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Cloud retrieval algorithm for GOME-2:

FRESCO+

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1. INTRODUCTION

Clouds strongly affect the trace gas retrievals by shielding, albedo enhancement and in-cloud absorptions. Because of the relatively coarse spatial resolution of the GOME-2 satellite instrument ($40 \times 80 \text{ km}^2$), only 5-15% of the pixels are cloud-free (Krijger et al., 2007). To be able to use the majority of GOME-2 pixels, cloud correction is necessary. To correct for cloud effects on trace gas retrievals, the most relevant cloud parameters are the cloud fraction and height (Koelemeijer and Stammes, 1999, Stammes et al., 2008). There are several cloud retrieval algorithms that have been developed for GOME and SCIAMACHY using the $\text{O}_2 A$ band (Koelemeijer et al., 2001, Kokhanovsky et al., 2005, van Diedenhoven et al., 2007) or using Polarisation Monitoring Devices (PMDs) (Grzegorski et al., 2006, Loyola et al. 2004). FRESCO (Koelemeijer et al., 2001) is a simple, fast and robust algorithm, which is also implemented in the GOME-2 level 1 data processor at EUMETSAT (Munro and Eisinger, 2004, Fournier et al., 2004; Wang and Stammes, 2007).

It is almost impossible to derive uniquely both cloud fraction and cloud optical thickness from the measured spectral reflectance of a single GOME-2 pixel. This is because cloudy scenes with the same cloud pressure may possess different cloud fractions and cloud optical thicknesses, which give rise to nearly the same reflectance in and around the oxygen A band. For cloudy scenes differing in this sense, however, cloud effects on the ozone column density retrieval are almost the same. Therefore, it is useful and necessary to introduce an effective cloud fraction, which is the cloud fraction derived from the satellite measurements, assuming an a priori chosen cloud optical thickness or cloud albedo. Then, the most relevant cloud parameters for trace gas column density retrieval reduce to effective cloud fraction and cloud pressure. Alternatively, separation of cloud fraction and cloud optical thickness could be done using PMD information, although ambiguity remains to some extent in that approach too.

The FRESCO method was originally developed for near real time ozone column retrieval from GOME (Piters et al., 1999). In Koelemeijer et al. (2001), the FRESCO method is described together with a sensitivity study and validation using ATSR-2 data. In Koelemeijer et al., (2002), a comparison is made between cloud pressures and effective cloud fractions of FRESCO and ISCCP on a monthly average basis. FRESCO+ is a new version of the FRESCO algorithm, in which single Rayleigh scattering is added in the reflectance database and the retrieval (Wang et al., 2008). Rayleigh scattering is mainly important for the almost cloud free part of the pixels. The FRESCO+ cloud pressure is more reliable than FRESCO for less cloudy scenes, say for effective cloud fractions < 0.15 . The FRESCO+ improvement is more relevant for tropospheric trace gas retrievals (like NO_2) than for total O_3 retrieval.

In this document a description of the FRESCO+ algorithm for GOME-2 (=FRESCO v5) is given and several improvements are described.

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2. ALGORITHM DESCRIPTION

2.1 Forward model

Information on cloud pressure and effective cloud fraction is derived from the reflectivity R in and around the $O_2 A$ band. The reflectivity is given by

$$R(\lambda) = \frac{\pi I(\lambda)}{\mu_0 E_0(\lambda)}, \quad (1)$$

where I is the Earth's reflected radiance ($W m^{-2} nm^{-1} sr^{-1}$) measured by GOME-2, E_0 the incident solar irradiance at the top of the atmosphere through a horizontal surface unit ($W m^{-2} nm^{-1}$) measured by GOME-2, and μ_0 the cosine of the solar zenith angle. Due to instrument temperature variations in orbit, the wavelength grid of the radiances and irradiances may be different for different measurements. Therefore, to calculate the reflectivity, the measurements of $I(\lambda)$ and $E_0(\lambda)$ are interpolated to a common grid, the so-called reference wavelength grid, which is also used in the simulations.

To simulate the reflectance spectrum of a partly cloudy pixel inside and outside the $O_2 A$ band, a simple atmospheric transmission model is used, in which the atmosphere above the ground surface (for the clear part of the pixel) or cloud (for the cloudy part of the pixel) is treated as an absorbing (due to oxygen) and purely Rayleigh scattering medium. Reflection occurs only at the surface or cloud top. The surface is assumed to be Lambertian; the cloud is assumed to reflect either Lambertian or with a BRDF based on Doubling-Adding and Mie calculations. The principle of the FRESCO+ algorithm is shown in Fig. 1 and 2. The reflectivity $R_{sim}(\lambda; \theta; \theta_0; \varphi - \varphi_0)$ at a wavelength λ , viewing zenith angle θ , solar zenith angle θ_0 , and relative azimuth angle $\varphi - \varphi_0$ is then given by

$$R_{sim}(\lambda, \theta, \theta_0, \varphi - \varphi_0) = cT_c A_c + (1 - c)T_s A_s + cR_c + (1 - c)R_s, \quad (2)$$

where c is the effective cloud fraction, the surface height, A_s the surface albedo, z_c the cloud height, and A_c the cloud albedo. $T(\lambda, z, \theta, \theta_0)$ is the direct atmospheric transmittance for light entering the atmosphere from the solar direction, propagating down to a level with height z , and then propagating to the top of the atmosphere in the direction of the satellite. The absorption and single Rayleigh scattering are taken into account in the light paths for T . $R_c(\lambda, z_c, \theta, \theta_0, \varphi - \varphi_0)$ and $R_s(\lambda, z_s, \theta, \theta_0, \varphi - \varphi_0)$ are the single Rayleigh scattering reflectances due to cloud and surface. $\varphi - \varphi_0$ is the relative azimuth angle of the observation w.r.t. the sun. The transmission and reflectance are calculated using line-by-line calculations through the entire

O_2 A band and convoluted with the instrumental response function. To speed up the algorithm the transmissions and single Rayleigh scattering reflectances are pre-calculated and stored in look-up-tables. A_s and z_s are taken from a surface albedo database and a surface height database, respectively. A_c is assumed to be 0.8 or the reflectance at 758 nm if the reflectance is larger than 0.8.

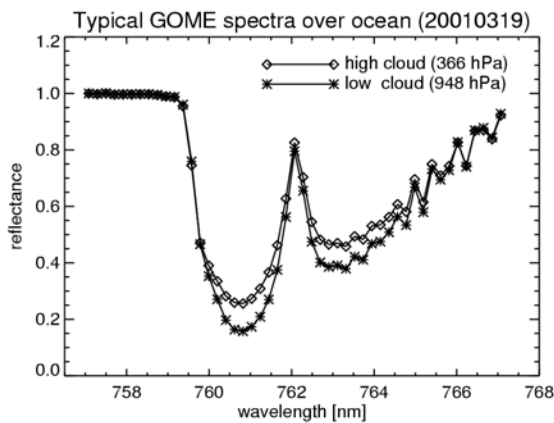


Figure 1. Typical O_2 A-band spectra measured by GOME. The spectra are normalized at 758 nm to show the relative depth of the band for clouds at different heights.

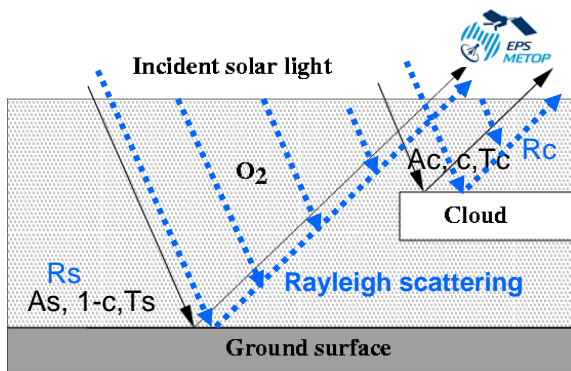



Figure 2. Atmospheric radiation model used in FRESCO+. The cloud and surface are both assumed to be Lambertian reflectors. Three light paths are considered: (1) from sun to surface to satellite, (2) from sun to cloud to satellite, (3) from sun to atmosphere to satellite according to single Rayleigh scattering (indicated in blue). Along all three paths O_2 absorption and Rayleigh scattering are included in the forward model simulations.

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2.2 FRESCO+ snow/ice mode

It can easily be shown that the derived effective cloud fraction becomes very sensitive to errors in A_s when A_s approaches A_c , which may occur for surfaces covered by snow. Hence, in that case it is almost impossible to accurately derive an effective cloud fraction and hence cloud pressure. Therefore, in snow/ice cases we assume $c=1$, and the measurements are fitted to the function (cf. Eq. 2):

$$R_{sim}(\lambda, \theta, \theta_0) = T_c(\lambda, z, \theta, \theta_0)A_c + R_c(\lambda, z, \theta, \theta_0, \varphi - \varphi_0). \quad (3)$$

The fit is solving for A_c and z , which are the albedo and height of the “lower reflecting boundary” (surface or cloud) of the atmosphere.

Presently, information on snow coverage is obtained from the global database of UV surface LER values, which was derived by Herman and Celarier (1997) from 14.5 years of Total Ozone Mapping Spectrometer (TOMS) data at 340 and 380 nm. According to their database, snow-free land and ocean have surface LER values in the UV smaller than ~ 0.2 .


2.3 Retrieval method

The retrieval method is based on minimizing the difference between a measured and a simulated spectrum, using the Levenberg-Marquart nonlinear least-squares method,

$$\chi^2 = \sum_{i=1}^N \left[\frac{R_{meas}(\lambda_i) - R_{sim}(\lambda_i)}{\varepsilon(\lambda_i)} \right]^2, \quad (4)$$

where $\varepsilon = \varepsilon_{meas} + \varepsilon_{sim}$ is the sum of the measurement and simulation errors, respectively. The simulation error is fixed on an estimated 1 percent. The summation is over the measurement points used by FRESCO+ in the wavelength interval between 758 and 766 nm, which comprises $N=15$ wavelengths. The free parameters in the fit are the effective cloud fraction and cloud height. The errors are calculated as the square root of the diagonal elements of the covariance matrix. The cloud pressure error is determined as $\Delta P = \max(|P_c - P(z_c - \Delta z)|, |P_c - P(z_c + \Delta z)|)$, with Δz the error in cloud height.

The subroutine used is MRQMIN from Numerical Recipes (Press et al., 1986).

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2.4 Databases and auxiliary data in FRESCO+

2.4.1 Transmission database

The transmission database has two look up tables now: one is the transmission database due to the oxygen absorption and single Rayleigh scattering, the other one includes the single Rayleigh scattering reflectance database except for the Rayleigh scattering phase function. The Rayleigh scattering phase function is calculated in the retrieval model directly. The transmission calculations are performed in two steps. In the transmission (T) and reflectance (R) calculations the effect of the Earth's sphericity is taken into account. Temperature and pressure profiles were assumed for a mid-latitude summer atmosphere (Anderson et al., 1986). The O_2 absorptions are calculated with a line-by-line method using HITRAN 2004. The transmission databases are calculated at 1 pm spectral resolution and convoluted with the instrumental slit function.


The depth of the oxygen A band depends on the absorption optical thickness, above the cloud, which is linear in cloud pressure. However, for practical reasons, the height z is used rather than the pressure P as the height variable in the model simulations and retrieval. Since the pressure-height relation in the model is generally different than in the real atmosphere, the retrieved cloud height is converted back to cloud pressure using the same atmospheric profile as was used in the simulations to yield the correct cloud pressure. In FRESCO+, a polynomial expansion is used to describe the height dependence of the transmission T , and the single Rayleigh scattering reflectance R_1 , (except for the Rayleigh scattering phase function):

$$T(\lambda, z, \theta, \theta_0) = \sum_{i=1}^N \alpha_i(\lambda, \theta, \theta_0) z^i, \quad (5)$$

$$R_1(\lambda, z, \theta, \theta_0) = \sum_{i=1}^N \beta_i(\lambda, \theta, \theta_0) z^i \quad (6)$$

where $N = 4$ was chosen to give negligible interpolation errors. The advantages of this approach are that (1) the simulation database can be much smaller, and (2) the derivative of the reflectance with respect to height can be obtained analytically (useful for Levenberg-Marquart fitting). Therefore, in the LUTs, T and R are represented by α_i and β_i ($i = 1, 4$), respectively, as a function of solar zenith angle (SZA), viewing zenith angle (VZA), and wavelength. The altitude grid for z is 0.5 km from 0 to 15 km. The formulas for the Rayleigh scattering phase function and single scattering reflectance are given in the Appendix (Sect. 6) and Wang et al. (2008).

Currently, in FRESCO+, three about 1-nm-wide wavelength windows are used, namely, 758-759 nm (continuum, no absorption), 760-761 nm (strong absorption), and 765-766 nm (moderate absorption). Each window comprises five GOME-2 wavelengths. It is important to note that the reflectances in these three wavelength windows contain nearly all independent information that is

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available in the O₂ A band for instruments with the spectral resolution of GOME-2. The detailed information about the transmission database and the tools to create the transmission database for GOME-2 is in the ‘GOME-2 FRESCO final report’ (Wang and Stammes, 2007).

2.4.2 Surface albedo database

2.4.2.1 GOME LER surface albedo

The surface albedo is deduced from a global surface Lambert-equivalent reflectivity (LER) database that was generated from GOME data of June 1995 - December 2000 (Koelemeijer et al., 2003). This database was generated as follows. For each GOME measurement the LER was determined, using the Doubling-Adding KNMI radiative transfer code (De Haan et al., 1987; Stammes, 2001). The LER is the calculated Lambertian surface albedo required to match the observed reflectance at the top of the atmosphere, assuming a Rayleigh scattering atmosphere. The LERs were binned by month and in grid-cells of 1 deg x 1 deg. The LER of the surface was then determined as the minimum LER in each grid-cell and each month. Effects of persistent clouds over ocean were corrected by replacing the values in such grid-cells by a weighted average of adjacent grid-cells. The GOME albedo climatology was generated for every month for several wavelengths, including 758 and 772 nm used by FRESCO+.

The data is decontaminated from the presence of desert dust aerosols using the GOME Absorbing Aerosol Index (Fournier et al., 2006). The surface albedo is refined at coastlines and made at 0.25°x0.25° resolution (Fournier et al., 2004; Wang and Stammes, 2007).

GOME surface albedo is the A_s in Eq. 1 used in the retrieval. The spectral dependence of the surface LER is taken into account by linearly interpolating between the surface LER values at 758 and 772 nm.


2.4.2.2 TOMS surface albedo for detection of snow/ice

The TOMS surface albedo (Herman and Celarier, 1997) is used to identify the presence of snow/ice at the surface for every pixel. Snow/ice coverage is assumed for a GOME-2 pixel if the TOMS database for that area and month gives a UV LER exceeding 0.2, and also when the LER at 758 nm is equal to or larger than the assumed cloud albedo.

2.4.3 Surface height database

The surface height is taken from the GTOPO30 database (made by the U.S. Geological Survey's EROS Data Center in Sioux Falls, South Dakota), downgraded to 0.25°x0.25° resolution.

References: data at <http://edcdaac.usgs.gov/gtopo30/gtopo30.asp>

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Documentation at <http://edcdaac.usgs.gov/gtopo30/README.asp>

2.4.4 Spectral wavelength grid

The LUTs for transmission and reflectance are made at a pre-defined wavelength grid. Therefore the spectral wavelength grid is also an auxiliary data set.

2.4.5 Atmospheric profile


The pressure-height relationship in the retrieval model and look-up tables is generally different than in the real atmosphere. Therefore, the retrieved cloud height is converted back to cloud pressure using the same atmospheric profile as was used in the simulations to yield the correct cloud pressure. The standard atmospheric profile for FRESCO+ is the mid-latitude summer profile (Anderson et al., 1986).

2.4.6 Cloud albedo

The cloud albedo is fixed to 0.8. However, when the measured reflectance outside the oxygen A band (at 758 nm) exceeds this value, the measured reflectance outside the band is used as cloud albedo.

It is also possible to use a BRDF cloud albedo based on Doubling-Adding and Mie calculations. The results are similar as albedo of 0.8 (Koelemeijer et al., 2001). Therefore, a Lambertian cloud albedo is the standard setting in FRESCO+.

It is important to stress that the effective cloud fraction derived using FRESCO thus pertains to an optically thick cloud: the cloud optical thickness that pertains to a cloud spherical albedo of 0.8 is ~ 33 . The choice for a cloud albedo of 0.8 is based on several considerations. First, the choice $A_c=0.8$ is optimized for ozone air mass factor calculations in the UV, when a ghost-column is added to the derived vertical column density to correct for ozone below the cloud. Second, in the FRESCO method we assume that absorption below the cloud may be neglected, which can be justified for optically thick clouds. Choosing a high cloud albedo ensures that the model assumptions are internally consistent. More detailed discussion about effective cloud fraction is in the paper by Stammes et al. (2008).

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3. VALIDATION

The FRESKO (v4) and FRESKO+ (FRESKO v5) cloud heights have been compared for SCIAMACHY with active remotely sensed cloud heights at the SGP/ARM site. The ARM cloud layer height distributions and the collocated SCIAMACHY FRESKO+ cloud heights are shown in Figure 3. In this plot we have further limited the FRESKO+ effective cloud fractions to values larger than 0.2 and the time periods of ARM cloud cover to periods longer than 30 minutes, which corresponds to geometric cloud fractions larger than 0.5. As shown in Figure 3(a), the FRESKO+ cloud height is close to the middle of the ARM cloud profiles. This agrees with the results of FRESKO+ for simulated spectra. As shown in Figure 3(b), the FRESKO+ cloud heights have an excellent correlation with the averaged ARM cloud profiles, with a correlation coefficient of 0.94. To demonstrate the improvement in FRESKO+, SCIAMACHY FRESKO and ARM cloud heights are shown in Figure 3(c, d). The criteria used for the selection of SCIAMACHY FRESKO and ARM data are similar as that for FRESKO+ and ARM, except that FRESKO effective cloud fractions are larger than 0.2. The different number of data in FRESKO and FRESKO+ is due to the different FRESKO and FRESKO+ effective cloud fractions. As shown in Figure 3(a, c) FRESKO+ retrieves lower cloud height than FRESKO, which agrees with the simulations and the statistics from GOME data. FRESKO+ significantly improves the cloud height retrievals for single-layer low clouds. In this case, FRESKO often does not converge and retrieves a cloud height close to the initial value of 5 km. The correlation coefficient of FRESKO and ARM cloud height is 0.79 (Wang et al., 2008).

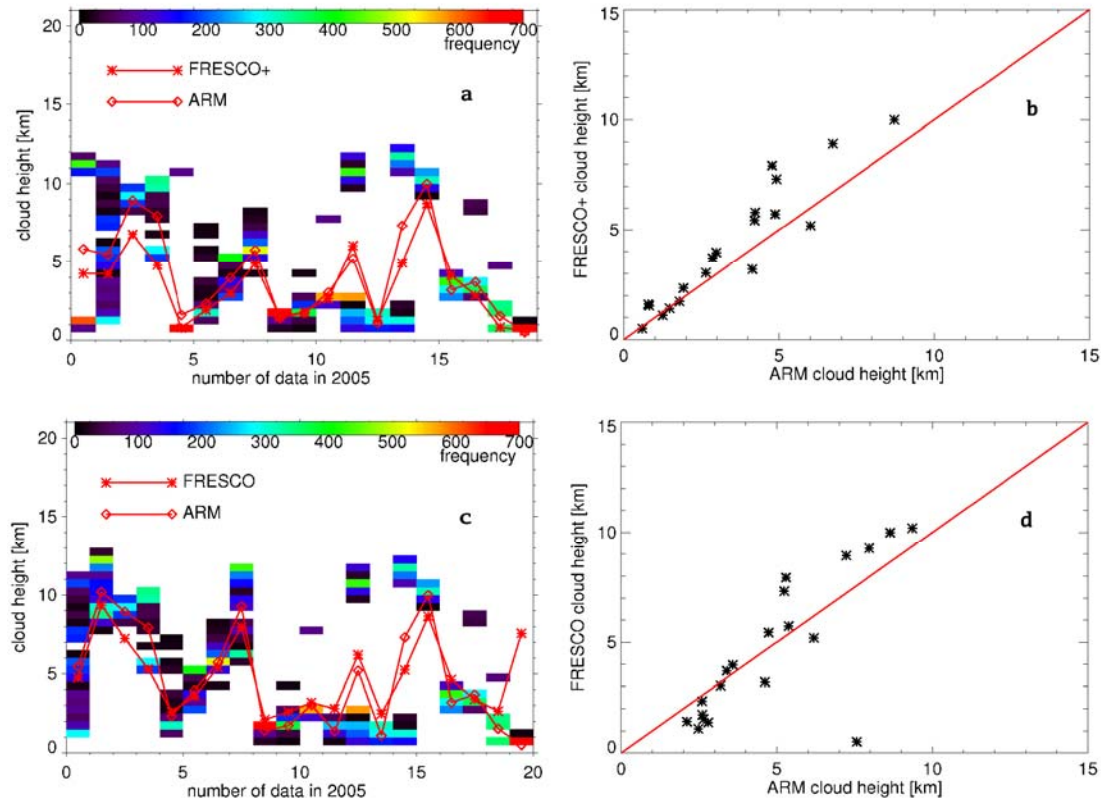



Figure 3. (a) Comparison between collocated SCIAMACHY FRESKO+ cloud heights and ground-based radar/lidar cloud profiles, for 18 days in 2005 on which SCIAMACHY overpasses of the SGP/ARM site occurred. The color indicates the occurrence of clouds as detected by the radar/lidar. (b) Correlation of FRESKO+ cloud height and the average cloud height from the radar/lidar profiles for the same data as in (a), with correlation coefficient of 0.94. (c) and (d) are similar as (a) and (b) but FRESKO data are used. The correlation coefficient between ARM and FRESKO cloud height is 0.79. Only effective cloud fractions larger than 0.2 are used.

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4. CONSTRAINTS, LIMITATIONS AND ASSUMPTIONS

4.1 Effective cloud fraction

The FRESCO+ effective cloud fraction is smaller than the geometric cloud fraction, because a Lambertian cloud albedo of 0.8 is used. This means that the effective cloud fraction is a radiometric cloud fraction for an optically thick cloud. The effective cloud fraction would become larger than 1 if the cloud in the pixel is brighter than 0.8. In this case the FRESCO+ cloud fraction is set to 1, and the cloud albedo is adjusted. The effective cloud fraction c can have small negative values ($-0.05 < c < 0$) from the Levenberg-Marquart fitting. This can happen for cloud-free scenes when the surface albedo from the database is higher than the actual surface albedo. In the fit the cloud fraction is allowed to vary between -0.05 and 1.1, in order to reach convergence. Because the simple cloud model and the surface albedo database are only an approximation of reality, we need some freedom in the allowed cloud fraction range to reduce the numerical problem. The change of the upper cloud fraction limit to 1.1 instead of 1, leads to a cloud pressure difference of less than 20 hPa; however, we cannot tell which pressure is more accurate. In the FRESCO+ output, the small negative values are clipped to 0.000, and the larger-than-1 values are clipped to 1.000. The FRESCO+ cloud fraction range in the output is therefore $[0, 1.0]$ ¹.


4.2 Cloud pressure

FRESCO+ uses a Lambertian cloud model, with no scattering inside and below the clouds. Therefore the cloud pressure in FRESCO+ is not the cloud top pressure. From the validation and comparison with DAK model simulations for scattering clouds we find: (1) FRESCO+ cloud height is lower than the cloud top height measured by Lidar/Radar or infrared passive satellite sensors such as MODIS. This has been found from validation with MODIS and Lidar/Radar measurements at the SGP/ARM site. (2) From DAK model simulations using scattering clouds we find that the FRESCO+ cloud height is close to the middle of the cloud or to the optical center of two-layer cloud systems. We note that FRESCO+ cloud height does not distinguish multi-layer clouds.

The FRESCO+ cloud pressure range is $[130.0, 1013.0]$ hPa². Cloud pressure is always lower than surface pressure and is higher than the pressure level of 15 km (which is 130 hPa in the MLS profile), because the altitude range for the LUTs is $[0, 15]$ km.

¹ The clipping to the range $[0,1]$ is not yet operational in the PPF.

² The clipping to the range $[130,1013]$ hPa is not yet operational in the PPF.

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4.3 Cloud albedo and pressure over snow/ice

In the snow/ice mode, FRESKO+ retrieves cloud albedo and cloud pressure. Actually these are scene albedo and scene pressure because FRESKO+ cannot separate between cloud and surface in this case. The scene albedo and pressure are parameters to be used in the air mass factor calculations for the trace gas retrievals. We do not recommend to use the cloud albedo and pressure over snow/ice for other purposes.

The retrieved cloud albedo in snow/ice mode should not be confused with the cloud albedo of 0.8. Especially for very bright scenes the scene albedo can have values > 0.8 .

4.4 Suggestions for application of the FRESKO+ cloud product

The FRESKO+ product is optimal for cloud correction in trace gas retrieval under the same Lambertian cloud assumption. This means that if one uses the FRESKO+ product as a cloud parameter in radiative transfer modelling for trace gas air mass factor (AMF) calculations, the cloud in the AMF calculations should be a Lambertian cloud, which will give the smallest error for the trace gas retrieval. We do not recommend to use FRESKO+ cloud fraction or cloud height directly if one assumes the cloud is a scattering media in the RTM model.


The FRESKO+ product can be used for determining cloud trends and variations on global or regional scales, using monthly averages.

4.5 Known problems and possible solutions

4.5.1 Surface albedo database

The surface albedo database derived from GOME (320 km x 80 km pixel size) is too coarse for SCIAMACHY and GOME-2. Therefore, some bright surface features such as mountains, hills in the Sahara desert show up in the global monthly mean maps of effective cloud fraction from SCIAMACHY. The same features will occur for GOME-2. The effect is not significant globally. However, one has to be careful with the effective cloud fraction data over bright surfaces, like deserts, where the surface albedo might be an issue.

A solution would be to make a new surface albedo database from GOME-2 itself. There is a sufficient amount of data (about 3 years) to make such a database.

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4.5.2 Snow/ice detection

Snow/ice is detected according to the TOMS surface albedo climatology (if $A_s \geq 0.2$ at 360 nm) or if $A_s \geq 0.8$ at 772 nm in the GOME albedo database. Therefore, FRESKO+ cannot detect snow/ice changes on a daily basis, especially at the places with lots of sea ice. The resolution of TOMS surface albedo database is also too coarse ($1^\circ \times 1^\circ$).

It is unlikely that snow coverage is assumed whereas in reality the scene is free of snow. On the other hand, it may occur that in reality snow coverage is present where no snow coverage is assumed. In that case, reflection by the surface is disguised by reflection by a low-level cloud layer. However, for the purpose of ozone column correction, this should have the same effect.

The solution could be to use other instruments on Metop for detecting snow/ice (AVHRR) or using the NISE snow/ice database for snow/ice detection.

4.5.3 Sun glint over ocean

FRESKO+ does not separate sun glint and real clouds. Therefore in the GOME-2 effective cloud fraction maps one can see the sun glint pattern in the eastern side of the swath. In trace gas retrievals the sun glint has a similar effect as clouds, namely an albedo effect. This can be corrected in the same way as clouds are corrected. It appears from FRESKO+ retrievals that the effective cloud fraction of sun glint is around 0.2, with a cloud pressure at surface pressure.

4.6 Additional suggestions for users of the FRESKO+ software

The previous sections were mainly focussed on the FRESKO+ principle and products. To implement the FRESKO+ software the following points have to be considered.

- 1) The FRESKO+ software does not have subroutines to read GOME-2 L1 data. Therefore the solar irradiance, earth radiance and the corresponding errors have to be provided as input.
- 2) The definition of relative azimuth angle can be different for different instruments. It can be checked by the calculation of sun glint position. For GOME-2 the sun glint should be at the east side of the swath over ocean, as can be seen from the effective cloud fraction maps. If the relative azimuth is wrong, the calculated sun glint position would be at west side of the pixels. The relative azimuth for the correct sun glint position is the correct one. The definition of the angles for GOME-2 is in the document "GOME-2 Level 1 product Generation Specification (EUMETSAT 2006)".

4.7 Range for FRESKO+ input and output parameters and exceptions

In Table 1 the settings and ranges of the input and output parameters for FRESKO+ are listed. A range is indicated by [,]. These settings hold for the FRESKO+ version at KNMI and at EUMETSAT (TBC).




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Table 1: Settings and ranges of FRESCO+ input and output parameters.

I/O/Code	Parameter	Value or range [,]	Comments
Input parameters	max. number of iterations in Levenberg Marquart fit	10	Usually 5 is enough
	Lambertian cloud albedo (not used if MIE_C1 is used)	Ac=0.800	In the code, Ac is reset to refl(1) if refl(1) > 0.8
	UV albedo threshold for snow/ice mode	uvalb=0.200	Detect snow/ice if (as360.ge.uvalb).or.(as758.ge.cldalb)
	minimum surface albedo 758 - 772 nm	asmin=0.010	if (as758.lt.asmin) as758=asmin if (as772.lt.asmin) as772=asmin
	first-guess effective cloud fraction	0.500	
	first-guess cloud top height [km]	5.000	
	first-guess cloud albedo	0.500	
	chi-square variation cut-off value	1.000e-5	
	error in simulated reflectivity	errsim=1.000e-2	Absolute error, the value can affect the fit especially when the fit is not good. sig(i) = errrefl(i) + errsim
	maximum allowed solar zenith angle	89.5	
maximum allowed measured reflectivity	4.5	If only nadir viewing, 1.5 is better	
Output parameters	Effective cloud fraction	c=[0, 1]	In the fit, c = [-0.05, 1.1] c=-1 indicates snow/ice mode
	Cloud pressure	pc=[surface pressure, 130 hPa]	Converted from cloud height zc [km] using fixed atmospheric profile (MLS).
	Cloud height (optional output)	[surface height, 15 km]	LUT is made up to 15 km
	Cloud albedo (for snow/ice mode)	[0, 1]	
Parameters inside the code	Errors of earthshine spectrum and irradiance spectrum	Read from L1 data	Absolute errors. erad, errorad: earthshine spectrum and its error. sirr, errsirr: solar irradiance spectrum and its error
	Error of reflectance	errrefl is calculated	errrefl(i)=refl(i)*sqrt((errorad(i)/erad(i))**2+(errsirr(i)/sirr(i))**2)
	Solar zenith angle SZA View zenith angle VZA	[28,89.5] deg [0,70] deg	Angles are defined at surface level. For definitions see Fig. 4 in appendix.

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	Rel. azimuth angle AZI	[0,180] deg	
	Surface albedo	Surface albedo database	If (as758.gt.refl(1)) as758=refl(1) and as772=refl(1)

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6. APPENDIX

In this appendix, the formulae for the FRESCO+ simulations of the O₂ A-band reflectance are given which is an update of the FRESCO formulae given by Koelemeijer et al. (2001).

6.1 Rayleigh scattering cross section and phase function

The Rayleigh scattering cross section, σ_R , is calculated with the formula (Bates, 1984):

$$\sigma_R = (32\pi^3 / 3N^2\lambda^4)(n_{air} - 1)^2 F'_K(air), \quad (A.1)$$


where $(n_{air} - 1)$ is the refractive index, and $F'_K(air)$ is the effective King correction factor. The effective King correction factors and refractive index for air are chosen at 750 and 800 nm from table 1 in Bates (1984), and are linearly interpolated between 750 and 800 nm.

The Rayleigh scattering phase function (without polarization) is given by,

$$F_R(\Theta) = \frac{3(1 - \rho_n)}{4(1 + \rho_n/2)} \left(\cos^2 \Theta + \frac{1 + \rho_n}{1 - \rho_n} \right), \quad (A.2)$$

$$\cos \Theta = -\cos \theta \cos \theta_0 + \sin \theta \sin \theta_0 \cos(\varphi - \varphi_0), \quad (A.3)$$

where Θ is the scattering angle, θ is the viewing zenith angle, θ_0 is the solar zenith angle, φ is the viewing azimuth angle, and φ_0 is the solar azimuth angle. ρ_n is the depolarization factor; at 750 nm $\rho_n = 0.02786$.

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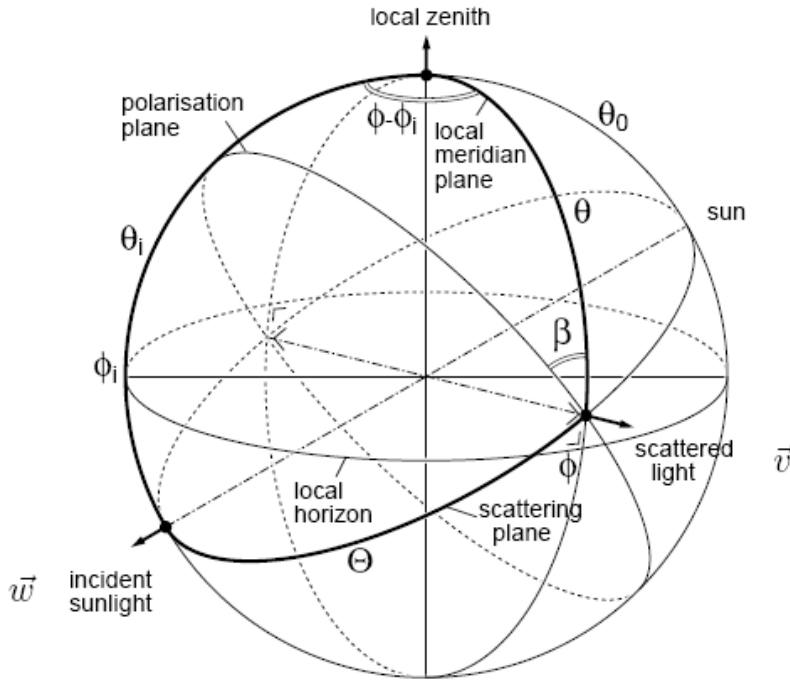


Figure 4. Definition of the solar and viewing geometry angles: SZA (θ_0), VZA (θ) and AZI ($\varphi - \varphi_i = \varphi - \varphi_0$) in FRESCO+. (Figure is from Tilstra et al., 2003)

6.2 Atmospheric optical thickness and transmission


The atmospheric optical thickness and transmission is determined by oxygen absorption and Rayleigh scattering. The absorption is calculated from the number density of O_2 molecules (n_{O_2}) and the O_2 absorption cross section, $\sigma_{O_2}(\lambda, T(z), P(z))$, along the light path; T, P are omitted from the notation from this point onwards. The absorption coefficient (in 1/m) is given by:

$$k_{abs}(\lambda, z) = n_{O_2}(z) \sigma_{O_2}(\lambda, z). \quad (A.4)$$

The Rayleigh scattering coefficient is calculated from the air density (n_{air}) and the Rayleigh scattering cross section ($\sigma_R(\lambda, z)$),

$$k_{sca}(\lambda, z) = n_{air}(z) \sigma_R(\lambda, z). \quad (A.5)$$

The total atmospheric optical thickness, τ , is the sum of the absorption and scattering contributions:

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$$\tau(\lambda, z_r, \theta, \theta_0) = \int_{z_r}^{\infty} (k_{abs}(\lambda, z) + k_{sca}(\lambda, z))(S_{sp}(\theta_0, z - z_r) + S_{sp}(\theta, z - z_r))dz, \quad (A.6)$$

Here: $S_{sp}(\theta_0, z - z_r)$ and $S_{sp}(\theta, z - z_r)$ are the spherical light path factors from the sun to the reflector and from the reflector to the satellite (Koelemeijer et al., 2001). z is height in the atmosphere, z_r is the altitude of the reflector (surface or clouds). θ_0, θ are the solar zenith angle and viewing zenith angle at surface height.

The transmission from TOA to z_r , assuming a reflector at altitude z_r , and back from z_r to TOA is now given by:

$$T(\lambda, z_r, \theta, \theta_0) = e^{-\tau(\lambda, z_r, \theta, \theta_0)}. \quad (A.7)$$

T is stored in a look-up-table.

6.3 Single Rayleigh scattering reflectance

The single Rayleigh scattering reflectance, R_R , is calculated with the formula (see Fig. 2) (Hovenier et al., 2005),

$$R_R(\lambda, z_r, \mu, \mu_0, \varphi - \varphi_0) = \frac{F_R(\mu, \mu_0, \varphi - \varphi_0)}{4\mu_0\mu} \int_{z_r}^{\infty} k_{sca}(z)T(\lambda, z, \mu, \mu_0)dz, \quad (A.8)$$


where $T(\lambda, z, \mu, \mu_0)$ is transmission, $\mu_0 = \cos\theta_0$, $\mu = \cos\theta$. We have to modify Eq. A.8 for the spherical light path:

$$R_R(\lambda, z_r, \theta, \theta_0, \varphi - \varphi_0) = \frac{F_R(\theta, \theta_0, \varphi - \varphi_0)}{4\cos\theta_0} \int_{z_r}^{\infty} k_{sca}(\lambda, z)T(\lambda, z, \theta, \theta_0)S_{sp}(\theta, z)dz. \quad (A.9)$$

Since we can neglect the wavelength dependence of the Rayleigh scattering phase function, F_R , in the O₂ A-band, we can multiply by the phase function in Eq. A.9 after the convolution with the slit function. Therefore the reflectances are stored in a look-up-table (LUT) as:

$$R_1(\lambda, z_r, \theta, \theta_0) = \int_{z_r}^{\infty} k_{sca}(\lambda, z)T(\lambda, z, \theta, \theta_0)S_{sp}(\theta, z)dz. \quad (A.10)$$

Another advantage of using Eq. A.10 is that the azimuth is not needed in the reflectance LUT, which now has the same parameters as the FRESCO+ transmission LUT. The factor

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$\frac{F_R(\theta, \theta_0, \varphi - \varphi_0)}{4 \cos \theta_0}$ is calculated in the FRESCO+ retrieval program according to the measurement geometry.

In the main text R_s and R_c are R_R for clear sky and cloudy cases, respectively. $R_c = R_R(\lambda, z_c, \theta, \theta_0, \varphi - \varphi_0)$, $R_s = R_R(\lambda, z_s, \theta, \theta_0, \varphi - \varphi_0)$, where z_c is the altitude of the cloud, and z_s is the surface height.