at the equator in 2 days.

The MERIS reflectance data is relatively well-calibrated and has an error of $< 4\%$. The maximal degradation was at 412 nm and is 5% as monitored by regular radiometric calibrations in flight (Delwart et al., 2003). MERIS reflectance data has been widely used in the fields of vegetation parameter retrieval (e.g. Dash and Curran, 2004), cloud data products (Rozanov and Kokhanovsky, 2004), land cover products (Bicheron et al., 2006) and other land applications (Verstraete et al., 1999). Several spectral channels of MERIS in the blue

region are similar to those in SeaWiFS. The measurements of TOA reflectance from these channels provide the unique information for the retrieval of aerosol data products for both dark and bright surface (Hsu et al., 2013).

One issue for MERIS data was the instrumental “smile” effect that covers the 760 nm O₂ A band, which is used for XBAER cloud screening (Mei et al., 2016a). This optical effect, typical for push-broom sensors using 2D CCD detectors, arises when the image of the straight entrance slit is projected via a grating onto a planar 2D CCD array. The “smile” effect leads to a shift of the wavelengths within the spectral range of the sensor. This spectral shift depends on the across track position of the detector pixel. This “smile” effect on the spectral position of the bands can be accounted for using a LUT method developed at IUP, UB (Personal communication, Wolfgang von Hoyningen-Huene, 2012; Malte Jäger, 2015). Thus, we believe the “smile” effect will not impact aerosol retrieval due to its impact on cloud screening.

4. Radiative transfer model - SCIATRAN

XBAER algorithm uses a LUT technique to solve the aerosol inverse problem. A radiative transfer model, which describes all relevant physical and radiative transfer adequately, is required. For XBAER, the LUT takes into account explicitly polarization and contains pre-calculated atmospheric path reflectance, total transmittance and spherical albedo for a set of representative aerosol types, AOTs and observation/illumination geometries. The grids/nodes in the LUT are similar to and adapted from MODIS-DT algorithm (Levy et al., 2013).

The XBAER LUT is calculated using the radiative transfer model SCIATRAN (Rozanov et al., 2014 and references therein). The development of SCIATRAN was driven by the need to simulate accurately the measurements of SCanning Imaging Absorption spectroMeter for Atmospheric CHartographY (SCIAMACHY) on board ENVIRONMENTAL SATellite (ENVISAT) (Burrows et al., 1995; Bovensmann et al., 1999). SCIATRAN is a comprehensive radiative transfer package, simulating all relevant processes in the atmosphere, land and ocean, in the spectral range from the ultraviolet to the thermal infrared (0.18–40 μm). It accounts for multiple scattering processes, absorption, polarization, thermal emission and ocean atmosphere coupling, and can model spectral and angular distributions of the intensity or the Stokes vector. Furthermore, SCIATRAN simulates either a plane-parallel or the computationally more expensive fully spherical atmosphere.

All relevant significant radiative transfer processes are accounted for in SCIATRAN: e.g. the Rayleigh scattering, scattering by aerosol and cloud particles, absorption by gaseous components, and bidirectional reflection by an underlying surface including Fresnel reflection from a flat or roughened ocean surface. The SCIATRAN software package also contains different methods to solve radiative transfer equation including finite difference and discrete-ordinates techniques, an extensive database of optical properties of atmospheric molecules and particle, and a specific module for solving inverse problems. In addition, SCIATRAN incorporates an efficient approach to calculate the so-called Jacobians, i.e. the derivatives of the intensity or Stokes vector with respect to various atmospheric and surface

parameters (Rozanov, 2006). A detailed description of SCIATRAN is given in Rozanov et al. (2014).

SCIATRAN is a valuable tool for a wide range of remote sensing applications, and has been compared and validated with respect to other RT codes (Lenoble et al., 2007; Lyapustin, 2005; Stamnes et al., 1988) and benchmarks (Mishchenko, 1990; Siewert, 2000). SCIATRAN is widely used and a user community of researchers exists.

5. Cloud mask

Except for special cases involving the retrieval of aerosol properties above clouds (Jethva et al., 2013), the retrieval of aerosol properties, primarily AOT, from singly angle viewing passive remote sensing instrument requires clear-sky (non-cloudy) conditions. The identification of cloud-contaminated scenes is thus an essential first step in any aerosol retrieval. Cloud screening of scenes is thus required. If that is too aggressive, it reduces the data coverage or possibly excludes scenes having optically relatively thick aerosol. Weak cloud screening and presence of sub-pixel scale clouds, often results in high-biased AOT. Consequently an “aerosol” cloud screening algorithm needs to find an optimal balance. Some instruments (e.g. MODIS) have infrared bands, which are used to detect the brightness temperatures of high thin clouds. However, MERIS does not have this capability, so the cloud screening algorithm must rely on the measurements of TOA reflectances in visible and Near-infrared (NIR) bands. In visible and near-IR wavelengths, clouds are bright and cloud scenes tend to have larger spatial variability than clear sky scenes (e.g. Martins et al., 2002). As a consequence, the BAER cloud screening algorithm uses intensity and spatial variability thresholds. While this was sufficient for detection of optically thick clouds, it did not optimally identify relative thin clouds. However MERIS also contains a spectral channel centered on the O₂ A band (channel 11 around 760 nm). This can be used to identify high, thin clouds (Gómez-Chova et al., 2007). In total, a multiple criteria cloud screening algorithm for XBAER (Mei et al., 2016a) has been developed. The algorithm utilizes:

- i. The TOA reflectance to distinguish cloud above relative dark surface.
- ii. The standard deviation of 412 nm within a 3×3 pixels spatial window was used to analyze the homogeneity around the scene. This assumes that aerosol away from its source is more homogeneous than cloud (Martins et al., 2002).
- iii. The ratio between TOA reflectance at 760 nm and 753 nm. This is used to determine cloud height information, because this ratio is dependent on the absorption of molecular oxygen. When cloud is in the scene, as it is at a higher altitude than the underlying surface, the O₂ column and thus also the ratio between TOA reflectance at 760 nm and 753 nm is larger.
- iv. The ratio between 760 nm and 753 nm is also used to detect the presence of thin cirrus, which is located at relatively high altitude.

A statistical method was used to determine the thresholds for all the criteria, more detailed information is found in Mei et al. (2016a). Briefly, the criteria for TOA reflectance at 412 nm, the standard deviation of 412 nm within a 3×3 pixels spatial window, the ratios

between 760 nm and 753 nm are selected to be 0.18, 0.0018, 0.315 and 0.5 respectively. The cloud spectral neutrality characteristic defined as the ratio of the TOA reflectance of channel 1 and channel 2 with threshold value of 1.06 is additionally used for cases where the TOA reflectance at 412 nm is in the range between 0.18 and 0.2 (Mei et al., 2016a).

After applying the criteria mentioned above, Fig. 1 shows an example of the impact of the cloud screening for a complicated cloud scene, provided by Gómez-Chova et al. (2007). The scene contains both thick and thin cloud (upper left panel in Fig. 1) and the “true” cloud mask (upper right panel in Fig. 1) is a manually created cloud mask result (Gómez-Chova et al., 2007). By taking into account the “twilight zone”, which is a belt of forming and evaporating cloud fragments and hydrated aerosols extending tens of kilometers from the clouds into the so-called cloud-free zone (Koren et al., 2007), an adequate and successful cloud mask for XBAER has been created.

Results for the cloud mask used in the BAER version are presented in the lower left panel of Fig. 1. As expected, there are good results for thick clouds and some issues for relatively thin clouds. The new XBAER cloud mask is presented in lower right panel of Fig. 1. Since the “twilight zone” is not included in the “true” cloud mask, the cloud mask in XBAER is expanded, especially in broken cloud scenes (Mei et al., 2016a). Overall we consider that the XBAER cloud screening mask works successfully.

6. Selection of the aerosol type

MERIS measurements do not have sufficient information content to determine all aerosol properties. Therefore, prescribed aerosol types are used based on priori assumptions. XBAER uses MODIS DT assumptions (e.g. as reported in Levy et al. (2007a)) and the expected aerosol type for a given region and season based on the analysis of AERONET observations.

A bimodal lognormal function (i.e. a combination of fine and coarse modes, differentiated by their effective radius) is generally adequate for modeling the particle size distribution (Remer and Kaufman, 1998; Dubovik et al., 2002). This assumption is widely used in satellite aerosol retrieval algorithms. Levy et al. (2007a) described a framework for connecting the aerosol micro-physical properties of refractive index and size distribution to AOT at 0.55 μm . This modeled the concept of “dynamic aerosol”, which assumes that the intrinsic properties of the ambient aerosol are related to aerosol loading (Remer and Kaufman, 1998). This is an effective parameterization of aerosols used in climate models and satellite remote sensing (Dubovik et al., 2002).

Levy et al. (2007a) performed a cluster analysis of the entire AERONET dataset of sun-sky inversions (Dubovik et al., 2002) up to 2010. In this manner, they created an “expected aerosol type” map for all locations at $1^\circ \times 1^\circ$ spatial resolution for each season. Levy et al. (2007a) identified three “fine-dominated” aerosol models, meaning that the size distribution was dominated by fine-mode sized particles. The fine models, are differentiated by their relative absorption (strong, moderate or weak). Some regions tended to be dominated by the strongly or weakly absorbing types (shown as in Fig. 2). Other regions were either

dominated by the moderately absorbing types or there was no clear dominance of the other two types. Border contours were drawn, taking into account mountainous terrain to separate aerosol regimes and information gleaned from additional studies (Levy et al., 2013).

In XBAER, we have adapted the approach developed by Levy et al. (2007a), but in addition used the MODIS Land Cover product (Friedl et al., 2002) to identify when aerosol is dominated by dust. The assumed aerosol properties for each of the fine-dominated models, along with the coarse-dominated dust model are taken from Levy et al. (2007a). Any of the three absorption aerosol types presented in Fig. 2 can re-produce different aerosol types such as continental clean, continental average, continental polluted etc., depending on their micro-physic properties (Hess et al., 1998). For instance, the SSA at 0.55 μm for continental average aerosol type in OPAC is 0.925 (Hess et al., 1998), which can be generated by moderately absorption MODIS aerosol type having SSA at 0.55 μm in the range [0.901, 0.962] depending on the AOT.

For SCIATRAN to simulate the top of the atmosphere reflectance, the following information is required as input: a) particle properties; b) a Mie code to calculate scattering properties; c) vertical profiles of i) aerosol particle number density, ii) air for Rayleigh scattering and iii) other absorbing constituents. The vertical profile of aerosol particle number density is needed to calculate the aerosol optical properties from the micro-physical properties. A sensitivity study investigating the aerosol height assumption shows negligible AOT error, especially for mid-visible wavelengths. Thus, in the XBAER algorithm, an “exponential vertical distribution” with height = 3.0 km is used.

The XBAER LUT calculated using SCIATRAN uses estimates of the atmospheric path reflectance, total transmittance and spherical albedo for given wavelengths, AOTs, aerosol types and geometries.

7. The parameterization of spectral surface reflectance, SSR

The estimation of the SSR is one of the key issues for the accurate retrieval of aerosol optical properties from TOA reflectance observed over land. In this section, a one-parametric approximation of SSR, the derivation of the spectral coefficients dataset, which is the basis of this approximation, and the evaluation of the approximation accuracy are described in detail. The spectral coefficients as described below are used in the XBAER algorithm.

7.1. Physical background

To derive a one-parametric approximation of SSR, it is assumed that the SSR for a given surface type at a given wavelength is determined by the use of a linear relationship (Tchente et al., 2010; Liu et al., 2014; von Hoyningen-Huene et al., 2003, 2011) to a particular and selected vegetation index (Hsu et al., 2013; Levy et al., 2013; Huete, 1998; Qi et al., 1994; von Hoyningen-Huene et al., 2003; Santer et al., 2007). After carefully performing a test with experimental and model data, it could be shown that the most appropriate linear relationship between SSR and vegetation index is achieved by employing SAVI, which is defined as:

$$\text{SAVI} = \frac{R(\lambda_{14}) - R(\lambda_7)}{R(\lambda_{14}) + R(\lambda_7) + L}(1 + L), \quad (1)$$

$$L = 1 - \frac{2R(\lambda_{14}) + 1 - \sqrt{(2R(\lambda_{14}) + 1)^2 - 8(R(\lambda_{14}) - R(\lambda_{14}))}}{2}, \quad (2)$$

where R is the SSR and the subscript for the wavelength denotes the MERIS channel numbers defined in Table 1. SAVI has first been proposed by Huete (1998) and further developed by Qi et al. (1994). The use of the parameter L , results in a better near-linear response with respect to SSR, as compared to NDVI. SAVI is equal to NDVI for values of $L = 0$ in Eq. (1).

Fig. 3 shows the dependence of SSR on SAVI for the wavelengths 412 nm (blue circles) and 885 nm (red circles), and were obtained from the land-cover-cci project (<http://www.esa-landcover-cci.org/>). The three panels in Fig. 3 show this relationship near three different AERONET sites: Rio Branco (vegetation), Paris (urban), and Bodele (desert). It can be seen from Fig. 3 that SSR can be approximated by a linear function of SAVI:

$$R = ax + b, \quad (3)$$

where a and b are regression coefficients (slope and intercept, respectively), and x is the value for SAVI. A statistical analysis of SSR data for the discrete channels of MERIS instrument shows that regression coefficients in Eq. (3) are obtained with the required accuracy for wavelengths beyond the red-edge, i.e., $\lambda > 720$ nm. However, the dependence of SSR on SAVI for the short wavelength such as 412 nm is weak (e.g. the blue circles are almost parallel to the x-axis in Fig. 3 and have correlation coefficients of 0.31, 0.01 and -0.18 for vegetation, urban and desert surface types respectively). This means that the estimation of the a and b coefficients for short wavelengths using Eq. (3) is not suitable for use in aerosol retrieval algorithms. To address this problem, a linear regression for SSR ratios instead of SSR is used. The ratio $R(\lambda_1)/R(\lambda_{14})$ between the SSR at wavelength 412 nm and 885 nm, as a function of SAVI, is also shown in Fig. 3 (the green circles). It follows that the ratio as expected shows much larger dependence on SAVI.

The SSR ratios depend on the vegetation amount/condition or “greenness” (Levy et al., 2007b). This is explained by two different effects: (1) for surface types where the SSR is dominated by vegetation, the SSR ratios are considered to be characteristic of the liquid water absorption and chlorophyll absorption of different vegetation states (Kaufman et al., 2002); (2) for surface where vegetation cover is not complete, the SSR ratios are related to the soil roughness, soil types and moisture content changes, which strongly influence the visible (i.e. red channel) and near infrared reflectances (Baret et al., 1993).

Combining the above considerations enables the SSR for the channels of the MERIS instrument to be represented in the form of following linear relationship:

$$R(\lambda_i) = a(\lambda_i)x + b(\lambda_i), i = 10, 12, 13, 14, \quad (4)$$

$$R(\lambda_i) = R(\lambda_{14})[a(\lambda_i)x + b(\lambda_i)], i = 1, 2, \dots, 9, \quad (5)$$

where the subscript i is the MERIS channel number (see Table 1), $a(\lambda_i)$ and $b(\lambda_i)$ are regression coefficients at the wavelength λ_i , x is the value of SAVI used in the case under consideration as regressor (independent variable), discrete wavelengths $\{\lambda_1, \dots, \lambda_9\}$ and $\{\lambda_{10}, \lambda_{12}, \lambda_{13}, \lambda_{14}\}$ are located in the spectral range before and after red-edge, respectively.

For a better understanding of the regression coefficients $a(\lambda_i)$ and $b(\lambda_i)$, let us consider first the surface reflectance with negligible small contribution of vegetation. In this case, SAVI is small (~ 0.05 for desert as seen from Fig. 3) and one can neglect with the term $x a(\lambda_i)$ as compared to $b(\lambda_i)$ in Eqs. (4) and (5). It follows that regression coefficient $b(\lambda_i)$ describes the non-vegetation contribution to the SSR at each grid point. For the wavelengths after red-edge $b(\lambda_i)$ represents spectral surface reflectance of the non-vegetation component, whereas for short wavelengths $b(\lambda_i)$ provides the surface reflectance spectral shape of non-vegetation component. The coefficient $a(\lambda_i)$ describes the difference between the vegetation and non-vegetation reflectance contribution in the grid at the location under consideration. Indeed rewriting the right-hand side of Eq. (4) in the following equivalent form: $xv(\lambda_i) + (1 - x)b(\lambda_i)$, where $v(\lambda_i)$ is the spectral reflectance of the vegetation component, one can state that $a(\lambda_i) = v(\lambda_i) - b(\lambda_i)$. We note that a similar idea has been successfully used to retrieve the surface properties over Africa (Tchente et al., 2010) and France (Liu et al., 2014) as well as in the BAER retrieval algorithm (von Hoyningen-Huene et al., 2003, 2011).

Eqs. (4) and (5) can be re-written in the vector form for simplification. The column vectors, for which the elements are the SSR or regression coefficient at a given wavelength, are introduced as following:

$$\begin{aligned} R_l &= [R(\lambda_{10})R(\lambda_{12})R(\lambda_{13})R(\lambda_{14})]^T, R_s \quad (6) \\ &= [R(\lambda_1)R(\lambda_2)\dots R(\lambda_9)]^T, \end{aligned}$$

$$\begin{aligned} A_l &= [a(\lambda_{10})a(\lambda_{12})a(\lambda_{13})a(\lambda_{14})]^T, A_s \quad (7) \\ &= [a(\lambda_1)a(\lambda_2)\dots a(\lambda_9)]^T, \end{aligned}$$

$$B_l = [b(\lambda_{10})b(\lambda_{12})b(\lambda_{13})b(\lambda_{14})]^T, B_s \quad (8)$$

$$= [b(\lambda_1)b(\lambda_2)\dots b(\lambda_9)]^T,$$

where subscripts “s” and “l” denote the short wavelengths (412.5, 442.5, 490, 510, 560, 620, 665, 681.25, 708.75 nm) and long wavelengths (753.75, 778.75, 865, 885 nm), respectively, and the superscript “T” denotes the transpose matrix. The desired one-parametric approximation for SSR and ratios is written as follows:

$$R_l = A_l x + B_l, \quad (9)$$

$$\frac{1}{R(\lambda_{14})} R_s = A_s x + B_s, \quad (10)$$

where R_l and R_s are the vectors containing SSR for a given pixel, x is SAVI calculated according to Eq. (1).

7.2. Preparation of global surface dataset

In order to use the one-parametric approximation given by Eqs. (9) and (10) in XBAER algorithm, the global dataset of spectral coefficients (vectors A and B) should be pre-calculated. These spectral coefficients are calculated using the global dataset of SSR provided by the land-cover-cci project. In the framework of this project, SSR dataset was retrieved by applying the standard atmospheric correction algorithm to the TOA reflectance measured by the MERIS instrument. The aerosol information used in this retrieval is that obtained from the MODIS product (Kirches et al., 2013).

The sampling selection of the SSR dataset used for the calculation of spectral coefficients has been determined for each $0.1^\circ \times 0.1^\circ$ grid cell on a monthly base data in the following manner:

- (1) The land surface was gridded to regular $0.1^\circ \times 0.1^\circ$ block;
- (2) Very dark and bright pixels (outliers) in the $0.1^\circ \times 0.1^\circ$ block were identified by using the statistical analysis and removed;
- (3) The linear regression between SSR and SAVI, and between SSR ratio and SAVI, as described by Eqs. (9) and (10) respectively were calculated;
- (4) For each month and each $0.1^\circ \times 0.1^\circ$ block, the resultant regression coefficients are saved in the form of two vectors A and B:

$$A = [A_s A_l] \quad (11)$$

$$= [a(\lambda_1)a(\lambda_2)\dots a(\lambda_9)a(\lambda_{10})a(\lambda_{12})a(\lambda_{13})a(\lambda_{14})],$$

$$B = [B_s B_l] \quad (12)$$

$$= [b(\lambda_1)b(\lambda_2)...b(\lambda_9)b(\lambda_{10})b(\lambda_{12})b(\lambda_{13})b(\lambda_{14})].$$

The estimated SSR for different surface types is calculated using the A and B vectors constructed above, as follows:

$$\hat{R}_l = A_l \hat{x}_l + B_l, \quad (13)$$

$$\hat{R}_s = (A_s \hat{x}_s + B_s)R(\lambda_{14}), \quad (14)$$

$$\hat{x}_s = \hat{x}_l = \text{SAVI}, \quad (15)$$

where parameters $\hat{x}_l$ and $\hat{x}_s$ are equal for long and short wavelengths and equal to SAVI as given by Eq. (1).

The SSR dataset used to generate the database is a not Lambertian reflectance, but Lambertian equivalent reflectance (Hsu et al., 2004), or surface directional reflectance (Kirches et al., 2013). In order to take the non-Lambertian effect into account, we need to derive the spectral coefficients database depending not only on the surface types but also on the solar/observation angles. However, in the current XBAER version, the non-Lambertian effect is ignored because its impact on the spectral coefficients dataset is of minor importance due to the following reasons:

- a. The non-Lambertian effect is of importance within a narrow range of observation angles near the so-called hot-spot direction, where surface reflectance shows significant enhancement. These cases are identified as outliers and removed as described in step (2) of the procedure to create A and B vectors.
- b. The linear regression described in step (3) and (4) utilizes all observations in the same month (i.e. we assume that the surface type is relative stable over the month) by averaging non-Lambertian reflectances under different solar/observation angles. This allows the spectral coefficients dataset to mitigate the impact of non-Lambertian effect.

Examples of A and B vectors, obtained for areas having different surface type (vegetation, city and desert) located near AERONET stations (Rio Branco, Paris and Bodele), are presented in Fig. 4. We can find that:

- a. The values of vector B are always positive and this agrees with our previous explanation that $b(\lambda_i)$ describes the non-vegetation contribution to the SSR.

- b. The values of vector A show as compared to B vector different spectral shapes for different surface types.
- c. A and B vectors are anti-correlated because a linear combination of these vectors should reproduce SSR with and without red-edge structure, depending on the value of SAVI. Thus the one-parametric approximation of SSR used in the XBAER algorithm is valid over both dark and bright surface.

Examples of the global distribution of A and B vectors on July for channel 1 (412 nm) and channel 14 (885 nm) are shown in Fig. 5. The pattern of the elements $a(\lambda_1)$ and $b(\lambda_1)$ (channel 1) presented in left panels of Fig. 5 are typical for the first 9 channels (ratio pattern) and the pattern of the elements $a(\lambda_{14})$ and $b(\lambda_{14})$ (channel 14) represent the last 4 channels (reflectance pattern). From the statistical analysis, for moderate land conditions (excluding ice and snow cover), A and B vectors are anti-correlated, as shown in Fig. 4. For example, the B vectors for both channel 1 and channel 14 are high while the A vectors are low for the bright surface regions such as Sahara. The opposite situation occurs over the Amazon regions.

7.3. Uncertainty estimation

To illustrate the dynamic capability of the surface parameterization method described above, two reference SSR spectra for 16 July 2008 and 2 July 2009 over three different AERONET sites (see Fig. 3) were selected from the land-cover database (red lines in Fig. 6) and are denoted by “Ref”. Two different methods have been employed to approximate selected reflectance spectra. For the method called “standard method”, the parameters x_l and x_s are both set to SAVI calculated according to Eq. (1). The second method we call “fitting method” and the parameters were calculated using the following expressions:

$$\hat{x}_l = \frac{R(\lambda_{14}) - b(\lambda_{14})}{a(\lambda_{14})}, \hat{x}_s = \frac{(R_s - R(\lambda_{14})B_s A_s)}{R(\lambda_{14})(A_s A_s)}, \quad (16)$$

We note that when using the “fitting method” the parameter x_l reproduces exactly the reference SSR at λ_{14} and the parameter x_s minimizes the following quadratic form:

$$\|R_s - R(\lambda_{14})(A_s x + B_s)\|^2 \rightarrow \min, \quad (17)$$

which represents the root mean square difference between approximation given by Eq. (14) and the reference SSR.

The SSR spectra calculated using parameters x_l and x_s according to the standard and fitting method are denoted by “Ref_s” (blue line) and “Ref_f” (green line), respectively in Fig. 6. The comparison of reference SSR spectra (red line) and spectra calculated employing the standard method (blue line) yields the following conclusions:

- a. Among the three selected surface types (vegetation, city and desert), the city type (Paris) shows the largest difference between reference and calculated SSR for all considered wavelengths, while the vegetation type shows the smallest difference.
- b. Good agreement can be found for the values of SSR at the shorter wavelengths for the desert surface type, but a relative large difference is obtained for longer wavelength.
- c. Fig. 6 also shows a little bit larger difference for the shortest wavelength (412 nm), which may be due to incomplete correction of aerosol in the atmospheric correction procedure used to create the land-cover dataset and can contribute uncertainty to the spectral coefficients dataset.

The obtained results are explained taking into account two main error sources arising by employing of the standard method, namely, the surface horizontal inhomogeneity and non-Lambertian effect. As described above, the impact of horizontal inhomogeneity and non-Lambertian effect were mitigated by spatial and temporal averaging when constructing the spectral coefficients dataset. However, these effects are presented in the single spatially and temporally high-resolved reference spectra. In particular, the large difference between reference and approximated SSR for the city surface type is caused mainly by the surface horizontal inhomogeneity, whereas the difference for desert surface type is explained by accounting for the non-Lambertian reflection effect.

To reduce the impact of these two error sources we use the fitting method instead of standard method. The SSR spectra obtained employing the fitting method is given in Fig. 6 by green lines. It can be seen that this yields significant improvement of the approximation accuracy.

The root mean square error of the fitting method for 2008 are 0.0026, 0.0201 and 0.0052 for vegetation, urban and desert surface conditions respectively, whereas the standard method leads to 0.0061, 0.0278 and 0.0111 for the same surface conditions. Thus, for the vegetation and desert surface conditions, the accuracy of SSR estimation using Eq. (15) is 2–3 times poorer than the result obtained with the fitting method. For the complicated urban case, the fitting method is about 40% superior to the standard method. As a result of these tests, the fitting method was selected for use in the operational run of XBAER algorithm.

Fig. 7 shows an example of global 7 days composited SSR for the 24th to 30th of July 2009 for MERIS channel 1 and channel 14 obtained using the surface spectral coefficients dataset, created in this study and the difference between the estimated SSR and land-cover-cci MERIS SSR product. In general, the SSR created with the spectral coefficients dataset agrees quite well with MERIS SSR product over both dark and bright surface. For the wavelength of 412 nm, the absolute difference is < 0.01 while for longer wavelength the difference is < 0.03 for majority cases depending on the surface type and observation geometry. Please note that the calculated SSR for channel 14 ($R(\lambda_{14})$) is obtained by fitting SAVI in the first 9 channels.

8. XBAER algorithm

To retrieve the AOT or τ , we used the following Eq. (18) to describe the reflectance at the top of atmosphere (Chandrasekhar, 1950; Kaufman et al., 1997a; Liou, 2002):

$$R^s(\lambda_i, \tau) = R_0(\lambda_i, \tau) + \frac{T(\lambda_i, \tau)R(\lambda_i)}{1 - r(\lambda_i, \tau)R(\lambda_i)}, \quad (18)$$

where $R_0(\lambda_i, \tau)$ is the TOA reflectances assuming black surface (atmospheric path reflectance), $T(\lambda_i, \tau)$ is the product of total (diffuse and direct) transmittance from the sun to the surface, $T^\downarrow(\lambda_i, \tau)$, and the total transmittance from the surface to the satellite, $T^\uparrow(\lambda_i, \tau)$, $r(\lambda_i, \tau)$ is the spherical albedo, $R(\lambda_i)$ is the Lambertian surface albedo. The explicit notations of the observation/illumination geometries are not included in Eq. (18) for simplification.

The main advantage of Eq. (18) is that it yields a solution of the multiple scattering radiative transfer problem only once for the atmosphere with black surface. The contribution of the surface reflectance is then easily calculated in the second term in the right hand side of Eq. (18). The Eq. (18) is correct for Lambertian surface while it is an approximation for non-Lambertian cases. Our estimations show that the difference between TOA reflectance simulated according to Eq. (18) and exact RT model including non-Lambertian effect increase with the increase of the wavelength and can reach in the worst cases (the hot-spot direction) up to 20–30% for channel 885 nm. Despite this disadvantage we use Eq. (18) in the retrieval process at present, the large errors are observed only within narrow angle range around the hot-spot direction. The non-Lambertian effect will be further taken into account using the newly developed correction model described in Mei et al. (2016b).

The TOA reflectance calculated according to Eq. (18) in the case of Lambertian surfaces is correct for both vertically homogeneous and vertically inhomogeneous medium (Chandrasekhar, 1950; Liou, 2002). However, in the case of vertically homogeneous medium, transmittance from the surface to the satellite can be calculated simultaneously with R_0 , $T^\downarrow(\lambda_i, \tau)$ and $r(\lambda_i, \tau)$, i.e., solving the standard atmospheric radiative transfer problem (solar illumination from above), whereas in vertically inhomogeneous medium, the total transmittance from the surface to the satellite has to be calculated under illumination of the atmosphere from below (Liou, 2002). This requires a separate solution of the radiative transfer equation with defined and specific boundary conditions. To speed up the calculation of LUT, we ignored the impact of vertical inhomogeneity and calculated $T^\uparrow(\lambda_i, \tau)$ solving the standard atmospheric radiative transfer problem (solar illumination from above). We recall that the vertical inhomogeneity of atmosphere is caused mainly by the mixture of Rayleigh and aerosol scattering within the tropospheric layers and by the ozone absorption in the stratospheric layers. Our estimations show that the impact of vertical inhomogeneity is small on TOA reflectance simulation for all the selected MERIS wavelengths. In particular, the difference between the TOA reflectance calculated using Eq. (18) and full radiative transfer model is $< 0.2\%$.

Accounting for that Eq. (18) can be solved analytically with respect to the Lambertian surface albedo, $R(\lambda_i)$, we formulate the inverse problem as follows. The measured TOA reflectance is transformed first into surface spectral reflectance, i.e. the “measured” SSR. This transformation is usually named atmospheric correction. Assuming that AOT and aerosol type are selected, ignoring the measurement and forward model errors and solving Eq. (18) with respect to the SSR, we have

$$R_{AC}(\lambda_i, \tau) = \frac{\Delta R(\lambda_i, \tau)}{T(\lambda_i, \tau) + r(\lambda_i, \tau) \Delta R(\lambda_i, \tau)}, \quad (19)$$

where $R_{AC}(\lambda_i, \tau)$ is the “measured” SSR, $R(\lambda_i, \tau) = R^m(\lambda_i) - R_0(\lambda_i, \tau)$, $R^m(\lambda_i)$ is the MERIS observed TOA reflectance for a given channel and τ is the AOT used to calculate atmospheric path reflectance, total transmittance and spherical albedo. Note that we used τ explicitly as argument of $R_{AC}(\lambda_i, \tau)$ to emphasize that the “measured” SSR is not the SSR of a real surface, but an estimation which depends on the selected AOT. Max-Planck-Institute Aerosol Climatology version 1 (MAC-v1) is used as the initial AOT, which will be described in Section 10. Assuming further that the one-parametric approximation given by Eq. (10) can be employed to approximate the “measured” SSR, the inverse problem with respect to parameters τ and x_s is formulated as

$$Q(\tau x_s) = \left\| R_{AC}(\tau) - R_{\lambda_{14}}(\tau)(A_s x_s + B_s) \right\|^2 \rightarrow \min \quad (20)$$

where the elements of the vector $R_{AC}(\tau)$ and $R_{\lambda_{14}}(\tau)$ are given by Eq. (19). Parameters, which provide the minimum of the formulated quadratic form, are obtained by solving the system of following equations:

$$\frac{\partial Q(\tau x_s)}{\partial x_s} = 0, \quad (21)$$

$$\frac{\partial Q(\tau x_s)}{\partial \tau} = 0. \quad (22)$$

Owing to the linear dependence of $\frac{\partial Q(\tau x_s)}{\partial x_s}$ on the parameter x_s , the solution of Eq. (21) is obtained in the form of following analytical expression:

$$x_s(\tau) = \frac{\left(R_{AC}(\tau) - R_{\lambda_{14}}(\tau) B_s A_s \right)}{R_{\lambda_{14}}(\tau) (A_s A_s)}. \quad (23)$$

Substituting $x_s(\tau)$ as given by Eq. (23) into Eq. (22), we have

$$\frac{\partial Q(\tau x_s(\tau))}{\partial \tau} = 0. \quad (24)$$

Thus, the solution of the formulated inverse problem is reduced to the solution of non-linear equation of single variable τ . In the framework of XBAER algorithm, Eq. (24) is solved iteratively employing the modification of Newton-Raphson method known as the secant method (Ben-Israel, 1966).

Fig. 8 shows a schematic flowchart describing the XBAER algorithm. The flowchart includes steps for the cloud screening, LUT information and surface spectral coefficients dataset. The output of XBAER includes both AOT (and related parameters like single scattering albedo (SSA)) and SSR.

The logical flow of the XBAER algorithm is as follows. For a given geographical position and satellite observation time, the predefined aerosol type, first guess of AOT, and A/B vectors of spectral coefficients dataset are selected. These parameters are used in the atmospheric correction according to Eq. (19) above is used to obtain the “measured” SSR at λ_{14} , $R_{\lambda_{14}}(\tau)$. In line with our assumptions described above, the “measured” SSR for all short wavelengths $\{\lambda_1, \lambda_2, \dots, \lambda_9\}$ is approximated by Eq. (10). AOT and x_s or effective vegetation index are obtained by minimizing the difference between “measured” SSR and SSR calculated using spectral coefficients database for the first nine channels of MERIS instrument.

9. Sensitivity study

A sensitivity study has been undertaken to investigate the influence of using an incorrect aerosol type and surface non-Lambertian effect. Assuming an effective and accurate cloud screening, errors associated with the determination of the SSR and the selection of aerosol type are the two dominant sources of error in the XBAER AOT product. The uncertainty in XBAER algorithm related to different surface and aerosol situations is illustrated in this section. As can be seen in Fig. 6, the city surface type is the most problematic case for XBAER to deal with. This is because of the range of non-Lambertian effect and the complexity of aerosol types.

Taking the above into account, we have chosen the AERONET site located near Paris (same as Fig. 3) for a sensitivity study. According to Fig. 2, the aerosol type over Paris for July is weakly absorbing. Consequently sensitivity study cases for the retrieval use the weakly absorbing aerosol type. Since the current XBAER retrieval algorithm is based on Lambertian assumption by utilizing Eq. (18), the non-Lambertian effect for the retrieval also need to be studied in this section.

The TOA reflectances have been simulated using a full radiative transfer model for the case of weakly absorbing aerosol type including and excluding surface reflection non-Lambertian effect using SCI-ATRAN for the two selected days shown in Fig. 6 and another day for

additional confirmation of the strong non-Lambertian effect. The MERIS observation geometry of 2 and 4, July 2009 as well as 16 July 2008 over Paris was used to perform the forward simulation. In particular, the solar zenith angle, viewing angle and relative azimuth were set to (32.32°, 28.7°, 30.65°), (18.18°, 31.63°, 25.97°), and (31.44°, 140.35°, 141.26°) respectively. The non-Lambertian property is strongest under the observation geometry of 16 July 2008 and 4 July 2009, which means that the sensitivity shown below represents a “worst” case for XBAER algorithm.

The SSR was defined according to Eq. (13) and (14), where parameters x_s and x_l were estimated by applying the XBAER algorithm to the MERIS measurement on the three days and A and B vectors were used from the previously determined spectral coefficients dataset for July over Paris. The non-Lambertian effects were simulated following the method of Bréon and Vermote (2012) in the framework of the modified representation of the kernel-based linear Ross-Li model, details can be found in Rozanov et al. (2014).

Fig. 9 shows the XBAER algorithm results retrieved from simulated TOA reflectances. XBAER AOT has < 1% retrieval error for the case of small AOT for Lambertian surface and weakly absorbing aerosol case, which are caused by the interpolation of LUT values. In contrast to the LUT interpolation errors, the non-Lambertian effect plays a significantly larger role for the relative error on small AOTs. Fig. 9 demonstrates that the non-Lambertian effect can increase the errors to 10% and higher depending on the AOT values. Although the relative uncertainty caused by non-Lambertian is large for small AOTs (34% for AOT = 0.1), but the absolute difference is actually 0.034, which is acceptable with the strong non-Lambertian effect under the simulation angles from MERIS mentioned above. If an incorrect aerosol type is selected, Fig. 9 shows that the errors can range from 10% to – 40% depending on AOT and geometry observations.

In contrast to the relatively benign impact of the non-Lambertian effect on the error of the AOT, the incorrect selection of aerosol type causes relatively large retrieval errors for large AOTs. The surface inhomogeneity is another important error source for XBAER algorithm, the previous study (e.g Tanre et al., 1996) as well as our investigation show that $10 \times 10 \text{ km}^2$ can be safely used as the default retrieval size.

10. Data

A reasonable first-guess of aerosol retrieval speeds up the retrieval procedure significantly and reduces the risk of non-convergence arising from local minima in the fitting procedure. In XBAER, a global aerosol climatology, the MAC-v1 from Kinne et al. (2013) was used for the first guess. The climatology contains the optical properties of both monthly and annual tropospheric aerosol with global coverage at a spatial resolution of $1^\circ \times 1^\circ$.

Aerosol Robotic Network (AERONET) is a federation of ground-based remote sensing aerosol networks, which provides the quality-controlled and long-term reference for global aerosol optical properties over > 600 stations (Holben et al., 1998). AERONET provides very strictly cloud screened level 2.0 AOT values, which was used for XBAER validation.

11. First results and validation

Fig. 10 shows a first comparison of XBAER and AERONET in-situ measurements for all global AERONET sites of July 2009. The validation contains various surface and aerosol types, which ensures a wide representativeness of the validation. The regression equation is $y = (0.92 \pm 0.07) + (0.05 \pm 0.01)x$ with correlation $R = 0.78$. The majority of the comparisons of AERONET and XBAER products are for low AOT values, some values being lower than 0.05. This value is similar to the accuracy of current satellite-derived AOT products and thus a current limitation. According to Fig. 10, it seems that the performance of the new cloud mask algorithm of XBAER also generally works well because there are few extremely high values of AOT from XBAER when AERONET AOTs are low. The comparison between XBAER AOTs and AERONET observations shows the good quality of the first XBAER results.

In order to analyze quantitatively the bias of XBAER AOTs compared with AERONET observations, the histograms of XBAER AOT bias of Global, Southern Hemisphere and Northern Hemisphere for July 2009 are presented in Fig. 11. The majority of the AOT differences between XBAER and AERONET are within the range ± 0.05 . Ignoring any effects of different absolute number for the location matches for Southern Hemisphere and Northern Hemisphere, the difference between XBAER and AERONET for Northern Hemisphere shows a larger variance range is observed compared to that in the Southern Hemisphere. The distributions of the retrieved AOT in both the Southern Hemisphere and Northern Hemisphere AOT are slightly skewed. This negative bias (an underestimation pattern) agrees with the results of the sensitivity study and is attributed to the non-Lambertian effect and aerosol absorption.

A more extensive and intensive validation of XBAER coupled with trend analysis is planned for a subsequent publication.

Fig. 12 shows the global monthly AOT of July 2009 for MODIS collection 6 (Levy et al., 2013), MISR (Kahn et al., 2010), AATSR (SU) (Holzer-Popp et al., 2013) and MERIS (XBAER) algorithm. MODIS/MISR on board of TERRA and AATSR/MERIS on board of ENVISAT has very similar overpass time (within 30 min difference), we expect that all four results should show similar patterns for large AOT from desert dust events, biomass burning and anthropogenic pollution. Differences in overpass time may explain some of the differences. However the knowledge of the reflectance measurements, sensor characteristics, algorithm assumptions and pre/post treatments such as cloud masking are likely to explain a large part of the differences.

According to Fig. 12, XBAER retrieval results agree well especially with the AATSR (both on ENVISAT satellite) AOT product for both dark and bright surface, except deserts and Amazon forest. For Amazon region, XBAER is similar to both the MODIS and MISR product. However, due to the surface brightness, the aerosol retrieval over desert regions is intrinsically more challenging. A comparison of AOT from MODIS-DeepBlue (Hsu et al., 2013), MODIS-MA-IAC (Lyapustin et al., 2011a) and MISR (Kahn et al., 2010) demonstrates that all products show different spatial and temporal patterns over the Sahara

(Lyapustin et al., 2011b). The differences are attributed to the surface and aerosol type treatments using in the respective retrieval algorithms. From validation studies, it is known that the AATSR AOT result is overestimated over desert regions (Grey et al., 2006). The current XBAER AOT over desert shows similarity with that from MODIS-DeepBlue algorithm. One explanation can be that SAVI values are very small over desert, thus the non-vegetation component (B vector) dominates the surface treatment, and XBAER becomes a DeepBlue-similar aerosol retrieval algorithm. XBAER shows large dust contribution over West Africa. Although the final AOT retrieval over ocean using XBAER is under development, we can still expect that the dust is blown from the east towards the Atlantic Ocean according to Fig. 12.

XBAER retrieved AOT, similar to that from MODIS and MISR, shows a special distribution pattern over India related to the special and unique meteorological conditions (Prasad and Singh, 2007), which is not presented in the AATSR retrieved AOT. XBAER AOT is similar to MODIS-DT product while MISR tends to be lower compared with MODIS (Mehta, 2015). XBAER and MODIS-DT over Amazon forest also show more similarities to one another. This may be explained by both retrievals using the same aerosol type treatment over those regions and both surface treatments deliver accurate surface parameterization.

The large contribution from biomass burning over Alaska observed by AERONET (Eck et al., 2009) and far eastern Siberia are also well identified in XBAER AOT and all other AOT products. These agree well with the sources being fires identified by the MODIS fire point map (<http://lance-modis.eosdis.nasa.gov/cgi-bin/imagery/firemaps.cgi>) and SCIAMACHY (Richter et al., 2005) and the Global Ozone Monitoring Experiment (GOME) (Richter and Burrows, 2002) NO₂ product for the corresponding time period. The other aerosol source region is East Asian and India (Yoon et al., 2014). East Asia has both desert dust and anthropogenic pollution. The amount of desert dust depends on the meteorological conditions. The anthropogenic sources depends on fossil fuel combustion and the release of sulfur dioxide, SO₂, and other pollutants.

12. Discussion

In this manuscript a new generic retrieval algorithm for AOT and SSR, called XBAER, is presented and explained. XBAER builds on the heritage of the BAER, DB and DT algorithms. XBAER has been applied to data from the MERIS instrument, which flew on Envisat. XBAER is valid for both dark and bright surface because of its use of an optimized monthly global SSR spectral coefficients dataset.

XBAER uses a new cloud mask algorithm, which has been successfully validated by comparison with manually created cloud mask results. The monthly global AOT maps show good agreement in spatial distribution pattern with current AOT products such as MODIS, MISR and AATSR. The comparison with AERONET measurements also shows that XBAER can provide promising results over both dark and bright surface. The first comparison with AERONET shows good agreement between the two data sets, with the regression yielding $y = (0.92 \times \pm 0.07) + (0.05 \pm 0.01)$ and correlation of $R = 0.78$.

The current XBAER cloud mask algorithm uses multiple criteria by utilizing the cloud brightness, cloud variability and cloud height information shows generally good results. However, the cloud mask over bright surfaces such as the Sahara regions tends to be too conservative. Some dust storms are masked i.e. identified as cloud because the current threshold criteria for the absolute value of the blue channel (412 nm), thus reducing the monthly mean values as shown in Fig. 10. The cloud mask thresholds will be further linked to the TOA reflectance and cloud optical thickness (COT), which can be obtained from TOA reflectance at 885 nm using analytical form (Kokhanovsky et al., 2006). Additional information obtained from RGB image and “BLUE value” (Dinter et al., 2009) will be also used. Such improvement can make the cloud mask more flexible for different surface type and aerosol condition, thus reduce the loss of heavy dust storm in XBAER.

The first surface spectral coefficients dataset do not yet take the scattering angle effects into account. This can be improved by using a regression for each scattering angle bins and the regression coefficient is then scattering angle dependent and describes the surface non-Lambertian effect more accurately. The spectral coefficients dataset can be further improved by using the full MERIS observation period (2002–2012). Since the spectral coefficients dataset is $0.1^\circ \times 0.1^\circ$ spatial resolution, small patterns inside a $0.1^\circ \times 0.1^\circ$ region cannot be well captured, which will be problematic for high-spatial resolution retrieval. Thus the MERIS land-cover product with spatial resolution of 300 m will improve the surface parameterization in the future work (Bicheron et al., 2006).

Another important issue is the dust aerosol type treatment. The current XBAER utilizes the MODIS-DT spheroid dust aerosol mode for regions like Sahara. This may be one of the reasons for the underestimation due to the non-sphericity of dust particles, which has strong impact on the aerosol phase function in the backward direction. The latest DeepBlue aerosol product shows the presence of absorbing mineral dust can be underestimated by using the normal dust type (Hsu et al., 2013). The use of the latest version of dust optical database from Optical Properties of Aerosols and Clouds (OPAC) 4.0 (Koepke et al., 2015) and the experimental observations like the Saharan Mineral Dust Experiment (SAMUM) (Dinter et al., 2009) will be investigated for the next version of XBAER focusing on the non-sphericity and absorbing properties of dust particles as well as the synergetic use of the absorbing aerosol index where it is available.

XBAER is planned to be applied to OLCI data, when it becomes available, to create a long-term record of AOT (and potentially other products) based on MERIS-OLCI retrievals. The long-term record will be used for creating a climate data record (Kinne et al., 2006), megacities studies (Yoon et al., 2014) and aerosol-cloud interaction researches.

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Fig. 1.

Comparison of different cloud mask algorithms. In the upper left panel is the RGB composite figure for the selected cloud scene; the upper right panel is the “true” cloud mask created by Gómez-Chova et al. (2007); the lower left panel shows BAER cloud mask; the lower right panel shows XBAER cloud mask. The XBAER cloud mask uses also the 3×3 adjacency pixels to minimize the “twilight zone” effect. If a pixel is detected as cloud, the surrounding 3×3 block will be automatically marked as cloud.

Fig. 2.

Aerosol types over land used in the XBAER algorithm designated at $1^{\circ} \times 1^{\circ}$ grid for different seasons. The four sub-figures represent four seasons. Upper row: left – December, January and February (DJF), right - March, April and May (MAM). Lower row: left - June, July and August (JJA), right - September, October and November (SON).

Fig. 3.

Plots of the relationship between SSR at 412 nm, SSR at 885 nm and the ratio of SSR at 412 nm and 885 nm and the value for SAVI for three different AERONET stations (Rio_Branco, Paris and Bodele) having different surface types (Vegetation, city and desert). “cc” refers to correlation coefficient.

Fig. 4.

Plots of the spectral coefficients dataset available for the three different AERONET stations (Rio_Branco, Paris and Bodele) having different surface types (vegetation, city and desert).

Fig. 5.

Plots of the global spectral coefficients dataset components for July. Left panels – MERIS channels 1. Right panels – MERIS channel 14 (Please note $a(\lambda_{14})$ over desert (dark blue) can be negative). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 6.

Plots of the approximated spectra for the reference surface spectra for the three different AERONET stations shown in Fig. 3. The upper row is for the 16th July 2008. The lower row is for the 2nd July 2009. The red, green and blue circles represent the SSR from land-cover cci (Ref), SSR fitted using Eq. (16) (Ref_f) and surface reflectance using standard SAVI (Ref_s). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 7.

Global 7 days composite SSR for MERIS channel 1 and channel 14 and the difference between XBAER estimated MERIS SSR and land-cover-cci MERIS SSR product for the period of the 24th to 30th of July 2009 for. Upper panels: left – XBAER estimated MERIS SSR for channel 1, right-XBAER estimated MERIS SSR for channel 14. Lower panels: left-the difference between XBAER estimated MERIS SSR and reference SSR for channel 1, right- the difference between XBAER estimated MERIS SSR and reference SSR for channel 14.

Fig. 8.
Flowchart, which pictorially describes the steps in the XBAER aerosol retrieval algorithm over land.

Fig. 9.

Plot of AOTs (550 nm) uncertainty versus AOT (550 nm) obtained from the sensitivity study of the XBAER algorithm and their dependence on the surface reflection type and aerosol model. (Red line - Lambertian surface; green line - BRDF effect for three different days; blue line - Moderately absorbing aerosol; black line - Strongly absorbing aerosol). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 10. Comparison of XBAER AOT with AERONET observation for 2009 July. R and N refer to the Pearson correlation coefficient and the number of locations used in the validation respectively. The dash lines are $\pm 20\% \tau \pm 0.05$.

Fig. 11.

Histogram of difference between XBAER AOT and AERONET observations for 2009 July separated into the following: global, Southern Hemisphere and Northern Hemisphere.

Fig. 12.

Comparison of retrieved global monthly mean AOT at 550 nm for July 2009. Upper row: left – MODIS, right – MISR. Lower row: left – AATSR (SU), right – MERIS (XBAER).

Table 1

The wavelength setting and corresponding applications of MERIS instruments in XBAER algorithm.

MERIS channel number	Centre wavelength $\pm$ bandwidth (nm)	Cloud screening	Surface parameterization	Aerosol retrieval
1	412.5 $\pm$ 10	✖	✖	✖
2	442.5 $\pm$ 10		✖	✖
3	490 $\pm$ 10		✖	✖
4	510 $\pm$ 10		✖	✖
5	560 $\pm$ 10		✖	✖
6	620 $\pm$ 10		✖	✖
7	665 $\pm$ 10		✖	✖
8	681.25 $\pm$ 7.5		✖	✖
9	708.75 $\pm$ 10		✖	✖
10	753.75 $\pm$ 7.5	✖		
11	760.625 $\pm$ 3.75	✖		
12	778.75 $\pm$ 15			
13	865 $\pm$ 20			
14	885 $\pm$ 10		✖	
15	900 $\pm$ 10			