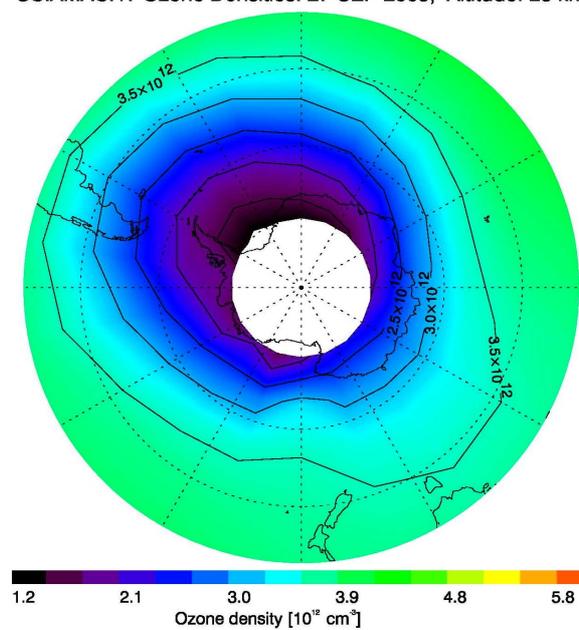# Algorithm document for SCIAMACHY *Stratozone* limb ozone profile retrievals

Date of origin: February 6, 2006

SCIAMACHY Ozone Densities: 27-SEP-2005, Altitude: 28 km

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1. Forward Model

The forward radiative transfer model used is the SCIARAYS model [*Kaiser and Burrows*, 2003]. It takes two orders of scattering into account and considers the sphericity of the atmosphere and atmospheric refraction. The atmosphere is assumed to be cloud-free. Stratospheric aerosols are taken into account as described in detail in the auxiliary data section.

2. Inversion Procedure

The ozone profile retrieval method employed here follows the method developed to retrieve stratospheric ozone density profiles from limb scattering measurements performed with SOLSE/LORE (Shuttle Ozone Limb Sounding Experiment/Limb Ozone Retrieval Experiment) [*Flittner et al.*, 2000], two limb viewing spectrometers flown on NASA's space shuttle mission STS-87 in 1997. A similar approach is also applied for operational ozone profile retrievals [von Savigny et al., 2003; Petelina et al., 2004] from limb scattering measurements with the OSIRIS (Optical Spectrograph and InfraRed Imager System) [Llewellyn et al., 1997] instrument on the Swedish-led Odin satellite. The method exploits the differential absorption between the center (λ_1 = 600 nm) and the wings (λ_2 = 525 nm/λ_3 = 675 nm) of the Chappuis absorption bands of ozone. Limb radiance profiles $I(\lambda_1,\text{TH})$ at these wavelengths are normalized with respect to a reference TH of TH_{ref} = 43 km: $I_N(\lambda,\text{TH}) = I(\lambda,\text{TH}) / I(\lambda,\text{TH}_{ref})$. The normalized limb radiance profiles are then combined to the Chappuis retrieval vector

$$\mathbf{y}(\text{TH}) = I_N(\lambda_1,\text{TH}) / (I_N(\lambda_2,\text{TH}) \times I_N(\lambda_3,\text{TH}))^{1/2}$$

which is fed into a non-linear Newtonian iteration version of optimal estimation (OE) [*Rodgers*, 1976] driving the spherical radiative transfer model SCIARAYS [*Kaiser and Burrows*, 2003]. SCIARAYS is not a full multiple scattering (MS) model, but takes 2 scattering orders into account. Yet, it was found that even with a single scattering (SS) model the retrieval errors are less than 2 % at and above the ozone density peak altitudes. Below

the ozone density peak the relative retrieval errors are bigger, but the absolute retrieval errors were found to be always lower then 2×10^{11} cm^{-3}. Since the contribution to the total limb radiance from the third and higher scattering orders is small compared to the first two orders, using only two scattering orders will result in retrieval errors of a few percent at the most within the 15 to 35 km altitude range. The altitude range between about 15 to 35-40 km is accessible with this technique. Below 15 km the line of sight optical depth becomes so large, that these altitudes cannot be "seen" from space in limb geometry, and above 35-40 km the absorption in the Chappuis bands becomes too weak.

The most recent versions of the Stratozone ozone profiles (i.e., versions 1.62 and 1.63) are also corrected for limb pointing errors using the tangent height retrieval code TRUE (Tangent height Retrieval by Uv-b Exploitation) [*Kaiser et al.*, 2004] Version 1.4.

The measurement covariance matrix is chosen to be diagonal with a standard deviation of 1%. The *a priori* covariance matrix is non-diagonal with exponentially decaying correlations between the altitude layers and a correlation length of L = 5 km. The standard deviation of the diagonal elements corresponds to 60 % of the *a priori*. Further information on the retrievals can be found in *von Savigny et al.* [2005a].

3. Auxiliary Data

The *a priori* ozone profile climatology is the UGAMP climatology [*Li and Shine*, 1995].

The surface albedo data base by *Matthews* [1984] is employed in the forward radiative transfer calculations. Furthermore, the empirical aerosol extinction profile model ECSTRA, originally developed by *Fussen and Bingen* [1999] for GOMOS stellar occultation measurements of atmospheric minor constituent profiles is employed here. In limb scattering geometry not only the aerosol extinction profiles are relevant, but also knowledge of the aerosol scattering phase function. For the retrievals a standard GOMETRAN stratospheric sulphate aerosol scattering phase function corresponding to a 75% H_2SO_4 / 25% H_2O mixture is used [*Rozanov et al.,* 1997].

4. Sensitivity and Error Analysis

von Savigny et al. [2005c] presented a comprehensive sensitivity analysis for ozone profile retrievals from limb scatter measurements with the Odin/OSIRIS instrument (Optical Spectrograph and InfraRed Imager System) using the same methodology. Although the instrument specific error contributions may differ between SCIAMACHY and OSIRIS ozone measurements, the fundamental issues, i.e. sensitivity to ground albedo, tropospheric clouds, stratospheric aerosols and pointing errors are identical. The total estimated error assuming a tangent height error of less than 500 m varies between about 8 % and 14 % within the 15 to 40 km altitude range, with incorrect knowledge of ground albedo, cloudiness and stratospheric aerosols as well as tangent height errors being the main sources of error. For SCIAMACHY ozone profile retrievals the main source of error are errors in the tangent height registration. An overview of the spatial and temporal variation of the SCIAMACHY limb pointing errors was given by *von Savigny et al.* [2005b].

5. Algorithm validation

The algorithm used is based on the algorithm originally developed by *Flittner et al.* [2000] and applied to SOLSE/LORE limb scatter measurements. It has then been implemented for the operational retrieval of ozone profiles from OSIRIS limb scattering observations [*von Savigny et al.*, 2003], and reliably delivers ozone profiles with very good vertical resolution (2 km). *Petelina et al.* [2004] showed that the retrieved OSIRIS profiles in most cases agree well within 10 % with coincident POAM III Ozone profile measurements. For the majority of months compared the agreement between 20 km and 32 km is better than 5 %.

The error estimate of about 8-14 % (allowing for a 500 m pointing error) is in good agreement with the comprehensive validation study published by *Brinksma et al.* [2005]. The authors

found agreement of the Stratozone (version 1.61 with a systematic –1.5 km tangent height correction) with Lidar and SAGE II solar occultation measurements within 3 – 6 % between 20 and 35 km with a standard deviation of 10 %. Note, that for individual comparisons the differences may be significantly larger.

Therefore, the algorithm has been tested for and applied to several satellite instruments (SOLSE/LORE, Odin/OSIRIS, SAGE III, and SCIAMACHY) and produced stratospheric ozone profiles of good quality.

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