9. Validation

With the support of ESA and a large number of international partners, an extensive SCIAMACHY validation programme has been developed jointly by Germany, The Netherlands and Belgium to face the complex requirements in terms of measured species, altitude range, spatial and temporal scales, geophysical states and intended applications. The successful preparation of the validation included (*Piters et al.* 2006)

- an organisational structure to coordinate this largescale validation campaign, to monitor continuously the validation results and to foster exchanges between the different validation parties,
- numerous independent validation measurements of all planned SCIAMACHY products, mostly performed in the first two years of operation, and
- the required manpower to analyse the data in the first two years of operation, for a large part funded by the national space agencies of the three instrument-providing countries.

While the extensive SCIAMACHY validation set-up was in place with the start of the mission, the validation itself had to be adjusted to the actual availability of operational SCIAMACHY data products in the ENVISAT ground segment. Since the first release of early SCIAMACHY data in summer 2002, the operational processors established at LRAC and D-PAC were upgraded regularly and some of the envisaged data products (level 1b spectra, O₃, NO₂, BrO and cloud data) have achieved a quality status which made validation worthwhile.

The product status in the early mission phases in particular and the requirement to ensure maximum product quality throughout the mission make it necessary that SCIAMACHY validation continues throughout the instrument's lifetime – and beyond, anticipating algorithm updates and reprocessing of data for many years to come.

9.1 Validation Strategy

The rationale of satellite validation is to ensure that geophysical quantities derived from in-orbit radiometric measurements meet quality requirements for the intended scientific studies and applications. Starting from this perspective of scientific usability, considering the major scientific objectives of the mission, and based on the GOME validation experience, the SCIAMACHY Validation and Interpretation Group (SCIAVALIG) elaborated a list of validation requirements (*SCIAVALIG 1998*) and a detailed validation plan (*SCIAVALIG 2002*). These documents underline the importance of

- performing correlative studies with well-characterised data obtained by complementary measurement systems and modelling tools, and
- validation as a diagnostic tool in the improvement of retrieval algorithms.

The methods developed and used for SCIAMACHY validation arise from the arguments and considerations in these documents.

Validation Concept

Satellite validation is often understood as a simple comparison exercise concluding to a once-and-for-all assessment of the difference between the satellite data being validated and a reference data set of 'validated' quality. Although such comparisons are indeed the basis for investigating the quality of the satellite data, they are by no means sufficient for assessing the usefulness of the data for its intended scientific applications. The simplified approach above is sufficient to determine whether satellite and correlative data agree within their respective error bars, and whether the accuracy and precision estimates of the satellite data drawn from a comprehensive error budget analysis of the retrieved value may be realistic. However, obtaining an agreement within the estimated error bars offers no guarantee that the retrieved values contain new information coming from the measurement itself, e.g. a good agreement might simply reflect the use of excellent first guess data. Therefore, beyond the calculation of differences between SCIAMACHY and correlative data sets, SCIAVALIG recommends the use of several validation methods, each with its own potential contribution to the overall assessment of the usefulness of the data.

It is important to investigate, both qualitatively and quantitatively, how well SCIAMACHY data represent known geophysical signals that are either observed by other measurement systems or deduced from our understanding of the atmosphere. Depending on the species and the type of product, e.g. total or tropospheric column or vertical profile, these signals may include effects like meridional and zonal structures, vertical structures, temporal cycles on seasonal, day-to-day and diurnal scales or special events of tropospheric pollution. Unpredictable events like the Antarctic vortex split of September 2002 and a few volcanic eruptions in 2003 and 2004 have been instrumental in testing the real capabilities of SCIA-MACHY (*Lambert et al.* 2004).

Geophysical (level 2) quantities are retrieved from SCIAMACHY level 1b data using auxiliary data, such as output from radiative transfer models, or climatologies. Simplifications or misinterpretations therein can result in systematic errors in the retrieved quantities that may depend on geophysical, instrumental or algorithmic parameters. It is important to investigate the influence of these parameter-dependent systematic errors on the intended scientific use. For example ozone loss assessments relying on successive SCIAMACHY measurements along isentropic trajectories might be affected by any dependence of ozone-related products on the solar zenith angle and the latitude, or by altitude registration biases associated with pointing errors of the instrument. Global and regional chemical family budgets might be altered by fictitious spatial structures and temporal signals generated by the retrieval algorithms and superimposed on the actual geophysical signals. Therefore, these retrieval-parameter dependent systematic errors should be tracked down systematically, and characterised in detail.

As a first stage, prior to performing full geophysical validation of a mature data product, validation has often played and still plays a diagnostic role in the improvement of retrieval algorithms. Careful investigation of comparison time series and the use of assimilation tools have been powerful in revealing internal inconsistencies in SCIAMACHY data, such as gaps, shifts, systematic biases between data acquired at two different viewing angles, drifts, cycles, etc. Intercomparison of SCIAMACHY data retrieved with independent algorithms, either directly or indirectly using correlative measurements as standard transfer, has also given new insights for potential improvement.

Representativeness in Comparison Studies

The comparison of remotely sensed geophysical quantities with correlative data is not straightforward. A major difficulty results from the convolution of atmospheric variability with the smoothing/scanning properties inherent to the remote sensing approach. Different observation techniques and retrieval methods yield different sampling of the atmosphere in time and in space, different averaging of its 3-D structure and different sensitivity to ancillary atmospheric and instrumental parameters. As a direct consequence of those differences in the perception of the atmospheric field, atmospheric structures and variability can critically corrupt the reliability of the comparison by introducing systematic biases and additional scatter. Similar considerations apply to the comparison of remote sensing measurements with modelling results. The most common methodology is the direct comparison of columns and profiles within an arbitrary time/space coincidence window spanning typically from 200 to 1000 km and from 1 hour to 2 days. The presumed advantage of such a selection window is that the variability caused by differences in air mass is reduced. As expected, it works satisfactorily for long-lived species with negligible variability in space and in time, and for which the retrieval has a moderate sensitivity to the vertical structure. When atmospheric variability increases, differences in smoothing and sensitivity increase the comparison noise. For the comparison of SCIAMACHY and correlative ozone column data, the same time/distance selection window can increase the 1σ comparison scatter from a few percent at middle latitudes to several ten percent near the polar vortex edge. Stronger effects, including systematic biases, have been observed for short-lived species, like NO2 and BrO. Therefore, more sophisticated methods have been developed to deal with this difference in representation. They comprise the use of

- radiative transfer tools to better determine the vertical and line-of-sight smoothing of both SCIA-MACHY and correlative data (modelling of slant columns, weighting functions, averaging kernels),
- modelling and assimilation tools to deal with transport and photochemical effects (including diurnal cycles),
- meteorological analyses to discriminate the effects of dynamic variability (e.g. use of backward trajectories, transformation to equivalent latitude and isentropic coordinates),
- complementary correlative data sources offering different smoothing/sampling properties, sensitivity and errors budgets in a synergistic way.

The latter aspect is of prime importance for SCIA-MACHY validation. The SCIAMACHY data products potentially support an assortment of scientific applications, covering regional to global scales, from the ground up to the mesosphere, from short-term to decadal time frames. The synergistic use of complementary validation sources deals with this variety of products and scales. Local studies carried out at single stations constitute the preferred approach to detailed investigation. They benefit from local research and excellent understanding of local geophysical particulars leading to full control and accurate error budgets of the instrumentation and the availability of adequate ancillary data. Complementary studies exploiting pseudo-global sources yield access to patterns, sensitivity and space/time structures on a global scale. The differences in spatial coverage between different satellite instruments may introduce artefacts, but the massive amount of possible collocations, at least for nadir viewing instruments, potentially improves the significance of statistical quantities.

9.2 Validation Organisation

The status as an AO instrument places the responsibility for SCIAMACHY validation with the AOP.

However, since ESA takes care of the operational SCIAMACHY data processor, ESA has also included the validation of SCIAMACHY into their ENVISAT validation programme. Therefore two complementary validation structures exist.

ESA Validation Structure

In 1997 ESA raised an AO for the use of ENVISAT data. After review of proposals by representatives of the instrument science advisory groups, additional activities had been added to improve coverage of the validation programme. The Principal Investigators of the approved projects dealing with the validation of SCIAMACHY, GOMOS and MIPAS were gathered in the Atmospheric Chemistry Validation Team (ACVT). SCIAMACHY validation is performed in the following subgroups:



Fig.9-1: A scheme of the SCIAMACHY validation organisational structures set-up by SCIAVALIG (light orange) and by ESA (pale blue). The validation scientists actually doing the work are supported by both organisations, if they have an approved AO proposal for SCIAMACHY validation (green). (graphics: DLR-IMF and KNMI)

- ACVT/GBMCD: Ground-based Measurements and Campaign Database subgroup
- ACVT/ESABC: ENVISAT Stratospheric Aircraft and Balloon Campaign
- ACVT/MASI: Models and data Assimilation, Satellite Inter-comparisons
- SCCVT: SCIAMACHY Calibration and Verification Team

The latter is a subgroup of the overall ENVISAT Calibration and Validation team.

The ESABC subgroup is more than a working group. ESA, DLR, and the French Space Agency CNES together financed dedicated campaigns for the validation of SCIAMACHY, MIPAS and GOMOS. These campaigns are referred to as *ESABC cam*-

paigns and are prepared and coordinated in the ESABC group. Preparation and results of other campaigns are only presented and discussed within the ESABC group. In addition, ESA developed a dedicated validation data centre, the ENVISAT Validation Data Centre (EVDC). This database is operated by the Norwegian Institute for Air Research (NILU) and integrated into its NILU Atmospheric Database for Interactive Retrieval (NADIR). The EVDC hosts all correlative results arising from the various validation campaigns (ground-based and ship-borne, balloon-borne, from aircraft and satellites) generated for all ENVISAT instruments by the various calibration/validation teams and allows all groups involved access to data generated by the other teams.

SCIAVALIG Structure

The organisation of the AOP part of SCIAMACHY validation is delegated to SCIAVALIG, a subgroup of the SCIAMACHY Science Advisory Group. SCI-AVALIG, being chaired by KNMI, BIRA-IASB and IUP Heidelberg, consists of an international scientific consortium of representatives from 12 institutes participating in the validation. Besides having established a list of validation requirements, SCIAVALIG also defined an essential 'core' validation programme and has set up an organisational structure for the continuous monitoring of validation results throughout the lifetime of SCIAMACHY. The core validation programme is mainly funded by the instrument providers and is embedded in the ESA AO programme via several AO projects. The 'national coordinators' of SCIAVALIG are responsible for the coordination of this programme.

SCIAVALIG established a product coordination system. For each SCIAMACHY data product a product coordinator maintains an overview of the validation results. Their task is not to coordinate the individual validation activities as such but to monitor the scientific process, collect the different validation



results and create a consistent view of the product quality. The product coordinators report their findings to SCIAVALIG, ACVT and scientists. They collect their information mainly via the SCIAMACHY validation discussion pages on Internet, via validation meetings and via e-mail. In addition, they have interaction with algorithm development teams and processor experts for an efficient translation from validation results towards algorithm changes.

9.3 Correlative Measurements

The core validation programme was complemented by a selection of AO projects from international partners. The major component of the SCIAMACHY val-

Station NO₂ BrO OCIO SO₂ H₂CO H₂O со СН₄ CO₂ T/p UV/CF/CTP/AAI **O**₃ N₂O Asia Tiksi Igarka Salekhard Zhigansk Markovo Yakutsk Magadan Vitim Ekaterinburg Krasnoyarsk Omsk Nikolaevsk Petropavlovsk Irkutsk Karaganda Yuzhno Sahalinsk Vladivostok lssyk Kul North America Greenbelt Wallops Island Table Mountain Kitt Peak Mauna Loa South America Merida Paramaribo Bauru Africa Nairobi Reunion Australia Wollongong Broadmeadows Lauder Antarctica Kerguelen Macquarie Marambio /ernadsky Dumont d'Urville Rothera Neumayer Halley Arrival Heights Belgrano South Pole UV/CF/CTP/AAI column profile column/profile

Fig. 9-2: Ground-based stations contributing to SCIAMACHY validation and associated SCIAMACHY data products. The last column includes UV, CF (cloud fraction), CTP (cloud top pressure) and AAI (absorbing aerosol index). (graphics: KNMI and DLR-IMF)

idation programme consists of comparison studies with correlative measurements acquired by independent instrumentations from various platforms, namely, ground-based stations and ships, aircraft, stratospheric balloons, and satellites.

Ground-based and Ship-based Instruments

Ground-based instruments provide the appropriate correlative data to fulfil four main tasks of the SCIA-MACHY validation programme:

- quick validation before public release of a new product or just after the release of a near-realtime product,
- detailed geophysical validation from Pole to Pole and for a variety of geophysical states, including

dependencies on measurement and atmospheric parameters such as SZA and temperature,

- verification of correctness of changes and preliminary quality assessment of the resulting data product after major improvement of a retrieval algorithm,
- long-term validation, including detection of trends and other time-varying features.

The list of stations providing correlative measurements for SCIA-MACHY validation is given in fig. 9-2. They are distributed globally but with a strong clustering in northern latitudes (see fig. 9-3). The nationally funded core validation programme, constituting the backbone of the validation, includes complementary types of instrumentation (see list in the next paragraph), yielding together nearly all targeted species, and operating at about forty stations distributed from the Arctic to the Antarctic and from South America to the Indian Ocean.

Based on long-lasting collaboration established mainly in the framework of WMO's Global Atmospheric Watch programme (GAW) – particularly within its affiliated ozonometric networks (see *Fioletov et al.* 1999 and references therein) – and the Net-



Fig. 9-3: Global distribution of validation sites. Symbols and colour codes are as follows: triangles = core validation station, blue = NDSC network, red = Russian/NIS M-124 network, purple = NDSC and Russian/NIS M-124 network, green = no network, yellow square or envelope = balloon launch site. (graphics: DLR-IMF with Earth map from NASA – Visible Earth)

work for the Detection of Stratospheric Change (NDSC, *Lambert et al.* 1999 and references therein), international partners also contribute through AO projects with a long list of instruments which add significantly to the geographical coverage of the groundbased instrumentation included in the core validation programme.

The ozone column amount is monitored at a variety of ground-based stations by Dobson and Brewer ultraviolet spectrophotometers and by Russian/NIS ultraviolet filter radiometers of the M-124 design. A network of about 30 DOAS instruments, all certified for the NDSC, monitor the column amount of species absorbing in the UV-VIS-NIR part of the spectrum such as O₃, NO₂, BrO, OClO, IO, HCHO, SO₂ and H₂O. Some of them have multi-axis observation capabilities yielding separation of the tropospheric and stratospheric columns. Seven Fourier Transform Infrared (FTIR) spectrometers, also carrying NDSC certification, report the vertical column amount and sometimes the vertical distribution of a series of species including O₃, NO₂, CO, CH₄, N₂O, CO₂, HCHO and H₂O. Six microwave radiometers measure the thermally induced rotational emission of selected species, such as O₃, H₂O and ClO. Groundbased ozone Differential Absorption Lidars (DIAL) and/or electro-chemical ozone sondes yield the vertical distribution of tropospheric and stratospheric ozone, at high and moderate vertical resolution. Aerosol and cloud properties are recorded by lidar and aerosol instruments.

In addition to the instruments operating continuously at ground-based sites, two instruments are operated on-board the German research vessel Polarstern to facilitate the validation of SCIAMACHY measurements in remote marine regions: a MAX-DOAS (Multi-Axis DOAS) and an FTIR instrument. The Polarstern made three cruises within the time period relevant for initial SCIAMACHY validation: the first between November 2001 and May 2002, the second between October 2002 and February 2003, the third between October 2003 and July 2004 (fig. 9-4, 9-5). The moveable MAX-DOAS experiment measured constantly during all three cruises and the investigation of large scale latitudinal cross sections of atmospheric trace gases was undertaken. The FTIR instrument was operating during the second and third campaign from Bremerhaven to Africa.

Airborne Campaigns

The German aircraft validation activities were concentrated on missions with the meteorological research aircraft Falcon 20 (D-CMET) operated by DLR. Many features make the Falcon an excellent aircraft for the validation experiment. Three large optical windows, two in the floor and one in the roof enable operation of large lidar experiments for both tropospheric and stratospheric research. Specially manufactured polyethylene windows allow remote sensing in the microwave spectral region. The aircraft carries a data acquisition system and an extensive instrument package capable of measuring position, altitude, static pres-



Fig. 9-4: The German research vessel Polarstern. (photo: E. Fahrbach)

sure and temperature. Within the SCIA-VALUE (SCIAMACHY Validation and Utilization Experiment) project two major campaigns with 28 flights were executed in September 2002 and February/ March 2003 (fig. 9-6). Both campaigns consisted of large-scale latitudinal cross sections from the polar regions to the tropics as well as longitudinal cross sections at polar latitudes. To validate SCIAMACHY, three different types of remote sensing instruments were installed on-board the Falcon 20 (fig. 9-7). The AMAX-DOAS (Airborne Multi-Axis DOAS) which is an experiment developed jointly by the Universities of Heidelberg and Bremen, is capable of measuring tropospheric and stratospheric columns of key gases such as O₃, NO₂, BrO and OClO absorbing in the UV-VIS wavelength range. ASUR (Airborne Submillimetre Radiometer) operated by the University of Bremen is a passive microwave sensor. A broad range of molecular lines can be detected containing the molecules that play an important role in the catalytic destruction of ozone. The frequency band includes emission lines of O₃, ClO, HCl, HNO₃, N₂O, H₂O, HO₂, CH₃Cl, NO, HCN and BrO. The Ozone Lidar Experiment (OLEX)



Fig. 9-5: Route of the Polarstern cruise during the *ANT XIX* campaign between November 2001 and May 2002. (graphics: DLR-IMF)

developed and operated by DLR completes the scientific payload of the Falcon. In the zenith viewing mode this instrument provides high resolution two-dimensional cross sections of ozone number densities, aerosol extinction and cirrus cloud cover information from about 2 km above aircraft flight level up to a height of 30 km (*Fix et al.* 2005).

The stratospheric research aircraft M55-Geophysika is also involved in ENVISAT validation. It performed two mid-latitude campaigns in July and October 2002 from a basis in Forli, Italy, and a high latitude campaign in January and March 2003 from Kiruna. For the ENVISAT validation flights, the M55 was equipped with two sets of instruments. The socalled *chemical flights* are performed with six in-situ and one remote sensing instrument, capable of measuring, among others, concentrations of H₂O, O₃, NO, NO_v, N₂O, CH₄, BrO and columns of O₃ and NO₂ (Kostadinov et al. 2003, Heland et al. 2003). For the the so-called *cloud/aerosol flights*, the remote sensing instrument was replaced by six instruments for the characterisation of aerosol and cloud properties. Although the in-situ instruments remained on-board, these flights were optimised for the cloud and aerosol properties.

Within the MOZAIC (Measurements of Ozone and water vapour by Airbus In-service aircraft) programme (*Marenco et al.* 1998) which started in 1994, five long-range Airbus A340 aircrafts are equipped with in-situ instruments measuring O₃, H₂O, CO and NO_y. They provide data from all over the world along the flight tracks at the upper troposphere, lower strat-



Fig. 9-6: Falcon flight tracks for the September 2002 (left) and February/March 2003 (right) SCIA-VALUE airborne campaigns. In red are the northern tracks (September 3-8, 2002 and February 19 – March 3, 2003) while the southern tracks (September 15-28, 2002 and March 10-19, 2003) are displayed in yellow. (graphics: DLR-IMF)



Fig.9-7: The Falcon aircraft with the viewing directions of the validation instruments. (image: *Fix et al. 2005*)

osphere altitude level from 9-12 km and down to the ground around 60 airports. These measurements are a unique dataset at the tropopause region and will be especially useful for development and validation of products distinguishing between troposphere and stratosphere. Other interesting data sets, which are not yet exploited for SCIAMACHY validation, may come from the CARIBIC (Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container) and NOXAR (Measurements of Nitrogen Oxides and ozone along Air Routes) programmes.

Balloon Campaigns

Balloon-borne measurements provide snapshot type vertical profile measurements of very high precision. The dedicated balloon campaigns for the atmospheric chemistry instruments MIPAS, GOMOS and SCIAMACHY are funded by ESA, DLR and CNES, with the costs and responsibilities shared according to an agreement between the three agencies. Part of this agreement is to use all balloon flights as far as possible for all three satellite instruments.

CNES provides the facilities and staff for launching scientific payloads with large stratospheric balloons from dedicated stations. The availability of the CNES equipment is an important constraint for the implementation of campaigns. Within the ACVT subgroup ESABC, the involved scientists from the balloon teams and representatives of the agencies met frequently to organise the ENVISAT validation balloon campaigns. The launch sites and campaign times were selected to cover mid-latitudes, northern latitudes and the tropics during several seasons as far as possible within the available resources. Up until May 2005, SCIAMACHY validation measurements were performed during 16 balloon campaigns from launch sites in Kiruna/Sweden, Aire sur l'Adour/France, Bauru/Brazil, Vanscoy/Canada, and Fort Sumner/New Mexico, US. Table 9-1 lists the payloads, launch dates and the measured species relevant to SCIAMACHY. Further ESABC supported campaigns are already planned in Brazil and Kiruna for the forthcoming years. They cover high latitudes in summer with normal conditions and in spring with the possibility of ozone depletion as well as mid-latitudes and tropical regions.

Explicitly funded for the validation of SCIA-MACHY are:

- the LPMA-DOAS (combining a Limb Profile Monitoring of the Atmosphere FTIR and a DOAS instrument),
- the TRIPLE (combining a resonance fluorescence ClO/BrO instrument, an in-situ Stratospheric Hygrometer – FISH, a cryogenic total air sampler – BONBON) and a tunable diode laser measuring H₂O and CH₄),
- and the MIPAS-B (MIPAS balloon version) gondolas.

These constitute the German contribution to the balloon-borne validation of ENVISAT. All three balloon payloads measured atmospheric profiles of O₃, NO₂, OClO, BrO, CH4, N₂O, H₂O, CO, CO₂, temperature and pressure which will allow validation of corresponding parameters measured by SCIAMACHY during collocated overpasses of the satellite.

Solar irradiances and limb radiances for level 1 validation are determined by radiometric calibration of the DOAS instruments on-board the LPMA-DOAS gondola.

Satellite Intercomparisons

Measurements of relevant parameters by independent instruments on-board other satellite platforms facilitate the required pole-to-pole validation for many of the SCIAMACHY products for all seasons. Several satellite instruments are available for comparison with results from the ENVISAT atmospheric chemistry experiments. In most cases satellite measurements provide near global coverage and, therefore, are well suited for global validation in space and time. Table 9-2 lists the satellite instruments used for the validation of SCIAMACHY products. SCIA-MACHY's precursor GOME on board ERS-2 follows ENVISAT with a delay of 30 minutes. Since the GOME channels are almost identical to the UV-VIS channels of SCIAMACHY, GOME is the first choice for validating UV-VIS nadir products. However, due

to a tape recorder anomaly on the ERS platform, GOME measurements are restricted to the North Atlantic sector and the north polar region since June 2003. TOMS and SBUV-2, as nadir looking instruments, provide total columns. HALOE, SAGE II/III and POAM III are solar occultation instruments providing trace gas profiles at sunset and sunrise. SABER observes infrared emissions in limb, retrieving ozone and water vapour profiles. OSIRIS also operates in limb mode, providing ozone profiles. SUSIM and SOLSTICE results are used for comparison with solar irradiance measurements, required to check the radiometric calibration of SCIAMACHY. In addition, intercomparisons are performed between the three atmospheric chemistry instruments on board ENVISAT, i.e. MIPAS, GOMOS and SCIAMACHY. More recent satellite instruments that will be used for intercomparisons are for example OMI, TES, and ACE.

9.4 Validation Results

The goal of validation is to generate a complete description of the quality of all SCIAMACHY products that fulfil specific criteria on availability, product and algorithm description and software version control. Given the current status and evolving nature of the data segment, this goal has not yet been achieved. Furthermore, a spaceborne mission like SCIA-MACHY requires continuous validation throughout the instrument's lifetime and even beyond when data is expected to be used in long-term climatological studies. The first years of validation have proven the overall concept and provided initial results. A detailed overview of the validation results for the years 2002-2004 is given by Piters et al. (2006) and references therein. Here, we summarise some of the main validation topics.

Level 2 Products from Nadir UV-VIS-NIR

O₃: The agreement of SCIAMACHY O₃ columns, processor version 5.01 and 5.04, to ground-based networks and satellite measurements is within 2-10%, SCIAMACHY on average somewhat lower. The bias significantly depends on solar zenith angle, season and viewing angle. Validation of SCIAMACHY O₃ columns generated by scientific algorithms show a good agreement with ground-based data, with a bias of 1-1.5% (usually a slight underestimation) and a RMS of about 5%.

NO₂: Validation of the SCIAMACHY NO₂ columns, processor version 5.01 and 5.04, indicate good agreement with correlative data over clean areas

Payload	Launch Dates	Launch Site	Target Species
MIPAS-B PI: Fischer	24-Sep-2002 07-Dec-2002 20-Mar-2003 03-Jul-2003	Aire sur l'Adour Kiruna Kiruna Kiruna	O ₃ , NO ₂ , N ₂ O, H ₂ O, CO, CO ₂ ; T/p
TRIPLE <i>PI: Fischer</i>	24-Sep-2002 06-Mar-2004 09-Jun-2004	Aire sur l'Adour Kiruna Kiruna	CO ₂ , CH ₄ , N ₂ O, NO ₂ , H ₂ O, BrO
LPMA-DOAS Pl: Camy-Peyret	18-Aug-2002 09-Mar-2003 23-Mar-2003 09-Oct-2003 24-Mar-2004	Kiruna Kiruna Kiruna Aire sur l'Adour Kiruna	O ₃ , NO ₂ , OCIO, BrO, CH ₄ , N ₂ O, H ₂ O, CO; T/p, irradiance
SAOZ-MIR <i>PI: Pommereau</i>	23-Feb/04-Mar-2003 26-Feb/06-Apr-2004	Bauru Bauru	O ₃ , NO ₂ , 2004: H ₂ O
SAOZ PI: Goutail	04-Oct-2002 18-Oct-2002 09-Jun-2004	Aire sur l'Adour Aire sur l'Adour Bauru	O ₃ , NO ₂ ; T/p
SAOZ+SAOZ-BrO <i>PI: Goutail/Pirre</i>	01-Oct-2002 23-Feb-2003 16-Mar-2003 30-Mar-2003 31-Jan-2004 05-Feb-2004	Aire sur l'Adour Bauru Kiruna Kiruna Bauru Bauru Bauru	O ₃ , NO ₂ , BrO; T/p
FIRS-2 <i>PI: Chance</i>	20-Oct-2002 20-Sep-2003 23-Sep-2004	Ft. Sumner Ft. Sumner Ft. Sumner	O ₃ , H ₂ O, N ₂ O, NO ₂ , 2003/2004: CO, CH ₄ , CO ₂ ; T
MANTRA PI: Strong	03-Sep-2002 25-Aug-2004	Vanscoy Vanscoy	O ₃ , NO ₂ , H ₂ O, N ₂ O, CH ₄ ; aerosol, T/p
SALOMON PI: Renard	19-Sep-2002 04-Mar-2002	Aire sur l'Adour Kiruna	O ₃ , NO ₂ , OCIO; aerosol
SPIRALE <i>PI: Pirre</i>	02-Oct-2002 21-Jan-2003	Aire sur l'Adour Kiruna	O ₃ , NO ₂ , CO, CH ₄
SDLA-LAMA <i>PI: Pirre</i>	08-Aug-2002	Kiruna	H ₂ O, CH ₄
ELHYSA <i>PI: Ovarlez</i>	11-Mar-2004	Kiruna	H ₂ O, CH ₄
AMON Pl: Renard	01-Mar-2003	Kiruna	O ₃ , NO ₂ , OCIO
μRADIBAL <i>PI: Brogniez</i>	08-Mar-2004	Kiruna	aerosol
LPMA-IASI PI: Renard	06-Aug-2002	Kiruna	total columns of H_2O , CO_2 , CO , O_3 , N_2O , CH_4

Table 9-1: Balloon launches for SCIAMACHY validation.

ESA			
GOME	Global Ozone Monitoring Experiment	ERS-2	columns: O ₃ , NO ₂ , SO ₂ , BrO, HCHO profiles: O ₃
AATSR	Advanced Along Track Scanning Radiometer	ENVISAT	spectral reflectance (555, 659, 865 nm), cloud cover, cloud top height
MERIS	Medium Resolution Imaging Spectrometer	ENVISAT	spectral reflectance (390-1040 nm), cloud cover, aerosol
NASA			
SUSIM	Solar Ultraviolet Irradiance Monitor	UARS	solar UV energy
HALOE	Halogen Occultation Experiment	UARS	profiles: O ₃ , NO ₂ , NO, CH ₄ , N ₂ O, CO ₂ , H ₂ O
TOMS	Total Ozone Monitoring Spectrometer	Earth Probe	columns: O ₃ , SO ₂ AAI
SAGE II & III	Stratospheric Aerosol and Gas Experiment II & III	ERBS & METEOR-3M	profiles: O ₃ , NO ₂ , H ₂ O, aerosols
SABER	Sounding of the Atmosphere Using Broadband Emission Radiometer	TIMED	profiles: O ₃ , H ₂ O
SOLSTICE	Solar Stellar Irradiance Comparison Experiment	UASR	solar UV spectral irradiance
MOPITT	Measurements Of Pollution In The Troposphere	EOS-TERRA	columns/profiles: CO
MODIS	Moderate Resolution Imaging Spectroradiometer	EOS-TERRA	cloud cover, cloud top pressure, aerosol
CNES			
Poam III	Polar Ozone and Aerosol Measurement III	SPOT-4	profiles: O ₃ , H ₂ O, NO ₂ , aerosols
SNSB			
OSIRIS	Optical Spectrograph and Infrared Imager System	ODIN	profiles: O ₃ , NO ₂
NOAA			
SBUV/2	Solar Backscatter Ultraviolet Ozone Experiment II	NOAA 14 & NOAA 16	profiles: O ₃

Table 9-2: Satellite instruments used in the core validation for intercomparison with SCIAMACHY.

in the southern winter/spring and northern summer. Large deviations are observed in other cases with a clear correlation with cloud fraction, ghost vertical column and air mass factor values. The scientific NO_2 stratospheric columns have good quality, but large differences exist between the different tropospheric NO_2 columns. Detailed validation and intercomparisons are ongoing.

BrO: SCIAMACHY scientific BrO columns coincide well with GOME retrievals and with groundbased UV-VIS measurements. The operational slant column, processor version 5.01, shows the same agreement except in summer for slant column values smaller than 1.5×10^{14} molec/cm², when it is systematically higher by 20% to 100%.

SO₂: Quantitative validation of scientific SCIA-MACHY SO₂ column is hampered by the lack of independent measurements. Routine measurements and campaigns near SO₂ sources are currently planned.

OClO: SCIAMACHY scientific OClO slant columns are consistent with GOME retrievals and AMAX-DOAS measurements.

 $\rm H_2O$: Validation of the scientific SCIAMACHY $\rm H_2O$ column shows a systematic bias of -0.05 g/cm² and a scatter of 0.5 g/cm² with respect to SSM/I measurements and ECMWF model values.



Fig. 9-8: Difference between the ozone columns retrieved from SCIAMACHY and from GOME with the same scientific algorithms. The relative differences are displayed in colour, as a function of the day since January 1st, 2003 (horizontal axis) and the latitude (vertical axis). Data is presented with a latitude resolution of 1 degree and time resolution of 1 day. The colour scale represents the ratio (SCIAMACHY-GOME)/GOME in %. The SCIAMACHY O₃ columns are retrieved by KNMI. (image: H. Eskes, KNMI)



Fig.9-9: Tropospheric NO₂ column obtained by SCIAMACHY together with the Falcon flight track in red showing where AMAX-DOAS measured almost simultaneously. In the inset tropospheric NO₂ columns from AMAX-DOAS are plotted versus those from SCIAMACHY. The SCIAMACHY tropospheric NO₂ columns are retrieved by IUP-IFE, University of Bremen. (image: *Heue et al. 2005*)



Fig.9-10: Intercomparison of BrO vertical columns retrieved from GOME, SCIAMACHY and ground-based DOAS measurements at Harestua, Norway, 60°N, 10°E. SCIAMACHY data products from the ESA NRT processor version 5.01 are shown together with scientific retrievals performed at BIRA-IASB. Airmass factors used to convert slant columns to vertical columns are calculated using same atmospheric profiles in all cases. (image: *Van Roozendael et al. 2004*)



Fig.9-11: Global mean and standard deviation of the difference between collocated SCIAMACHY and ECMWF water vapour columns for the year 2003. The SCIAMACHY H₂O columns are retrieved by IUP-IFE, University of Bremen. (image: *Noël et al. 2005*)



Fig. 9-12: Averaged O₃ profiles with their standard deviations (dashed lines) and errors (shaded areas) for 145 collocated measurements from SCIAMACHY (blue) with 6 different lidars (yellow). An altitude shift of -1.5 km has been applied to the SCIAMACHY data. The SCIAMACHY O₃ profiles are retrieved by IUP-IFE, University of Bremen. (image: *Brinksma et al. 2006*)

CF and CTP: The operational SCIAMACHY cloud fraction correlates well with scientific retrievals. The scientific cloud top pressure compares well with MODIS.

AAI and AOT: SCIAMACHY scientific Absorbing Aerosol Index compares well with TOMS and the SCIAMACHY scientific Aerosol Optical Thickness agrees reasonably well with MERIS.

Level 2 Products from Nadir SWIR

Correlative studies have been conducted using

- ground-based data from a pole-to-pole network of 12 FTIR instruments and from the FTIR operated during two cruises of the Polarstern vessel from Bremerhaven to Africa,
- CO column data from the EOS-Terra MOPITT satellite,
- CO and CH₄ data from the TM3 (KNMI) and TM5 (IMAU) models, and
- ancillary data such as fire maps produced by ERS-2 ATSR and EOS-Aqua MODIS.

The general potential of SCIAMACHY SWIR products is demonstrated, in particular its capabilities to detect source/sink areas of CO, CH₄ and CO₂ and to track their transport. Provisional precision estimates for SCIAMACHY CO (20–30%) and CH₄ (1–2%) vertical columns are not far away from the nominal requirements and can already be used in a variety of applications. Even so, inverse modelling analyses seem to indicate that nominal precision requirements are a firm precondition for the potential improvement of existing emission catalogues. The current estimated precision for N_2O is 20%. It is expected that this will be improved in the near future. For CO_2 , current validation is too limited to give firm conclusions. The tropics need special attention.

Level 2 Products Retrieved from Limb UV-VIS – Profiles

O₃: Validation of the OL processor version 2.5 O₃ profiles with ground-based instruments and satellites showed that 20% of the profiles have unrealistic values. The other 80% display no systematic deviations above 24 km but are significantly underestimated below 24 km by 15%. Scientific O₃ profiles have also been generated by IUP-IFE, University of Bremen with software version 1.61. These profiles were validated for five months spread over 2004 with groundbased and satellite data. The systematic bias of the IUP-IFE profiles, after a downward shift of 1.5 km was applied to account for the reported tangent height bias (see chapter 6.3), is -3% with respect to lidars, averaged between 16 and 40 km, and -6% with respect to SAGE II over the same latitude range.

 NO_2 : A comparison of the OL processor version 2.5 NO_2 profiles with collocated and photochemically corrected SAGE II (vs. 6.2) measurements indicate that the quality of the retrievals strongly depends on latitude and/or solar zenith angle.

BrO: The direct comparison of photochemically uncorrected BrO profiles from balloons and from SCIA-MACHY limb spectra provide promising results in the middle stratosphere. Further validation is necessary, that will include photochemical corrections for balloon observations along calculated airmass trajectories.