ATMOSPHERIC TRACE GAS SOUNDING WITH SCIAMACHY

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ABSTRACT

SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric CHartographY) is a contribution to the ENVISAT-1 satellite, which is to be launched in late 2000. The SCIAMACHY instrument is designed to measure sunlight transmitted, reflected and scattered by the Earth's atmosphere or surface. The instrument measures simultaneously from the UV to the NIR spectral spectral region (240 – 2380 nm). Observations are made in alternate nadir and limb viewing geometries and also for solar sunrise and lunar moonrise occultation. Inversion of the SCIAMACHY measurements will provide the following: the amount and distributions of some important trace gases O_3, BrO, OClO, ClO, SO_2, H_2CO, NO_2, CO, CO_2, CH_4, H_2O, N_2O, p, T, aerosol, and radiation flux profiles, cloud cover and cloud top height. Combination of the near simultaneous limb and nadir observations enables the tropospheric column amounts of O_3, NO_2, CO, CH_4, H_2O, N_2O, SO_2, and H_2CO to be detected. SCIAMACHY will provide new insight into the global behaviour of the troposphere and the stratosphere.

INTRODUCTION

SCIAMACHY (Scanning Imaging Absorption Spectrometer for Atmospheric Chartography) is a space-based spectrometer designed to measure both the extraterrestrial irradiance and sunlight which is transmitted, reflected or scattered by the Earth's atmosphere or surface. It will provide information about the amounts and distribution of numerous atmospheric constituents by inversion of the ratio of the upwelling radiance to the extraterrestrial irradiance. The instrument was proposed in 1988 by the SCIAMACHY Science Team (Burrows *et al.*, 1988). SCIAMACHY is funded by Germany, The Netherlands, and Belgium as a national contribution to ESA's ENVISAT-1 satellite which will be launched in late 2000. A smaller version of SCIAMACHY, the Global Ozone Monitoring Experiment (GOME), is currently operating successfully on the ERS-2 satellite (see e.g. Burrows *et al.*, 1999).
SCIAMACHY will measure both the solar irradiance and the Earthshine radiance continuously between 240 nm and 1750 nm and at two spectral windows in the NIR (1940 nm to 2040 nm and 2265 nm to 2380 nm) with a high radiometric accuracy and spectral stability. The characteristics of the SCIAMACHY instrument are summarised in Table 1. A picture of the SCIAMACHY Optical Bench Module is shown in Figure 1.
The primary scientific objective of the SCIAMACHY mission is to improve our global knowledge and understanding of the Earth's atmosphere from the mesosphere to the troposphere. This will enable the origin of any changes in atmospheric composition, resulting either from anthropogenic activity or natural phenomena, to be established. As ENVISAT will fly during the period when it has been predicted that the stratospheric halogen loading will decrease, a special emphasis will be placed on the investigation of stratospheric ozone (with foci on the behaviour of the 'ozone hole' and on mid-latitude ozone). One unique application for SCIAMACHY is the global study of tropospheric pollution arising from both industrial activity and biomass burning. Similarly the observation and interpretation of

Table 1. Characteristics of the SCIAMACHY Instrument

UV-Vis-NIR imaging double spectrometer, cooled and temperature stabilised	
Spectral range	240 – 2380 nm
Spectral resolution	0.2 – 1.5 nm
Straylight suppression	$< 10^4$
Relative radiometric accuracy	$< 1\%$
Absolute radiometric accuracy	< 2–4%
Spectral stability	0.015 – 0.005 nm
Dynamic range	$10^7 - 10^8$

special events like volcanic eruptions, solar proton events, and related regional and global phenomena will be of great importance.

This study describes the SCIAMACHY data products and aspects of the algorithms used to derive these products. A more detailed description of the instrument and the mission can be found in Burrows *et al.* (1995) and Bovensmann *et al.* (1999).

MEASUREMENT STRATEGY

SCIAMACHY will perform measurements in nadir, limb, and solar/lunar occultation geometry.

In nadir mode the atmospheric volume directly under the instrument (i.e. the spacecraft) is observed. The spatial resolution of nadir observations depends on the solar geometry, i.e. the intensity of the incoming light, and its spectral range. For all major atmospheric constituents, a typical spatial resolution of ≈ 60 km $\times$ 30 km (across/along track) will be achieved.

In limb mode the instrument observes the edge of the atmosphere. At different tangent altitudes scans of up to 960 km in horizontal across track direction will be performed having a vertical resolution of approximately 3 km.

As can bee seen from Figure 2, alternating limb and nadir measurements will cover the majority of the sunlit part of the orbit. This strategy is intended to provide an optimal amount of information from the lower atmosphere. This approach is discussed in more detail below.

During each sunrise solar occultation measurements will be performed. The same geometry as in limb mode will be used, but with the sun in the instrument's field of view. The vertical resolution will be similar to the limb case. As the ENVISAT-1 orbit will be sun-synchronous, solar occultation measurements will cover a latitudinal range at the tangent points between 90°N and 65°N over the year. When the moon is visible for SCIAMACHY (which will be the case for about one week per month) lunar occultation measurements will also be performed every second orbit. These measurements will cover latitudes between 30°S and 90°S. On the eclipse side several calibration measurements will be performed, including dark current measurements and measurements with the on-board lamps. The measurement pattern described above will result in a global coverage at the equator after 6 days.

RETRIEVAL METHODS

This section provides a short overview of the retrieval methods which have been proposed for application to SCIAMACHY data to derive atmospheric information from the measured spectra. Details about the operational algorithms are laid down in the Algorithm Theoretical Baseline Document (Spurr, 1998).

DOAS

The concept underlying the Differential Optical Absorption Spectroscopy (DOAS) is the separation of the measured signal into slowly varying components, which result from Rayleigh and Mie scattering and broadband absorption, and a rapidly varying component, comprising the differential absorption structures. The broadband spectral features are approximated by a low-order polynomial, which is subtracted from the data. Differential reference cross sections are then fitted to the resultant spectrum for selected wavelength regions. This results in the so-called slant column (i.e. the density integrated along the mean light path) which may be converted into a vertical total column density by the use of an air mass factor (AMF) derived from a radiative transfer calculation. DOAS is only appropriate for regions

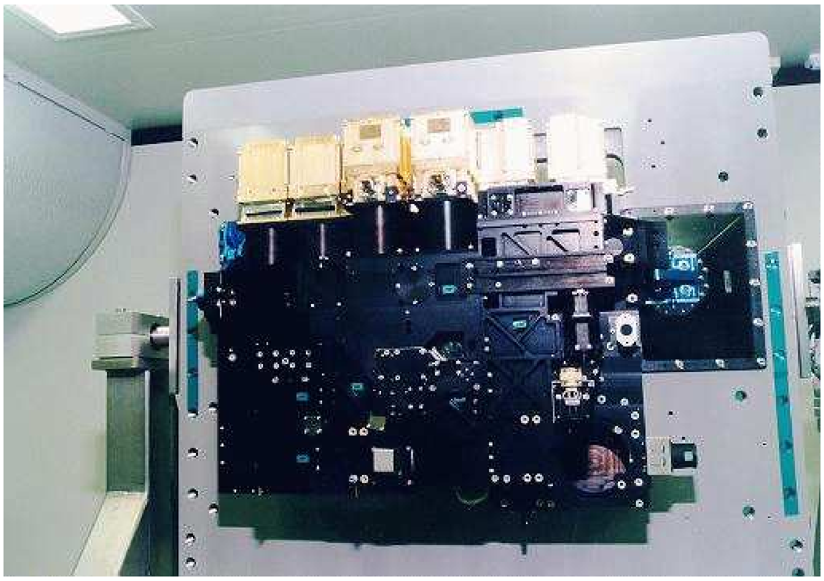

Fig. 1. SCIAMACHY Optical Bench Module.

having relatively weak absorptions where the AMF is to a good approximation constant. The main application of DOAS is the derivation of total columns. DOAS was originally developed for long path tropospheric observations (see e.g. Brewer *et al.*, 1973; Perner and Platt, 1979) but it has proven to be applicable also for both ground based zenith sky and space-based nadir measurements (Burrows *et al.*, 1999). DOAS is a generic term, originally applied to UV spectral region. However the general approach or its optimised variants are equally successful assuming the above limitations in visible or infrared spectral windows.

<u>FURM</u>

The <u>FU</u>ll <u>R</u>etrieval <u>M</u>ethod (FURM) uses a radiative transfer model to calculate the radiance for a specific atmospheric state and viewing geometry. Subsequently in the inversion, this radiance is matched in an iterative procedure to the measured radiance by modification of selected atmospheric parameters. The retrieval of height resolved information from nadir sounding UV sensors was first proposed by Singer and Wentworth (1957). It was successfully exploited by the SBUV instruments (Bhartia *et al.*, 1996). This method is based on the wavelength dependence of the penetration depth of light within the atmosphere. During the development of the SCIAMACHY proposal the potential use of the temperature dependence of the Huggins bands to provide more information about O_3 in the lower atmosphere was suggested (see e.g. Chance *et al.*, 1991, 1997, for a discussion of this approach). In practice the vertical resolution of a trace gas profile from such retrievals is determined by the effective penetration depth of light in the atmosphere, the a-priori or inferred knowledge of atmospheric temperature and pressure profiles, and the signal to noise of the instrument (see e.g. Rozanov *et al.*, 1992; Munro *et al.*, 1992). The FURM and similar algorithms have been applied successfully to GOME data using GOMETRAN (Rozanov *et al.*, 1997) as the favoured radiative transfer model (Eichmann *et al.*, 1997; Munro *et al.*, 1998). These algorithms attempt to use the full information content within the data. This is limited by radiative transfer through the atmosphere and instrumental noise. As a result of its inherent flexibility the FURM approach may also be used for stratospheric/upper tropospheric profiles from limb and occultation measurements (limited by the presence of clouds) and for the retrieval of other atmospheric parameters such as information about aerosols and clouds. FURM calculations are in general rather time consuming, and they require a-priori information from climatological data bases. Therefore FURM will only be used for scientific case studies. For a more detailed description of the FURM approach and an application to GOME data see Hoogen *et al.* (1999).

<u>Limb and Occultation Profile Retrieval</u>

Two approaches for retrieval of vertical profiles from limb or occultation geometry are currently under consideration. The first and probably most accurate method is the ‘global fitting’ approach in which modelled radiances are iterated

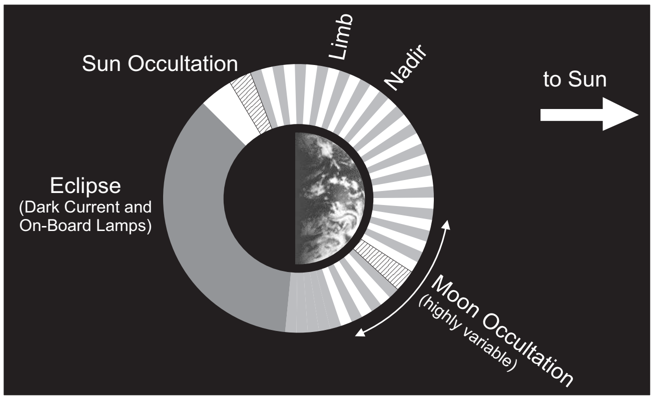

Fig. 2. Typical sequence of SCIAMACHY measurements performed during one orbit.

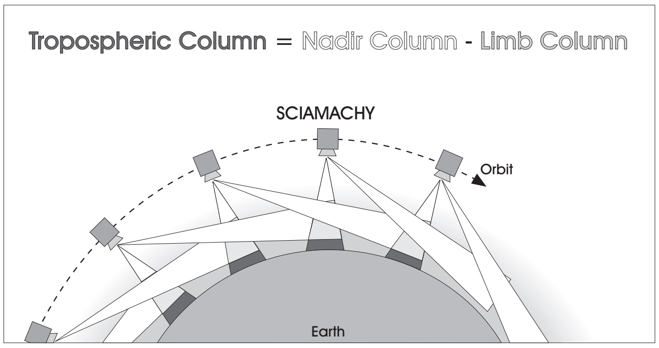

Fig. 3. Derivation of tropospheric columns.

to match the measured values simultaneously for all atmospheric layers. The second method is the 'onion peeling' approach in which each limb measurement is fitted individually starting from the top of the atmosphere. Subsequently, the columns of the lower layers are computed considering the results for the upper layers. 'Onion peeling' is probably computationally faster than 'global fitting' but less favoured because contributions to the measured spectrum from altitudes below the tangent height are not considered. However, as algorithm development for limb and occulation profile retrieval is still in an early phase, both the 'onion peeling' and 'global fitting' options are kept open.

Tropospheric Columns

The derivation of tropospheric columns from SCIAMACHY will be performed by subtracting the stratospheric column derived from limb measurements from the nadir total column (see Figure 3). This approach is similar to the residual technique used to determine tropospheric ozone columns from the combination of TOMS total nadir columns with SAGE II occultation profiles or SBUV nadir profiles (Fishman *et al.*, 1990, 1996). Using the alternating limb/nadir scheme described above almost the same atmospheric volume is observed by the same instrument within 8 min first in limb and then in nadir viewing geometry. This strategy minimises two important sources of systematic error for tropospheric measurements. As a result it will be possible to derive tropospheric columns down to the scattering layer (Earth's surface or the cloud top) not only for O_3 but also for NO_2, CO, CH_4, H_2O, N_2O, SO_2, H_2CO, and BrO.

OPERATIONAL DATA PRODUCTS

All operational data products will be regularly processed, quality controlled and archived. The SCIAMACHY operational products are structured in different levels. From the raw Level 0 data (counts as function of pixel position) calibrated radiance and irradiance spectra are calculated; these Level 1 data serve as input for the retrieval models which extract the geophysical information, e.g. columns/profiles of atmospheric trace gases. These are Level 2 data. An overview on SCIAMACHY operational Level 2 trace gas products and their potential precision is given in Table 2. These precision estimates are based on several sensitivity studies performed by a number of people over the last years. This is explained more deeply by Bovensmann *et al.* (1999). The values given are supported by previously unpublished estimates of precisions based on recent studies undertaken at the University of Bremen (M. Buchwitz, private communications) which assume that the total information content in the spectra is used. Therefore these estimates represent an upper limit of the data product precision. Atmospheric pressure and temperature profiles and information about aerosols and clouds will also be retrieved on an operational basis. For the aerosol data product it is forseen to generate an absorbing aerosol index (AAI) and an aerosol optical thickness (AOT) value using experiences from GOME aerosol retrieval (see e.g. Guzzi *et al.*, 1997, 1998; Koppers *et al.*, 1997; Popp *et al.*, 1997).
There will be two types of operational data products: Near Real-Time (NRT) and Off-Line (OL) products. NRT data products will be available within a few hours after the measurements. OL data products will be produced using improved ancillary data that become available after spectrum acquisition, e.g. analysed temperature and pressure fields. The NRT data processor will be installed at ESA's ground stations (Kiruna, Frascati) and as a reference system at DLR-DFD. The OL processor will be hosted by DLR-DFD. All trace gas products listed in Table 2 will be available

Table 2. SCIAMACHY Operational Trace Gas Products and Precision Estimates

Molecule	Total Columns	Stratospheric Profiles	Molecule	Total Columns	Stratospheric Profiles
O_3	1 %	10 %	N_2O	5 %	10 %**
NO_2	2 %	10 %	CO	5–10 %	10 %**
H_2O	1 %	10 %	BrO	5 %	50 %**
CO_2	1 %	10 %	SO_2*	10 %	—
CH_4	1–3 %	10 %	OClO*	20 %	—
			H_2CO*	20 %	—

* observed under special conditions (tropospheric pollution, ozone hole)

** recommended by scientists, under negotiation with agencies

as OL data. In addition, NRT total columns will be computed for all listed gases except for CO_2. There will be no NRT limb retrievals.

In addition, scientific products from occultation and limb measurements (e.g. O_2, $O_2(^1\Delta_g)$, NO, and ClO) and derivation of higher level products (such as tropospheric columns) are planned from process studies on a non-operational basis.

SUMMARY

SCIAMACHY is a space-based spectrometer measuring almost continuously from the UV to NIR spectral region in nadir, limb, and occultation geometry. It will provide highly-resolved radiance and irradiance spectra and mesospheric/stratospheric profiles/columns of O_3, NO_2, H_2O, CO_2, CH_4 N_2O, BrO, CO, O_2, $O_2(^1\Delta_g)$, and NO. SO_2, H_2CO, ClO, OClO profiles/columns may be derived under special conditions. Moreover, information about clouds, aerosols, atmospheric temperature and pressure will be obtained.

The combination of near-simultaneous nadir and limb measurements will provide tropospheric columns of O_3, NO_2, CO, CH_4, H_2O, N_2O, SO_2, H_2CO, and BrO down to the Earth's surface or the cloud top.

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