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Validation of SCIAMACHY in-flight measured irradiances, radiances and selected ENVISAT tracegas products by comparison with measurements from independent satellite instruments

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ABSTRACT

A prerequisite for achieving a sufficient quality of high-level data products, particularly trace gas concentrations, is the radiometric calibration and characterisation of SCIAMACHY. The major aim of this project is thus the validation of SCHIAMACHY solar irradiance and limb and nadir radiance measurements (level-1 operational data products) by comparison with independent satellite measurements (SOLTICE, SUSIM, OSIRIS) and radiative transfer calculations during the first two years of operation in space. In addition, selected trace gas profiles (O_3, NO_2, H_2O, CH_4, and OClO) and total columns (O_3 and NO_2) from SCHIAMACHY, and in addition from GOMOS and MIPAS, are to be validated with other space borne sensors (GOME, HALOE, SAGE II, TOMS and SABER) in order to assess the level-2 data retrieval accuracy and its dependence on the radiometric calibration of the level-1 spectral data. The validation of both level-1 and level-2 data products in combination forms the baseline for the evaluation of all higher-level data products. The results from this project shall provide the required information to modify the level 1 and level 2 data processing in order to guarantee the high quality of the SCIAMACHY data products during the entire ENVISAT mission.

INTRODUCTION

The three ENVISAT instruments GOMOS, MIPAS, and SCIAMACHY provide information of a large family of trace constituents, which play an important role in atmospheric chemistry and in climate change issues. A prerequisite of scientific use of the trace gas data is to achieve a high accuracy in the derived trace gas products. Spectral data (level 1b data) are inverted to derive trace gas concentration profiles and columns using different techniques depending on the viewing geometry and wavelength range. The quality of higher level data products critically depends on good radiometric and polarimetric characterisation of the spectrometer before launch on ground (pre-flight calibration) and during the entire lifetime of the instrument (dynamic inflight calibration and characterisation). This is the most important requirement for the usefulness of satellite data for long term monitoring of atmospheric species. Currently several high quality solar irradiance data are available which can be utilised for the comparison with SCIAMACHY. The use of independent satellite measurements to validate SCIAMACHY trace gas products has the great advantage that the pole-to-pole coverage for all seasons is available and that the validation activities are not limited to a certain period and location. Nadir and limb viewing instruments (GOME (the Global-Ozone-Monitoring-Experiment), TOMS (Total Ozone Mapping Spectrometer), SCIAMACHY, SBUV-2 (second generation of Solar Backscatter UV irradiance) cover the entire surface within a few days, the exact number of days depending on the across-track scanning angle and the altitude of the satellites. For instance, GOME is operating from an altitude of about 800 km (near polar orbit) and has a maximum scan angle of 32°, thus the entire earth surface is scanned after three days [1]. SCIAMACHY achieves global coverage after six days combining the limb and nadir observations [2]. Solar occultation measurements have a repeat cycle of slightly more than a month (HALOE (Halogen Occultation Experiment) and SAGE II (Stratospheric Aerosol and Gas Experiment II Instrument)). All latitudes are covered within a month period.
In this study primarily SCHIAMACHY level 1 and level 2 data (Table 1) will be validated with the use of independent established satellite instruments. Later on the same SCHIAMACHY data products will be intercompared to some other new satellite instruments. In addition to that, some level 2 data products of the two other ENVISAT instruments, GOMOS and MIPAS, will be validated and intercompared to the same independent satellite instruments. These validation activities will result in recommendations for improving level-1 and level-2 data processing and will benefit future satellite projects such as the second and third generation of GOME aboard METOP (launches in 2003 and 2008). This paper gives an overview over the workplan and techniques used in the validation and intercomparison.

Table 1: Operational SCIAMACHY data products which will be validated in this study

Level 1 products	Level 2 products
Limb/nadir radiances	Trace gas profiles (O_3, NO_2, H_2O, CH_4, OClO)
Solar irradiances	Total columns (O_3, NO_2)
Polarisation measurements	

WORK PLAN OF SATELLITE VALIDATION

Level 1 data validation

There are several different types of SCIAMACHY Level 1 products, solar irradiances, earthshine radiances (measured in both limb and nadir viewing geometry), and the fractional polarisation of the radiance. Furthermore, SCIAMACHY will perform solar and lunar occultation measurements. Because SCIAMACHY measurements cover a large spectral range, from the UV to the NIR, several calibration sources have to be considered including on-ground and satellite based measurements (Table 2) as well as theoretical calculations. All calibration activities will be performed on a case-study basis. For comparison, all reference data have to be transformed to the same spectral resolution and geophysical conditions (e.g. distance Earth-Sun, solar cycle).

Solar Irradiance

SCIAMACHY solar irradiances are important as a reference for earthshine measurements and provide highly accurate solar spectra over the large wavelength range of 240 - 2400 nm which are linked to the radiometric standard of GOME (Global Ozone Monitoring Experiment) and SBUV (Solar Backscatter UV irradiance) type instruments. This large spectral region is currently not covered by any other individual space-borne instrument. Therefore it is planned to use in addition to satellite sensors McMath-Pierce Fourier Transform Spectrometer solar irradiance measurements obtained at the Kitt Peak National Solar Observatory as a solar irradiance validation source [3]. These data cover the whole spectral range of SCIAMACHY and are available via ftp from the National Solar Observatory Digital Library. A high-resolution solar spectrum by Kurucz based on Kitt Peak data is also part of the MODTRAN distribution [4]. The probably most promising validation source for SCIAMACHY is GOME. Solar irradiance and radiance measurements of GOME cover the same UV and visible wavelength region and have approximately the same spectral resolution as corresponding measurements by SCIAMACHY. This comparison will link SCIAMACHY measurements to the radiometric standard of GOME and SBUV type instruments. Other satellite based measurements (e.g. daily UV measurements of SOLSTICE (Solar-stellar irradiance comparison experiment) or SUSIM (Solar Ultraviolet Spectral Irradiance Monitor)) will also be considered, depending on the availability of these data during the SCIAMACHY mission.

Nadir Radiance

Because of the high variability of observed ground scenes the calibration of nadir radiances is difficult. GOME measurements are planned to be used for similar ground pixels in the calibration of SCIAMACHY nadir radiances; because of its similarity both in design and observational geometry to SCIAMACHY GOME provides the best possibility to produce comparable data. Fig. 1 shows an example of earthshine radiance spectra measured by GOME. In the infrared part of the spectrum which is not covered by GOME measurements, model calculations shall be performed using the spherical and pseudo-spherical radiative transfer codes CDI [5] and SCIATRAN, the latter an extension of the GOMETRAN model [6].

Limb Radiance

SCIAMACHY limb radiances shall be compared with limb measurements by the OSIRIS (Optical Spectrograph and InfraRed Imager System) instrument. OSIRIS is part of the payload of the Swedish satellite ODIN and consists of an imaging spectrograph covering the spectral range between 280 nm and 800 nm and three near-infrared telescopes operating at 1.27 micrometers. The optical resolution is about 1 nm in the UV-VIS wavelength region and 10 nm in the IR. A sequence of IR limb radiance as a function of tangent height is shown in Fig. 2.

Table 2: Data products of Level 1 validation measurements by comparison with various satellite sensors and their expected accuracy, spectral range, and vertical resolution [1], [6-11]

Instrument	Data Products	Accuracy	Range	Resolution
GOME	Irradiance	3-5%	240-795 nm	0.2-0.4 nm
	Nadir Radiance	-	-	-
OSIRIS	Irradiance	≈ 5%	280-800 nm	1-2 nm
	Limb Radiance		15-60 km	>1 km
SBUV-2	Irradiance	<3%	240-400 nm	1.1nm
SOLSTICE	Irradiance	<3%	240-400 nm	0.2 nm
SUSIM	Irradiance	<3%	240-400 nm	1.1 nm
SAGE III	Occultation Radiance		280-1030 nm	1-2 nm

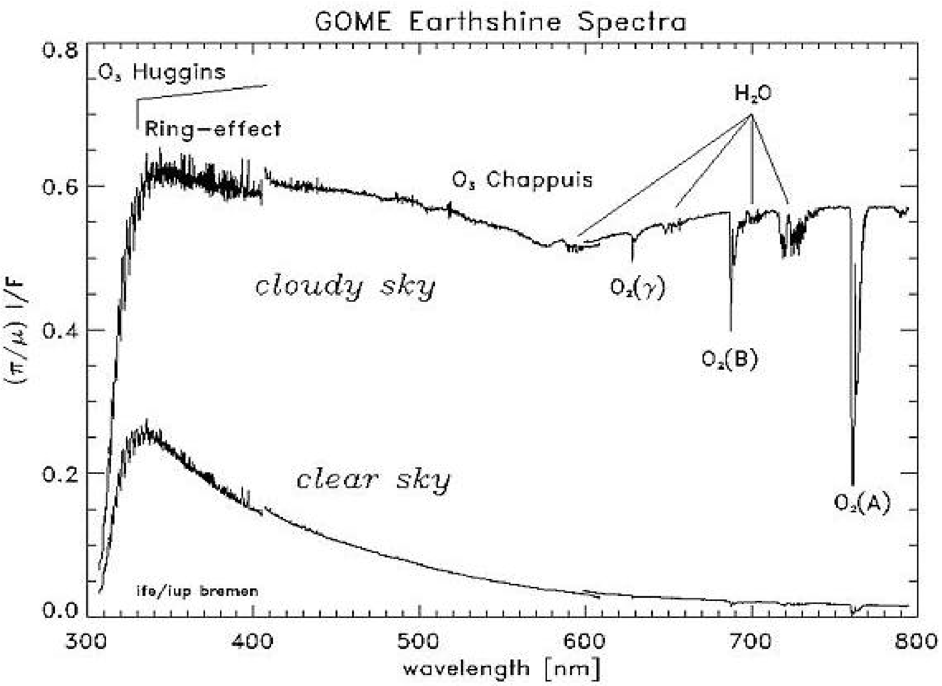

Fig. 1: Example of earthshine spectra measured by GOME [1]

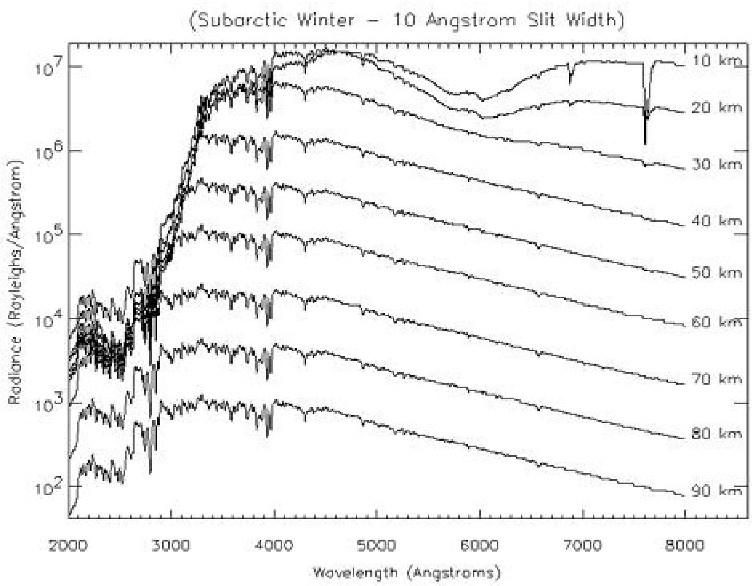

Fig. 2: Typical on-orbit limb spectra that will be measured with OSIRIS. These spectra were calculated using the MODTRAN code for high latitude winter conditions and convolved with a 10 Angstrom slit function (Picture by Univ. Saskatchewan).

In order to gain information about spectral regions covered by SCIAMACHY but not by OSIRIS, radiative transfer model calculations with CDI and/or SCIATRAN shall be performed.

Solar Occultation

Solar and lunar occultation spectra of SCIAMACHY can be directly compared with equivalent spectra provided by SAGE III (the Stratospheric Aerosol and Gas Experiment III Instrument; [12]). The spectral resolution is about a factor of five smaller than that of SCIAMACHY.

Polarisation

Because no internal light source of well-known polarisation is available, a direct in-flight monitoring of the polarisation properties of the instrument is not feasible. Therefore, only cross-checks using natural atmospheric sources of polarised light can be performed. Several possibilities to verify the polarisation correction shall be investigated:

1. a theoretical study shall show if and how limb measurements may be used in this context. The main idea is to take limb measurements for tangent altitudes above about 30 km, i.e. altitudes where Rayleigh scattering dominates and the polarisation characteristics can be calculated. However, it has to be considered that light from below the tangent altitude contributes to the limb signal because of multiple scattering effects.
2. looking at moon occultation spectra, which should show a polarisation as a function of lunar phase. Since the relation between lunar phase and polarisation is currently not sufficiently known, a lunar polarisation data base from the SCIAMACHY data themselves have to be build up before performing such an analysis.
3. using the fact that the sun is a non-polarised light source for polarisation cross checks. For observations of the direct sun above the atmosphere, which are e.g. performed regularly at the end of the solar occultation window, the polarisation correction algorithm should then yield a fractional p of 0.5. Unfortunately, the unpolarised nature of the sunlight is already used in the operational 0-1b processing, so that this cross check will be of limited use only.

Level-2 Data Validation

For the validation of level-2 data products satellite data from GOME/ERS-2, HALOE/UARS, SAGEII/ERBS, TOMS/ Earthprobe will be available; intercomparisons of these data are planned to the new satellite instruments SABER/TIMED, QuikTOMS/Taurus and SBUV2/NOAA-16 which have been recently launched or will be in the near future. Table 3 gives a summary of the data products to be validated by comparison with the various satellite sensors and the expected accuracy.

Level 2 trace gas validation with coincident independent satellite measurements will be carried out during all major validation phases as defined by ESA (Table 4). Monthly means and seasonal dependencies will be determined and synoptic mapping will be used. Before launch of SCIAMACHY a database of satellite data used for calibration is created and algorithms to find coincidences between SCIAMACHY and the other instruments are developed. The trajectory model to identify the collocation of air masses will be optimised. During the core validation phase (commissioning phase) comparison to other satellite instruments will concentrate on those validation instruments which have after many years of operation and several algorithm upgrades achieved a high quality standard in their data products. These are mainly GOME, TOMS, the UARS instruments HALOE and SAGE II. The results of these validations will be concluded in recommendations for improving trace gas retrieval. During the main validation phase and long term validation phase (starting thereafter) the list of validation instruments will be extended to the new instruments, which have been or will be launched close to ENVISAT launch time. The new instruments available for trace gas cross correlation studies are, except for SAGEIII aboard METEOR3 which will be used for validation by [12], SABER/TIMED, QuikTOMS and SBUV2/NOAA-16.

Table 3: Altitude, measurement type, accuracy, range and vertical resolution of validation measurements [1],[9],[13-17]

Instrument	Data Products	Altitude	Measurement type	Accuracy	Range	Resolution
GOME	O_3, NO_2 columns	800 km	nadir	5-15%	-	-
	O_3 profiles			10%	0-50 km	6-10 km
HALOE	O_3, NO_2, CH_4, H_2O profiles	585 km	occultation	10-20%	15-60 km	>2.5 km
SAGE II	O_3, NO_2, H_2O profiles	610 km	occultation	5-15%	15-60 km	>2 km
TOMS	O_3 columns	500 km	nadir	5%	-	-
SBUV-2	O_3 profiles	870 km	nadir	10%	5-60 km	6-10 km
SABER	O_3, H_2O profiles	625 km	limb	10-15%	15-65 km	2 km
TOMS-5	O_3 columns	800 km	nadir	5%		

In the long term validation phase validation and intercomparison activities are continued in order to assess the data quality and to document improvements of updates of the retrieval algorithms. A data base for quick evaluation of algorithm development progress will be created which may be used after future regular updates of operational algorithms. In addition, a scientific case study on the ozone chemistry and dynamics in the northern hemisphere will be carried out using ozone concentrations from the ENVISAT observations and trajectory models in order to determine chemical depletion rate of ozone for the three arctic winters 2001-2003.

Identifying collocated measurements
Since GOME/ERS-2 and ENVISAT are flying within the same orbit only 30 minutes a part, results will be easily comparable. However, the different observation geometry of the various ENVISAT instruments have to be considered. The simplest method for deriving collocations for comparisons between data of two different satellites is to look for *coincident measurements*. Two measurements are defined as coincident if they were taken within a certain time and within a certain distance to each other. Work has already been conducted where ozone profiles from GOME were compared to HALOE [18]. In this study coincident measurements of the two satellite instruments were taken within the same day and using a 160 km collocation tolerance between the tangent height of HALOE and the centre of the nearest GOME ground pixel. This requirement ensures that the tangent point is covered by the GOME ground pixel. 2151 matches between the two sensors had been available during 1998 (Fig. 3). Fig. 4 shows the comparison of GOME ozone profiles with HALOE profiles during spring 1998 at 60°-80°N. For long lived substances, like ozone in the lower stratosphere, gradients in their horizontal distribution evolve from transport processes. Meridional transport is strongest in the winter hemisphere. At the edge of the polar vortex high ozone values arise which sharply decrease to both sides; thus the validation at the border of different air masses is rendered more difficult.

A *trajectory model* enables to retrace the origin of air masses up to 10 days. By this method different air masses of two coincident measurements can be identified and collocated measurements within the same air mass can be found. An easier method for tracing the origin of air masses is the determination of potential vorticity (PV) distribution. In addition to the criteria given for potential and temporal coincidences an upper limit for the difference in PV can be defined. Instead of calculating zonal means, a presentation in the equivalent latitude system is advantageous. The later co-ordinate system is defined by the PV distribution.

Tabelle 4: Time schedule of validation and intercomparison of level-2 trace gas data products from SCIAMACHY (S), GOMOS (G) or MIPAS (M) with level-2 data from various satellite instruments data

Phase	Independent satellite instrument	Trace gas products	ENVISAT instrument validated	notices
Commissioning Phase	GOME (n)	O_3-profiles	S (n,l), M (l), G (o)	
		O_3-columns	S (n)	
		NO_2-columns	S (n)	
	TOMS (n)	O_3-columns	S (n)	
		NO_2-columns		
	HALOE (o)	O_3-profiles	S (n,l), M (l), G (o)	
		NO_2-profiles	S (l), G (o)	
		CH_4-profiles	S (l), M (l)	
		H_2O-profiles	M (l)? oder S(l)?, G (o)	
	SAGE II (o)	O_3-profiles	S (n,l), M (l), G (o)	
		NO_2-profiles	S (l), G (o)	
		H_2O-profiles	M (l)? oder S(l)?, G (o)	
Main Validation Phase*	SABER (l)	O_3-profiles	S (n,l), M (l), G (o)	night/daytime O_3 as G
		H_2O-profiles	S(l)?, G (o)	
	SBUV/2 (n)	O_3-profiles	S (n,l), M (l), G (o)	
		O_3-columns	S (n)	
	QuikTOMS (n)	O_3-columns	S (n)	
Longterm Validation**	Scientific case study on O3-chemistry and dynamics in the northernhemisphere			

Here: l = limb, n = nadir, o = occultation and *= tasks which have to be done in the Commissioning Phase also will be done here, **= tasks which have to be done in the Commissioning and Main Validation Phase also will be done here

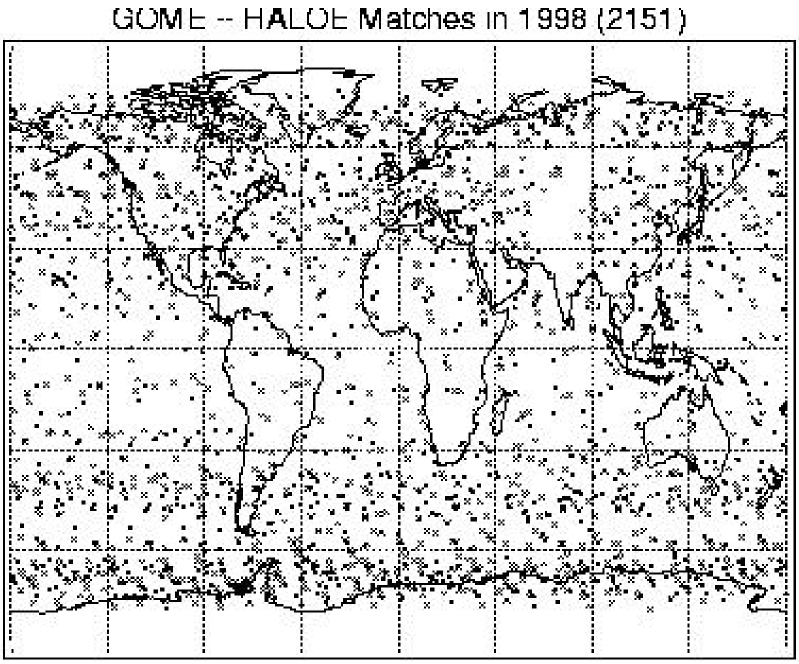

Fig. 3: Locations of coincident measurements of GOME and HALOE in 1998 [18]. Coincident measurements were defined as measurements taken within the same day and using a 160 km collocation tolerance. A total of 2151 collocated measurements were found

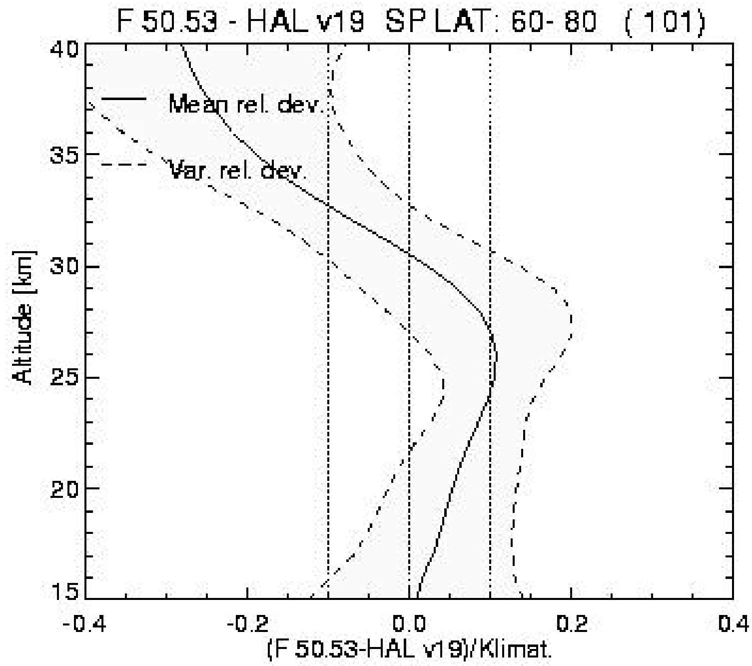

Fig. 4: Mean relative deviation and variance of mean relative deviation of the comparison of GOME ozone profiles with HALOE profiles in April-June 1998 at 60°-80°N. In the lower stratosphere the mean relative deviation is 5% with a variance of about 10% [18]

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