

Chapter 9 Validation

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Abstract Satellite validation has to ensure that geophysical quantities derived from in-orbit radiometric measurements meet quality requirements for the intended scientific studies and applications. It is not a ‘once a mission lifetime’ task, but requires regular proof measurements throughout the in-orbit phase. An extensive SCIAMACHY validation programme has been developed jointly by Germany, The Netherlands and Belgium, with the support of ESA and a large number of international partners. Due to its status as an AO instrument SCIAMACHY is embedded in two collaborating validation structures, ESA’s Atmospheric Chemistry Validation Team and the SCIAVALIG, a subgroup of the SCIAMACHY Science Advisory Group. In the first years of the mission intensive independent measurement campaigns were organised, setting the basis for a continuous validation programme over the instrument lifetime, harmonised with the steadily improving operational processors and the scientific algorithms. All validation activities have to obey well-established validation principles including a thorough analysis when comparing geophysical parameters derived from SCIAMACHY with correlative measurements. Such measurements use all available means – from ground, ships, aircraft and balloons. Additionally the SCIAMACHY measurements were compared with results from other space-borne atmospheric sensors. Meanwhile validation has confirmed the current accuracy

for a wealth of retrieved parameters. The list includes O₃, NO₂, BrO, OCIO, SO₂, HCHO, CHOCHO, H₂O, CO, CO₂, CH₄, cloud fraction and cloud top pressure, aerosol index and aerosol optical thickness.

Keywords Validation • Trace gases • Ground station networks • Shipborne campaigns • Airborne campaigns • Balloon-borne campaigns • Satellite intercomparisons

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

- An organisational structure to coordinate large-scale validation campaigns, to monitor continuously the validation results, and to foster exchanges between the different validation parties
- Numerous independent validation measurements of all planned SCIAMACHY products, performed intensively in the first 2 years of operation and continued on sustainable basis afterwards
- Adequate manpower to analyse the data in the first 2 years of operation, for a large part funded by the national space agencies of the three instrument-providing countries
- Sustained support from the national agencies and from ESA to ensure – after the two first years – continuity of the organisation, measurements and analysis manpower over the lifetime of the instrument

While the extensive SCIAMACHY validation setup was in place with the start of the mission, the analysis itself had to be adjusted to the actual availability of operational SCIAMACHY data products in the ENVISAT ground segment as

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well as data products derived by involved science teams. Since the first release of early SCIAMACHY data in summer 2002, the operational processors were upgraded regularly. More and more of the envisaged data products did achieve good quality (level 1b spectra, O₃, NO₂, BrO and cloud data). Also the science data products were successfully improved on a regular basis thus enabling meaningful validation of O₃, NO₂, BrO, SO₂, OClO, HCHO, CHOCHO, CH₄, CO, H₂O, CO₂, and aerosols.

The requirement to ensure maximum product quality throughout the mission and to achieve best possible consistency with follow-on missions made it necessary to continue SCIAMACHY validation throughout the instrument's lifetime – and even beyond, anticipating that algorithm updates, reprocessing of data and the development of new data products will continue after the in-orbit life of SCIAMACHY.

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 underlined the importance of

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

The methods and practices developed and used for SCIAMACHY validation arise from the arguments and considerations in these documents. Over the years, they have been refined according to the developing SCIAMACHY validation experience, and enriched through exchanges of scientific and organisational nature occurring in international forums and projects.

Validation Principles

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 dataset of 'validated' quality. The reality is somewhat different. Data comparisons are indeed the basis for investigating the quality of the satellite data. Provided that the satellite and the correlative measurements offer the same perception of the atmospheric profile, its variability and its gradients – so that comparison errors remain small – the simplified approach outlined above is sufficient to determine whether the satellite and correlative data agree within their respective error bars, hence, whether the theoretical bias and precision estimates of the satellite data may be realistic. If the two measurements sample and smooth differently the atmospheric field and its variations, the verification of theoretical error bars through data comparisons is much more complex in the presence of atmospheric structures and variability. Furthermore, straightforward comparisons are by no means sufficient for assessing the usefulness of the data for their intended scientific applications. In addition obtaining an agreement within the estimated error bars offers no guarantee that the retrieved values do contain enough information coming from the measurement itself. For example a good agreement at altitudes where the satellite cannot measure at all for physical reasons, e.g. in the lower troposphere masked by thick clouds, might simply reflect the use of an excellent climatology as first guess data and of appropriate retrieval constraints. Therefore, beyond the calculation of differences between SCIAMACHY and correlative datasets, SCIAVALIG recommended the use of complementary validation methods, each with its specific contribution to the overall assessment of the usefulness of the data.

Throughout the validation it is important to investigate, both qualitatively and quantitatively, how well SCIAMACHY data capture 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 data product, e.g. total or tropospheric column or vertical profile, these signals may include meridional and zonal structures, geographical structures linked to the distribution of emission sources and to the orography, vertical structures, long-term trends, temporal cycles on seasonal, day-to-day and diurnal scales, and special events of tropospheric pollution. Unpredictable events like the Antarctic vortex split of September 2002 (von Savigny et al. 2005), the solar proton events of October and November 2003 (Rohen et al. 2005), and a few volcanic eruptions (Afe et al. 2004), have been instrumental in testing the real capabilities of SCIAMACHY.

Level 1b spectra measured by SCIAMACHY contain information from the target species (usually absorption features) along the optical path. However, the optical path of light through the atmosphere is controlled by many factors, e.g. the solar elevation, the satellite viewing angles, and the

presence of clouds, aerosols, and interfering species. Geophysical quantities (level 2 data) are retrieved from SCIAMACHY spectra (level 1b data) using auxiliary information such as absorption cross sections, output from radiative transfer models and climatologies. Consequently, the sensitivity of SCIAMACHY retrievals to the real atmospheric state depends on measurement, instrumental, and algorithmic parameters. Simplifications or misinterpretations therein can result in systematic errors in the retrieved quantities. It is necessary to study the influence of these parameter-dependent systematic errors on the intended scientific use. For example, polar 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, and 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. These retrieval dependent systematic errors need to be tracked down systematically and characterised in detail. To achieve this, a good communication is needed between retrieval and validation experts.

As a first stage, prior to performing the thorough geophysical validation of a mature data product, ad hoc algorithm verification and validation studies performed on a selected subset of data have often played and still play an important diagnostic role in the maturity of retrieval algorithms. In support, the use of data assimilation tools has been powerful in revealing internal inconsistencies in SCIAMACHY datasets, such as gaps, shifts, systematic biases between data acquired at different viewing angles, temporal drifts, abnormal cycles, etc. Intercomparison of SCIAMACHY data retrieved with independent algorithms, either directly or indirectly using correlative measurements as a standard transfer, has also given new insights for algorithm improvements.

Comparison Errors and Representativeness

From a metrological point of view, the comparison of remotely sensed geophysical quantities with correlative measurements is not straightforward. A major difficulty results from the convolution of atmospheric variability and structures with the smoothing/scanning properties inherent to the remote sensing approach. Different observation platforms, measurement techniques and retrieval methods yield different sampling of the atmosphere in time and in space, different averaging of its variations and structures, 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 noise. Similar considerations apply to the comparison of remote sensing measurements with in situ measurements and with modelling results.

The first step of a comparison process consists in selecting the satellite and correlative data offering the best collocation in time and space. Ideally, data should not be selected for comparison if their time and space mismatches are associated with atmospheric gradients and variability exceeding the individual errors bars of the measurements. In practice, such an ideal coincidence of the data is rarely available due to the above considerations, and a compromise has to be found between – on one hand – representativeness and statistical significance of the datasets to compare – and on the other hand – accuracy of the comparison process. The most common selection practice is to compare satellite and correlative data within an arbitrary time/space coincidence window, spanning typically from 200 to 1000 km and from 1 h to 2 days. 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 example using the same time/distance selection window, the 1σ standard deviation between an ozone column derived from SCIAMACHY and correlative data can increase from a few percent at mid-latitudes to several 10% near the polar vortex edge. Stronger effects, including systematic biases, have been observed for short-lived species, especially those exhibiting large meridian gradients and a diurnal cycle like NO_2 and BrO . In addition to time and space mismatches, differences in vertical and horizontal smoothing of the atmospheric variability can result in large discrepancies between satellite and correlative data. In particular, data products with a poor vertical resolution are often affected by the so-called ‘vertical smoothing error’, which must be considered appropriately when interpreting comparisons with data obtained at better vertical resolution. Altitude registration uncertainties due to pointing errors of the instrument and attitude uncertainties of the ENVISAT platform are a source of vertical mismatch for limb data validation.

According to the needs, more sophisticated methods have been developed to deal with differences in representation and representativeness. They comprise the use of

- Radiative transfer tools to better characterise the vertical and line-of-sight smoothing of both SCIAMACHY and

correlative data: modelling of apparent slant column densities, of weighting functions and of averaging kernels (see Chapter 7)

- Chemical-transport 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. the use of backward trajectories and the transformation of coordinates (latitude, longitude, time) to flow-tracking coordinates like equivalent latitude and potential temperature
- Complementary correlative data sources offering different smoothing and sampling properties, sensitivity and errors budgets in a synergistic way

The latter aspect is of prime importance for SCIAMACHY validation. The SCIAMACHY data products do support an assortment of scientific applications and thematic domains, 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 can deal with this variety of products and scales. Local studies carried out at single stations constitute the preferred approach to detailed investigations. They benefit from local research and excellent understanding of local geophysical features leading to full control and accurate error budgets of the instrumentation and the availability of adequate ancillary data. Complementary studies exploiting pseudo-global sources like monitoring networks yield access to error patterns, sensitivity, and atmospheric structures on the global scale. Satellite-to-satellite comparisons, using MIPAS and GOMOS data as well as observations from other satellites, extend network-based validation ranges to higher altitudes and more regular geographical sampling. The differences in geographical coverage and in latitude/time sampling between different satellite instruments may introduce artefacts, but the massive amount of possible co-locations, at least for nadir viewing instruments, considerably improves the significance of statistical quantities and the representativeness in terms of atmospheric states.

9.2 Validation Organisation

The status as an announcement of opportunity (AO) instrument places the responsibility for SCIAMACHY validation with the AO provider. Since ESA takes care of the operational SCIAMACHY data processor, the validation of SCIAMACHY has also been included by ESA into their ENVISAT validation programme. Therefore two collaborating complementary validation structures co-exist. The overall organisation is sketched in Fig. 9.1.

ESA Validation Structure

In 1997 ESA raised an Announcement of Opportunity (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 sub-groups:

- ACVT/GBMCD: Ground-based measurements and campaign database
- ACVT/ESABC: ENVISAT stratospheric aircraft and balloon campaign
- ACVT/MASI: Models and data assimilation, satellite inter-comparisons
- SCCVT: SCIAMACHY Calibration and Verification Team (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 campaigns and have been 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), hosting the validation database. 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, as well as 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.

Eight years after the launch of ENVISAT, this validation organisation still exists and subgroup participants work together episodically, not only for the preparation of Atmospheric Chemistry Validation of ENVISAT (ACVE) conferences but also to ensure sustainability of ENVISAT validation on the long-term. For this purpose, for delta validation of data processor upgrades and multi-mission consistency between ENVISAT and other atmospheric composition satellites, ESA supports a few long-term validation projects, which interact with algorithm maturation activities carried out in the framework of the SCIAMACHY Quality

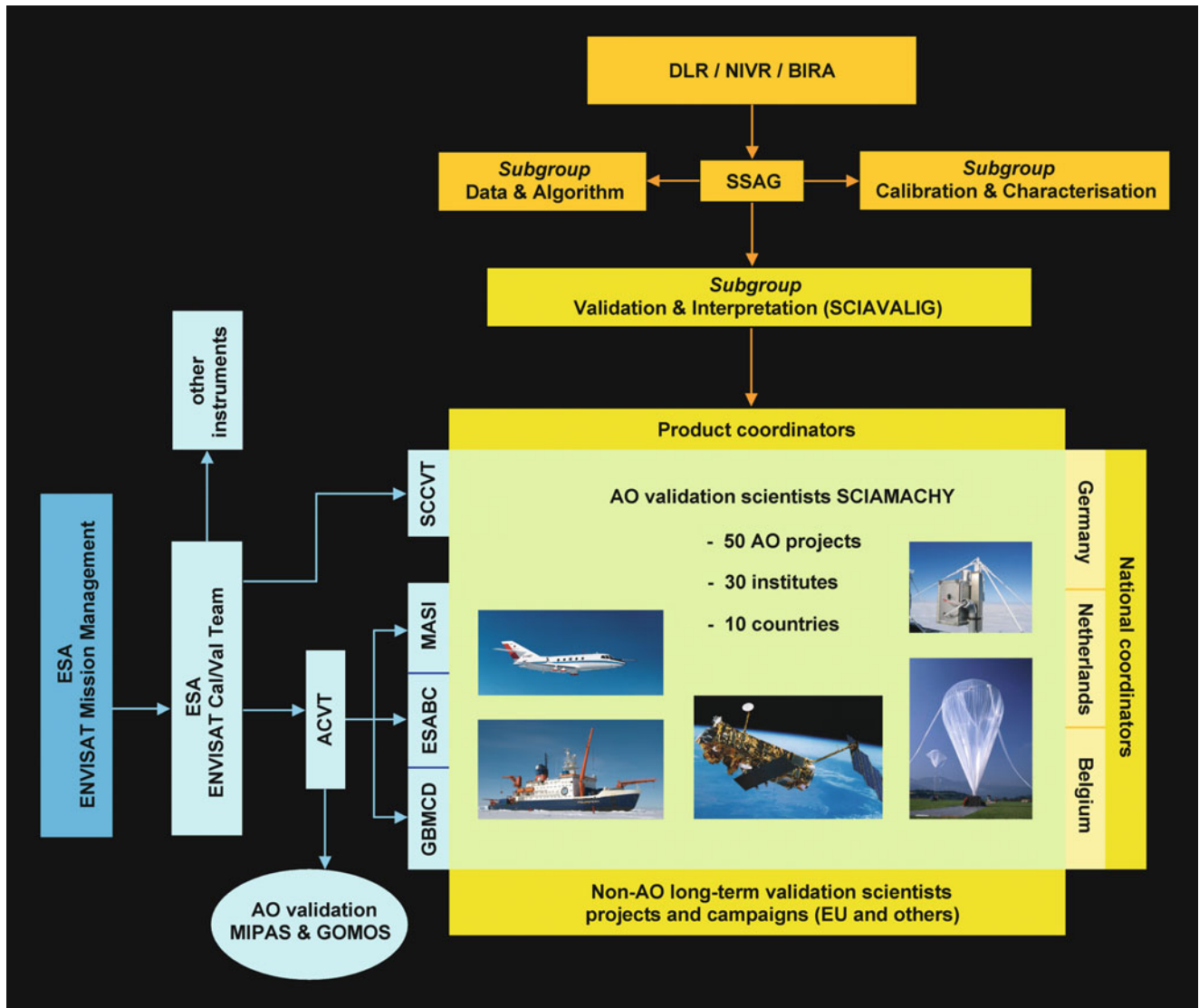


Fig. 9.1 A scheme of the SCIAMACHY validation organisational structures setup by SCIAVALIG (light orange) and by ESA (pale blue). The validation scientists actually doing the work are supported by both organisations, if they have an approved AO proposal for SCIAMACHY validation (green) (Courtesy: KNMI/DLR-IMF).

Working Group (SQWG). The ESA multi-mission oriented validation projects exploit major, continuously operated validation sources such as ground-based networks of the Network for the Detection of Atmospheric Composition Change (NDACC) and the Total Carbon Column Observing Network (TCCON) as well as independent satellite data. These ESA activities are complemented by national validation projects under the auspices of the SCIAMACHY AOP, e. g. balloon campaigns dedicated to improve the retrieval under specific atmospheric conditions.

SCIAVALIG Structure

The organisation of the AOP part of SCIAMACHY validation is delegated to SCIAVALIG, a subgroup of the SCIAMACHY Science Advisory Group (SSAG). SCIAVALIG, being co-chaired by KNMI, BIRA-IASB and IUP-IFE, University of Bremen, 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 set up an organisational structure for the continuous monitoring of validation results throughout the lifetime of SCIAMACHY and for the delta validation, necessary in case of processor upgrades. The core validation programme is mainly funded by the instrument providers and has been embedded in the ESA AO programme via several AO projects involving ‘national coordinators’ of SCIAVALIG.

SCIAVALIG established a coordination system related to products and validation methods. For each SCIAMACHY data product a ‘product coordinator’ was selected who maintains an overview of the validation results. The coordinator’s task is monitoring the scientific process, collecting the different validation results and providing a consistent record of the product quality. Product coordinators report their findings to SCIAVALIG, ACVT, and external scientists. In addition, they are invaluable advisors to algorithm development teams, the SCIAMACHY QWG, and to processor experts for an efficient translation of validation results into algorithm improvements.

9.3 Correlative Measurements

The core validation programme was complemented by a selection of AO projects from international partners and, in the long term, by supporting projects by ESA and various national institutions. The major component of the SCIAMACHY validation programme consisted of comparison studies with correlative measurements acquired by independent instrumentations from various platforms, namely, ground-based stations, ships, aircraft, stratospheric balloons, and satellites. The reference dataset collected within this initial effort is and remains the basis for every comparison. However, distinguishing between instrument ageing effects and real atmospheric trends requires continuous instrument monitoring and dedicated reference measurements throughout the mission.

Ground-Based Instruments

Ground-based instruments provide the appropriate correlative data to fulfil four main tasks of the SCIAMACHY 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 dependences on measurement, instrument and atmospheric parameters

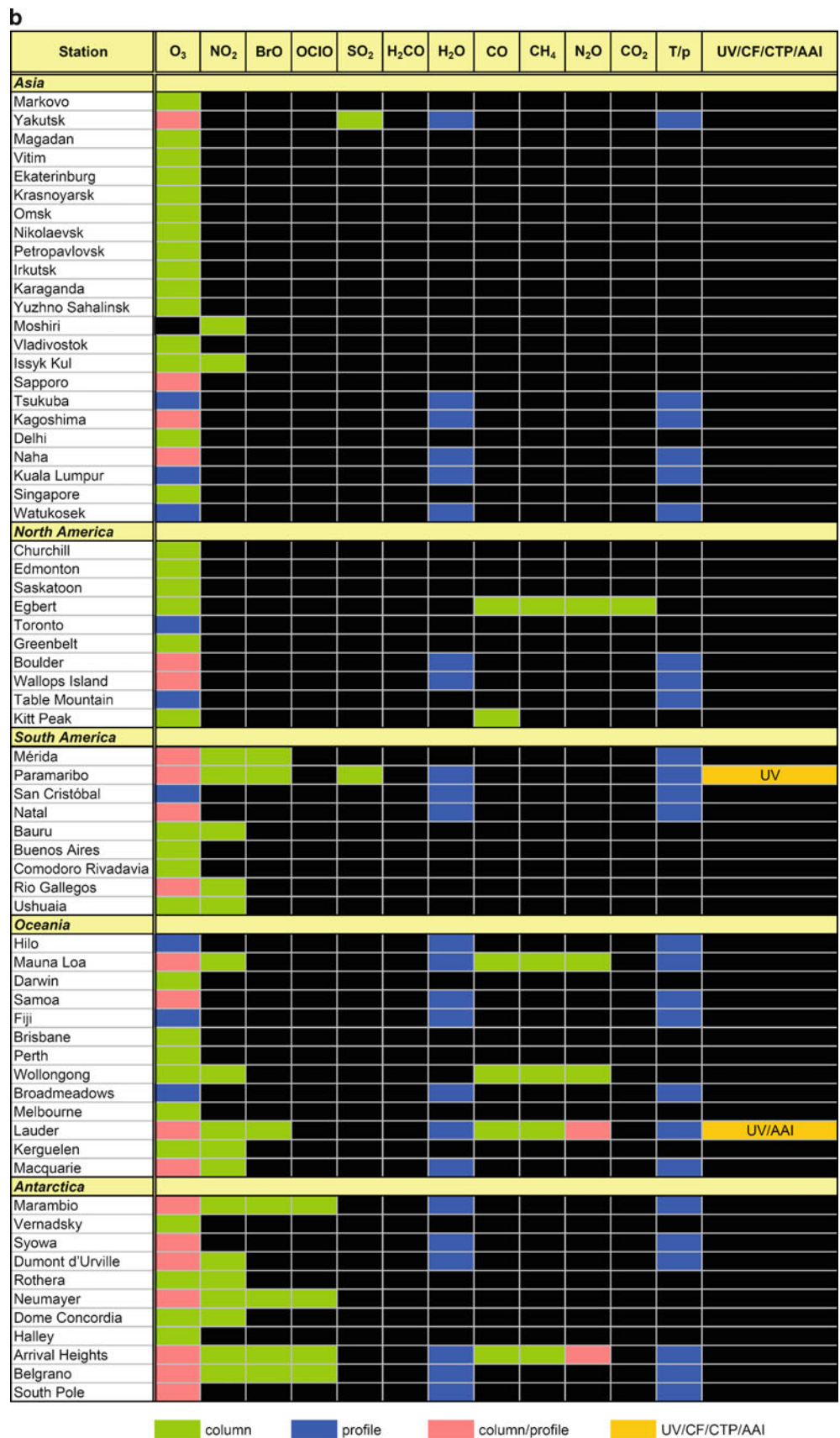
such as solar zenith angle, viewing angle and atmospheric temperature

- Verification of correctness of changes and preliminary quality assessment of the reprocessed data after a major improvement of a retrieval algorithm
- Long-term validation, including detection of drifts, cyclic errors and other time-varying features

The list of stations providing correlative measurements for SCIAMACHY validation is given in Fig. 9.2. These stations 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 ground-based validation, includes complementary types of instrumentation, yielding together nearly all targeted species, operating at about forty stations distributed from the Arctic to the Antarctic and from South America to the Indian Ocean.

Based on long-lasting collaborations established mainly in the framework of monitoring networks contributing to WMO’s Global Atmospheric Watch programme (GAW) – particularly the affiliated ozonometric networks (see Fioletov et al. 1999 and references therein) and the NDACC, formerly the NDSC (see Kurylo and Zander 2001; Lambert et al. 1999 and references therein) – international partners also contribute through AO projects and long-term validation projects with a long list of instruments which add significantly to the geographical coverage of the ground-based instrumentation included in the core validation programme. The ozone column amount is monitored at a variety of ground-based stations by Dobson and Brewer UV spectrophotometers and by Russian/NIS UV filter radiometers of the M-124 design. A network of about 30 DOAS instruments, all certified for the NDACC, 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. About ten Fourier Transform Infrared (FTIR) spectrometers, also NDACC certified, monitor the vertical column amount and, where possible, the vertical distribution of a series of species including O₃, NO₂, CO, CH₄, N₂O, CO₂, HCHO, and H₂O. Many of the NDACC FTIR teams are also expanding their measurement capabilities to the NIR, in an effort to join the network of TCCON stations. Six NDACC microwave radiometers measure the thermally induced rotational emission of selected species in the stratosphere and lower mesosphere, such as O₃, H₂O, and ClO. Differential Absorption Lidars (DIAL), certified for NDACC, and 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.

Fig. 9.2 (Continued)



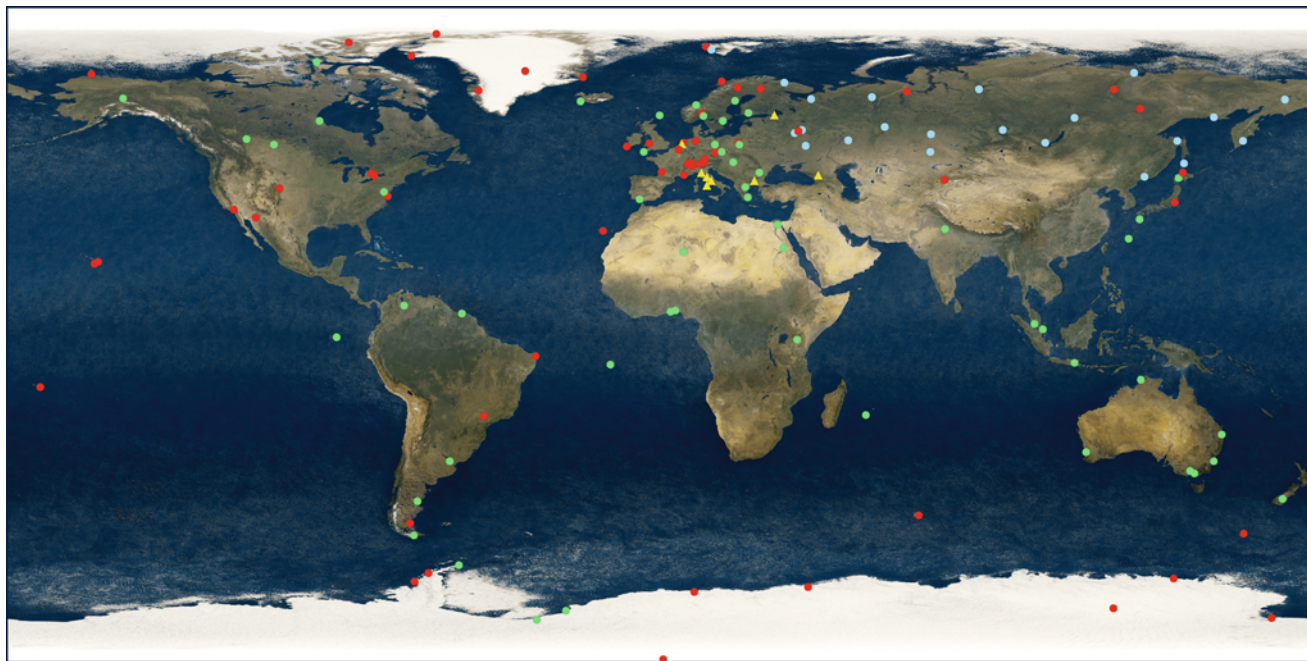


Fig. 9.3 Global distribution of validation sites. Symbols and colour codes indicate the prime network as follows: *red circles* – NDACC, *blue circles* – Russian/NIS M-124, *green circles* – GAW, *yellow triangles* – others (Courtesy: DLR-IMF/SRON/KNMI).

Triggered by new challenges in atmospheric research and the always higher accuracy requirements of satellite validation, several international measurement field campaigns took place in Europe in the last years with the specific objective to improve our understanding of the error bars of the respective types of measurement, of the intrinsic differences between these measurements, and of their potential synergies. At the same time they served identifying the best means to understand and validate observations from satellites. Some of the campaigns were supported by SCIAMACHY validation partners and by ESA. These comprised the SAUNA campaigns in Sodankylä (Finland) in 2006 and 2007 with the focus on ozone measurements at high latitudes, low solar elevations and large ozone column ranges. Other examples were the campaigns DANDELIONS in 2005 and 2006 (Brinksma et al. 2008) and CINDI in 2009, all taking place in Cabauw/The Netherlands. Their focus was on NO_2 and on other tropospheric measurements including species such as O_3 , HCHO, CHOCHO, BrO and aerosols.

Shipborne Campaigns

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 (Figs. 9.4 and 9.5). The moveable MAX-DOAS experiment measured not only constantly during these initial cruises but also during further *Polarstern* expeditions from 2005–2009. The FTIR instrument was operating during the second and third campaign from Bremerhaven to Africa. The unique *Polarstern* dataset was and is most useful for all investigations concerning large scale latitudinal cross sections of atmospheric trace gases.

Besides dedicated validation measurements on-board the *Polarstern*, data acquired during primarily research-oriented ship campaigns were also made available for the validation of SCIAMACHY. An example is the TransBrom campaign in autumn 2009 with the German research vessel *Sonne*. During the TransBrom cruise through the Pacific Ocean from Tomakomai/Japan to Townsville/Australia the exchange of halogens between the ocean and the lower and upper atmosphere was investigated. Two MAX-DOAS and an FTIR instrument delivered important validation data in the rarely covered tropical Pacific area.

Airborne Campaigns

The German aircraft validation activities were concentrated on missions with the meteorological research aircraft Falcon



Fig. 9.4 The research vessel *Polarstern* (Photo: G. Chapelle/Alfred Wegener Institute for Polar and Marine Research).

20 (D-CMET) operated by DLR, partially in cooperation with ESA campaigns involving the Russian research aircraft M55-Geophysika. Many features make the Falcon an excellent aircraft for validation. 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 pressure, and temperature. Within the SCIA-VALUE project (SCIAMACHY Validation and Utilization Experiment) two major campaigns with 28 flights were executed in September 2002 and February/March 2003 (Fig. 9.6). Both campaigns provided 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 O_3 , NO_2 , BrO, and OCIO, all absorbing in the UV-VIS wavelength range (see Fig. 9.8). 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 O_3 , ClO, HCl, HNO_3 , N_2O , H_2O , HO_2 , CH_3Cl , NO, HCN, and BrO. The Ozone Lidar Experiment (OLEX), 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

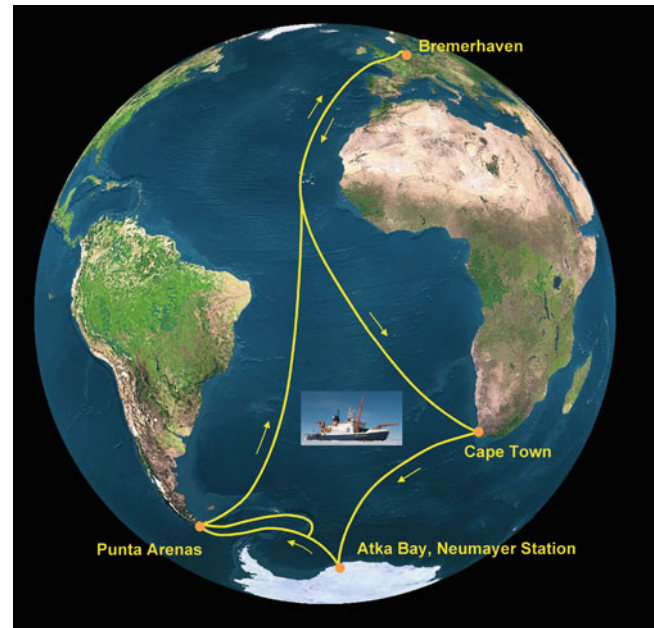


Fig. 9.5 Route of the *Polarstern* cruise during the ANT XIX campaign between November 2001 and May 2002 (Courtesy: DLR-IMF).

information, from about 2 km above the aircraft flight level up to a height of 30 km (Fix et al. 2005).

The stratospheric research aircraft M55-Geophysika has also been involved in ENVISAT's validation. It performed two mid-latitude campaigns in July and October 2002 from a base in Forli/Italy and a high latitude campaign in January and March 2003 from Kiruna. For the ENVISAT validation flights, the M55-Geophysika was equipped with two sets of instruments. The so-called 'chemical flights' were performed with six in situ and one remote sensing instruments, capable of measuring, among others, concentrations of H_2O , O_3 , NO, NO_y , N_2O , CH_4 , BrO, and columns of O_3 and NO_2 (Kostadinov et al. 2003, Heland et al. 2003). For the so-called 'cloud/aerosol flights', the remote sensing instrument was replaced by six instruments dedicated to the characterisation of aerosol and cloud properties. Although the in situ instruments remained on-board, these flights were optimised for the cloud and aerosol investigations.

Within the MOZAIC programme (Measurements of Ozone and water vapour by Airbus In-service aircraft, Marengo et al. 1998) which started in 1994, five long-range Airbus A340 aircrafts were equipped with in situ instruments measuring O_3 , H_2O , CO, and NO_y . They provide data from all over the world along their flight tracks in the upper troposphere/lower stratosphere at an altitude level from 9–12 km down to the ground in the vicinity of about 60 airports. These measurements are a unique dataset at the tropopause region and are especially useful for the development and validation of products distinguishing between troposphere and stratosphere. Other interesting datasets, which are not yet exploited for

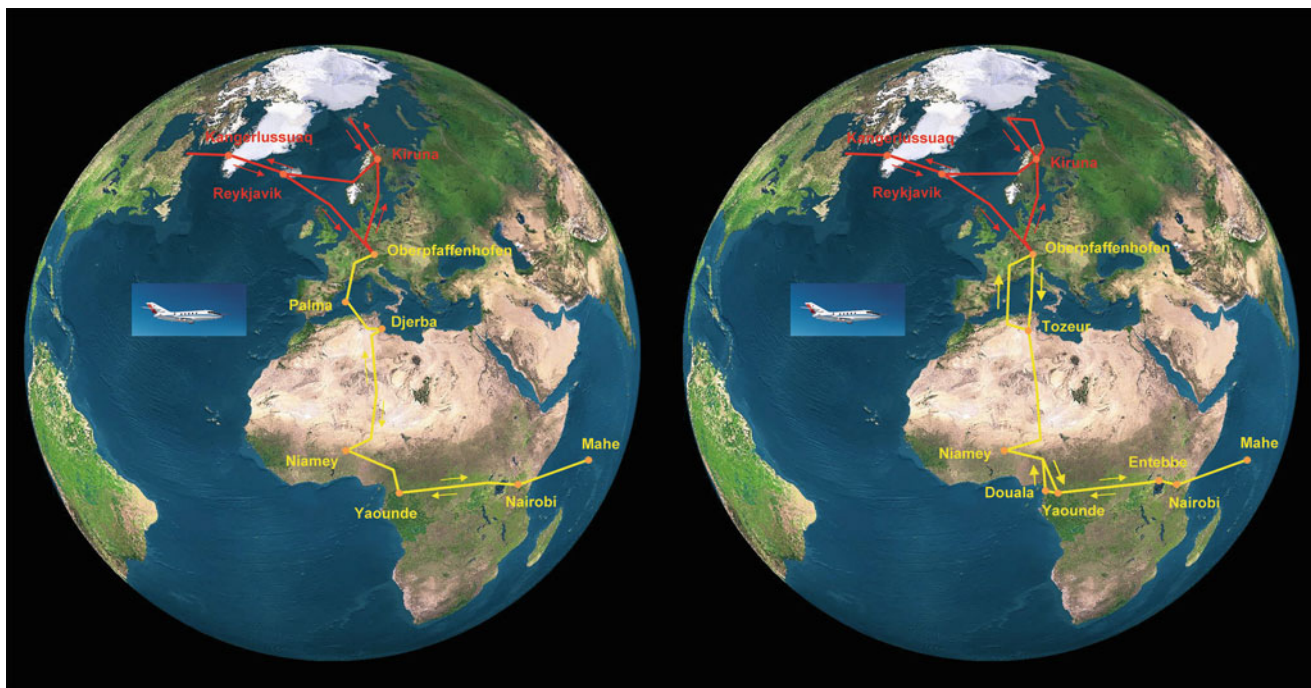


Fig. 9.6 Falcon flight tracks for the September 2002 (*left*) and February/March 2003 (*right*) SCIA-VALUE airborne campaigns. In red are the northern tracks (3–8 September 2002 and 19 February – 3 March 2003) while the southern tracks (15–28 September 2002 and 10–19 March 2003) are displayed in yellow (Courtesy: DLR-IMF).

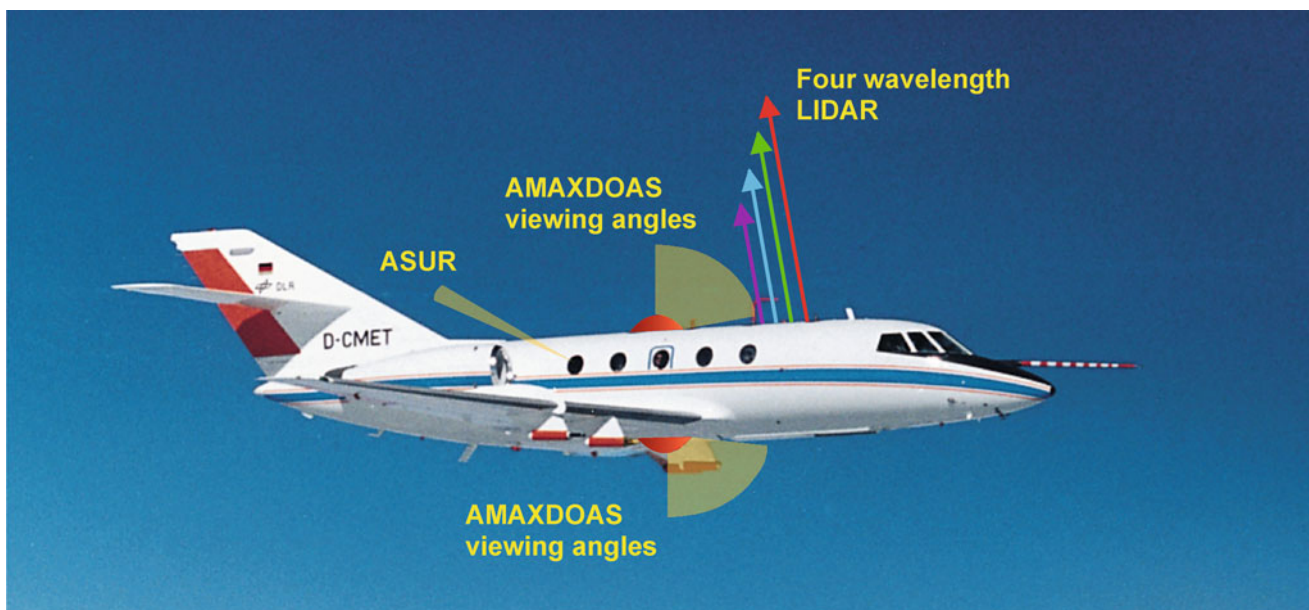


Fig. 9.7 The Falcon aircraft with the viewing directions of the validation instruments (Courtesy: Fix et al. 2005).

SCIAMACHY validation, may come from the programmes CARIBIC (Civil Aircraft for the Regular Investigation of the Atmosphere Based on an Instrument Container, Brenninkmeijer et al. 2007) and NOXAR (Measurements of Nitrogen Oxides and Ozone along Air Routes).

Since 2005 data from several scientifically driven airborne campaigns also contributed to SCIAMACHY's validation and algorithm improvements (Martin et al. 2006). One of them is led by ICARTT (International Consortium of Atmospheric Research on Transport and Transformation)

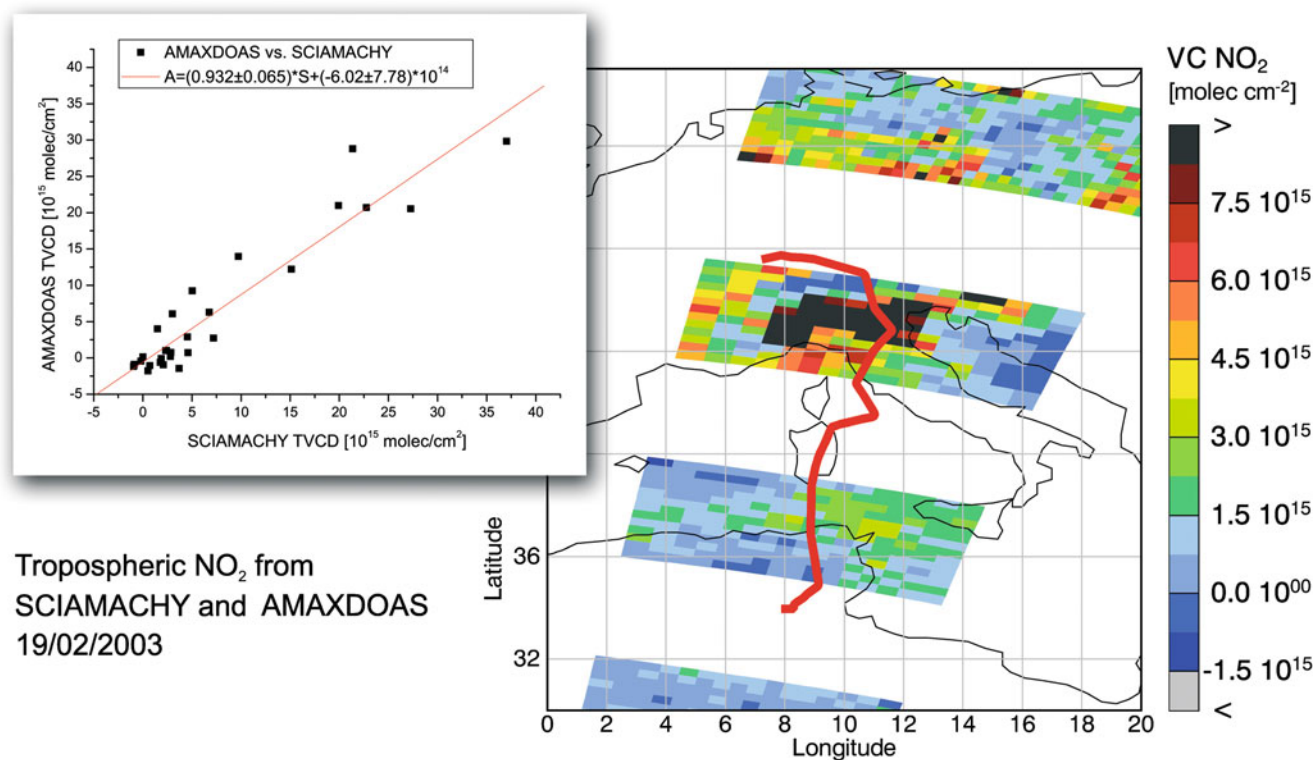


Fig. 9.8 Tropospheric NO_2 column obtained by SCIAMACHY together with the Falcon flight track (in red) showing where AMAX-DOAS measured almost simultaneously. In the inset tropospheric NO_2 columns from AMAX-DOAS are plotted versus those from SCIAMACHY. The SCIAMACHY tropospheric NO_2 columns are retrieved by IUP-IFE, University of Bremen (Courtesy: Heue et al. 2005).

combining several regional research projects independently developed by various international groups in the US and in Europe. The purpose of their cooperation is to derive a better understanding of the evolution of anthropogenic emission injected into the atmosphere. The major participants of the consortium are NOAA with their programme *New England Air Quality Study – Intercontinental Transport and Chemical Transformation* (NEAQS – ITCT 2004) program, NASA with their campaign *Intercontinental Chemical Transport Experiment – North America* (INTEX-NA) and, on European side, the project *Intercontinental Transport of Ozone and Precursors – North Atlantic Study* (ITOP) project. These regional undertakings studied local air quality by executing several aircraft flights in the New England area, the Northern Atlantic, and Western Europe. Another example is POLARCAT (Polar study using aircraft, remote sensing, surface measurements and modelling of climate, chemistry, aerosols and transport) which, from 2007–2008, investigated the transport of air pollution to the Arctic and its effect on atmospheric chemistry and climate. The measurements, taken with airborne sensors carried on several platforms, were closely coordinated with satellite overpasses including ENVISAT thus permitting validation of satellite observations of tropospheric species and aerosol parameters.

Balloon-Borne Campaigns

Balloon-borne measurements provide snapshot type vertical profile measurements of high precision. For the initial phase of intensive validation, the dedicated balloon campaigns for the atmospheric chemistry instruments GOMOS, MIPAS, and SCIAMACHY were funded by ESA, DLR, and CNES, with the costs and responsibilities shared according to an agreement between the three agencies. Part of this agreement was to use all balloon flights as far as possible for all three satellite instruments. CNES provided the facilities and staff for launching scientific payloads with large stratospheric balloons from dedicated stations. The availability of the CNES equipment was 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 campaigns (Fig. 9.9). The launch sites and campaign times were selected to cover mid-latitudes, northern latitudes, and the tropics during several seasons, including the possibility for ozone depletion conditions in spring, as far as possible within the available resources.



Fig. 9.9 Launch of the TRIPLE payload in Aire sur l'Adour in September 2002. (Photo: W. Gurlit, IUP-IFE, University of Bremen).

Explicitly funded for the validation of SCIAMACHY were:

- LPMA-DOAS: Combining a Limb Profile Monitoring of the Atmosphere FTIR and a UV-VIS DOAS instrument
- TRIPLE/TWIN: Combining sensors such as a resonance fluorescence ClO/BrO instrument – HALOX-B, an in situ Stratospheric Hygrometer – FISH, a cryogenic total air sampler – BONBON, and, occasionally, a tunable diode laser measuring H₂O and CH₄
- MIPAS-B: MIPAS balloon version

These constitute a part of 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 allow validation of corresponding parameters measured by SCIAMACHY during co-located overpasses of the satellite. Solar irradiances and limb radiances for level 1 validation were determined by radiometric calibration of the DOAS instruments on-board the LPMA-DOAS gondola.

In the initial phase of balloon-borne validation until mid 2005, many balloon campaigns (see Tables 9.1 and 9.2), dedicated to SCIAMACHY validation measurements, were performed from launch sites in Kiruna/Sweden, Aire sur

Table 9.1 SCIAMACHY validation specific payloads used in balloon campaigns (after Piters et al. 2006 and Oelhaf et al. 2009)

Payload	Launch dates	Launch site	Target species
MIPAS-B	September 2002	Aire sur l'Adour	O ₃ , NO ₂ , N ₂ O, H ₂ O, CO, CO ₂ , T/p
	December 2002	Kiruna	
	March 2003	Kiruna	
	July 2003	Kiruna	
	June 2005	Teresina	
	June 2008	Teresina	
TRIPLE +TWIN	September 2002	Aire sur l'Adour	CO ₂ , CH ₄ , N ₂ O, NO ₂ , H ₂ O, BrO
	March 2003	Kiruna	
	June 2003	Kiruna	
	June 2005	Teresina	
	June 2008	Teresina	
	March 2009	Kiruna	
LPMA- DOAS	August 2002	Kiruna	O ₃ , NO ₂ , OClO, BrO, CH ₄ , N ₂ O, H ₂ O, CO, T/p, irradiance
	March 2003	Kiruna	
	October 2003	Aire sur l'Adour	
	March 2004	Kiruna	
	June 2005	Teresina	
	June 2008	Teresina	
	September 2009	Kiruna	

l'Adour/France, Bauru/Brazil, Vanscoy/Canada, and Fort Sumner/New Mexico, US. Most of the individual flights lasted typically less than 1 day. However a few long duration trajectories were also included (Borchi and Pommereau 2007). These provided a large number of coincidences between spaceborne, including SCIAMACHY, and balloon-borne measurements as demonstrated by, e.g. the validation of water vapour profiles exploiting results from a 39 day long flight in the frame of the HIBISCUS campaign in February/March 2004 in Bauru/Brazil (Montoux et al. 2009).

When this phase was terminated, data suitable for SCIAMACHY validation were still acquired during additional balloon flights. These had either different atmospheric chemistry objectives or were intended for ENVISAT validation in general. Balloon launch sites included the locations listed above together with Teresina/Brazil and Niamey/Niger. One of them was performed in May/June 2008 within the SCOUT-O3 project in collaboration with an ENVISAT validation campaign, operated from Teresina, a site already visited by CNES and balloon scientists for an earlier ENVISAT validation campaign in June/July 2005. The balloon payload also comprised, in different combinations, the instruments funded for the dedicated SCIAMACHY validation such as MIPAS-B, TRIPLE, and LPMA/DOAS.

Satellite Intercomparisons

Correlative measurements by independent instruments on-board the same and other satellite platforms add significantly to the required pole-to-pole validation of

Table 9.2 Further balloon-borne experiments suitable for ENVISAT and/or SCIAMACHY validation

Payload	Launch dates	Launch site
SAOZ-MIR	February–March 2003	Bauru
	February–April 2004	Bauru
SAOZ	August 2002	Kiruna
+SAOZ-BrO	October 2002	Aire sur l'Adour
+SAOZ-H2O	February 2003	Bauru
	March 2003	Kiruna
	January 2004	Bauru
	February 2004	Bauru
	June 2004	Aire sur l'Adour
	August 2004	Vanscoy
	May 2005	Aire sur l'Adour
	October 2005	Aire sur l'Adour
FIRS-2	August 2006	Niamey
	October 2002	Ft. Sumner
	September 2003	Ft. Sumner
MANTRA	September 2004	Ft. Sumner
	September 2002	Vanscoy
SALOMON	September 2004	Vanscoy
	September 2002	Aire sur l'Adour
	March 2004	Kiruna
	June 2004	Aire sur l'Adour
	January 2006	Kiruna
SPIRALE	June 2007	Aire sur l'Adour
	August 2009	Kiruna
	October 2002	Aire sur l'Adour
	January 2003	Kiruna
	June 2005	Teresina
SDLA-LAMA	January 2006	Kiruna
	June 2008	Teresina
	August 2009	Kiruna
ELHYSA	August 2002	Kiruna
	September 2003	Aire sur l'Adour
	January 2003	Kiruna
AMON	March 2004	Kiruna
	August 2009	Kiruna
	March 2003	Kiruna
μRADIBAL	March 2004	Kiruna
	August 2009	Kiruna
LPMA-IASI	August 2002	Kiruna
	June 2005	Teresina
	March 2006	Kiruna
	June 2008	Teresina
	August 2009	Kiruna

SCIAMACHY. A few satellite instruments provide nearly global coverage at nearly daily frequency and, therefore, are well suited for global validation of SCIAMACHY data products in space and time. Complementarily, other satellites cover only a portion of the globe, often evolving with the season, but with a more regular geographical sampling and higher altitude range than the sampling and range achievable by ground-based instrumentation. Table 9.3 lists the satellite instruments used for the core validation of SCIAMACHY data products in the early phase of the mission. Some of

these sensors are now no longer in operation (marked by a ‘*’ below), others are still functioning. Additional instruments joined the fleet of spaceborne atmospheric instruments recently.

SCIAMACHY's precursor GOME on board ERS-2 follows ENVISAT with a delay of 30 min. Because the GOME channels are almost identical to the UV-VIS channels of SCIAMACHY, GOME was the first choice for validating UV-VIS nadir products. Over 15 years after launch, GOME is still a suitable validation source for SCIAMACHY. However, since a tape recorder anomaly in June 2003, GOME measurements are restricted to the North Atlantic sector and to the visibility sector of a few worldwide ground antennas. Launched in October 2006 on-board EUMETSAT's EPS/METOP-A, an improved version of GOME, GOME-2, precedes ENVISAT by 30 min and became the first choice for validating UV-VIS nadir measurements acquired after March 2007. Operational since 2004, OMI provides similar nadir UV-VIS data products, but with a relatively large time difference of about 5 h.

TOMS* and SBUV-2, other nadir looking instruments, deliver ozone total column and profile data. The solar occultation sensors HALOE*, SAGE II*/III*, POAM III* and ACE provide trace gas profiles at sunset and sunrise. SABER observes infrared emissions in limb, retrieving ozone and water vapour profiles at high altitudes. Also operating in limb mode, OSIRIS acquires vertical profiles of several UV-VIS absorbing species. In the infrared, MOPITT and TES generate nadir products. SUSIM and SOLSTICE results are used for comparison with solar irradiance measurements while MERIS and AATSR spectral reflectances are confronted with SCIAMACHY reflectance data. Both comparisons are 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.

9.4 Validation Results

The goal of validation is to generate a clear description of the quality of all SCIAMACHY data to allow users to readily evaluate the fitness of the data for their purpose. Besides providing evidence of traceability to established standards in terms of bias, precision and uncertainties, quality assessment of a data product also involves specific criteria on data availability, product and algorithm description, as well as software version control. Given the evolving nature of algorithm development together with defining new products, this goal has to be pursued continuously, but likely is never completely achieved. Since the Commissioning Phase of the instrument, more than 50 products were created, in part retrieving identical

Table 9.3 Satellite instruments used for SCIAMACHY validation in the early phase of the mission (2002–2004)

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 (390–1,040 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
MLS*	Microwave limb sounder	UARS	Profiles: O ₃
TOMS	Total ozone mapping spectrometer	Earth Probe	Columns: O ₃ , SO ₂ AAI
SAGE II* and III*	Stratospheric aerosol and gas experiment II and III	ERBS and 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	UARS	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
NRL			
POAM III*	Polar ozone and aerosol measurement III	SPOT-4	Profiles: O ₃ , H ₂ O, NO ₂ , aerosols
CSA/SNSB			
OSIRIS	Optical spectrograph and infrared imaging system	ODIN	Profiles: O ₃ , NO ₂
NOAA			
SBUV/2	Solar backscatter ultraviolet ozone experiment II	NOAA 14 and NOAA 16	Profiles: O ₃

Instruments marked “*” stopped operations around 2005

parameters with different algorithms. Most of them are science products, i.e. produced on a non-routine basis by the involved scientific institutes. Twelve products are currently provided and distributed operationally by the ESA ENVISAT ground segment. Upcoming new algorithms, changing scientific attention with respect to regional atmospheric particularities or trends as well as the monitoring of instrument changes require continuous validation throughout the instrument’s lifetime and even beyond, e.g. when data is expected to be used in long-term climatological studies.

The first years of the SCIAMACHY mission have proven the overall validation concept and provided initial results. A detailed overview of the validation results for the years 2002–2004 was given by PETERS et al. (2006) and references therein. Since then, data products and their validation have been updated and upgraded on many occasions. As a result of the intensive work of the SQWG the new version 5 of the SCIAMACHY Ground Processor (SGP) has become operational in 2010. It improves data products delivered and operationally provides new data products. This version expands on the previous processor SGP V3.01 whose products have been validated in the recent years as described below. In addition, as a consequence of the creative work of the SCIAMACHY scientific retrieval teams, improved and new scientific products became available and were validated by mission participating institutions. A regularly updated summary of the

validation status of operational and science data products can be found on <http://www.sciamachy.org/products/>.

Level 1 Irradiance and Reflectance UV-VIS-NIR-SWIR

The spectral solar irradiance is the most important extraterrestrial energy input into the Earth-Atmosphere system. SCIAMACHY measures the spectral solar irradiance from 214 to 2380 nm, with small gaps around 2000 and 2200 nm, on a daily basis. Skupin et al. (2005) demonstrated that after careful radiometric calibration, the solar spectral irradiance measured by SCIAMACHY agrees with other independently acquired datasets such as SIM, SOLSPEC, SOLSTICE, and SUSIM typically within 2–3%.

The solar radiation leaves the Earth’s atmosphere after reflection at the surface and/or scattering in the atmosphere. Normalising this radiation by the incoming solar irradiance leads to the Sun-normalised spectral reflectance, an important parameter characterising the Earth’s energy budget and being also the basis for some level 2 data products. Kokhanovsky et al. (2008) compared the top-of-atmosphere sun-normalised spectral reflectance measurements from SCIAMACHY, based on the up-to-date level 1b calibration, to

those from MERIS and AATSR, all three operating on ENVISAT. They agree typically within 2–3% in the visible wavelength range, even taking into account the large spread in different reflectivity regimes from close to 1.0 over snow to close to 0.05 over the oceans. This agreement is within the calibration errors for the individual instruments and demonstrates the substantial progress made – due to SCIAMACHY's improved calibration – when compared with earlier intercomparisons (von Hoyningen-Huene et al. 2007; Tilstra and Stammes 2007).

Level 2 Products from Nadir UV-VIS-NIR

Ozone (O_3): The agreement of SCIAMACHY SGP V3.01 O_3 columns with correlative data from ground-based networks and satellites is within 0–2%, with a small underestimation of up to 5% at high solar zenith angles. The bias depends on solar zenith angle, season, viewing angle, and cloud fraction. Although dominated by comparison errors, the 3–10% scatter of the discrepancies seems to vary with the cloud optical depth derived from SCIAMACHY O_2 A-band spectra. When comparing on the long-term to ground-based stations, the difference in O_3 total column may show a small temporal drift, around 0.5% per year (Lerot et al. 2009). The drift will become smaller in the processor version 5, as instrument degradation is taken into account in the related level 1b product. The sign and amplitude of this trend seems to be variable from station to station (Fig. 9.10). SCIAMACHY O_3 columns generated by scientific algorithms also show a good agreement compared to ground-based data, with a bias of 1–1.5% (usually a slight underestimation) and a RMS of about 5% and the same trend as the operational product.

Nitrogen dioxide (NO_2): Validation of the SCIAMACHY SGP V3.01 NO_2 columns indicates good agreement to within $1\text{--}5 \times 10^{14}$ molec/cm² with correlative data (from ground-based UV-VIS and FTIR, and from the GOME and GOME-2 satellite sensors) over areas free of tropospheric NO_2 , although slightly low biased in the Southern Hemisphere, by about 5×10^{14} molec/cm² on average. The low bias exhibits a seasonal cycle and varies smoothly with latitude. Larger deviations are observed in cases of tropospheric pollution and have a clear correlation with cloud fraction and Air Mass Factor. The scientific NO_2 stratospheric columns also show good quality (Gil et al. 2008) as illustrated in Fig. 9.11. Large differences exist between the different tropospheric NO_2 column algorithms (Brinkma et al. 2008). Results of the CINDI 2009 intercomparison field campaign, still under investigation, are expected to bring more quantitative validation statements on tropospheric NO_2 . Also first attempts were made to compare tropospheric NO_2 from SCIAMACHY with airborne (Martin et al. 2006) and boundary layer

(Boersma et al. 2009) in situ measurements. In the latter case satellite data were linked to concentrations relevant for air quality applications.

Bromine oxide (BrO): While the previous operational processor SGP V3.01 did not include BrO as a deliverable trace gas, BrO columns are provided with the current level 2 processor version 5. BrO columns retrieved with scientific algorithms agree well with those obtained from GOME, GOME-2 and from ground-based measurements. This indicates that also the operationally generated results will be of good quality. For example, comparisons between ground-based BrO vertical columns measured over Reunion-Island (20.9°S, 55.5°E) and total BrO columns derived from SCIAMACHY nadir observations in a latitudinal band centred around 21°S present a good level of consistency (Theys et al. 2007).

Chlorine dioxide ($OCIO$): Qualitatively, SCIAMACHY scientific $OCIO$ slant columns reproduce well $OCIO$ features measured by ground-based UV-VIS and airborne AMAX-DOAS spectrometers. They also agree well with GOME scientific retrievals. Quantitatively, the SCIAMACHY data show a relatively large offset and scatter compared to the GOME data. The accuracy of the SCIAMACHY $OCIO$ column retrieval appears to be much better at low column amounts of less than 0.5×10^{14} molec/cm², close to the detection limit. Oetjen et al. (2009) demonstrated excellent agreement between SCIAMACHY $OCIO$ slant columns and MAX-DOAS ground based data around 1×10^{13} molec/cm² or even lower (see Fig. 9.12).

Sulphur dioxide (SO_2): Quantitative validation of SCIAMACHY columns of SO_2 is hampered by the lack of independent measurements. Routine measurements near emission sources are currently being developed. A few international airborne campaigns were organised, e.g. INTEX and a campaign over Eastern China, during which SO_2 columns from SCIAMACHY and from OMI were validated with co-located in situ measurements. Validations conclude yearly average errors ranging from 10^{15} molec/cm² over clean ocean areas to 25×10^{15} molec/cm² over polluted regions (e.g. eastern China). This corresponds to errors of less than 10% in the first case and up to 35–70% in the second case (Lee et al. 2009).

Formaldehyde ($HCHO$): As in the case of SO_2 , the quantitative validation of SCIAMACHY columns of $HCHO$ requires independent measurements which are only rarely available. Comparisons to ground based DOAS measurements over Cabauw/The Netherlands and Nairobi/Kenya agree within their error bars with the tropospheric column derived from SCIAMACHY data (Wittrock et al. 2006). De Smedt et al (2008) compiled an error assessment of the $HCHO$ product, indicating total errors of 20–40% for monthly and zonally averaged $HCHO$ vertical columns.

Glyoxal ($CHOCHO$): Since glyoxal was for the first time detected from space with SCIAMACHY, quantitative vali-

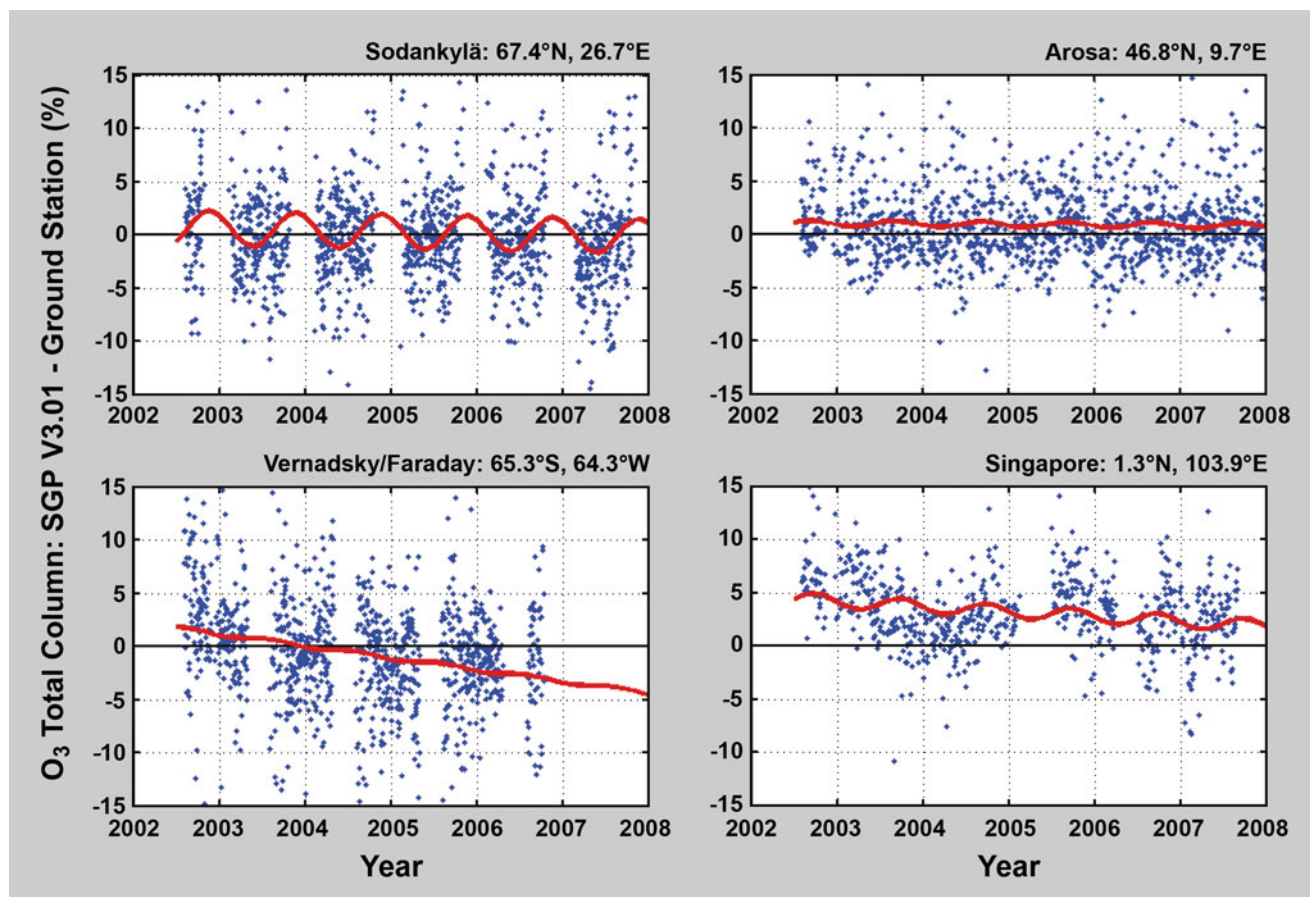


Fig. 9.10 The difference between total O₃ columns retrieved from SCIAMACHY and selected ground stations for the years 2002–2008. The red curve indicates seasonal variability and long-term trends obvious in the comparison. The trends range between -0.15% and -1.1% per year (Courtesy: adapted from Lerot et al. 2009).

dation of columns is even harder to accomplish due to the lack of independent measurements. Ground based DOAS measurements again from Cabauw/The Netherlands and Nairobi/Kenya indicate an agreement within the error bars for the tropospheric SCIAMACHY column (Wittrock et al. 2006). How the quality of such data relates to various chemical environments (urban, rural, ocean) is discussed by Vrekoussis et al. (2009) when comparing SCIAMACHY derived CHOCHO with in situ ground-based observations.

Water vapour (H₂O): Validation of the scientific SCIAMACHY AMC-DOAS water vapour columns V1.0 shows a systematic bias of -0.1 to -0.5 g/cm² with respect to co-located balloon-sonde observations (cryogenic frost point hygrometer) and SSM/I satellite observations, as well as ECMWF analyses (Fig. 9.13). This bias is attributed to the fact that SCIAMACHY retrievals are essentially cloud-cleared (Noël et al. 2005; Noël et al. 2007). The scatter on such comparisons, about 0.5 g/cm², is quite large due to the significant atmospheric variability of water vapour in the

troposphere. Somewhat larger deviations are present between SCIAMACHY and SSM/I water vapour data over oceans.

Cloud Fraction (CF), Cloud Top Pressure/Cloud Top Height (CTP/CTH): The SCIAMACHY processor estimates the fractional cloud coverage (CF) using the OCRA algorithm, and then the cloud top height (CTH) or pressure (CTP) together with the cloud optical thickness (COT) using SACURA. The CF correlates well with scientific retrievals and with MODIS observations. From intercomparisons with ground-based cloud radar for single-layer cloud fields Kokhanovsky et al. (2009) concluded, that the uncertainty of the SACURA CTH retrieval is less than 0.34 km for low-level clouds and 2.22 km for high-level clouds with an underestimate in CTH on average for all clouds.

Absorbing Aerosol Index (AAI), Aerosol Optical Thickness (AOT): The SCIAMACHY scientific AAI compares well with TOMS results. Also the SCIAMACHY scientific AOT agrees reasonably well with MERIS data.

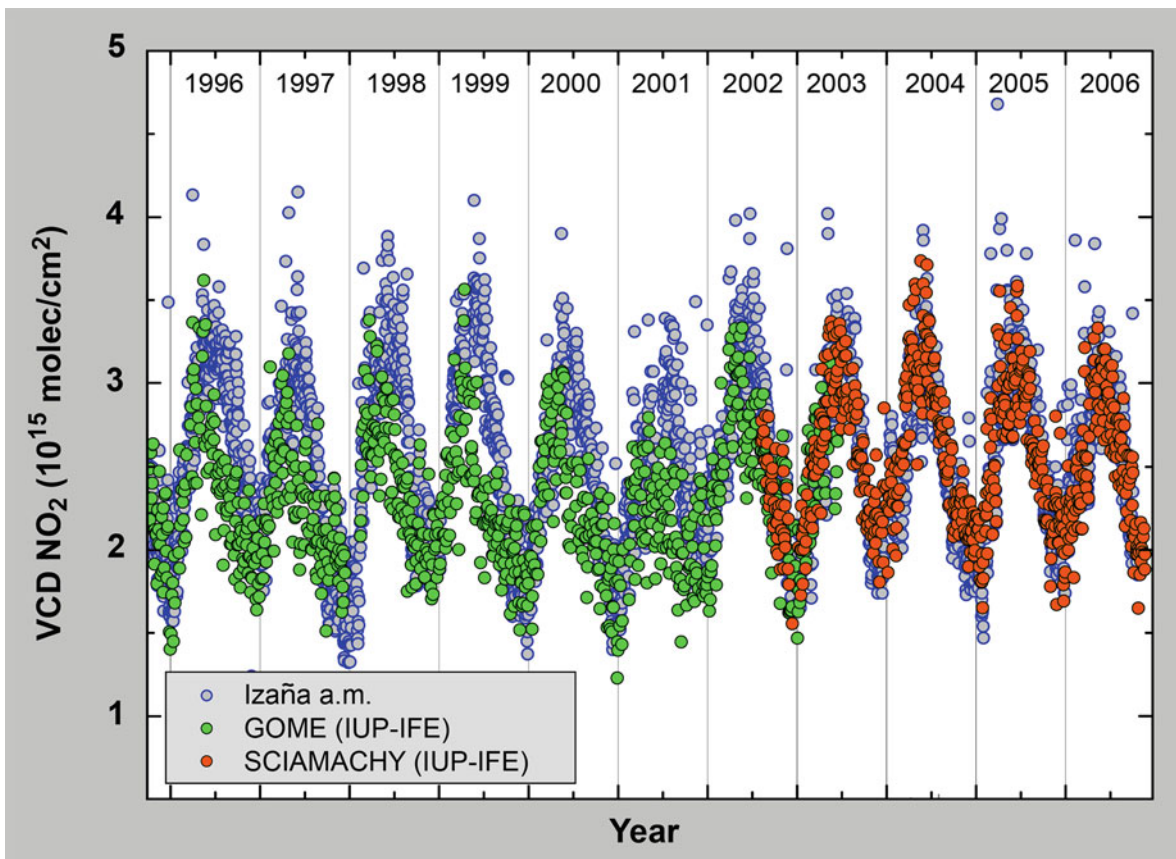


Fig. 9.11 NO₂ vertical column densities from SCIAMACHY nadir measurements (*red*) compared with ground-based morning data from Izaña (*grey*) and VCD from GOME (*green*). The GOME and SCIAMACHY VCD have been retrieved with a scientific algorithm from IUP-IFE, University of Bremen (Courtesy: Gil et al. 2008).

Level 2 Products from Nadir SWIR

The general potential of SCIAMACHY SWIR products had already been demonstrated, in particular its capabilities to detect areas of sources of CO, CH₄ and CO₂ and to track their long-range transport. Various algorithm versions have been validated by comparing their output with results from:

- Ground-based CO, CH₄, and CO₂ data from Fourier Transform Spectroscopy (FTS) via the pole-to-pole network of 12 NDACC-certified FTIR instruments (see e.g. Dils et al. 2006, 2007).
- Ship-based FTIR data taken during the bi-yearly cruises of the *Polarstern* vessel from Bremerhaven to Africa
- CO column data from the EOS-Terra MOPITT satellite
- CO and CH₄ data from the TM4 (KNMI), TM5 (IMAU), INCA (LSCE), and CTM2 (Oslo University) models
- Ancillary data such as fire maps produced by ERS-2 ATSR and EOS-AQUA MODIS

Observations from the Japanese TANSO/GOSAT satellite mission, launched in January 2009, are expected to

contribute significantly to further characterise SCIAMACHY and GOSAT data quality.

Carbon monoxide (CO): Pre-launch estimates for the precision of scientific retrievals of SCIAMACHY nadir CO vertical columns amounted to 10% over land. The scientific CO data product derived with the WFM-DOAS algorithm has been compared with MOPITT (Buchwitz et al. 2007) and ground-based FTS measurements (Dils et al. 2006) finding a scatter of the CO product relative to the FTS retrievals of typically 20% for daily averages around the FTS sites, i.e. close to what was expected. Main reason for the somewhat larger scatter is the fact that not all CO lines can be used in the retrieval due to detector degradation. The mean bias is typically approximately 10%. Recently de Laat et al. (2010) analysed the quality of the SCIAMACHY CO data set for the years 2003 to 2007. Their main finding was that for stations not affected by local emissions or altitude effects, differences between SCIAMACHY and ground based FTS measurements are close to or within the SCIAMACHY CO total column precision of 0.1×10^{18} molecules/cm² (~5–10%) of the SCIAMACHY CO columns (de Laat et al. 2010).

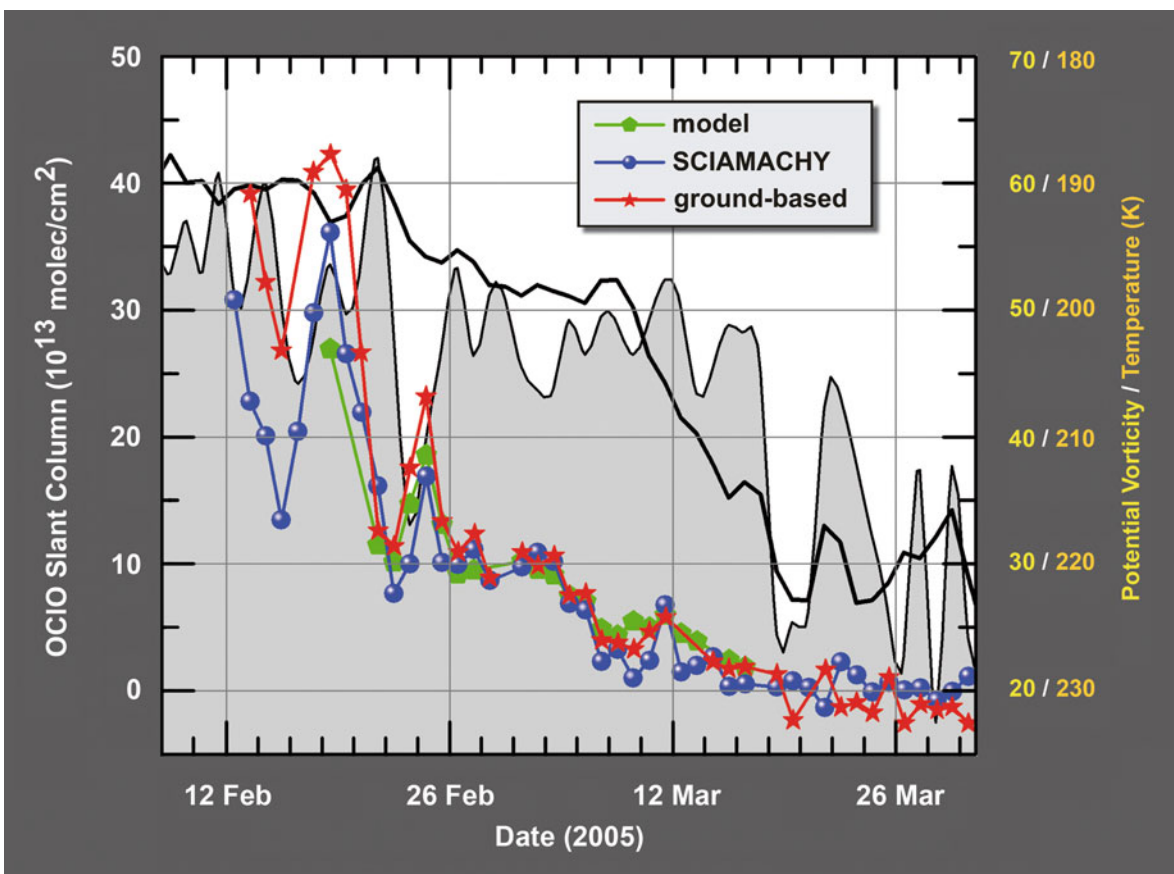


Fig. 9.12 OCIO slant columns retrieved from SCIAMACHY data (blue) compared with ground-based measurements (red), sampled at the time of ENVISAT overpass, over Ny-Ålesund (79°N, 12°E) in spring 2005 and model data (green). Also shown are potential vorticity (shaded area) and temperature (black solid line) at the 475 K isentropic surface (Courtesy: adapted from Oetjen et al. 2009).

Initial results, illustrated in Fig. 9.14, demonstrate good agreement with CO columns from MOPITT. The data was already used in a variety of applications, like inverse modelling of emissions (Kopacz et al. 2010; Tangborn et al. 2009). CO is included in the operational processor version 5 released in 2010.

Methane (CH₄): High precision and accuracy of greenhouse gas measurements are a firm precondition for the potential improvement of existing emission catalogues by inverse modelling. With about 1–2% the pre-launch precision estimates for scientific retrievals of SCIAMACHY nadir CH₄ vertical columns were not far off the nominal requirements for such applications. A huge effort was spent in the last years to improve the precision and accuracy of real retrievals to finally reach the goal that SCIAMACHY CH₄ data is used for emission estimates (see Chapter 10). From the comparison with FTS and model (TM5) data and supported by an error analysis of the WFM-DOAS retrieval algorithm, the SCIAMACHY XCH₄ data set (column averaged mixing ratio) can be characterised globally by a single ground pixel retrieval precision of about 1.7% and a systematic low bias of

about 1% (Schneising et al. 2009). Methane FTS observations, acquired over Paramaribo/Suriname, exhibit good agreement for the measured ratio of CH₄/CO₂ with SCIAMACHY results and represent the first validation of SCIAMACHY retrievals in the tropics using ground-based remote sensing techniques (Petersen et al. 2010).

Carbon dioxide (CO₂): As in the case of CH₄, the precision of scientific retrievals of SCIAMACHY nadir CO₂ vertical columns were estimated before launch to be 1–2%. Schneising et al. (2008) reported indeed that the XCO₂ dataset can be characterised globally by a single measurement retrieval precision (random error) of 1–2% (see Fig. 9.15), a systematic low bias of about 1.5%, and by a relative accuracy of about 1–2% for monthly averages at a spatial resolution of about 7° × 7°. In areas of enhanced atmospheric scattering due to aerosol or cirrus clouds the systematic errors could be higher. It is expected that in the near future the ongoing expansion of ground-based FTIR spectrometers to the near-infrared will improve capabilities for the validation of satellite greenhouse gas data products such as CO₂.

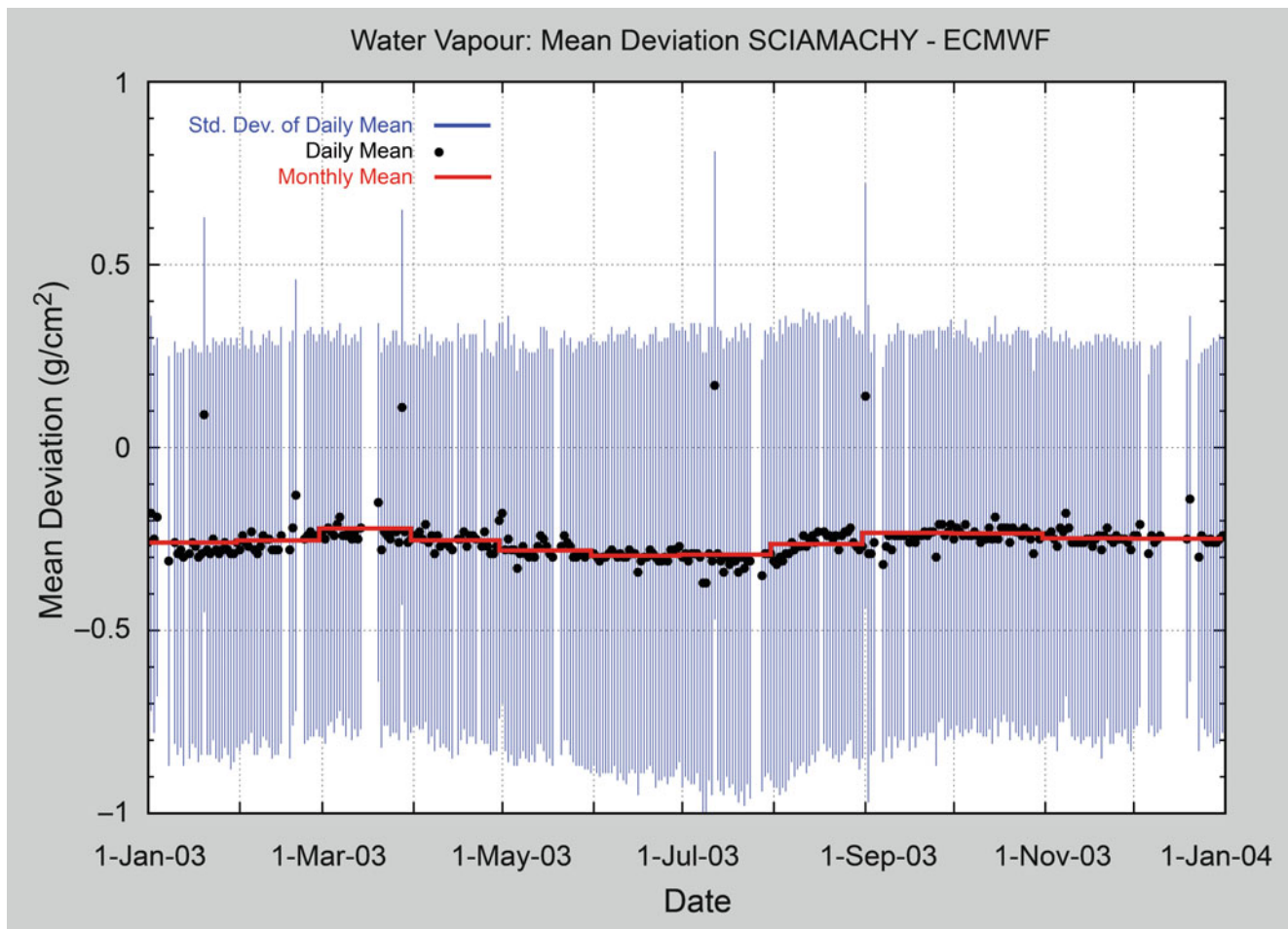


Fig. 9.13 AMC-DOAS V1.0 total column water vapour compared with model data provided by the European Centre for Medium-Range Weather Forecasts (ECMWF) over land and ocean for 2003. The comparison has been performed with co-located daily global averages on a $0.5^\circ \times 0.5^\circ$ grid (Courtesy: S. Noël, IUP-IFE, University of Bremen).

Level 2 Products from Limb UV-VIS

Ozone (O_3): Vertical profiles of the ozone concentration retrieved from SCIAMACHY limb UV-VIS measurements with the SGP version V3.01 have been validated extensively against observations from ground-based networks (of ozone-sondes, lidars, and microwave radiometers) and satellites, e.g. HALOE, SAGE-II, MLS (Fig. 9.16), ODIN, ACE, GOMOS, and MIPAS. Validations indicate that SCIAMACHY has a low bias (up to 10 %) around the ozone maximum and below, even after implementation of the limb pointing corrections. Due to the limited sensitivity of the retrievals below 20 km and above 40 km, the retrieval errors increase considerably past these altitudes. O_3 profiles retrieved with a scientific limb retrieval algorithm (Sonkaew et al. 2009) were additionally validated against ground-based and satellite data. Between 16 and 40 km the systematic bias of the retrieved profiles ranges within 5–10% compared to lidars

and SAGE-II and is even smaller when MLS data are taken into account. Jones et al. (2009) assessed the quality of several long-term stratospheric O_3 satellite data records. They examined monthly average ozone values from various satellites for nine latitude and altitude bins covering 60°S – 60°N and 20–45 km from the time period 1979–2008. The analysed data were from SAGE I/II, HALOE, SBUV/2, SMR (Submillimeter Radiometer), OSIRIS and SCIAMACHY. This investigation identified that instrumental drifts are not relevant for SCIAMACHY data in the mid northern latitudes, but become relevant for long-term trend assessment in the tropics and southern mid-latitudes. When comparing the SCIAMACHY O_3 profiles with observations from the ACE FTS solar occultation sensor the agreement is on average within 4% (Dupuy et al. 2009).

Nitrogen dioxide (NO_2): After photochemical correction for the time difference between SCIAMACHY limb data acquired in the morning and correlative solar occultation

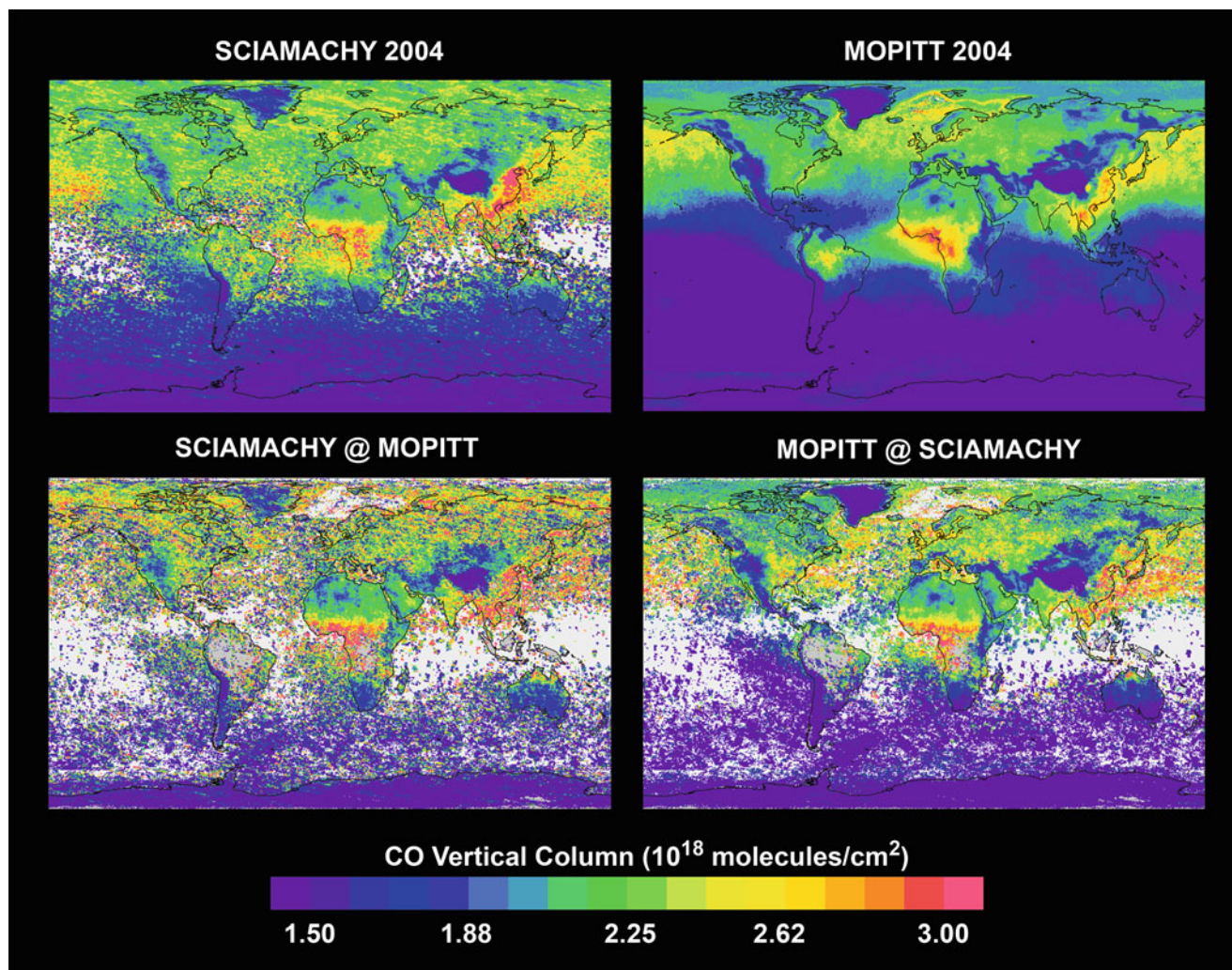


Fig. 9.14 Comparison of CO vertical columns for the year 2004 derived with SCIAMACHY (*top left*) and MOPITT (*top right*). The bottom row shows spatial coincidences between both sensors (Courtesy: Buchwitz et al. 2007).

profile measurements performed at twilight by other missions, SCIAMACHY limb NO_2 profiles retrieved with SGP V3.01 coincide well – on average at about 10–15% – with profiles derived by other spaceborne sensors. Comparisons with NO_2 profiles measured by ACE FTS (Kerzenmacher et al. 2008) show an even better coincidence (4% average). Further improved NO_2 retrieval algorithms are in preparation and are aiming at better results in the lower stratosphere towards the tropopause. Figure 9.17 illustrates, as an example, the results of such an algorithm when applied to SCIAMACHY limb data with an agreement of better than 10% for even a single balloon-borne measurement.

Bromine oxide (BrO): Figure 9.18 displays 5 years of SCIAMACHY BrO profiles, retrieved with a scientific algorithm (Rozanov et al. 2005), and how they match with ground-based UV-VIS profile measurements in Harestua/Norway (60°N, 11°E). SCIAMACHY and ground-based UV-VIS

columns integrated over the 15–27 km range are in good agreement, with SCIAMACHY columns being lower than ground-based columns by $2\% \pm 20\%$. Both datasets reflect markedly the seasonal variability of the BrO column (Hendrick et al. 2009). Dorf et al. (2006) showed – using photochemical corrections for balloon observations along calculated air mass trajectories – that the SCIAMACHY BrO profiles coincide on average within approximately 20% with the balloon data.

Chlorine dioxide (OCIO): Experimental OCIO profile measurements were compared to non-co-located balloon data from earlier campaigns. The values of the SCIAMACHY OCIO data and their variability are similar to those from the balloon-borne measurements, indicating that SCIAMACHY is providing geophysical meaningful OCIO profiles. In addition, comparisons of SCIAMACHY OCIO with ClO from ODIN SMR – both species are photo-chemically related – are supporting these findings (Kühl et al. 2008).

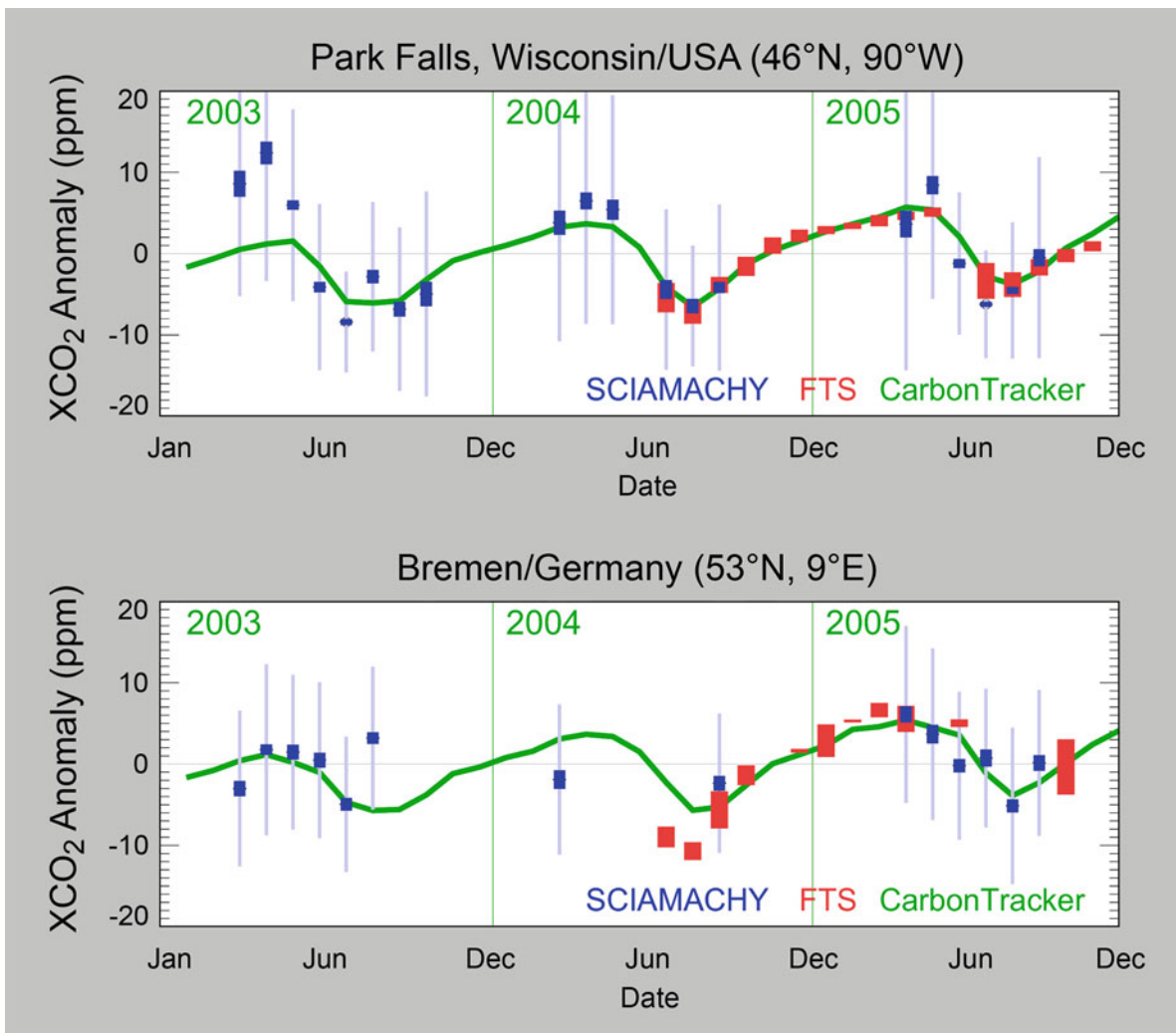


Fig. 9.15 Comparison of SCIAMACHY XCO₂ (blue) with ground based Fourier Transform Spectroscopy (FTS) measurements (red) for Park Falls (top) and Bremen (bottom). Also included are corresponding CarbonTracker results (green). Shown are comparisons of XCO₂ anomalies, i.e. the corresponding mean values have been subtracted. All quality filtered SCIAMACHY measurements within a radius of 350 km around the ground station are considered for the comparison (Courtesy: Schneising et al. 2008).

Fig. 9.16 Zonal mean O_3 from SCIAMACHY vertical profiles averaged from 2005 to 2008. Only co-located daily measurements with MLS have been used, where the criteria for co-locations are 100 km spatial and 10 h temporal difference. Co-locations with MLS measurements during night with solar zenith angles $>90^\circ$ have been excluded (Courtesy: S. Mieruch, IUP-IFE, University of Bremen).

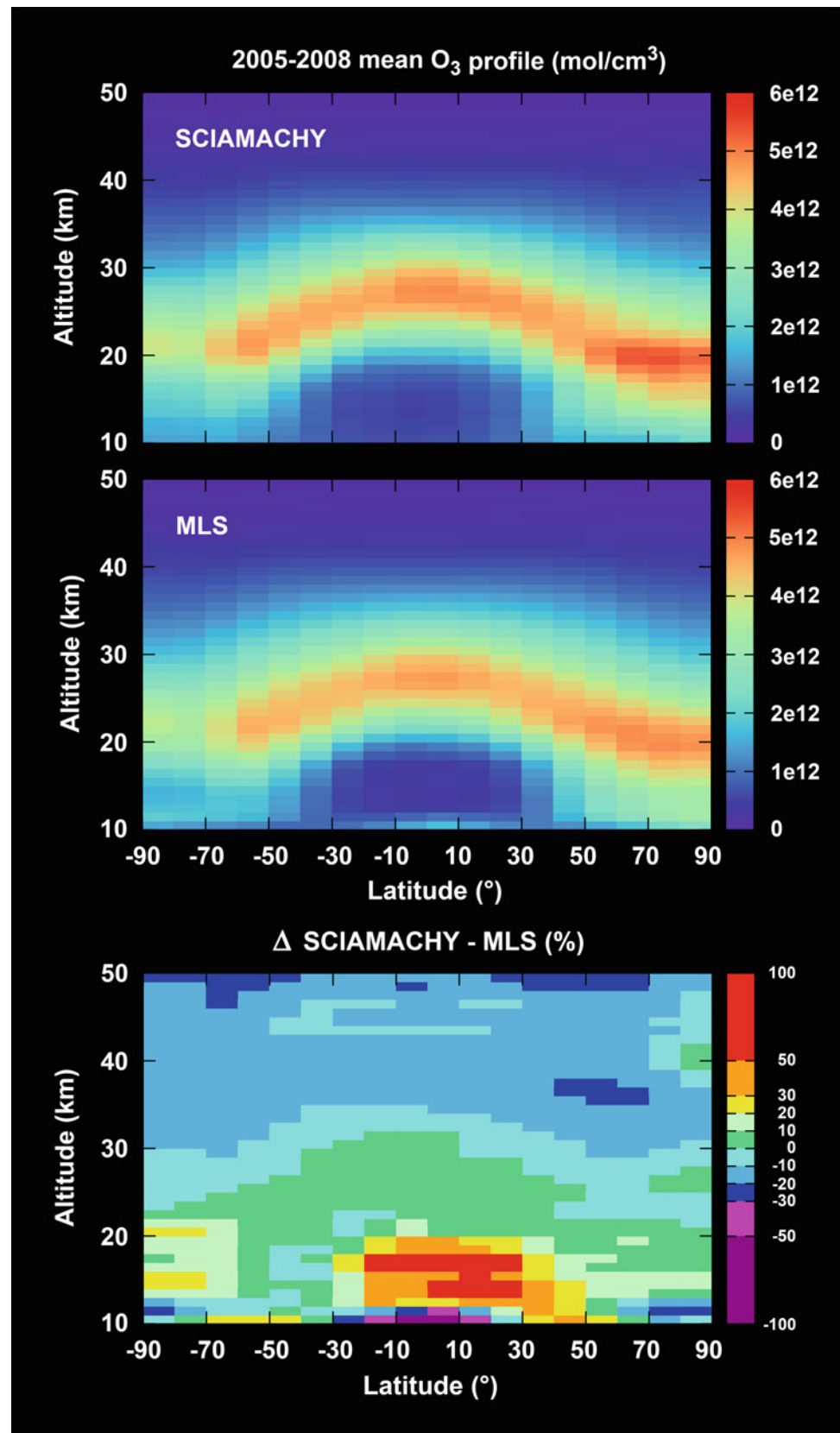


Fig. 9.17 Comparison between a SCIAMACHY NO₂ profile (blue) retrieved with the SCIATRAN V3.1 algorithm and co-located balloon NO₂ measurements at Kiruna (red). The grey shaded area shows the uncertainty of the balloon measurements, whereas the yellow region indicates the altitude range where both instruments are considered to probe similar air masses (Courtesy: R. Bauer IUP-IFE, University of Bremen).

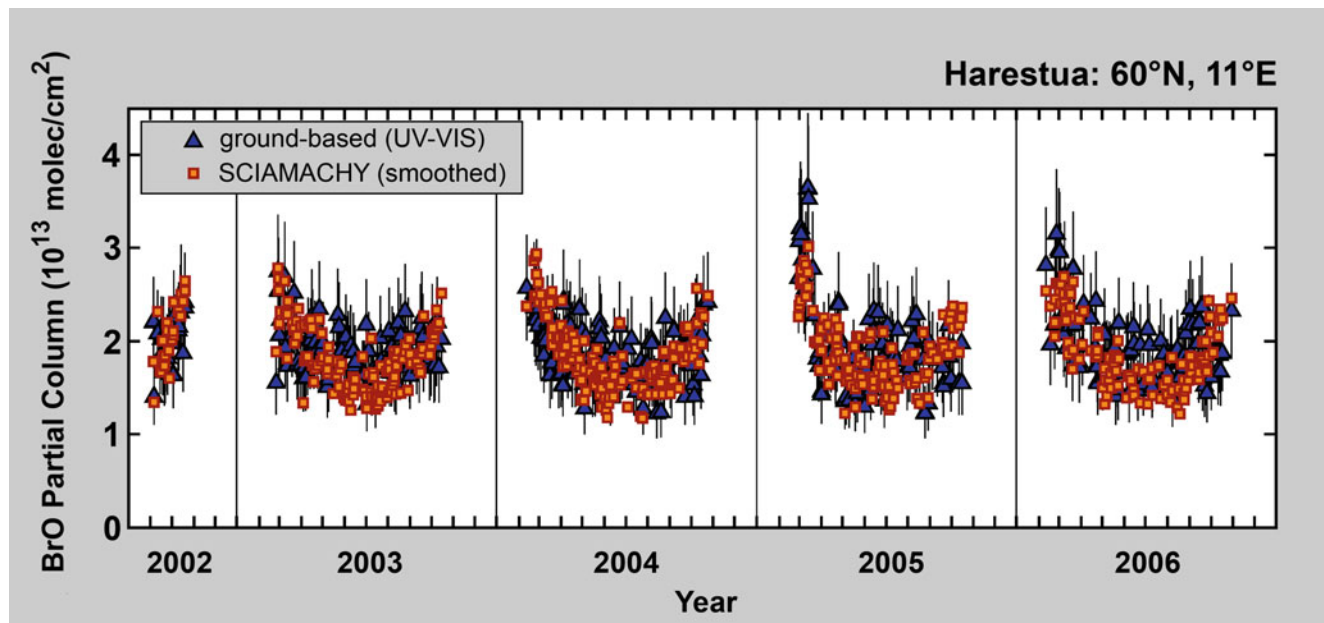
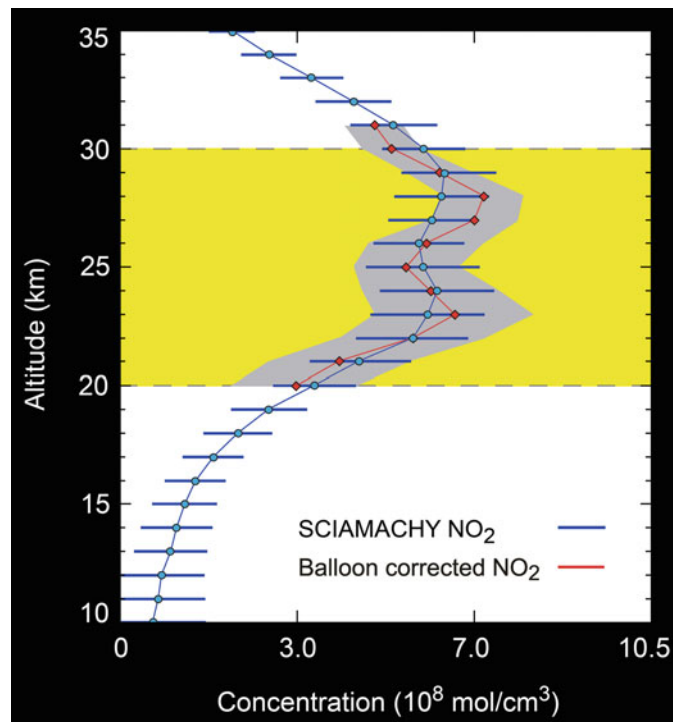


Fig. 9.18 Intercomparison of the 15–27 km BrO partial columns calculated from SCIAMACHY limb and ground-based UV-VIS profiles at Harestua/Norway for 2002–2006 (morning coincidences). To reduce comparison errors due to differences in vertical smoothing of the vertical profile, SCIAMACHY profiles were smoothed using coincident ground-based UV-VIS averaging kernels (Courtesy: adapted from Hendrick et al. 2009).

Water vapour (H_2O): Recently it was successfully demonstrated to derive H_2O concentrations in the upper troposphere and lower stratosphere region from SCIAMACHY limb measurements. Montoux et al. (2009) used data from the HIBISCUS campaign in Bauru/Brazil in the February/March 2004 period for validating satellite water vapour measurements in the southern tropical and subtropical UTLS region. Preliminary analysis suggests that the SCIAMACHY results reproduce the atmospheric variability of water vapour around the tropopause and indicate a dryer atmosphere by 20% when compared to HALOE.

A common issue to all limb viewing instruments is the accurate determination of the limb pointing and in particular of the tangent height. New corrections in tangent height registration and of misalignment parameters, already implemented in SGP V3.01 (Gottwald et al. 2007), yielded a reduction in the east-west offset and in the bias of the altitude registration of the limb profile products, being now smaller than about 200 m (see Section 6.5).

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