**Sentinel-3 snow and ice (SICE-3) products**

Algorithm Theoretical Basis Document

Version 5.1

October 1, 2022

1. A. Kokhanovsky (1), B. Vandecrux (2), A. Wehrle (2),

O. Danne (1), C. Brockmann (1), J. Box (2)

1. Brockmann Consult GmbH, Chrysanderstr.1 , 21029 Hamburg, Germany
2. Geological Survey of Denmark and Greenland (GEUS)  
   Øster Voldgade 10, 1350 Copenhagen, Denmark

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# Introduction

This document describes the theoretical basis of the algorithms used to determine properties of snow and ice from the measurements of the Ocean and Land Color Instrument (OLCI) onboard Sentinel-3 satellites (see also <http://snow.geus.dk/>). The previous version of the code used for the retrieval of snow properties and its documentation can be found at <https://github.com/GEUS-SICE/pySICE>. The detailed description of the retrieval algorithm is given by Kokhanovsky et al. (2018, 2019, 2020a).

Snow is composed of ice crystals in contact with each other and surrounded by air. Snow can include impurities such as dust, soot, algae (e.g., Skiles et al., 2018), here referred to as ‘pollution’. Snow can also contain liquid water. The volume concentration of snow grains is usually around 1/3 with 2/3 of the snow volume occupied by air (Proksch et al., 2016). The concentration of pollutants is often low, that is, below 100 ng/g especially in polar regions (Doherty et al., 2010).

The algorithms described here are dedicated to the retrieval of snow optical properties such as snow spectral and broadband albedo and also snow microstructure (snow specific surface area and effective optical grain size). We propose a snow mask and a technique to retrieve the concentration of pollutants in snow, which is possible only for the cases with relatively heavy (above 1ppmv) pollution load (Warren, 2013).

## Ocean and Land and Colour Instrument

Ocean and Land and Colour Instrument is a 21band spectrometer that measures solar radiation reflected by the Earth’s atmosphere and surface with a ground spatial resolution of 300 m (see Table 1.1). The OLCI swath width is 1270 km. OLCI is installed on both Sentinel-3A and Sentinel-3B satellite platforms operated by the European Space Agency (ESA) in service to the European Union Copernicus Programme. The Sentinel-3 A and B orbit at 802 km altitude, 98.6 orbital inclination and a 10:00 UTC sun-synchronous equatorial crossing time. The Sentinel-3 C instrument will be launched in 2024.

Table 1.1 Band characteristicsof the Sentinel-3 Ocean and Land Colour Instrument (OLCI)[[1]](#footnote-1)

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Band** | **λ centre (nm)** | **Width (nm)** | **Band** | **λ centre (nm)** | **Width (nm)** | **Band** | **λ centre (nm)** | **Width (nm)** |
| 1 | 400 | 15 | 8 | 665 | 10 | 15 | 767.5 | 2.5 |
| 2 | 412.5 | 10 | 9 | 673.75 | 7.5 | 16 | 778.75 | 15 |
| 3 | 442.5 | 10 | 10 | 681.25 | 7.5 | 17 | 865 | 20 |
| 4 | 490 | 10 | 11 | 708.75 | 10 | 18 | 885 | 10 |
| 5 | 510 | 10 | 12 | 753.75 | 7.5 | 19 | 900 | 10 |
| 6 | 560 | 10 | 13 | 761.25 | 2.5 | 20 | 940 | 20 |
| 7 | 620 | 10 | 14 | 764.375 | 3.75 | 21 | 1 020 | 40 |

## Generated Products

The products of the SICE algorithms are listed in Table 1.2. The effective grain diameter (EGD) is derived at 865 and 1020nm*,* where the influence of atmospheric light scattering and absorption processes on top-of-atmosphere signal as detected on a satellite over polar regions is weak and can be ignored in the first approximation.

Table 1.2 SICE: Snow and ice products

|  |  |  |  |
| --- | --- | --- | --- |
|  | **Snow product name** | **Units** | **Expected range** |
| 1 | Snow fraction | - | 0 - 1 |
| 2  3  4 | Spectral spherical snow albedo  Spectral planar snow albedo  Spectral surface reflectance  (for all OLCI channels) | - | 0 - 1 |
| 5 | Broadband snow albedo  (plane and spherical, for three spectral ranges) | - | 0 – 1 |
| 6 | Snow specific surface area | m2 kg-1 | 2-200 |
| 7 | Snow grain diameter | mm | 0.07-2 mm |
| 8 | Concentration of pollutants  (part per million weight) | ppmw  (10-6) | 2-500 |
| 9 | Normalized difference snow index (NDSI) | - | - |
| 10 | Normalized difference bare ice index (NDBI) | - | - |
| 11 | Effective radius of dust grains | micron | 5-50 |
| 12 | Effective absorption length | mm | 1.4-40 |
| 13 | Reflectance of a nonabsorbing snow | - | 0.7-1.2 |
| 14 | Absorption Angström exponent of snow impurities | - | 0.9-10 |
| 15 | Impurity load parameter | 1/m | 0.1-1 |
| 16 | Mass absorption coefficient of dust particles at 660nm | /g | 0.01-0.1 |
| 17 | Mass absorption coefficient of dust particles at 1000nm | /g | 0.0005-0.005 |
| 18 | ECMWF total ozone column (TOC) given in OLCI files | DU | 200-600 |
| 19 | Retrieved TOC | DU | 200-600 |
| 20 | Normalized root-mean-square differences of registered and modelled TOA spectra using all OLCI channels | % | 0-5 |
| 21 | The same as above except outside oxygen and water vapor absorption bands | % | 0-5 |
| 22 | Relative difference between OLCI and retrieved TOCs | % | 0-12 |
| 23 | Type of underlying surface  (1-clean snow, 2- polluted snow, 3-partially snow covered) | - | - |
| 24 | Type of impurities (0 – no impurities, 1- black carbon, 2- dust) | - | - |
| 25 | Bare glacier ice index (1- glacier clean ice, 2- glacier polluted ice, 0- otherwise) | - | - |
| 26 | Snow index (0-no snow, 1-snow) | - | - |
| 27 | OLCI spectral index (OSI) | - | - |

## Summary of assumptions

We derive snow properties using the following assumptions:

* horizontally homogeneous plane parallel snow layer;
* vertically homogeneous layer;
* semi-infinite layer. Therefore, there is no need to account for the reflective properties of underlying surface;
* close - packed media effects are ignored.
* geometrical optics under weak light absorption approximation can be used to derive local optical snow characteristics.
* impurities (dust, soot, etc.) are located external to ice grains.
* the single light scattering angular pattern is spectrally neutral in the OLCI spectral range.
* the effects of slopes and snow roughness are not accounted for.

The output for the snow products is provided if the derived diameter of grains is larger than 0.14mm. The diameters of ice grains in clouds and snow occupy different size bins. Therefore, it is assumed that ground scenes with EGD below 0.14mm are contaminated by clouds. The partially snow - covered ground pixels are considered as explained below.

# Snow and ice property retrievals

## Definitions

### Geometry of the system

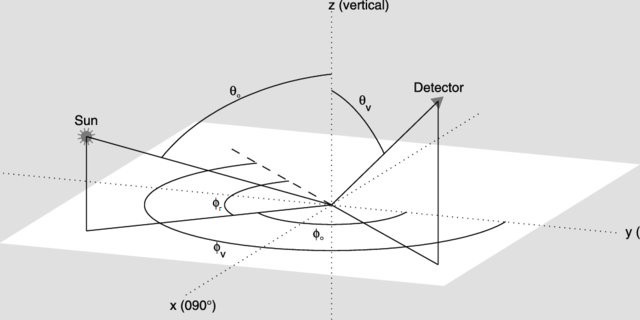


Figure 2.1.1 Definition of the solar zenith angle , azimuth angle , viewing zenith angle and relative azimuth angle . Illustration adapted from Hudson et al. (2006). The OLCI relative azimuth angle is equal to .

The angles describing the solar and satellite positions around the point observation are presented in Figure 2.1.1. From these we derive the cosine of the solar zenith angle , the cosine of the viewing zenith angle and the scattering angle :

|  |  |  |
| --- | --- | --- |
|  |  | (2.1.1) |

### Reflectance, spherical and plane albedos

The **top-of-atmosphere reflectance** is defined as:

|  |  |  |
| --- | --- | --- |
|  |  | (2.1.2) |

where, is the intensity of reflected light, is the solar flux at the top-of-atmosphere. Many satellite instruments simultaneously measure both and and allow the derivation of the top-of-atmosphere reflectance. In the absence of cloud, the **bottom-of atmosphere reflectance or snow reflectance** is defined by Eq. (2.1.2) when applied at the bottom of the atmosphere.

The reflectance depends on atmospheric effects due to molecular and aerosol scattering and absorption of solar radiation. For retrieval of surface optical properties, these effects must be removed.

The ***plane albedo*** is defined as the integration of bottom-of atmosphere reflectance *R* across all viewing azimuth angles (assuming that the solar azimuth angle is equal to zero) and zenith angles:

|  |  |  |
| --- | --- | --- |
|  |  | (2.1.3) |

The ***spherical albedo*** is found by integration of *R* over all incident angles :

|  |  |  |
| --- | --- | --- |
|  |  | (2.1.4) |
|  |  |  |

## Retrieval overview

The retrieval process consists of the following steps:

* cloud screening;
* ground scene classification;
* retrievals for 100% and also partially snow/ice-covered ground pixels.

We first convert the spectral OLCI top of the atmosphere radiance to reflectance using the [SNAP](http://step.esa.int/main/toolboxes/snap/) Rad2Refl module.

## Cloud screening

Cloud screening is performed using the following procedures. If the EGD is smaller than the threshold value (THV) of 0.14, then it is assumed that the ground scene is covered by cloud or diamond dust. The results for ground pixels with RMSE differences between initial and modelled (using retrieved parameters) OLCI reflectances (at 16 OLCI channels almost free of gaseous absorption, see Table 1.1) are larger than 5% are not provided in output in the postprocessing stage. They are assumed to be covered by other types of surfaces or partially covered by clouds. The same is true for the pixels, where retrieved total ozone column (TOC) differs by more than 25% from the TOC provided in OLCI files. All values of THVs mentioned in this section can be changed depending on the user requirements.

## Ground scene classification

The land mask is used. Therefore, ground pixels containing oceanic surfaces are not processed.

If R(400nm) is smaller than 0.2, the retrievals are not performed because ground scenes are dark and not covered by snow or bare ice.

The normalized difference bare ice index is calculated as:

|  |  |
| --- | --- |
|  | (2.4.1) |

The bare ice is classified in two steps. First, dark bare ice is identified where NDBI is less than 0.65 and R (400nm) is less than 0.75 (bare ice index equal to 2). Then for cases the dark bare ice flag (2) is not set, the bare ice flag is assumed to be equal to 1 (100% bare ice – covered pixel), if NDSI is larger than 0.33. Summing up, the bare glacier ice index is equal to 1(2) for the case of clean (polluted) bare ice. Otherwise, it is equal to zero.

Also we provide OLCI spectral index:

(2.4.2)

This index shows the range of variability of the snow OLCI reflectance, being closer to 1 for snow surfaces (as compared to bare ice). It follows:

. (2.4.3)

The normalized difference snow index (NDSI) is calculated as:

(2.4.4)

A pixel is considered snow-covered (snow index is equal to 1) if NDSI is smaller than 0.1 and R(400nm) is larger than 0.75. Otherwise, snow index is equal to zero.

The indices (***I, K, N***) are used for the ground scene classification. They are provided in the output of the algorithm. However, they are calculated after processing of OLCI pixels with respect to the determination of their microstructure, albedo, and impurity characterization. The indices can be used for the assessment of the quality of the retrievals.

## Snow property retrieval

**2.5.1 Completely snow - covered ground scenes**

In this section we describe a technique for snow property retrievals, which accounts for atmospheric scattering effects and can be used both for clean and polluted snow. Therefore, *a priori* knowledge on the snow pollution level is not required. It is assumed that the ground scene is completely covered by snow and the measured top-of-atmosphere reflectance can be presented in the following form:

(2.5.1)

(2.5.2)

where absorption, is the atmospheric reflectance for the case of black underlying surface, is the atmospheric spherical albedo for the black underlying surface, is snow spherical albedo, is the gaseous transmittance, is total atmospheric transmittance for black underlying surface. The functions can be calculated using the radiative transfer theory for a given distribution of aerosol particles in atmosphere with account for multiple light scattering effects. The analytical approximation for the calculation of these functions under assumption that the phase function of atmospheric aerosol can be modelled as double Henyey - Greenstein phase function in absence of light absorption by aerosol particles is given in Appendix 1. Taking into account that atmospheric aerosol load is rather weak in polar regions, the errors related to the modelling of functions with the use of approximation described in Appendix 1 does not influence the results of retrievals considerably. The theoretical foundations of snow spectral reflectance modelling are given in Appendix 2. Appendix 3 is aimed at gaseous transmittance function modelling. It should be pointed that Eq. (2.5.1) is also an approximation. Generally, the gaseous absorption effects and multiple light scattering in vertically inhomogeneous atmosphere should considered in the framework of the solution of the radiative transfer equation. We concentrate our snow property retrievals on the OLCI channels only weakly affected by the gaseous absorption. Therefore, the use of Eq. (2.5.1) is justified.

Eq. (2.5.2) follows from the first principles in the case of Lambertian underlying surfaces. The snow is not exactly Lambertian reflector. Therefore, we substitute in the nominator by the value of the snow reflection function . Such a substitution partially accounts for the non-Lambertian nature of snow reflectance and provides correct limit for the measured reflectance for the idealized case of absence of atmosphere between satellite and ground ( = by definition in this case). Therefore, we shall assume that

(2.5.3)

for optically thin polar atmosphere with underlying snow surface. The snow reflectance function can be modelled using the following approximation at OLCI channels (Kokhanovsky, 2021):

*()= () ,* (2.5.4)

where

*exp* (2.5.5)

is the snow spherical albedo. The meaning of all parameters and functions in Eqs. (2.5.4), (2.5.5) is explained in Table 2.1. The derivation of Eq. (2.5.5) is presented in Appendix 2.

Table 2.1. The meaning of various parameters in Eqs. (2.5.4)-(2.5.5) (see Appendix 2).

|  |  |  |
| --- | --- | --- |
| Parameter | Meaning | Equation |
|  | Cosine of viewing zenith angle |  |
|  | Cosine of solar zenith angle |  |
|  | Relative azimuthal angle |  |
| *()* | The reflectance of snow at the idealized assumption that there is no light absorption in snow |  |
|  | Anisotropy function | *()* |
|  | The escape function |  |
|  | The normalized wavelength () |  |
|  | The impurity load parameter |  |
| *m* | The impurity absorption Angström parameter |  |
| *L* | The effective absorption length |  |

It follows from Eqs. (2.5.3) - (2.5.5) that the underlying snow – atmosphere reflectance outside gaseous absorption bands is determined by the four underlying snow and impurity parameters (), on illumination/observations conditions and atmospheric characteristics (. The snow parameters listed above do not depend on the wavelength in a good approximation (see Appendix 2). The atmospheric characteristics strongly depend on the wavelength primarily due to the spectral dependence of molecular and aerosol optical thickness, which decreases with the wavelength. Both aerosol and molecular optical thickness is smaller than 0.01 at the OLCI wavelengths larger than 865nm for clean polar atmospheres in most of cases. In particular, Six et al (2005) have found that the aerosol optical thickness is smaller than 0.01 at 870nm at Dome C in Antarctica. Tomasi and Petkov (2005) have found that the molecular optical thickness is smaller than 0.01 in polar regions at wavelength larger than 850nm.

Therefore, in a good approximation one can assume that OLCI reflectance as observed at channels 865nm and 1020nm is not affected by atmospheric light scattering effects. These channels are also outside gaseous absorption bands. Also light absorption by snow grains is much larger as compared to light absorption by small amounts of pollutants in polar snowpack. Therefore, we can assume that the second term in Eq. (2.5.5) can be ignored in the near IR. Then the parameters () can be derived from Eqs. (2.5.3) - (2.5.4) analytically. In particular, we can write for the measured reflectance at the pair of near infrared OLCI channels only weakly affected by the atmospheric scattering and absorption effects in clean polar atmospheres:

*exp (-𝜉 ), exp (-𝜉 ),* (2.5.6)

where indices signify the OLCI wavelengths. In this work we have used the OLCI channels located at almost free of gaseous absorption. The spectral calibration can be applied for all OLCI channels ahead of retrievals (see Table 3.1 in Appendix 3).

It follows from Eqs. (2.5.6) neglecting weak atmospheric scattering effects:

, () , (2.5.7)

where , *W*=1/ Taking into account the data for ice refractive index (Warren and Brandt, 2008) one derives:.

One can see that OLCI measurements at two near infrared channels make it possible to determine the parameters and and, therefore, one can also estimate spectral spherical albedo of clean snow at any wavelength using Eq. (2.5.5). Simultaneously, one can determine the bottom of-atmosphere (BOA) clean snow surface reflectance (see Eqs. (2.5.4), (2.5.5)). The plane albedo can be derived as (Kokhanovsky, 2021):

*=* (2.5.8)

The effective absorption length (EAL) *L* can be used to determine the effective grain diameter (EGD) and the snow specific area (SSA) as shown in Table 2.2. The broadband palne albedo of clean snow is given by the following equation:

*a+b exp(),* (2.5.9)

where

Table 2.2 The relationship between the values of EGD, SSA and EAL.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Quantity | Symbol | Equation | Parameters | Source |
| EGD | *d* | *pL* | *p=0.0625* | Kokhanovsky et al. (2019) |
| SSA | 𝜎 | *q*/*L* | *q=0.1047* | Kokhanovsky et al. (2019) |

Therefore, the technique specified above makes it possible to derive all essential clean snow parameters for the case of 100% snow covered ground OLCI scenes.

In the case of polluted snow, the parameters (*m*, γ) can be derived fitting OLCI measurements in the visible (outside gaseous absorption bands) and calculations according Eqs. (2.5.3) - (2.5.5). The aerosol optical thickness is small in polar regions. Therefore, it is difficult to derive its value accurately. Therefore, we use the following approach to derive the pair (*m*, γ). We assume that the molecular and aerosol optical thicknesses can be presented as:

, (2.5.10)

, (2.5.11)

where =ζexp(-h/), ζ=0.008735, *n*=4.08, *h* is the underlying surface height, scale height (6 km) and it is assumed that the wavelength is measured in microns. There are different approximations for the spectral molecular optical thickness In particular, one can use Eq. (2.5.10) with *n*=4.0932 and The values of and are assumed in the retrieval process using the characteristic values of these parameters in the region studied. Currently, these parameters are fixed:

(2.5.12)

One can use the climatological values of these parameters in the retrieval process, if needed. The aerosol phase function is approximated by the double Henyey – Greenstein phase function as explained in the Appendix 1. In this case the only unknown parameter in Eq. (2.5.3) is the spherical albedo , which can be derived solving the transcendent equation:

(2.5.13)

where . Eq. (2.5.13) follows from Eq. (2.5.3). This equation can be solved analytically at ξ=1:

(2.5.14)

and also at ξ=2:

(2.5.15)

We solve this equation numerically for the case of arbitrary value of ξ at the wavelengths . Then we use Eq. (2.5.5) to derive the parameters (*m*,γ). Namely, it follows from Eq. (2.5.5) under assumption that light absorption by snow in the visible can be neglected:

*exp (- ), exp (- ).* (2.5.16)

If the derived value of at 400nm is larger than 0.99, it is assumed that snow is clean and parameters (γ,*m*) are not retrieved. If the value of is smaller than 0.99, than the parameters (γ,*m*) are retrieved from Eq. (2.5.16) under assumption that *L* is known (retrieved from measurements at 865 and 1020nm as explained above). Namely it follows:

 , (2.5.17)

/*L* , (2.5.18)

where ,  . One can see that the parameters (*q*, γ) can be derived from OLCI measurements at four wavelengths almost not affected by gaseous absorption ( 400, 490, 865, 1020nm). This makes it possible to derive

* spectral spherical albedo;
* spectral plane albedo;
* spectral bottom of atmosphere reflectance at any observation and illumination geometry;
* effective grain diameter;
* snow specific surface area;
* reflectance of nonabsorbing snow layer .

In addition, the value of can be used to identify the type of pollution. It is known that the value of for black carbon (BC) is close to 1. We shall assume that the pollutant is BC, if 0.9m1.2. Otherwise the pollution by dust is assumed. The concentration of pollutants can be derived using the following approximate formula (see Appendix 2):

(2.5.19)

where the normalized impurity absorption coefficient at the wavelength 1μm γ is derived as explained above , *c=* is the relative volumetric concentration of snow impurities, is the volumetric concentration of snow pollutants, is the volumetric concentration of ice grains, is the absorption enhancement factor (Kokhanovsky and Zege, 2004; Libouis et al., 2014), is the volumetric absorption coefficient of impurities at the wavelength defined as the ratio of average absorption cross section of particles to their average volume (Kokhanovsky et al., 2021c). We shall assume that The external mixture of ice grains and impurities is assumed.

One can see that the quality of retrievals of the concentartion of pollutants *c* depends on the availability information on the value of the volumetric absorption coefficient of impurities at the selected wavelength

The derived concentration of pollutants is equal to the ratio of volumetric concentrations of pollutants and ice grains in snow. To determine the relative mass concentration of pollutants , one must multiply the value of c by the ratio 𝜁 of densities of pollutants and ice:

𝜁=, (2.5.20)

where and we assume that for black carbon and for dust, which gives: 𝜁=2.1 for BC and 𝜁=2.9 for dust. Namely, it follows:

(2.5.21)

The parameter 𝜁 can vary depending on the type of BC and dust.

In the case of BC, it is assumed that ( see Appendix 2) :

(2.5.22)

where the value of imaginary part of BC refractive index varies depending on the origin and age of BC. We shall assume that The parameter *D* depends on the real part of BC particles and also on their shape. We assume that this parameter is equal to 1.3 for BC. We can also introduce volumetric mass absorption coefficient:

, (2.5.23)

where is the soot density.

The derivation of the value of case of dust impurities is much more involved. In particular, the value of depends on the shape and size distribution of dust particles in snow matrix. It depends on the position of dust particles (inside of ice grains, outside, or both). Also refractive index and colour of atmospheric dust depends on the origin of dust layers. This makes it difficult to retrieve the dust concentration as compared to the BC concentration retrieval.

The value of ( for dust aerosol at has been parameterized with respect to the absorption Angström parameter *m*

, (2.5.24)

where is in *1/mm* , and the model of spherical dust particles is assumed. The size of dust particles can be estimated from the value of *q* as well (Kokhanovsky et al., 2021a):

 (2.5.25)

where and is expressed in microns.

The pollution type index is set to 1 for dust and 2 for soot.

**2.5.2 Partially snow - covered ground scenes**

The case of partially - snow covered ground scenes can be reduced to the case described above using the linear mixing approximation (LMA). It follows in the framework of LMA that the bottom of atmosphere reflectance  can be presented as a linear combination of reflectances from various portions of the ground scene:

, (2.5.26)

where  is the reflectance of the j-*th* portion of the ground scene and is the weight of this portion to the total signal and *N* is the number of various types of surfaces in the ground scene. The value of  can be approximated by the ratio of the surface area of the j-*th* portion to the surface area of the whole ground scene. Let us assume that *N=2.* Then it follows:

, (2.5.27)

where  is the snow fraction, is the snow reflectance, is the reflectance of the snow-free background surface. We shall consider a special case of partially water or sediment – covered glacier with snow patches. In this special case the last term in Eq. (2.5.27) can be neglected and one derives from Eq. (2.5.27):

, (2.5.28)

The value of *f* can be estimated using OLCI measurements at 400nm: *f=* . We shall use the approximation for the value of  for the clean snowpack given in Appendix 2. The derived value of *f* at *400nm* makes it possible to determine the snow reflectance of the fraction of ground scene completely covered by snow at any wavelength:

. (2.5.29)

The derived value of can be used to determine clean snow parameters from measurements at 865 and 1020nm (EAL,  ) as discussed above.

We assume that the surface type index **M** is equal to 3 (partially snow – covered ground scene) in case *f* is below than 0.99. The value of **M** is equal to 1 for clean 100% snow-covered ground scenes ( *f* is larger than 0.99 and spherical albedo at 400nm is above 0.98) and it is equal to 2 for polluted (*f* is larger than 0.99 and spherical albedo at 400nm is smaller than 0.98) 100% snow-covered ground scenes.

The retrievals for partially snow – covered pixels are performed in case the reflectance R(400nm) is smaller than 0.75. This THV can be adjusted depending on the requirement of users.

## Broadband albedo

The considerations discussed above make it possible to determine ( and , respectively) for each of the wavelength corresponding to OLCI channels and also beyond OLCI measurements interval. The derived spectral albedo can be used to integrate the planar and spherical broadband albedo (BBA) over any wavelength interval [:

|  |  |  |
| --- | --- | --- |
|  | , | (2.6.1) |
|  |  |  |

where is the incident solar flux at the snow surface, is plane (*p*) or spherical (*s*) albedo depending plane or spherical BBA. Currently, shortwave (), UV-visible () and near IR spherical/plane BBA are being retrieved but additional ranges may be added in the future depending on user demand. Broadband albedo are only weakly sensitive to the variation of . The spectrum of incident solar flux at the snow surface is therefore assumed to be identical in all pixels and is approximated by the following analytical equation:

|  |  |  |
| --- | --- | --- |
|  |  | (2.6.2) |

where 3.238e+1, -1.6014033e+5, 7.95953e+3, 11.71 , and 2.48. The coefficients have been derived using the code SBDART (Ricchiazzi et al., 1998) in the spectral range 330-2400 nm at the assumptions given in Table 2.3. It is assumed that at the wavelengths 300-330nm due to strong ozone absorption in this spectral range.

Table 2.3. Assumptions used in SBDART to derive the solar flux at the surface

|  |  |
| --- | --- |
| Parameter | Value |
| water vapor column | 2.085 g m-2 |
| ozone column | 0.35 atm-cm |
| tropospheric ozone | 0.0346 atm-cm |
| aerosol model | rural (Shettle and Fenn, 1979) |
| vertical optical depth of boundary layer at 550nm | 0.1 |
| altitude | 825 m a.s.l. |
| solar zenith angle | 60 degrees |
| snow albedo at the surface | calculated using spherical grains of 0.25 mm diameter |

To avoid numerical integration as shown in Eq. (2.6.1), we build functions of the wavelength that approximate the retrieved over three intervals:

1. Over 300-709 nm, we approximate spherical and planar albedo by a polynomial of the second order fitted to the retrieved 400 nm), 560 nm), and 709 nm).
2. Over 709-865 nm, we approximate spherical and planar albedo by a polynomial of the second order fitted to the retrieved 709 nm), 753 nm), and 865 nm).
3. Over 865-2400 nm, we approximate the spherical and planar albedo with an exponential function fitted to the retrieved 865 nm), and 1020nm).

These assumptions make it possible to derive the value of BBA analytically.

First, for all three intervals, the denominator of Eq. (2.6.1) can be calculated as:

|  |  |  |
| --- | --- | --- |
|  | , | (2.6.3) |

Over the intervals , either equal to 300-709 nm or 709-865 nm, the spherical albedo can be expressed using its polynomial approximation:

|  |  |  |
| --- | --- | --- |
|  |  | (2.6.4) |

where *a, b* and *c* take different values whether they are fitted to derived or . With this formulation of , the numerator in Eq. (2.6.1) can be expressed in the following form:

|  |  |  |
| --- | --- | --- |
|  | , | (2.6.5) |

where

|  |  |  |
| --- | --- | --- |
|  | , | (2.6.6) |

and

|  |  |  |
| --- | --- | --- |
|  |  | (2.6.7) |

For wavelengths in the 865-2400 nm range, we use the exponential approximation for :

|  |  |  |
| --- | --- | --- |
|  |  | (2.6.8) |

where and take different values whether they are fitted to derived or . The numerator in Eq. (2.6.1) can be expressed in the following form:

|  |  |  |
| --- | --- | --- |
|  |  | (2.6.9) |

The same procedure as discussed above can be also used for clean snow. However, in this particular case we use more simple equation for the shortwave plane broadband albedo as suggested by Kokhanovsky (2021b):

*a+b exp(),* (2.6.10)

where In the case of UV-visible BBA Eq. (2.6.10) is simplified:

*exp(),* (2.6.11)

where ε=7.86 The NIR BBA follows from Eq. (2.6.10) at *a*=0.2335, *b*=0.56, and The expression for the spherical albedo follows from Eq. (2.6.10), (2.6.11) at *u*=1 (Kokhanovsky, 2021b).

## Quality of retrievals

The quality of retrievals can be assessed making the intercomparison of the retrieved and measured OLCI spectra. The retrieved OLCI spectrum can be calculated as follows:

(2.7.1)

where is the atmospheric reflectance for the case of black underlying surface, is the atmospheric spherical albedo for the black underlying surface, is snow reflectance, is snow spherical albedo, is the gaseous transmittance calculated as discussed in Appendix 3, is total atmospheric transmittance. The functions are calculated using the radiative transfer theory for a given distribution of aerosol particles in atmosphere with account for multiple molecular light scattering effects. The analytical approximation for the calculation of these functions under assumption that the phase function of atmospheric aerosol can be modelled as double Henyey - Greenstein phase function in absence of light absorption by aerosol particles is given in Appendix 1. It follows for the snow reflectance

*()=* (2.7.2)

where

*exp* (2.7.3)

is the snow spherical albedo. The parameters (*L*, ) are retrieved using measurements at 400, 490, 865 and 1020nm as explained above.

The quality of retrievals is assessed from the analysis of the values of the root-mean-square difefrence (RMSD) of the OLCI spectral reflectance determination:

, (2.7.4)

where *N* is the either number of all OLCI channels (*N*=21) or the number of selected OLCI channels almost free of gaseous absorption (*N*=16, all OLCI channels except 3 channels at oxygen A-band and 2 channels at water vapor band, see Table 1.1). The parameters and and (in percent) are reported in the output of the retrieval routine. Here is the average OLCI reflectance at 16 (21 channels). The output is provided if *.*EGD, which enhances the cloud mask routine. We also derive the total ozone column (TOC) using OLCI observations as described by Kokhanovsky et a. (2020b). If the retrieved TOC differs from that provided in OLCI files by more than 12%, the output of snow parameters is not provided (the contamination of pixel by clouds is supposed). The threshold values of corresponding parameters can be changed, if needed.

## Examples of retrievals

* + 1. **Antarctica**

We have applied the algorithm to the OLCI/S-3B data for the selected area in Antarctica (81-82S, 120-130E, January 31, 2020, 22:26UTC). The results of the application of the algorithm are shown in Fig.2.8.1. The statistical distributions of the derived parameters are shown in Fig. 2.8.2. The average values of the retrieved parameters for valid retrievals are given in Table 2.4. As expected for the interior of the Antarctic ice sheet, no snow pollution has been found using the algorithm applied. The valid retrievals are selected using the threshold values of the difference between measured and simulated OLCI spectra (for 16 channels almost free of oxygen and water vapor absorption), the difference Δ between the retrieved total ozone columns and those provided in OLCI files and assuming that EGD>0.14. They are specified in Table 2.5. Unfortunately, we can not validate the results given in this section using ground observations. However, it is known that the effective diameter of grains is almost uniformly in the range 0.2-0.4 mm in the interior of ice sheet in Antarctica (Gay et al., 2002). Our results (see Table 2.4 and Fig. 2.8.2a) confirm the conclusions of Gay et al. (2002) study. It has been found that the coefficient of variance of EGD is around 13% for the huge area studied (more than 100km along latitude and longitude). The average snow specific area is around 22 . It corresponds to the case of aged snow (without distinct ice crystals) according to the classification of Domine et al. (2007). Such type of snow is to be common in the interior of the Antarctic ice sheet. Pirrazzini (2004) reports the values of BBA equal to 0.8 at Concordia (approximately 75S, 123E) on January 26-29, 1997 and Kuipers Munneke et al. (2008, 2009) report BBA equal to 0.81 at 75S and 0E ( Amundsenisen station at the East Antarctic Plateau) which is close to the value 0.8114 (see Table 2.4) reported by us. Therefore, one can see that our findings are in accordance with previous research based on ground observations.

Table 2.4. The average values of the retrieved parameters (the values in brackets correspond to the results of the previous version of the algorithm (Kokhanovsky et al., 2020) for the same area)

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | Average | Standard deviation | Coefficient of variance, percent |
| EGD, mm | 0.3060 (0.3597) | 0.04 (0.06) | 13.1 (16.7) |
| SSA, | 21.75(18.78) | 2.82(4.1) | 13.0 (21.8) |
| BBA | 0.8114(0.8394) | 0.0047(0.02) | 0.6 (2.4) |

Table 2.5. The threshold values for valid retrievals

|  |  |
| --- | --- |
| Parameter | THV |
| Σ, % | <5 |
| Δ, % | <12 |
| EGD, mm | >0.14 |

1. b)

Chart

Description automatically generatedChart

Description automatically generated

c)

Chart

Description automatically generated

Fig.2.8.1 Retrieved spatial distributions of EGD (mm) (a), SSA() (b), and BBA (c) in the range 81-82S, 120-130E (January 31, 2020, 22:26UTC) using OLCI/S-3B observations over Eastern Antarctica. The blue color in the left upper part of the panel (c) is the artifact of the retrievals due to the presence Dome C station. Similar features are seen in panels (a), (b).

![Chart

Description automatically generated](data:image/png;base64,iVBORw0KGgoAAAANSUhEUgAABnIAAAT6CAMAAABWGg2qAAADAFBMVEUAAACAAAAAgACAgAAAAICAAIAAgIDAwMDA3MCmyvBAIABgIACAIACgIADAIADgIAAAQAAgQABAQABgQACAQACgQADAQADgQAAAYAAgYABAYABgYACAYACgYADAYADgYAAAgAAggABAgABggACAgACggADAgADggAAAoAAgoABAoABgoACAoACgoADAoADgoAAAwAAgwABAwABgwACAwACgwADAwADgwAAA4AAg4ABA4ABg4ACA4ACg4ADA4ADg4AAAAEAgAEBAAEBgAECAAECgAEDAAEDgAEAAIEAgIEBAIEBgIECAIECgIEDAIEDgIEAAQEAgQEBAQEBgQECAQECgQEDAQEDgQEAAYEAgYEBAYEBgYECAYECgYEDAYEDgYEAAgEAggEBAgEBggECAgECggEDAgEDggEAAoEAgoEBAoEBgoECAoECgoEDAoEDgoEAAwEAgwEBAwEBgwECAwECgwEDAwEDgwEAA4EAg4EBA4EBg4ECA4ECg4EDA4EDg4EAAAIAgAIBAAIBgAICAAICgAIDAAIDgAIAAIIAgIIBAIIBgIICAIICgIIDAIIDgIIAAQIAgQIBAQIBgQICAQICgQIDAQIDgQIAAYIAgYIBAYIBgYICAYICgYIDAYIDgYIAAgIAggIBAgIBggICAgICggIDAgIDggIAAoIAgoIBAoIBgoICAoICgoIDAoIDgoIAAwIAgwIBAwIBgwICAwICgwIDAwIDgwIAA4IAg4IBA4IBg4ICA4ICg4IDA4IDg4IAAAMAgAMBAAMBgAMCAAMCgAMDAAMDgAMAAIMAgIMBAIMBgIMCAIMCgIMDAIMDgIMAAQMAgQMBAQMBgQMCAQMCgQMDAQMDgQMAAYMAgYMBAYMBgYMCAYMCgYMDAYMDgYMAAgMAggMBAgMBggMCAgMCggMDAgMDggMAAoMAgoMBAoMBgoMCAoMCgoMDAoMDgoMAAwMAgwMBAwMBgwMCAwMCgwMD/+/CgoKSAgID/AAAA/wD//wAAAP//AP8A//////9Y0jREAAAAAWJLR0T/pQfyxQAAAAlwSFlzAAAXEQAAFxEByibzPwAAIABJREFUeNrt3UFu4nyawGFHilSBZUXZchakuUAptZtWcoTmKujrzSitOcJUr6a95BpRjpDSdC9QvGqJwQaDjcE4xKb/hue3GFU5fBmaeut9ykBMtFhIknSOIg+BJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnIkSQJOZIk5EiShBxJEnIkSciRJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnIkSQJOZIk5EiShBxJEnIkSciRJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnIkSQJOZIk5EiShBxJEnIkSciRJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnIkSQJOZIk5EiShBxJEnIkSciRJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnIkSQJOZIk5EiShBxJEnIkSciRJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnIkSQJOZIk5EiShBxJEnIkSciRJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnIkSQJOZIk5EiShBxJEnIkSciRJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnIkSQJOZIk5EiShBxJEnIkSciRJAk5kiTkSJKEHEkSciRJyJEkCTmSJORIkoQcSRJyJEnICbTkJppvf/PrMYqi8cugcIPZ03DnUPVIsxtJkq6bnFG0ISd5jvJeFpVjbwePNLuRJOnKyZlEG3KSh2jbdLARKe/10JFmN5IkXTc5qTg5OZNcmrv7jRTx+lh2aL7/SLMbSZKumpz1018rE5Kb0mnLeFA6liwPTfceaXYjSdJVkxPfRwVyZsPoNn+xPzXjfXW2kh9LD833HWl2I0nSFZOTvXQznj/kJEyKL7uMVr8ZFY6tvl490uxGkqRrJucmfb0ledh7FrKCovTFOH2KrHqk2Y0kSddNzvRjB4xF8SznPVNpvPnBmuyJt+qRZjeSJF01Od+y/7uXnPXREhcZJNUjzW4kSbpmckq47LR+/b/0pFh2y+qRZjeSJCFnrwiFN6whR5KQ0yE56bHpAjmShJyuyUnyHwRFjiQhp1Ny0iPjzZVskCNJyOmKnII4XZITSVKnIacH5Mzuo+2bmrt7k7S/DZKgc/XkLLU4xEWrPwrq74Ik5Fw7OdmHDhz4YqsXvPF3QRJyrpyc9BNzSp/iubruzeaLr/uONLtRlZwO/xC6nbRuv32Pv7sHxgNzRY87cr5OTnqO8176amcfXoAcm9UD47sj56rJSV/Hed/5aumz1lJGqkea3Qg5NqsHxndHDnI25KS/qjwFln849WzzidLVI81uhByb1QPjuyMHObkJ8c4Lb6uTk9H2wNqj6pFmN0KOzeqB8d2Rg5wVOdmHhFbJSZ7z3+fvK6geaXYj5NisHhjfHTnIWZNzs5ecxWL2NIyi8UvhBZnqkWY3Qo7N6oHx3ZFz1eT8ux4n5NisHhjkIAc5yLFAPDDuOnKQgxz3/Zrvu7vuviMHOQbZfXfXTYz7jhzD4L7b2+66+44cGWT33V1339135BgG991dd9fdd+Qgx323t9119x05yDHI7ru7bmLcd+QYBvfd3nbX3XfkyCC77+66++6+I8cwSLJlkGMYJMmWQY5hkGTLIMcwSLJlkCPkSLJlkGMYJNkyyDEMkmTLIMcwSLJlkGMYJNkyyBFyJNkyyDEMkmwZ5BgGSbJlkGMYJNkyyDEMkmwZ5Ag5kmwZ5BgGSbYMcgyDJNkyyDEMkmwZ5BgGSbYMcgwDciTZMsgxDJJsGeQYBkmyZZBjGCTZMsgxDJJsGeQYBo+UJFsGOYZBki2DHMMgSbYMcgyDJFsGOYZBki2DHMPgQZBkyyDHMEiyZZBjGCTJlkGOYZBkyyDHMEiyZZBjGCTJlkGOYZBkyyDHMEiSLYMcwyDJlkGOYZBkyyDHMEiSLYMcwyDJlkGOYZAkWwY5hkGSLYMcwyDJlkGOYZAkWwY5hkGSLYMcwyBJtgxyDIMkWwY5hkGSLYMcwyBJtgxyDIMkWwY5hkGSbBnkGAZJtgxyDIMkWwY5Vz0MqzwUkjpaL8hRZSY8YpJsF+QYCkm2C3IMhSTZLsj5zFB4ECTZMsgxDJJsGeQYBkmyZZBjGCTZMsgxDJJsGeQYBkmyZZBjGCTZMsgxDJJkyyDHMEiyZZBjGCTZMsgxDJJkyyDHMEiyZZBjGCTJlkGOYZBkyyDHMEiyZZBjGCTJlkGOYZBkyyDHMEiSLYMcwyDJlkGOYZBkyyDHMEiSLYMcwyDJlkGOYZAkWwY5hkGSLYMcwyDJlkGOYZAkWwY5hkGSLYMcwyBJtgxyDIMkWwY5hkGSLYMcwyBJtgxyDIMkWwY5hkGSbBnkGAZJtgxyDIMkWwY5hkGSbBnkGAZJtgxyDIMk2TLIMQySbBnkGAZJtgxyDIMk2TLIMQySbBnkGAZJsmWQYxgk2TLIMQySbBnkGAZJsmWQYxgk2TLIMQySZMsgxzBIsmWQYxgk2TLIMQySZMsgxzBIsmWQYxgkyZaxSA2DJFsGOYZBki2DHMMgSbYMcgyDJFsGOYZBkpDTu3uc3ETz7e9mT8MoGr8MFnWHTr0RciQh57rJGUVbcpLnaN3b4UOn3gg5kpBz5eRMogI5o2jT68FDp94IOZKQc93kpOJsyImXv54OFou7+83B6qFTb4QcSci5anLWT3+tTUhu8lOSZHmSMt1/6NQbIUcScq6anPg+KpKzPDW5HWz1me89dOqNkKOD/atZHighp8fkJA/LP5Hx/GFDwqjwustk9evqoVNvhBx9URzmCDm9Jucmfb0l2ZCz/dXqzGW679CpN0KOvkyOR0rI6TU5048iGEuCxpufopkN06fGqodOvRFyVENOe7eSkBMqOd/K5zYlG1ZqVA+deiPkCDlCzjWTsxbhofBW5+nO4eqhU2+EHCFHyEEOcoQcIQc5yBFykCPkIAc5Qo6Qg5xekVPO3w/kIEdfNubq9gpyTiQHOshBjloWBzkhk3PuN0kjR8gRcq6WnHP/KChyhBwh53rJccEbIUcXRRByAiYnvRjne354e8XOnUOn3gg5Qo6Qg5wHH14g5Ag5yDk3OeUPVsvMqB469UbIEXKEHOQUXneZrD8+erb9+OjqoVNvhBwhR8hBTsGE0fadHq8HD516I+QIOUIOcrbkJM+5E2+HD516I+QIOUIOcorPfM2ehlE0fim++lI9dOqNkCPkCDlXTY5hEHJkyyDHMAg5yJEtgxzDIOTIlkGOYRByJOQIOUKObBnkGAYhR7YMcgyDkIMc2TLIMQxCjmwZ5BgGIUdCjpAj5MiWQY5hEHJkyyDHMAg5yJEtgxzDIOTIlkGOYRByJOQIOUKObBnkGAYhR7YMcgyDkIMc2TLIMQxCjmwZ5BgGIUdCjpAj5MiWQY5hEHJkyyDHMAg5yJEtgxzDIOTIlkGOYRByJOQIOUKObBnkGAYhR7YMcgyDkIMc2TLIMQxCjmwZ5BgGIUdCjpAj5MiWQY5hEHJkyyDHMAg5yJEtgxzDIOTIlkGOYRByJOQIOUKObBnkGAYhR7YMcgyDkIMc2TLIMQxCjmwZ5BgGIUe2DHKEHCFHtgxyDIOQI1sGOYZByEGObBnkGAYhR7YMcgyDkCNbBjlCjpAjWwY5hkHIkS2DHMMg5CBHtgxyDIOQI1sGOYZByJEtgxwhR8iRLYMcwyDkyJZBjmEQcpAjWwY5hkHIkS2DHMMg5MiWQY6QI+TIlkGOYRByZMsgxzAIOciRLYMcwyDkyJZBjmEQcmTLIEfIEXJkyyDHMAg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![Chart, histogram

Description automatically 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![Chart, histogram

Description automatically 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Fig.2.8.2 Statistical distributions of retrieved parameters

* + 1. **Greenland**

We also retrieved snow properties using old and new versions of the SICE software over Greenland for July 27 (day 210) 2019. The pixels have been selected in random way in the region 27-67W, 62-80N. The comparisons between retrievals have been performed only for the grain diameters in the range 0.2-0.6mm. Lower values of EGD could be due to the contamination of pixels by clouds. Larger values could be due to 3-D effects/glitter. The differences in the retrieved values of EGD, SSA, and BBA are presented in Fig. 2.8.3 as the function of the longitude. It follows from Fig. 2.8.3, 2.8.4 and also from data presented in Table 2.6 that the derived value of EGD and BBA are reduced (by 16 and 3%, respectively). The value of SSA is larger by 17.5% as compared to the previous version. These differences are due to update in the coefficient of the transformation from EAL to EGD and also due to update of the equation for the BBA.

![Chart, scatter chart

Description automatically 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LDSIH3qh10WP1M8vF4IP37M37JKdYahA58EbVycYfXqpLINfnuc0DSk7/eksNIgfebBx+CeT4OxwFG7twE5EDfz2dCyMDxu7H367+gksNIge+Q+Z8Sq7E/2KpQeTAkMP35/V1o/dfLTWIHABEDgCIHABEDgCIHABEDgAiBwBEDgAiBwBEDgAiBwCRAwAiBwCRAwAiBwCRA4DIAQCRA4DIAQCRA4DIAUDkAIDIAUDkAIDIAUDkACByAEDkACByAEDkACByABA5ACByABA5ACByABA5AIgcABA5AIgcABA5AIgcAEQOAIgcAEQOAIgcAEQOACIHAEQOACIHAEQOACIHAJEDACIHAJEDACIHAJEDgMgBAJEDgMgBAJEDgMgBQOQAgMgBQOQAgMgBQOQAIHIAQOQAIHIAEDn+BACIHABEDgCIHABEDgAiBwBEDgAiBwBEDgAiBwCRAwAiBwCRAwDH+j+P27tcsYC+RAAAAABJRU5ErkJggg==)

Fig.2.8.3. The differences in the retrieved values of EGD, SSA and BBA (in percent) between two versions of the code.

Table 2.6. The average values of the retrieved parameters according to new and old versions of the algorithm

|  |  |  |  |
| --- | --- | --- | --- |
| Parameter | New version | Old version | Relative difference, % |
| EGD, mm | 0.3307 | 0.3953 | -16.1 |
| SSA, | 20.95 | 17.55 | 17.5 |
| BBA | 0.7932 | 0.8117 | -2.9 |

![Chart, scatter chart

Description automatically 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Fig.2.8.4 The correlation between new and old values of the retrieved EGD. The coefficient of correlation is 0.9221 and the linear correlation equation can be presented as follows: *y=0.74x+0.04.*

The retrieval results of main parameters (BBA, SSA, EGD) in the vicinity of the EGP site on August 2, 2019 are shown in Fig. 2.8.5 It follows that all parameters are within expected range of variability. The coefficient of variance (CV) of retrieved and measured TOA reflectance (for channels not affected by gaseous absorption) is given in Fig. 2.8.6. It follows that the CV is below 5%, which shows that our retrievals make it possible to predict not only BOA but also TOA reflectance.

The difference between retrieved total ozone column and that provided in OLCI files is given in Fig. 2.8.7. The areas with large differences of both TOC datasets could be due to the presence of clouds or violations of assumptions used in the algorithm. Therefore, these differences can be also used in post - processing.

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Fig. 2.8.5 The retrieval of snow parameters in the vicinity of the EGP site.

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Fig. 2.8.6 The coefficient of variance of the retrieved TOA reflectance as compared to that measured by OLCI ( for free of gaseous absorption channels) for the case shown in Fig. 2.7.5.

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Fig.2.8.7 The relative difference of the retrieved total ozone column and total ozone column provided in OLCI files.

## The validation of the algorithm for snow and ice albedo

***Broadband albedo***

In this section we describe the validation of the algorithm for the broadband albedo retrieval using OLCI comparing the retrieval results with local BBA measurements in the framework of the Programme for Monitoring of the Greenland Ice Sheet (PROMICE) (Fausto et al., 2021). The locations of PROMICE stations are given in Fig. 2.9.1.

Horizontally levelled up- and down-facing Kipp & Zonen CNR1 or CNR4 pyranometers record incoming and upcoming solar radiation (in W m−2). These data are used to calculate the short wave broadband albedo. The measurement height is at the sensor boom level of 2.7 m over the ice surface. Short-wave radiation is measured by the pyranometers within plastic meniscus domes, allowing minimal water droplet adhesion. The manufacturer reports that sensor uncertainty is 10 %. In practice, this sensor uncertainty has been found to be 5 % for daily totals in Antarctica ([van den Broeke et al.](https://essd.copernicus.org/articles/13/3819/2021/#bib1.bibx43), [2004](https://essd.copernicus.org/articles/13/3819/2021/#bib1.bibx43)). Short-wave radiation measurements are corrected for sensor tilt following [van As et al.](https://essd.copernicus.org/articles/13/3819/2021/#bib1.bibx37) ([2011](https://essd.copernicus.org/articles/13/3819/2021/#bib1.bibx37)) in post-processing.

The intercomparison of the broadband albedo measured by ground-based instrumentation and derived from OLCI measurements is shown in Fig. 2.9.2-2.9.4. The measurements have been collocated both in space and time domains. We also show the results derived from MODIS and also from the previous version of the algorithm. Only cloud free cases (PROMICE cloud index below 0.33) have been used in the comparisons. One can see that OLCI provides more stable values of BBA as compared to MODIS. The differences of PROMICE and new algorithm BBA values are generally smaller as compared to the MODIS BBA values and also ones derived from the previous version of the algorithm (see Table 2.7 and also Fig. 2.9.5). The average bias of OLCI BBA retrievals and PROMICE ground observations is smaller than 0.05 for the most of cases studied with smaller biases for clean snow surfaces. This difference can occur not only due to experimental errors of ground - based and satellite instruments but also due to the assumptions used in the process of the retrieval and scene inhomogeneity (300m OLCI measurements versus point PROMICE pyranometer measurements). The presence of instrument itself may also lead to some decrease of ground-measured BBA. Overall, the absolute accuracy of satellite retrievals is good. The differences between ground – based and OLCI retrievals are inside of the interval of accuracy required for climate models (0.02-0.05) (Dickinson, 1983; Henderson-Sellers et al., 1983; Sellers et al., 1995) on a global scale. A smaller uncertainty of is required for regional climate simulations (Dickinson, 1995). Such an uncertainty is difficult to achieve taking into account typical experimental errors of measurements and processing software. Nevertheless, an accuracy better than is achieved for almost all cases specified in Table 2.8 for OLCI BBA retrievals using new version of the code (without account for OLCI gains).

The sites EGP and KAN\_U are located far from the ocean (see Fig. 2.9.1) and characterized by quite large value of average surface albedo (0.8) as derived from different types of measurements (see Fig.2.9.2, 2.9.3). The elevation of the KAN\_U site is 1.84km. The EGP PROMICE station is located even at a higher level (2.66km).

We show the absolute BBA differences (satellite – ground) for the three PROMICE sites in Fig.2.9.4. We conclude that temporal changes of surface albedo are less pronounced for the EGP site. This is due to its higher location, larger distance to the ocean as compared to the other sites and also due considerable difference in latitude (about 9 degrees difference with EGP being more to the North, see Fig.2.9.1). Interestingly, PROMICE data provide almost the same BBA (0.8) for the EGP and KAN-U sites. Peng et al. (2018) have found that PROMICE data is biased low as compared to VIIRS satellite albedo retrievals. We have arrived to the same conclusion as far as OLCI retrievals are of concern for retrievals over EGP site. KAN-U and SCO-U BBA biases could be both positive and negative.

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Fig.2.9.1 Map of Greenland showing the PROMICE weather station locations (Gausto et al., 2021).

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Fig. 2.9.2. The intercomparison of BBA measured on ground (PROMICE EGP) and derived using the present algorithm (SICE-3) for different years (upper panel – 2018, lower panel-2019). The values of the broadband albedo derived from MODIS observations and previous version of the algorithm (SICE-old) are also shown.

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Fig. 2.9.3. The intercomparison of BBA measured on ground (PROMICE SCO U) and derived using the present algorithm (SICE-3) for different years ( upper panel – 2018, lower panel-2019). The values of the broadband albedo derived from MODIS observations and previous version of the algorithm (SICE-old) are also shown.

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Fig. 2.9.4. The intercomparison of BBA measured on ground (PROMICE KAN U) and derived using the present algorithm (SICE-3) for different years ( upper panel – 2017, lower panel-2018). The values of the broadband albedo derived from MODIS observations and previous version of the algorithm (SICE-old) are also shown.

The intercomparison of satellite and ground BBA measurements for the SCO\_U site (elevation 0.67km) with smaller yearly average ground albedo (0.5-0.6) is shown in Fig. 2.9.3. During winter time the site is covered by snow and BBA is close to 0.8. The melt season starts early June at this site, which is well captured by both satellite and ground measurements. The lowest values of BBA (0.3-0.4) are reached in July with further increase in September due to the drop of temperatures and subsequent snowfall events. As seen from Fig. 2.9.3 and also from Fig. 2.9.5, the largest disagreement between satellite and ground measurements occur during melting season, when the scene is very heterogeneous and may contain ice/snow, water ponds, crevassing, supraglacial water, cryoconite, algae and bare ground in various proportions. One can see that the new version of the SICE algorithm provides more accurate results for a darker ground as compared to the previous versions with the average biases below 0.02 for years 2017-2019 (0.08 for the previous version of the algorithm). Also biases are smaller as compared to the MODIS BBA retrievals (0.05). Such an accuracy is sufficient for running global climate models and agrees with requirements for other satellite missions with respect to the snow BBA determination (e.g., Joint Polar Satellite System requirement (Peng et al., 2018)).

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Fig. 2.9.5a The absolute BBA differences (satellite – ground) derived using the present/old OLCI algorithm and MODIS for zears 2018, 2019 at EGP PROMICE site.

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Fig. 2.9.5b The absolute BBA differences (satellite – ground) derived using the present/old OLCI algorithm and MODIS for years 2017, 2018 at KAN -U PROMICE site.

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Fig. 2.9.5b. The absolute BBA differences (satellite – ground) derived using the present/old OLCI algorithm and MODIS for years 2018, 2019 at SCO-U PROMICE site.

Table 2.7. Statistical data ( yearly average BBA: 1- PROMICE, 2- current algorithm, 3- previous version of the algorithm, 4- MODIS retrievals; yearly average relative difference (RD) between satellite and PROMICE BBA: 5- current algorithm, 6- previous version of the algorithm, 7- MODIS retrievals; yearly average absolute difference (AD) between satellite and PROMICE BBA: 8- current algorithm, 9- previous version of the algorithm, 10- MODIS retrievals) for 2017, 2018, and 2019 at three PROMICE stations (EGP, SCOU-U, KAN-U). N gives the number of collocated measurements by PROMICE, OLCI/S-3 and MODIS/Terra/Aqua (free of clouds).

Year N  **BBA** **RD, % AD**

**1 2 3 4** **5 6 7** **8 9 10**

EGP

2017 119 0.7825 0.7904 0.8274 0.8363 0.1174E+01 0.5943E+01 0.7045E+01 0.7909E-02 0.4494E-01 0.5382E-01

2018 35 0.7897 0.7925 0.8323 0.8489 0.1260E+00 0.5398E+01 0.7504E+01 0.2747E-02 0.4254E-01 0.5920E-01

2019 48 0.7900 0.7930 0.8304 0.8523 -0.6470E+00 0.5127E+01 0.7878E+01 0.3058E-02 0.4033E-01 0.6227E-01

SCO-U

2017 88 0.5149 0.5311 0.5824 0.5415 0.2764E+01 0.1370E+02 0.5267E+01 0.1628E-01 0.6751E-01 0.2661E-01

2018 55 0.6137 0.6182 0.6905 0.6594 0.1260E+00 0.1304E+02 0.8082E+01 0.4428E-02 0.7676E-01 0.4567E-01

2019 69 0.6047 0.5982 0.6406 0.6197 -0.6470E-00 0.6716E+01 0.1272E+01 -0.6547E-02 0.3586E-01 0.1501E-01

KAN-U

2017 63 0.7795 0.7689 0.8080 0.8019 -0.1169E+01 0.3863E+01 0.2918E+01 -0.1059E-02 0.2849E-01 0.2240E-01

2018 25 0.7866 0.7809 0.8230 0.8312 -0.6212E-04 0.4730E+01 0.5798E+01 -0.5655E-02 0.3644E-01 0.4464E-01

2019 42 0.8105 0.8105 0.7809 0.7631 -0.4686E+01 -0.1612E+01 -0.4204E+01 -0.5734E-01 -0.2964E-01 -0.4745E-01

***The spectral albedo***

We have compared the spectral albedo retrieved using the algorithm described above with ground albedo measurements in the vicinity of DOME C in Antarctica (69.3762S, 139.0162E) on December 25, 2016. A good correspondence of measured and retrieved albedo has been found (see Fig. 2.9.6). The satellite measurements have been performed at the solar zenith angle 61.5 degrees. However, ground measurements have been performed at the SZA equal to 64.8 degrees. Therefore, the satellite - retrieved snow plane albedo has been corrected for this small difference in SZA using the following equation, which follows from Eq. (2.5.8):

*=* (2.8.1)

Here, is the cosine of SZA at the time of satellite measurements and is the same parameter except at the time of ground measurements. The retrieved EGD for this case is 0.36mm and BBA is equal to 0.8. Both parameters are characteristic for clean snow surfaces in the vicinity of DOME C station in Antarctica.

The second example of the intercomparison of satellite and ground – based retrievals of the snow plane albedo using developed software is shown in Fig. 2.9.7 for the case of dust – loaded snow at Col du Lautaret site in French Alps (45° 2′ 4″ N, 6° 24′ 18″ E). The measurements have been performed on April 17, 2018 at SZA equal to 55.27 degrees. The snow pollution originated from the Sahara is clearly seen at the site at the moment of measurements (see Fig.2.9.8).

The ground measurements are corrected for the solar zenith angle (41.25 degrees) corresponding to the satellite measurements and also for the slope effects (3 degrees slope). The scircles and stars represent satellite measurements of snow plane albedo with OLCI S-3A gains applied/not applied ( see Appendix 3). One can see that the retrieved plane albedo (with and without gains) is close to the ground measured albedo with results including OLCI gains closer to the ground measurements. The difference can occur due to imperfect atmospheric correction (the aerosol optical thickness has been assumed to be equal to 0.07, which is a realistic assumption for the elevation of the site (2km) and Angström exponent has assumed to be equal 1.3) and also due to the scene inhomogeneity both with respect to the snow grain size and pollution load (see Fig. 2.9.8).

The albedo of polluted snow decreases with decrease of the wavelength in the spectral range 400-600nm as seen in Fig. 2.9.7. This decrease can be attributed to various pollutants present in snowpack. The parameters of pollutants and snow retrieved by us for the case shown in Fig. 2.9.7 are listed in the first two lines (derived with and without OLCI gains) of Table 2.8. The last line contains the parameters derived using ground measurements (one month later) in Italian Alps. One can see that the retrieved parameters are similar. This points out to the same aerosol source location (Sahara as suggested by Dumont et al. (2017) and Di Mauro et al. (2019)). The spectral dust mass absorption coefficient derived by us from spaceborne observations of polluted snow is given in the first two lines of Table 2.9. One can see that our data are consistent with those reported by Caponi et al. (2017). In particular, we derived that the absorption Angström exponent in the range 2.2-3, which is close to the value of 2.9 suggested by Caponi et al. (2017) for the dust from Sahara.

Table 2.8. The retrieved snow and pollutants parameters at two dates and two locations in European Alps. The results derived for French Alps have been obtained using spaceborne observations. The results for Italian Alps (Kokhanovsky et al., 2021b) have been derived from ground – based spectral albedo observations. The retrievals with the gains applied are given in brackets.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Date | Location | *m* | *γ, 1/mm* | *L,mm* | , 1/mm | *d, mm* | , ppm | , μm |
| 17.04.2018 | Col du Lautaret  (French Alps) | 3.04  (2.16) | 1.53e-4  (3.74e-4) | 17.5  (23.9) | 9.61  (8.96) | 1.1  (1.5) | 82.6  (217.0) | 11.5  (18.1) |
| 17.05.2018 | Torgnon (Italian Alps) | 2.5 |  | 25.6 | 9.11 | 1.6 | 77.4 | 15.2 |

Table 2.9. The retrieved spectral mass absorption coefficient (MAC) of dust (first line – no gains, second line – with gains applied). The last line corresponds to the measurements provided by Denjean et al. (2016) and also Caponi et al. (2017). The underlined numbers on the last raw are derived using the data for the MAC at 428nm and the absorption Angström exponent for the Saharan dust equal to 2.9 provided in Table 5 of the Caponi et al. (2017) paper.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Wavelength, nm | 428 | 532 | 660 | 850 | 1000 |
| MAC, | 47.7  (21.1) | 24.6  (13.2) | 12.8  (8.3) | 5.9  (4.8) | 3.6  (3.4) |
| MAC, (*Caponi et al., 2017*) | 37 | 20 | 11 | 5 | 3 |

![Chart

Description automatically 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Fig. 2.9.6 The intercomparison of satellite ( symbols) and ground – based (line) plane albedo measured at Dome C ( Antarctica) on December 25, 2016 ( courtesy of M. Lamare and G. Picard).

Chart, scatter chart

Description automatically generated

Fig. 2.9.7 The plane albedo measured at the Col du Lautaret site in French Alps on April 17, 2018 (crosses, only results for OLCI channels are shown). The ground measurements are corrected for the solar zenith angle (41.25 degrees) at the satellite overpass and also for the slope effects (3 degrees slope). The other symbols represent satellite measurements of snow plane albedo with OLCI S-3A gains applied/not applied.



Fig. 2.9.8. The Solalb light collector shown over a polluted snowpack at Col du Lautaret, French Alps (Kokhanovsky et al., 2019)

### Appendix 1. Atmospheric radiative transfer

The top-of atmosphere (TOA) reflectance over a Lambertian surface with albedo can be presented in the following way:

(A.1)

Here, is the top of atmosphere (TOA) reflectance, albedo, and total transmittance (Kokhanovsky et al., 2005), respectively, for the artificial atmosphere without gaseous absorbers, is the gaseous transmittance. The snow is close to the Lambertian surface in the visible. However, there are differences. Therefore, to account for the non-Lambertian effects we substitute the snow albedo in the nominator of Eq. (A.1) by the snow spectral reflectance .

The value of can be presented in the following way using the Sobolev approximation (Sobolev, 1975):

(A.2)

where single scattering contribution

(A.3)

and multiple light scattering contribution is approximated as

(A.4)

where

,, (A.5)

,, (A.6)

(A.7)

Here, is the cosine of the solar zenith angle (SZA), is the cosine of the viewing zenith angle (VZA) , is the scattering angle defined as

, (A.8)

is the relative azimuthal angle (equal to 180 degrees minus OLCI relative azimuthal angle), is the sine of the SZA, is the sine of the VZA, is the atmospheric optical thickness, is the phase function, is the asymmetry parameter. The value of *g* is determined by the following expression:

. (A.9)

The approximate account for aerosol absorption effects is performed multiplying (see Eq. (A.3) by the single scattering albedo The accuracy of Eqs. (A1)-(A3) can be further improved using the truncation approximation as discussed in (Katsev et al., 2012).

The transmission function is approximated as follows:

, (A.10)

where the value of is calculated using the following approximation (Katsev et al., 2012):

. (A.11)

Here,

(A.12)

is the so – called backscattering fraction.

The atmospheric spherical albedo is found using the approximation proposed by Sobolev. Namely, he gives the following expression for the atmospheric plane albedo

, (A.13)

where

. (A.14)

The spherical atmospheric albedo is defined as

. (A.15)

The substitution of Eq. (A.13) to Eq. (A.15) gives after integration:

, (A.16)

where

 (A.17)

and

 (A.18)

is the exponential integral. The exponential integral has the following properties:

, (A.19)

 (A.20)

where is the Euler’s constant. Therefore, one can see that  as 𝜏 as it should be for nonabsorbing case considered here. Also, taking into account that  as 𝜏0 we have: 0 and  as 𝜏0 as it should be at small values of optical thickness. One can use the following approximations for the exponential integral (Abramowitz and Stegun, 1964):

, (A.21a)

, (A.21b)

where

. (A.21c)

The vectors ***b****,* ***q****,* ***s*** have the following components:

***b***=(-0.57721566,0.99999193,-0.24991055,0.05519968,-0.00976004,0.00107857),

***s***=(0.250621, 2.334733,1.0), ***q***=(1.681534, 3.330657,1.0). (A.21d)

The atmospheric optical thickness is smaller than 0.3-0.5 for polar atmospheres and we use the following approximation for the function  in the nominator of Eq. (A.16) in this work:

. (A.21e)

The reflection function and atmospheric spherical albedo depends on the atmospheric optical thickness, which can be presented in the following form:

. (A.22)

The molecular optical thickness can be approximated as (Hansen and Travis, 1974; Iqbal, 1984):

, (A.23)

where the wavelength is in microns. The parameters (*q,* ) are subject to variations depending on the atmospheric state. We use as default values the following parameters at the normal pressure and temperature: . We derive the value of molecular optical thickness at another pressure level *p* using the following expression:  where , *p* is the site pressure, . The site pressure is calculated using the following equation: *z* is the height of the underlying surface provided in OLCI files. It is assumed that the scale height *H* is equal to *6km*. The correct value of can be derived from the information on the pressure profile at a given location ( e.g., from the ECMWF re-analysis).

We also have the following option for the parameters in Eq. (A.23): *q*=0.0053 and as suggested by Tomasi and Petkov (2005) for polar regions.

It follows for the aerosol optical thickness (AOT) ( Angström, 1929):

, (A.24)

where , the pair represents the Angström parameters. We did not make an attempt to derive the value of over snow. These values must be assumed ahead of retrievals ( e.g., using aerosol climatology (Kinne, 2019), ground measuremnets or aerosol forecasts) . The statistical results for the values over various Greenland AERONET stations are given by Kokhanovsky et al. (2020). It follows that over Greenland the value of is in the range 0.025-0.125. The AERONET monthly statistics shows that is in the the range 1.0-1.6 over Greenland (Kokhanovsky et al. (2020)). Therefore, we assume the value of

The phase function can be presented in the following form for nonabsorbing aerosol case:

, (A.25)

where

(A.26)

is the molecular scattering phase function and is the aerosol phase function.

The aerosol phase function can be presented in the following form:

, (A.27)

(A.28)

We shall assume that

(A.29)

It follows for the asymmetry parameter:

(A.30)

and, therefore,

. (A.31)

The parameter varies with the location, time, aerosol, type, etc. We shall assume that it can be approximated by the following equation:

. (A.32)

The coefficients in this equation (as derived from multiple year AERONET observations over Greenland (Kokhanovsky et al., 2020a)) are:

(A.33)

The parameter *c* can be found from Eq. (A.30):

. (A.34)

Let us derive the analytical approximation for the backscattering fruction B given by Eq. (A.12). The Henye-Greenstein phase function can be presented in the following form:

, (A.35)

where G is the asymmetry parameter and *x* is the cosine of the scattering angle. The integral

(A.36)

can be evaluated analytically:

, (A.37)

where *C* is the integration constant. It follows from Eqs. (A.12), (A.29) that the backward fraction is

. (A.38)

One can see that

(A.39)

as G

Also we can derive:

(A.40)

and

, (A.41)

where

### Appendix 2. The approximate equation for the reflectance of light from a semi – infinite snow layer

The reflectance for a non-absorbing surface can be approximated, as discussed by Kokhanovsky (2005), by the following expression:

|  |  |  |
| --- | --- | --- |
|  |  | (A2.1) |

where *A* = 1.247, *B* = 1.186, *C* = 5.157, and

|  |  |  |
| --- | --- | --- |
|  | . | (A2.2) |

Here θ is the scattering angle in degrees.

The value of can be used to calculate the snow bottom of atmosphere reflectance at any OLCI channel using the following approximation (Zege et al., 1991: Kokhanovsky and Zege, 2004; Kokhanovsky et al., 2007; Kokhanovsky, 2021):

*()= () ,* (A2.3)

where

*(*), (A2.4)

, (A2.5)

*exp* (A2.6)

where

A2.7)

is the probability of photon absorption (PPA) by an elementary volume of snowpack, *g* is the average cosine of scattering angle in snow. The value of *g* depends on the real part of ice refractive index and also on the shape of ice grains. It is close to ¾ for ice crystals in snow in the visible (Kokhanovsky, 2021). The dependence of *g* on the ratio of the size of ice grains to the wavelength can be neglected due to the fact that the ice grains are much larger as compared to the wavelength in the spectral range covered by OLCI. Also the spectral variation of the real part of ice refractive index and, therefore, the average cosine of scattering angle for OLCI channels can be neglected. The PPA can be calculated as follows

. (A2.8)

The extinction coefficient of snow can be calculated as

, A2.9)

where  is the average extinction cross section of particles,

 (A2.10)

is the number concentration of ice grains, is the volumetric concentration of ice grains and  is the average volume of ice grains. The density of snow  can be derived as:

, (A2.11)

where is the density of ice. The average extinction cross section of large ice grains is equal to the double value of its projected geometrical cross section  (Kokhanovsky, 2021). Therefore, one derives:

. (A2.12)

An important point is that the value of  does not depend on the wavelength and refractive index of particles. Therefore, one derives for the snow extinction coefficient:

, (A2.13)

where =/2 is the characteristic length. It is related to the characteristic extinction length  in snow by the following equation:

. (A2.14)

Due to low concentration of impurity particles and their small sizes, the influence of pollutants of the value of snow extinction coefficient can be neglected in most of cases. This is not the case for the absorption coefficient, which can be calculated as follows for polluted snow:

 (A2.15)

Here  is the absorption coefficient for ice grains and  is the absorption coefficient for impurity particles and external mixture of ice grains and pollutants have been assumed. Light absorption by ice grains at OLCI channels is e weak and, therefore, the average absorption cross section is proportional to the volume of ice particles:

. ( A2.16)

Therefore, absorption coefficient of ice grains = can be presented as

. ( A2.17)

where *B* is the shape factor. It depends on the shape of ice crystals but not on their size. Therefore, one derives for the value of PPA:

, ( A2.18)

where Λ=*B.* We shall assume that

, ( A2.19)

where is the volumetric concentration of pollutants, *q* is the Angström absorption exponent (AAE), and  is the volumetric absorption coefficient of pollutants at the wavelength :

. ( A2.20)

Taking into account that

 ( A2.21)

where  is the number concentration of impurity particles and  is the average absorption cross section of impurity particles, one derives:

, (A2.22)

where is the average volume of impurity particles. Therefore, one derives:

, (A2.23)

where

 (A2.24)

is the impurity load parameter,  is the relative volumetric concentration of impurities. The value of the relative impurity mass concentration is related to *c* by the following equation:

 (A2.25)

where =/,  is the density of impurity particles and is the ice density. Therefore, it follows for the impurity load parameter:

. (A2.26)

Finally, one derives:

, (A2.27)

where

= (A2.28)

is the effective absorption length (EAL).

One can see that the polluted snow spherical albedo, polluted snow plane albedo , and polluted snow reflection function in the spectral range covered by OLCI can be approximated using just three unknown parameters (γ, *q, L*). In the case of pure snow, just one parameter is needed (EAL). In the retrieval procedure one may assume that the value of , which is spectrally neutral constant, is not known as well. Then the use of approximate Eq. (A2.1) is avoided and there are four unknown constants (γ, *q,* , *L*).

The relative mass concentration of pollutants can be estimated using the retrieved value of γ (see Eq. (2.26)):

, (A2.29)

where

 . (A2.30)

This requires an assumption on the value of *B* and also the volumetric absorption impurity coefficient . We assume that the value of *B*=1.8 (Kokhanovsky and Zege, 2004). The volumetric absorption coefficient  depends on the type of impurities. It follows for the black carbon (Kokhanovsky et al., 2019):

, (A2.31).

where we assume that D=1.3, =0.47 (Kokhanovsky et al., 2019) and =1μm. Then it follows: =7.68. Assuming that the absorption Angström parameter is equal to 1, we derive at the wavelength 0.55 *:* . Introducing the mass absorption coefficient , where black carbon density =1.9g/, we derive:  , which is close to the value of =7.5 for black carbon impurities suggested by Bond et al., 2006 and Bond and Bergstrom (2006).

Then it follows:

 (A2.32)

for black carbon.

It is known that the value of *q* is close to one for BC particles, which are much smaller as compared to the wavelength (Bond et al., 2013). Therefore, we shall assume that snow is primarily polluted by BC particles, if the retrieved value of *q* is smaller than 1.2 (and larger than 0.9). Otherwise, the pollution of snow by dust particles is assumed. In the case of dust particles, the value of the mass absorption coefficient depends on the size/shape of particles and origin of dust (chemical composition) (Di Mauro et al., 2015, 1019, 2021; Dumont et al., 2017; Tuzet et al., 2017; Skiles et al., 2018; He and Flanner, 2020). In this work we use the estimation of as proposed by Kokhanovsky et al. (2021b) in the assumption of spherical shapes of particles. Namely it follows

, (A2.33)

, (A2.34)

where is presented in *1/mm* , . The effective diameter of dust particles

, (A2.35)

 is the average diameter of dust grains and  is the average cross section area, can be estimated from the value of *q* as well (Kokhanovsky et al., 2021):

 (A2.36)

where and is expressed in microns.

The effective snow grain diameter

 (A2.37)

is derived from the value of EAL. Namely, it follows:

 (A2.38)

where

. (A2.39)

Kokhanovsky (2006) has found that the value of the scaling constant ε=*B*/(1-g) is close to 9 on average for natural snow. We shall use the value of ε =9 in this study. Then it follows:

 (A2.40)

The derived value of is used to estimate the snow specific surface area  (Kokhanovsky, 2021):

 (A2.41)

where =6/.

### Appendix 3. Atmospheric gaseous transmittance

The gaseous transmittance is calculated as the product of the gaseous transmittance due to oxygen, ozone and water vapour:

. (A.3.1)

The contribution of other gases is neglected.

*Ozone transmittance function*

The ozone transmittance function is defined as

, (A.3.2)

|  |  |
| --- | --- |
|  |  |

where *m*= is the air mass factor derived in the geometrical approximation and is the ozone vertical optical depth (VOD) at the wavelength , defined as:

|  |  |  |
| --- | --- | --- |
|  |  | (A.3.3) |

Here is the ozone absorption cross-section at the height *z* and the wavelength is the number of ozone molecules at the height *z*. The ozone VOD depends on the vertical profiles of (z) and It is known that both temperature and pressure ( and, therefore, height) dependence of the ozone absorption cross section in the visible is weak and can be ignored. Then it follows:

|  |  |
| --- | --- |
|  | (A3.4) |

where

|  |  |
| --- | --- |
|  | (A3.5) |

is the total ozone column (TOC). We estimate TOC using OLCI measurements at 620nm:

(A.3.6)

where 3.9806 per molecule (Gorshelev et al., 2014; at 193K). Eq. (A3.6) can be also presented in the following form:

(A.3.7)

where *K*=9349.3 Dobson Units (DU) and we have accounted for the fact that 1DU=2.687. The ozone VOD at 620nm can be derived from Eq. (A3.2):

(A.3.8)

where the value of is derived from the ratio of OLCI reflectance at 620nm to the modelled OLCI reflectance at 620nm in absence of gaseous absorbers. Therefore, the ozone transmittance can be calculated as:

. (A.3.9)

Eq. (A.3.9) can be also presented in the following way:

, (A.3.10)

where is the reference ozone VOD derived at a reference total ozone(see Table A.1) and / .

We note that one should account for the instrument spectral response function because the measurements are performed not at a single wavelength but in narrow spectral range Therefore, the value of will differ for different instruments even if measured at the same central wavelength (see Figure A.1). The spectral ratio of the ozone VOD to its value at 620nm is given in Table A.3.2, where we also show the spectral calibration coefficients We note that one should account for the instrument spectral response function because the measurements are performed not at a single wavelength but in narrow spectral range Therefore, the value of will differ for different instruments even if measured at the same central wavelength (see Figure A.1). The spectral ratio of the ozone VOD to its value at 620nm is given in Table A.3.2, where we also show the spectral calibration coefficients *c(λ)* and imaginary

refractive indexat all OLCI channels.

Table A.1 The vertical optical depth (VOD) of ozone at OLCI channels at the reference total ozone column equal to 404DU. The results are derived assuming particular temperature, pressure and ozone concentration profiles as discussed in Kokhanovsky et al. (2020b). In particular, the a-priori vertical profiles (temperature, ozone concentration) were selected according to a climatological database obtained from a 2D chemical transport model developed at University of Bremen (month: August, latitude: 75N (zonally averaged)) (Sinnhuber et al., 2009). The width of OLCI channels has been accounted for. The value of VOD does not change with the variation of profiles significantly in the spectral range studied. The channels with relatively strong absorption by ozone are given in bold blue colour.

|  |  |
| --- | --- |
| **Wavelength,nm** | **Ozone VOD** |
| 400.000 | 1.3782E-004 |
| 412.500 | 3.0488E-004 |
| 442.500 | 1.6457E-003 |
| **490.000** | **8.9359E-003** |
| **510.000** | **1.7505E-002** |
| **560.000** | **4.3471E-002** |
| **620.000** | **4.4871E-002** |
| **665.000** | **2.1016E-002** |
| **673.750** | **1.7162E-002** |
| **681.250** | **1.4663E-002** |
| 708.750 | 7.9830E-003 |
| 753.750 | 3.8797E-003 |
| 761.250 | 2.9238E-003 |
| 764.375 | 2.7922E-003 |
| 767.500 | 2.7297E-003 |
| 778.750 | 3.2560E-003 |
| 865.000 | 8.9569E-004 |
| 885.000 | 5.1888E-004 |
| 900.000 | 6.7158E-004 |
| 940.000 | 3.1278E-004 |
| 1020.00 | 1.4088E-005 |

Chart

Description automatically generated

Figure A.1. Optical depth of the total ozone column as a function of wavelength. The OLCI bands are highlighted in blue.

Table A.2 The spectral functions , c(λ), The first (second) number in the third column corresponds to the OLCI S-3A(B) gain at a given channel (Mazeran and Rueskas, 2020). The third number is the result of vicarious calibration of the OLCI(https://forum.earthdata.nasa.gov/viewtopic.php?t=1273). The first column has been used during retrievals.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| wavelength, nm |  |  |  |  |
| 400 |  | 3.071e-3 | 0.9755/0.9946/0.9597 | 6.27e-10 |
| 412.5 |  | 6.795e-3 | 0.9749/0.9901/0.9723 | 5.78e-10 |
| 442.5 |  | 3.668e-2 | 0.9689/0.9922/0.9716 | 6.49e-10 |
| 490 |  | 0.1991 | 0.9718/0.9862/0.9692 | 1.08e-9 |
| 510 |  | 0.3901 | 0.9757/0.9890/0.9764 | 1.46e-9 |
| 560 |  | 0.9688 | 0.9800/0.9911/0.9795 | 3.35e-9 |
| 620 |  | 1.0 | 0.9783/0.9977/0.9771 | 8.58e-9 |
| 665 |  | 0.4684 | 0.9786/0.9968/0.9754 | 1.78e-8 |
| 673.5 |  | 0.3825 | 0.9791/0.9972/0.9734 | 1.95e-8 |
| 681.25 |  | 0.3268 | 0.9801/0.9980/0.9760 | 2.1e-8 |
| 708.25 |  | 0.1779 | 0.9855/1.0/1.0056 | 3.3e-8 |
| 753.75 |  | 8.646e-2 | 0.9855/1.0/0.9829 | 6.23e-8 |
| 761.25 |  | 6.538e-2 | 1.0/0.9968/1.0 | 7.1e-8 |
| 764.375 |  | 6.238e-2 | 1.0/0.9972/1.0 | 7.68e-8 |
| 767.5 |  | 6.083e-2 | 1.0/0.9980/1.0 | 8.13e-8 |
| 778.75 |  | 7.256e-2 | 0.9877/0.9978/0.9899 | 9.88e-8 |
| 865 |  | 1.996e-2 | 0.9860/1.0/1.0 | 2.4e-7 |
| 885 |  | 1.156e-2 | 0.9866/1.0/1.0182 | 3.64e-7 |
| 900 |  | 1.497e-2 | 1.0/1.0/1.0 | 4.2e-7 |
| 940 |  | 6.971e-3 | 1.0/1.0/1.0 | 5.53e-7 |
| 1020 |  | 3.140e-4 | 0.9132/0.9406/1.0 | 2.25e-6 |

*Oxygen and water vapor transmittance function*

Eq. (A3.2) is quite accurate for the ozone because the most of ozone molecules are concentrated in the relatively thin atmospheric layer positioned in stratosphere. The concentration of oxygen molecules decreases with height. Therefore, the oxygen VOD depends considerably on the height of underlying surface.

We shall assume that the oxygen transmittance in the oxygen A-band can be modelled as:

(A.3.11)

where *s* is the parameter, which accounts for the fact that the gaseous transmittance in other OLCI oxygen A-band channels is larger than that at 761.25nm. In particular, we have used the following factors derived empirically from the analysis of large volume of OLCI measurements: *s*(764.375nm)=0.532 and *s*(767.5nm)=0.074. is derived as the ratio of the TOA OLCI reflectance at to the modelled TOA OLCI reflectance for the idealized atmosphere free of gaseous absorption.

We have used a similar approach for the water vapor transmission function. Namely we have derived  as the ratio of the TOA OLCI reflectance at to the modelled TOA OLCI reflectance for the idealized atmosphere free of gaseous absorption. Then we have used the following approximation for the determination of the water vapor transmission function at 900nm:

(A.3.12)

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1. [*https://sentinel.esa.int/web/sentinel/user-guides/sentinel-3-olci/resolutions/radiometric*](https://sentinel.esa.int/web/sentinel/user-guides/sentinel-3-olci/resolutions/radiometric)*.* Channels affected by oxygen and water vapor absorption are given in red color. [↑](#footnote-ref-1)