

# **SCIAMACHY 1b to 2 OL Processing**

1

# **Algorithm Theoretical Basis Document**

# Semi-Analytical CloUd Retrieval Algorithm for SCIAMACHY/ENVISAT

ENV-ATB-IFE-SCIA-0003

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2

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# Change Record

Issue	Rev.	Date	Page	Description of Change
1.0		15/11/05	all	completely new
2.0		08/02/2008	11,16	New thresholds are introduced to increase the number
				of pixels processed by SACURA



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### 1 Introduction

### **1.1 Purpose and Scope of Document**

SCIAMACHY is a joint project of Germany, The Netherlands and Belgium for atmospheric measurements. SCIAMACHY has been selected by the European Space Agency (ESA) for inclusion in the list of instruments for Earth observation research for the ENVISAT polar platform, launched in 2002.

This document gives scientific background and technical information about the Semi-Analytical CloUd Retrieval Algorithm SACURA, and its implementation at DLR-IMF as part of the SCIAMACHY off-line processor. SACURA implemented at DLR has basically the purpose to provide information for corrections of vertical columns of trace gases. Therefore relevant products are Cloud Top Height (CTH) and Cloud Optical Thickness (COT). However, in its original concept SACURA provides more then both parameters. This document focuses on scientific background information for these two parameters. Additionally, limitations of the algorithm are explained. Validation results for CTH are described as well as input and output file formats.

Beyond given information here the reader is referred to an extensive bibliography at the end of this document.

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### **1.2 Document Overview**

The present document provides information about

- **Clouds**: this section contains general information about clouds and remote sensing of clouds in particular.
- **Cloud Top Height**: this chapter shows how to derive the relevant cloud parameter mathematically and gives information about auxiliary data and the retrieval of the cloud fraction.
- The following section points out the *Limitations* of the method to derive the CTH/COT
- The section *Validation* gives brief information about the status of the validation of the CTH
- Interface information can be found in *Format of input and output*.
- Chapter *Documents* lists applicable documents and references.
- The last section lists *Abbreviations and Acronyms*



## 2 Clouds

Clouds play an important role in the Earth climate system [R-35, R-39]. The amount of radiation reflected by the Earth-atmosphere system into outer space depends not only on the cloud cover and the total amount of condensed water in the Earth atmosphere but also the size of droplets  $a_{ef}$  and their thermodynamic state is also of importance.

The information about microphysical properties, cloud top height and spatial distributions of terrestrial clouds on a global scale can be obtained only with satellite remote sensing systems. Different spectrometers and radiometers [R-4, R-12, R-20, R-49], deployed on space-based platforms, measure the angular and spectral distribution of intensity and polarization of reflected solar light. Generally, the measured values depend both on geometrical and microphysical characteristics of clouds. Thus, the inherent properties of clouds can be retrieved (at least in principle) by the solution of the inverse problem. The accuracy of the retrieved values depends on the accuracy of measurements and the accuracy of the forward radiative transfer model.

In particular, it is often assumed that clouds can be represented by homogeneous and infinitely extended in the horizontal direction plane-parallel slabs [R-15, R-17, R-18, R-19, R-47, R-48, R-54, R-55, R-28]. The range of applicability of such an assumption for real clouds is very limited as is shown by observations of light from the sky on a cloudy day. For example, the retrieved cloud optical thickness  $\tau$  is apparently dependent on the viewing geometry [R-40, R-41]. This, of course, would not be the case for an idealized plane-parallel cloud layer. However, both the state-of-art radiative transfer theory and computer technology are not capable to incorporate 3-D effects into operational satellite retrieval schemes. As a result, cloud parameters retrieved should be considered as a rather coarse approximation to reality.

However, even such limited tools produce valuable information on terrestrial clouds properties. For example, it was confirmed by satellite measurements that droplets in clouds over oceans are usually larger than those over land [R-17]. This feature, for instance, is of importance for the simulation of the Earth's climate [R-63].

Concerning trace gas retrievals in the UV-vis, clouds are considered as "contamination". The part of the column, which is below the top of the clouds, cannot be detected by the satellite. This ghost vertical column has to be estimated from climatological vertical profiles and is added to the vertical column retrieved. It is determined by integrating the profile from surface-up to the **cloud top height**. Partial cloudiness within the field of view can be taken into account using fractional cloud cover.

The Semi-Analytical CloUd Retrieval Algorithm (SACURA) was designed for the retrieval of various cloud parameters and combines basically three approaches:

- Cloud top height is derived from measurements in the oxygen A-absorption band as recommended by Yamamoto and Wark (1961) [R-68]. Such an approach has been used extensively by many authors [R-37, R-14, R-22, R-23, R-36]. In addition, we retrieve the cloud geometrical thickness from the fit of the measured spectrum in the oxygen A-band and optical thickness using the wavelength 755 nm outside of the band.
- 2. Specific parameters are based on the asymptotical solution of the radiative transfer equation for a special case of disperse media, having a large optical thickness.



Apart  $a_{ef}$  and  $\tau$  (cloud optical thickness is also derived in approach 1), we also retrieve the liquid water path *w* [gm<sup>-2</sup>], the cloud albedo *r*, and the column concentration of droplets *N* [m<sup>-2</sup>], using well-known relationships between these quantities. In particular, the relation between cloud optical thickness and cloud albedo follows:

 $r = 1-1 / (1.072 + 0.1125 \tau).$ 

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3. Furthermore, the cloud thermodynamic state is obtained using different spectral signatures of liquid water as compared to ice in the spectral range 1550-1670nm [R-45, R-50, R-21, R-1].

Due to the relevance of cloud top height (and cloud optical thickness) for trace gas retrievals this document is dedicated to the first issue. The other approaches are not part of this documentation.



### 3 The cloud top height

The determination of the cloud top height *h* using SACURA is based on the measurements of the top-of-atmosphere (TOA) reflection function *R* in the oxygen A-band [R-33, R-59, R-60]. The spectral dependence  $R(\lambda)$  of the cloud with the optical thickness five for the nadir observation and the solar angle equal to 60° is shown in Fig. 1 for various cloud top heights. This Figure shows that the cloud reflection function is extremely sensitive to the cloud top height in the centre of the oxygen absorption band. To find the value of *h*, we first assume that the TOA reflectance *R* can be presented in the form of a Taylor expansion around the assumed value of cloud top height equal to h<sub>0</sub>:

$$R(h) = R(h_0) + \sum_{i=1}^{\infty} a_i (h - h_0)^i,$$
(1)

Where  $a_i = R^{(i)}(h_0)/I!$ . Here  $R^{(i)}(h_0)$  is the *i*-derivative of *R* at the point  $h_0$ . The next step is the linearization, which is a standard technique in the inversion procedures [R-57, R-59, R-60, R-53]. We found that the function R(h) is close to a linear one in a broad interval of the argument change [R-32]. Therefore, we neglect non-linear terms in Eq. (1). Then it follows:

$$R = R(h_0) + R'(h_0)(h - h_0),$$
(2)

where  $R' = \frac{dR}{dh}$ . We assume that *R* is measured at several wavelengths in the oxygen Aband. Then instead of the scalar quantity *R* we can introduce the vector  $\vec{R}_{mes}$  with components  $(R(\lambda_1), R(\lambda_2), ..., R(\lambda_n))$ . The same applies to other scalars in Eq. (1). Therefore, Eq. (2) can be written in the following vector form:

$$\vec{y} = \vec{a}x \tag{3}$$

where  $\vec{y} = \vec{R}_{mes} - \vec{R}(h_0)$ ,  $\vec{a} = \vec{R}'(h_0)$ , and  $x = h - h_0$ . Note that both measurement and model errors are contained in Eq. (13). The solution  $\hat{x}$  of the inverse problem is obtained by the minimizing the following cost function [R-53]:

$$\Phi = \left\| \vec{y} - \vec{a} x \right\|^2 , \qquad (4)$$

where  $\| \|$  means the norm in the Euclid space of the correspondent dimension. The value of  $\hat{x}$ , where the function  $\Phi$  has a minimum can be presented as

$$\hat{x} = \frac{\left(\vec{y}, \vec{a}\right)}{\left(\vec{a}, \vec{a}\right)} = \frac{\sum_{i=1}^{n} a_i y_i}{\sum_{i=1}^{n} a_i^2} , \qquad (5)$$

where (,) denotes a scalar product in the Euclid space, *n* is the number of spectral channels, where the reflection function is measured.

Therefore, from known values of the measured spectral reflection function  $R_{mes}$  (and also values of the calculated reflection function R and its derivative R' at  $h = h_0$ ) at several wavelengths, the value of the cloud top height can be found from Eq. (5) and equality:  $h = \hat{x} + h_0$ . The value of  $h_0$  can be taken equal to 1.0 km, which is a typical value for low level clouds [R-13]. The main assumption in our derivation is that the dependence of R on h can be presented by a linear function on the interval x [R-32].



The SACURA code finds both the cloud top height h and the cloud geometrical thickness l simultaneously. This requires the minimization of the following cost function (see Eq. (4)):

$$\Phi = \left\| \vec{y} - \hat{A}\vec{X} \right\|^2 \tag{6}$$

The elements of the matrix  $\hat{A}$  are correspondent weighting functions [R-53]. The solution of the inverse problem is given by the vector-parameter  $\vec{X}$ . This vector has 5 components, which give corrections to the initially assumed cloud top height and cloud geometrical thickness, the correction to the initially assumed half-width of the spectrometer spectral response function, the shift parameter, and the squeeze parameter. Clearly, first two parameters give us final values of the pair (h, l) to be retrieved. The third parameter allows adjusting the assumption on the instrument response function. Last two parameters allow reducing errors related to the displacement of the experimentally measured spectrum due to the errors of the spectral calibration and the Doppler shift. We have developed two versions of the retrieval algorithm. One is based on the exact radiative transfer calculations of the reflection function *R* and another one is based on the approximate representation of *R* by the following equation [R-32, R-33, R59, R-60]:

$$R = R_0 + T_1 R_c T_2, (7)$$

where  $R_0$  gives the reflection function of the part of atmosphere above the cloud,  $R_c$  is the cloud reflection. Functions  $T_i$  (i = 1, 2) give transmission coefficients from the sun to a cloud and from the cloud to a satellite, respectively. Approximate equations for all functions in Eq. (7) are given by Kokhanovsky and Rozanov, 2004 [R-32]. We have used the correlated k-distribution method to account for the high-frequency oscillations of the oxygen molecule absorption cross section  $\sigma_a$  [R-38, R-7, R-8]. The temperature and pressure dependence of

 $\sigma_a$  for a given location of measurements was accounted for using the standard atmosphere model built in SCIATRAN [R-58]. We have used the most recent version of the HITRAN molecular spectroscopic database to get data on cross sections  $\sigma_a$  [R-56].

For the operational retrievals, we have used the retrieval technique based on the approximate representation of R (see Eq. (7)). It allows speeding up the retrieval process considerably.

SACURA is capable to retrieve cloud geometrical thickness as well. However, the meaning of this parameter for multi-layered systems is not clear. The wavelength window<sup>1</sup> selected for this approach has been set to 754 - 775 nm (for SCIAMACHY this means channel four and currently cluster 26).

<sup>&</sup>lt;sup>1</sup> Additional wavelength windows (424 - 527 and 1550 – 1670 nm) are considered when taking into account approaches two and three (see introduction).





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Fig. 1: The spectral dependence of the cloud reflection function in the oxygen A-band calculated for several cloud top heights at the nadir observation and the solar angle equal to 60 degrees. It was assumed that the optical thickness is equal to 5, the surface albedo A=0, and the cloud geometrical thickness l=250m. The Cloud C.1 droplet size distribution [R-11] was used in calculations of local optical properties including the phase function, the single scattering albedo, and the extinction coefficient. The atmospheric model used in calculations is described in more detail by Kokhanovsky and Rozanov (2004) [R-32] (1-exact calculations using SCIATRAN [R-58], 2- the analytical radiative transfer model as described by Kokhanovsky and Rozanov (2004) [R-32]).

#### 3.1 Auxiliary data

The ground albedo, the ground height, atmospheric temperature and pressure profiles and oxygen molecule cross sections needed for the retrievals are taken from the SCIATRAN database (see http://www.iup.physik.uni-bremen.de/sciatran). At DLR-IMF ground height (topography) and surface albedo are coming from different sources (GTOPO30 and other).

#### 3.2 The cloud fraction

For both implementations, the local one from IUP-IFE and the one at DLR-IMF, the cloud fraction *c* has been derived using OCRA algorithm as described by Loyola and Ruppert, 1998; Loyola, 2000, 2004; and Tuinder et al., 2004 [R-42, R-43, R-44, R-65].

It is based on the analysis of several SCIAMACHY PMD measurements. The reflectance over a partially cloudy field is presented as  $R=c R_c+(1-c) R_a$ , where  $R_a$  is the reflection function of the background continental atmosphere defined in the framework of SCIATRAN and  $R_c$  is the cloud reflection function. This allows finding:

$$R_c = c^{-1} R - c^{-1} (1 - c) R_a$$
.

(8)

Eq. (8) enables the reduction of a partially cloudy case to the case of completely cloud covered scene.



### 4 Limitations

Large parts of the algorithm are based on radiative transfer (RT) calculations. In order to speed up the RT-code a pseudo-spherical approach was used to into account the sphericity of the atmosphere. For this reason reliable results can only be obtained where the solar zenith angle is  $\leq 80^{\circ}$ .

The algorithm for the previous version of the code was restricted to the case of optically thick clouds (the cloud optical thickness  $\geq 5$ ). The current version retrieves CTH (but not COT) for thinner clouds as well. It is planned to be supplemented in the future by the exact radiative transfer calculations at  $\tau < 5$  [R-47]. However, it should be stressed that the optical thickness is highly correlated with the geometrical thickness of clouds. For instance, it was shown [R-13] that clouds having  $\tau < 5$  have the geometrical thickness less than 200m on average. It is difficult to expect that such clouds are homogeneous in the horizontal direction. This requires the horizontal photon transport [R-10, R-51].

However, this is not considered in standard retrieval procedures [R-2, R-47, R-51]. Backscans, are practically much larger than usual SCIAMACHY ground pixels (30\*60 km<sup>2</sup>) for this reason the scene albedo is likely to be inhomogeneous. Additionally, cloud fragmentation can be expected to be larger.

Although both aerosol [R-26] and molecular [R-6] scattering and absorption are neglected, their influence is minimized by a careful selection of spectral channels. Also, the influence of molecular and aerosol scattering is of importance mostly for  $\tau$  < 5 and in UV[R-67] (not for the oxygen A-band spectral region).

The applicability of the algorithm proposed for the optical thickness retrieval is limited both from the side of small ( $\tau < 5$ ) and large ( $\tau > 100$ ) values of the optical thickness [R-28]. However, the appearance of such clouds in the Earth's atmosphere is rare as indicated by Trishchenko et al. (2001) [R-64]. For the effective radius retrieval, however, there is no upper boundary for large  $\tau$ . This is due to the fact that the reflection of light depends on the size of droplets even for an infinitely thick absorbing cloud.

The algorithm flags each data set with quality levels. Accounting for these flags is crucial and should always be performed. The quality flags can have values from 0 to 5 with the following meaning:

- 0: no retrieval
- 1: cloud top height constrains not fulfilled
- 2: cloud bottom height constrains not fulfilled
- 3: retrieval constrains not fulfilled
- 4: no convergence -
- 5: retrieval OK

Flag 0: abnormal retrieval or clear sky pixel. This flag can be used together with the cloud fraction as the base for a cloud screening (see results from Lotz and Vountas, 2006 [R-45]). Flags 1-3: The retrieval led to a atypical result (e.g. in case of vertically inhomogeneous clouds).

In Lotz and Vountas (2006) [R-45] it could be shown that removing records flagged with "0" is already sufficient to remove abnormal retrievals or those over clear sky. Therefore it is recommended to account only for those retrievals flagged as 1-5. Modelled retrievals flagged with 1-4 had an average error of -0.5km/+0.5km. Retrievals flagged with 5 have average errors of -0.25 km/+0.25 km.



## 5 Validation

The validation of SACURA is ongoing activity. Up to date only the validation of the cloud top height product has been performed. The validation was based on single lidar and radar [R-33] measurements as far as the application of SACURA to SCIAMACHY is of concern.

These comparisons show up to 0.5-1.0 km differences in the SACURA-retrieved cloud top heights. However, it must be remembered that lidars and radars provide measurements at single points whereas the SCIAMACHY pixel size is 30\*60 km<sup>2</sup>. SACURA as applied to GOME, which has a similar spectral but lower spatial resolution, shows quite good correspondence as compared to ATSR-2 thermal infrared measurements. We expect to have a similar accuracy of SACURA as applied to SCIAMACHY data as compared to AATSR measurements. The comparison with AATSR retrievals is a matter of ongoing research. The correlation plot of SACURA-derived CTHs as compared to IR ATSR-2 measurements is shown in Fig. 2 (left).



Fig. 2: (left) Correlation plot between CTHs obtained using SACURA and thermal IR measurements of ATSR-2. (Right) Histogram of biases of SACURA GOME - derived CTHs as compared to those derived using thermal IR measurements of ATSR-2.

SACURA-derived CTH are on average by 0.5 km higher as compared to collocated IR measurements (see Fig. 2, right).

Fig. 3 confirms that biases are larger for thicker clouds. This may indicate the problem with multi-layered cloudiness. All retrievals using SACURA are performed in the assumption of a homogeneous single cloud layer composed of water droplets.



Fig. 3: Dependence of the SACURA bias  $B_s$  on the cloud geometrical thickness (CGT).



### 6 The format of input and output

The software delivered to DLR-IMF for the implementation of Sacura needs five Sacura-NG consumable input files:

- SCIA\_cfrac.dat (cloud fractions) Contains re-formated cloud fractions: No header lines are given.
  - 1. column: cloud fractions []
  - 2. column: start time [MJD] (Modified Julian Day)
  - 3. column: integration time [1/16 sec]
- 2. SCIA\_geolo.dat

Contains information about the complete geolocation for each ground pixel: No header lines are given.

1. column: sequence number: state readout [statenumber x 1000 + readoutnumber]

- 2. column: latitude center [deg]
- 3. column: longitude center [deg]
- 4. column: solar zenith ang. [deg]
- 5. column: viewing zenith angle (loszen) [deg]
- 6. column: viewing azimuth angle (losaz) [deg]
- 7. column: latitude ne [deg]
- 8. column: longitude ne [deg]
- 9. column: latitude se [deg]
- 10. column: longitude se [deg]
- 11. column: latitude nw [deg]
- 12. column: longitude nw [deg]
- 13. column: latitude sw [deg]
- 14. column: longitude sw [deg]

#### 3. SCIA\_initi.dat

Contains info about states and readouts and is self-explanatory.

4. SCIA\_nadir.dat

state-based input radiance spectra:1. column: wavelength [nm]2-Nth column: radiance for each of allreadouts per state.This is repeated for each state of the orbit.

- 5. SCIA\_solar.dat
- 6. Re-formatted Scia input irradiance spectra.
  - 1. column: wavelength [nm]
  - 2. column: irradiance



The central output file is *SCIA\_retri.dat*. The file contains 12 columns which are described in the following table:

Column	Field name	Description	Example value
1	Seq	Sequence number	5115
2	Lac	Latitude of center coordinate [deg]	77.50
3	Loc	Longitude of center coordinate [deg]	-57.46
4	Gh	Ground height [km]	2.07
5	Alb	Reflectance	0.91
6	Sza	Solar zenith angle [deg]	87.99
7	Tau	Cloud optical thickness (B)	27.54
8	Cbh	Cloud bottom height [km]	2.00
9	Cth	Cloud top height [km]	4.28
10	Cfr	Cloud fraction (coming from OCRA)	0.46
11	Rms	Root mean square	0.2323E-01
12	Sts	Retrieval status	2



# 7 Thresholds and constrains of SACURA

The retrieval algorithm for the current SACURA version is slightly differs from that of the previous one. SCIAMACHY measurements enter cloud fraction retrieval algorithm OCRA. This algorithm enables the determination of cloud fraction. For cloud fractions smaller than 0.05 (**0.2 in the previous version**) no retrievals are performed. It is assumed that pixel is clear then. For larger cloud fractions, the cloud reflectance at 758nm is retrieved in the framework of independent pixel approximation using Eq. (8). The algorithm checks if the cloud reflectance is a positive number. Only then retrievals are performed. First the cloud optical thickness is determined. If the determined value of COT is larger or equal to 5, then the retrieved value of cloud optical thickness is used in the retrieval of cloud top height and also cloud bottom height by SACURA. For the retrieved values of COT smaller than 5.0 retrievals of cloud boundaries are performed fitting the oxygen A-band spectrum in the assumption that COT=5. This is because the error of SACURA for the retrieval of cloud optical thickness is large at small COT. If the difference in CTHs retrieved from two subsequent iterations is smaller than 0.2km, then the iterations are stopped. In the previous version of the code there were no retrievals of CTH at COTs smaller than 5.

The rms of oxygen A-band fit using derived COT, CTH and CBH is reported in output. Alternatively, iterations are stopped, if rms is smaller than 0.5%. The errors of retrieved cloud optical thickness are large also at COT larger than 100. Therefore, the retrieved value of cloud optical thickness is set to 100, if values of COT larger than 100 are retrieved. The same is done also if negative values of the cloud optical thickness are derived. For cloud fractions larger than 0.95, Eq. (8) is not used and it is assumed that the cloud fraction is equal to 1.0. SACURA uses the following constrains in the solution of the two-parameter inverse problem: -1.1km  $\leq$  CTH<1.7km

• 0.8km≤CGT<9.0km

In addition, the derived CBH is reported. The retrieved values of CBH are reported only in the range [0.2km, 16.8km]. For smaller and larger values of retrieved CBH, the correspondent limiting values are given to the output.



### 8 Documents

#### 8.1 Applicable Documents

- [A-1] ENVISAT Product Specification Volume 15
- [A-2] IECF Technical Description, PO-TN-ESA-GS-1142
- [A-3] SCIAMACHY Level 0-1b Data Processing: Detailed Processing Model (DPM), ENV-DPM-DLR-SCIA-0006
- [A-4] SCIAMACHY Level 0-1b Data Processing Tools: SciCal DPM, ENV-DPM-DLR-SCIA-0071

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## 9 Abbreviations and Acronyms

A list of abbreviations and acronyms which are used throughout this document is given below:

AO	Announcement of Opportunity
CBH	Cloud Bottom Height
CGT	Cloud Geometrical Thickness
СОТ	Cloud Optical Thickness
DFD	Deutsches Fernerkundungsdatenzentrum
DLR	Deutsche Forschungsanstalt für Luft- und Raumfahrt e.V.
DOAS	Differential Optical Absorption Spectroscopy
ENVISAT	Environmental Satellite
ERS	European Remote Sensing Satellite
ESA	European Space Agency
ESRIN	European Space Research Institute
ESTEC	European Space Centre of Technology
GOME	Global Ozone Monitoring Experiment
GS	Ground Segment
IFE	Institut für Fernerkundung der Universität Bremen
IMF	Institut für Methodik der Fernerkundung, DLR e.V.
IPF	Instrument Processing Facility
IUP	Institut für Umweltphysik der Universität Bremen
OCRA	Optical Cloud Recognition Algorithm
NRT	Near Real Time
SACURA	Semi-Analytical CloUd Retrieval Algorithm
SCIAMACHY	Scanning Imaging Absorption Spectrometer for Atmospheric Chartography
SSAG	SCIAMACHY Scientific Advisory Group
UV	Ultra-Violet
UV-vis	UV visible