SCIAMACHY Validation Workshop

6-8 December 2004, Bremen

Summary Report

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Introduction

This document is a summary report of the SCIAMACHY validation workshop, held on 6-8 December 2004 in Bremen. It is based on the presentations and the discussions during the workshop. The workshop was kindly hosted by ACCENT-Troposat 2, who provided support for meeting expenses and travel and accommodation costs for a number of the invited participants. The main objective of this workshop was to establish the status of our knowledge of the quality of the currently available operational and non-operational SCIAMACHY products.

Outline of the workshop

The agenda of the workshop is attached as Annex A. The workshop started with a general session with information on the status of the instrument, the operational processor, the scientific products, and available support for validation (Sessions I and II). It was followed by the final German Validation Team meeting, with 16 presentations of the results of the nationally funded validation projects (Sessions III to V). The rest of the workshop consisted of product-based sessions on respectively: O_3 and NO_2 columns (VI), H_2O columns (VII), aerosol (VIII), clouds (IX), O3 profiles (X), and CO, CH4, CO2, and N2O columns (XI). Apart from individual presentations on the validation and retrieval of these products, each session contained a discussion on the current status of the products.

Participants

Participation to the workshop was open for everybody and all abstracts submitted were scheduled for an oral presentation. The number of participants was about 60, of which 40 gave a presentation. Most of the participants were validation scientists. In addition there were retrieval experts, and representatives of ESA and DLR.

General comments and recommendations

Ample time was allotted for discussions, so that both general and product specific comments and recommendations could be made. Here is a list of all general comments and recommendations gathered during the workshop.

- Level-2 OL products need to be processed and distributed, especially profiles of ozone and NO_2.
- The OL processor requires complete new validation, e.g. comparison and analysis also for the products already available from NRT.
- For all operational products it has to be clearly visible which contents are retrieval results, which are derived results and which are modeled or external values (for example number density versus VMR in Level-2 OL products)

- Implementation of an up-to-date algorithm comparable to GDP 4.0 or better is recommended for SCIAMACHY nadir products, especially ozone and NO_2 columns.
- Improvement of the radiometric calibration is needed for those products that use absolute reflectance, like aerosol products. Known solutions should be implemented.
- Parameters that are known to be of insufficient quality should not be included in the delivered operational product (for example current columns retrieved from the IR channels).
- A validation reference set has to be reprocessed prior to reprocessing the whole mission.
- Reprocessing speed of Level-1 and Level-2 products has to be improved considerably. Reprocessing should be at least a factor 10 faster than real time, so that 3 years of data are processed within 3 months.
- Reprocessing on historic data should be done consecutively in time. Current big gaps in the availability of data, even for Level-0 and Level-1 products, should be closed soon.
- Reprocessing should be based on consolidated data and performed with one processor version. Inconsistent datasets strongly hamper the validation tasks.
- Representatives of the developers of the operational processors (ESRIN/DLR) should attend major validation meetings.
- Information of the validation (and general scientific) community of the ongoing work on the operational products has to be improved, especially about schedules and changes of schedules for the delivery of data.
- An atmospheric science advisory committee on ESA ENVISAT level with members from the GOMOS, MERIS, MIPAS, and SCIAMACHY science teams is proposed.
- First reprocessed and global datasets of operational products will be available in 2005, for many anticipated atmospheric parameters even later. Detailed validation of these dataset is an extensive task. This effort has to be adequately funded.
- Long-term validation of SCIAMACHY is essential for the scientific success of instrument. This has to include the collection and usage of collocated measurement over the lifetime of the instrument to continuously monitor the instrument. This effort has to be adequately funded.

Session summaries

Session I: SCIAMACHY instrument and ground-segment status

Heinrich Bovensmann (IFE) gave an overview of the status of the instrument, the operations, and the scientific use of the data. He concluded that the instrument has a high spectral and radiometric stability. Degradation in the is low: about 2% per year in the UV, less than 0.5% per year in channels 3-6. The ice on channels 7 and 8 is still present: after each decontamination period the ice layer gradually builds on the detector, decreasing the radiative throughput. The limb pointing accuracy seems to be improved since December 2003, validation should quantify this. The use of the data, especially of the so-called scientific products (i.e. non-operational products), is increasing

Paul Snoeij (ESA) presented the current status for the SCIAMACHY processors and a plan for delivering operational products to the validation scientists. Forward calibration with the IECF is operational since 8 May 2004, all calibration data before that date is now reprocessed. The current operational NRT processor is 5.04, a bug-fixed version of 5.01. The OL processor will be operational soon with software version 2.5. The currently planned improvements to the processor will be first implemented in the OL processor (planned for Spring 2005). The data dissemination is now via nominal channels. The level 2 data is available via three complementary ftp sites. The time-schedule for the upgrades of the processors is currently under discussion between ESA and DLR. The complete consolidated level 0 dataset is estimated to be available in the beginning of 2005. The verification of the level 1b processor upgrade, originally planned for December 2004 / January 2005, is delayed because the IECF needs to undergo some changes first (e.g., calculation of sun mean reference should be adapted).

Sander Slijkhuis (DLR) reported about the changes w.r.t. the NRT level 0-1b processor version 5.04 now implemented in the prototype at DLR. The changes are:

- memory effect correction for channels 1-5,
- non-linearity correction for channels 6-8,
- in-orbit dark for channels 6-8 for consolidated products,
- theoretical U values for all PMDs,
- integration time correction for channels 6-8,
- improved channel 1 straylight correction,
- sun ADSs now with 2 records: calibrated and uncalibrated,
- decontamination flag: y or n for 8 channels in SPH,
- correction of bug in Doppler-shift for ASM solar reference,
- correction of 0.2^{o} azimuth mispointing of SCIA w.r.t. ENVISAT.

After verification, these will be implemented also in the operational processor, somewhere in 2005.

The OL version 2.5 will become operational very soon. The only difference for nadir products with respect to NRT 5.04 is an upgrade of the cloud detection algorithm: line-of sight dependence of reflectance database is removed. The difference fro limb products with respect to OL 2.1 is a change of the NO2 profile covariance matrix, and a latitude dependent selection of retrieval layers.

The OL processor is currently being upgraded. The coming version will have a DOAS algorithm comparable to GDP 3.0 (already implemented in prototype), and also some adaptations for nadir-NIR, and for limb-UV/vis. The second upgrade (planned for mid 2005) will have a DOAS GDP 4.0, the IFE algorithm for water vapour, and a cloud top pressure retrieval. The number of UV/vis-limb products might be extended.

Günter Lichtenberg (SRON) reported on the status of the calibration. New radiometric calibration parameters were calculated by IFE, and verified by the verification team. The systematic offset in radiance and irradiance was shown to be much less. However, the new parameters introduce some spectral features, which might influence the DOAS retrievals. Therefore, it was proposed to use the uncalibrated solar spectrum taken over the ASM diffuser for DOAS retrievals, and the calibrated solar spectrum over the ESM diffuser for retrievals where absolute radiometric accuracy is needed. The other open issues are: polarisation correction, light leak in channel 7, implementation of a dynamical bad&dead pixel mask (BDM). Details on the present calibration issues can be found on

Gijs van Soest (KNMI) showed large scale comparisons between SCIAMACHY reflectances in the UV and RTM data. He finds that ESRIN NRT data, SCI_NL__1PNPDE*, before March 2004 (software version 4.0x), has a wrong calibration, explicitly showing up in channel 1. He also investigated the new IFE radiometric key data and finds that the irradiance looks reasonable, the reflectance offset is improved, but many spectral features are introduced and the reflectance is sometimes very noisy.

Session II: Scientific products and validation support

In this session the SCIAMACHY scientific products and their first applications were presented by **Thomas Wagner**, **Andreas Richter**, **Michael Buchwitz** and **Christian von Savigny**. **Klaus Bramstedt** and **Ankie Piters** presented the validation and product web sites, and the tools available for the validation community.

Session III-V: German SCIAMACHY Validation Team

The 5th German Validation Team (GSVT) meeting was the final meeting of the German SCIAMACHY validation community, as the German projects will run out of funding at the end of the year 2004/ beginning 2005. Each project presented its work and results, which were obtained over the entire time of funding. In summary, interesting and important results were shown by the German scientists. Over the first two and a half years, the German SCIAMACHY validation team has set up a unique dataset of collocated measurements for the validation of SCIAMACHY and further instruments onboard ENVISAT. This dataset has also been used for interesting scientific work in atmospheric research, documented by publications in the ACP special issue "Probing the atmosphere in three dimensions for SCIAMACHY" and further publications. Despite the ongoing delays of operational SCIAMACHY products, the German scientists showed important first validation results for the available products. Many validation results are shown for so-called scientific products, retrieved by several institutes (IUP Bremen and Heidelberg, KNMI, SRON, BIRA-IASB and others) from SCIAMACHY spectra, showing the capabilities of the SCIAMACHY instrument as well as the validation efforts of the German community.

Session VI: O_3 and NO_2 columns

O_3 column validation

Henk Eskes (KNMI) reports on retrieval, validation and assimilation of SCIAMACHY O_3 columns performed at KNMI. Starting from the heritage of several retrieval algorithms (OMI-DOAS, TOGOMI, TOSOMI, ESA ITT for improved GOME O_3 columns), he describes the main innovations of the current algorithms and gives concrete illustrations of the effect on the retrieved O_3 columns: improved treatment of rotational Raman scattering (RRS) and Ring effects, improved radiative transfer, use of TOMS v8 O_3 climatological database, calculation of empirical Air Mass Factor (AMF), and calculation of effective absorption cross-sections based on ECWMF temperature analyses. After those retrieval details, Eskes illustrates the validation performed over De Bilt (Netherlands) and also from pole to pole using ground-based network data. Comparisons show no clear meridian/seasonal bias of KNMI's SCIAMACHY O_3 columns on an average. Data assimilation results are then reported, based on the TM3DAM model driven by ECMWF fields. RMS of differences between TOSOMI and assimilated O_3 fields are about 3% on an average.

To conclude, Eskes informs the audience that data are distributed via the TEMIS web site (www.temis.nl) and to ECMWF.

Astrid Bracher (IFE) reports on the comparison of SCIAMACHY v5.01/5.04 O_3 and NO_2 column products with GOME products generated at IFE/IUP with the GOME-WF-DOAS algorithm. After a comparative description of the two types of algorithms (SCI_NL v5.0x and WFDOAS) and an explanation of the main improvements implemented in WFDOAS (RRS, ozone temperature correction, improved cloud cover and effective scene height, surface reflectance), she reports on comparisons between GOME-WFDOAS and ground-based network O_3 column data, showing no significant meridian/seasonal bias and an average agreement ranging from within 1% at low and middle latitudes to +4 to +8% at the wintertime pole. Comparison between SCIAMACHY v5.01/5.04 and GOME for April 16, 2004, conclude to a small underestimation of GOME by SCIA from South Pole to 23°N and a small overestimation from 23°N to North Pole. Comparisons carried out over the January-June 2003 period confirm the dependences on season, latitude, SZA and total ozone reported at ACVE-2 by the ACVT SCIA O_3 validation subgroup. On the opposite, similar types of comparison between SCIAMACHY v5.01/5.04 and GOME GDP 3.0 NO_2 column data, over the same first half of 2003, conclude to a worse agreement than the one reported at ACVE-2 with only the Commissioning Phase validation orbits (sampling sporadically the period from July to November 2002) and the algorithm verification orbits. Comparisons with the SCIAMACHY orbits currently available conclude to a meridian dependence and, in Winter-Spring in the Northern Hemisphere, to a strong SZA dependence.

On behalf of **Antje Dethof** (ECMWF), Ankie Piters reports on the monitoring and assimilation of SCIAMACHY data performed at ECMWF. Assimilated fields based on SCIAMACHY ozone column data processed either with SCI_RV__2P 5.01/5.04 or TOSOMI are compared to the original observations. Passive monitoring shows that problems with ESA NRT SCI_RV__2P data occur before April 2004 (they seem to be fixed after 27 April 2004) and also after 15 October 2004. Data coverage may be an issue for data assimilation as some data are not available in NRT (improved since August2004). Monitoring sometimes reveals significant differences between ESA and KNMI retrievals. In the second part of the talk, several illustrations show how the assimilation of SCIAMACHY TOSOMI O_3 columns by the ECMWF system can improve the fit of ECMWF O_3 column and profiles to independent data (namely, EP-TOMS, balloon-borne ozonesondes, and NOAA-16 SBUV/2). TOSOMI O_3 columns have been included in the operational ECMWF system since 28 September 2004.

Discussion on O_3 column validation

To initiate the general discussion on SCIAMACHY O_3 column validation, **Jean-Christopher Lambert** (BIRA-IASB) presents an overview of the methods and results reported so far by the community in preparation of, and during the workshop, and in recent validation reports and scientific publications. Results reported at ACVE-2 for some seasons and latitudes are consolidated, demonstrating that the O_3 column data product generated by SCIAMACHY IPF 5.01/5.04 offers the level of quality that can be expected from a processor based on GOME GDP 2.4. Nevertheless, from mid-October till maybe the end of the year (to be verified as relevant SCIAMACHY data become available), larger errors than those detectable at the time of ACVE-2 appear

both for 2003 and 2004. Those errors correlate with cloud fraction, GVC and AMF, and they do not show up at some NH mid-latitudes and at the Equator, explaining some apparent differences in comparison results.

In the mean time, validation of new GOME O_3 column retrieval algorithms (GDOAS, GDP 4.0, GODFIT, TOGOMI, WFDOAS) has demonstrated the possibility to cut SZA/season/latitude dependences of the GOME O_3 column product down to the "1% level", that is, to the level of accuracy reachable with well-maintained and calibrated ground-based sensors when their known dependences on air mass, temperature etc. are corrected for. Those algorithms have also proven to be stable and insensitive to instrumental degradation over the entire GOME lifetime, enabling accurate O_3 trend monitoring. Everyone agrees that one of those improved O_3 column algorithms should replace as soon as possible the current version 5.04 of the SCIAMACHY operational algorithm (based on GDP 2.4). Sander Slijkhuis (DLR-OP) announces that, to his knowledge, DLR has the intention to implement, by mid-2005, GDP 4.0 in the Off-Line SCIAMACHY Data processor. As it is crucial that data release of this OL upgrade starts well before ACVE-3, the recommendation is made to Paul Snoeij, the ESA Representative at the workshop, to schedule the event accordingly. In the mean time, in view of the important problems discovered recently with SCIAMACHY IPF 5.04 (e.g. unreliable O_3 columns after 15 October 2003), it is strongly recommended to upgrade again the near-real-time processor to a version 5.05 which should have related bugs fixed.

The general feeling is that current SCIAMACHY IPF 5.01/5.04 O_3 data are sufficiently well characterised. Needs for additional investigation should be communicated to the validation scientist. A new validation round will be necessary as soon as either IPF 5.05 (IPF 5.04 corrected for recently found errors) or the upcoming version inspired from GDP 4.0, are implemented in the operational chain. Common validation methods are suitable for the current quality of SCIAMACHY IPF 5.04 O_3 data. The anticipated 1%-level of quality of the future GDP 4.0-like SCIAMACHY product has for consequence that ground-based comparisons using raw (unconsolidated) data as archived in near real time in worldwide databases might lack of accuracy for validation purposes. Validation teams must be aware of this fact and take appropriate actions when carrying out network-based validation studies.

An important conclusion is that, as expected from the GOME heritage, the limited list of ACVE-2 orbits, and *a fortiori* a few verification orbits, lead to incomplete / erroneous quality assessments.
Any (delta) validation should rely at least on the dedicated list of orbits identified in 2003. The unexpected latitude/season pattern of the IPF 5.01/5.04 errors demonstrates, once again, that a few 'representative' stations are definitely not enough and that validation of a long-term, global product must address global aspects in the long term. It is underlined that user feedback is an important source of validation as well, as directed towards the real use of the data, and that at least for this reason communication/exchange channels should be maintained.

NO_2 column validation

On behalf of **Nadege Blond** (KNMI), Henk Eskes reports on the comparison of SCIAMACHY NO_2 tropospheric columns with CHIMERE air-quality modelling results. The talk starts with a detailed description of the SCIAMACHY slant column

spectral fitting performed at BIRA-IASB, followed by the conversion to tropospheric column performed at KNMI. This conversion uses cloud information derived from FRESCO, the assimilation of slant columns to derive the stratospheric "background" reference, and modelling results to assess the tropospheric profile shape needed for tropospheric AMF calculations. A NO_2 temperature correction is also applied, that could explain differences reported at ACVE-2 by Lambert et al. between SCIAMACHY NO_2 stratospheric column products generated by KNMI and the ones generated by several other groups. The talk gets on with a description of the CHIMÈRE model for operational air-quality forecast, the validation of its lowermost values with respect to surface observations, and the methodology adopted here for the confrontation with SCIAMACHY tropospheric columns (cloud-free SCIAMACHY pixels, convolution of CHIMÈRE profile data with SCIAMACHY averaging kernels). The study concludes for 2003 to very small biases between SCIA and CHIMÈRE and also between CHIMÈRE and surface observations, and to correlation coefficients of typically 0.7.
The resolution of SCIAMACHY and CHIMÈRE are comparable. Extended NO_2 plumes are captured similarly, but details show differences in seasonality (CHIMÈRE reports higher values in winter), for individual days, in distribution, and in the amount of details.

Discussion on NO2 column validation

To initiate the general discussion on SCIAMACHY NO_2 column validation, **Jean-Christopher Lambert** (BIRA-IASB) presents an overview of the methods and results reported so far by the community in preparation of, and during the workshop, and in recent validation reports and scientific publications. Validation methods developed for GOME perform well for SCIAMACHY stratospheric NO_2. For some seasons and latitudes, SCIAMACHY IPF 5.01/5.04 is affected by larger errors that those detectable at the time of ACVE-2, which correlate with cloud fraction, GVC and AMF. Comparison results vary from one station/campaign to another, partly because SCIAMACHY errors are not constant with respect to time and latitude. Reprocessing with a bug-fixed version 5.05 of IPF is strongly encouraged. The general feeling is that current SCIAMACHY IPF 5.01/5.04 NO_2 data are sufficiently well characterised. A new validation round will be necessary as soon as IPF 5.05, or even a better version inspired from at least GOME GDP 3.0, are implemented in the operational chain. Validation methods for tropospheric NO_2 remain an open issue, as they need "validation" and standardisation.

Both individual and coordinated validations are carried out also for scientific products generated by BIRA-IASB, IUP/Bremen, IUP/Heidelberg, KNMI, and SAO. Differences in their respective NO_2 products can often be explained by differences in retrieval settings. No significant changes are to date between GOME GDP 3.0 and GDP 4.0. GOME GDP 2.7 after 2001 is strongly affected by instrumental degradation. New level-1 calibration implemented in 2002 solves the problem for GDP 3.0, GDP 4.0 and scientific algorithms, which all perform well.

After this overview, Andreas Richter (IFE/IUP) informs the audience that there is a paper of GOME versus CHIMERE confirming that the model CHIMERE is performing very well. As for the validation of O_3 columns, several attendees support the idea that (delta) validation should rely at least on the dedicated list of orbits identified in 2003. Recent results show that ACVE-2 orbits and *a fortiori* verification

orbits (aimed mainly at optimising retrieval settings) lead to incomplete / erroneous quality assessments. It is agreed that the statement "operational NO_2 column is ok" derived at ACVE-2 with a limited set of orbits should be taken back in any SCIAMACHY IPF 5.04 quality disclaimer. Ulrich Platt (IUP/Heidelberg) underlines the importance of quality disclaimers, among others to avoid damageable rumours. The question arises whether the operational processing should stop when such major problem occurs. The general discussion shows that agencies are not wise to do so. Stefan Noel (IFE/IUP) asks about enlarging the validation reference set. Ankie Piters and Jean-Christopher Lambert remind that there is already a clear recommendation on this valrefset from SCIAVALIG. SCIAVALIG will sit around the table with ESA to find out how we can deal with the problems concerning the (re-)processing and distribution of data sets suitable for (delta-) validation. Finally, Achim Friker (DLR-Bonn) proposes that there should be a point where ESA and DLR sit together for upgrading IPF (=NRT). For the time being it is planned that only the OL processor will be upgraded.

Session VII: H_2O columns

Stefan Noel from IFE-Bremen gave a presentation on the SCIAMACHY water vapor column retrieval using AMC-DOAS. The Air Mass Corrected (AMC) DOAS retrieval method has been applied successfully to GOME and SCIAMACHY data. The retrieval has been applied to all available SCIAMACHY nadir data for 2003 and automatic retrieval takes place for all 2004 SCIAMACHY NRT level 1 data. The retrieved SCIAMACHY H_2O columns show a good correlation with SSM/I and ECMWF data for one day in 2003. On average there is a good agreement with SSM/I and somewhat better with ECMWF data. Small SCIAMACHY H_2O columns seem to be lower and high SCIAMACHY H_2O columns larger than correlative data. The deviations are difficult to quantify because of large scatter, which is mainly due to high spatial and temporal variability of water vapour. The large scatter is a general problem in the validation of water vapour products. Because of this the focus of the study by S. Noel is on long-term analysis of correlation and mean. The mean deviation of the SCIAMACHY daily mean values with SSM/I and ECMWF are respectively –0.2 g/cm^2 and –0.05 g/cm^2. The SCIAMACHY monthly mean values look reasonable but some features need further investigation.

Discussion on H_2O column validation

Scientific products

The operational product/algorithm is not mature enough for validation (because of problems channels 7&8). The following institutes are providing or developing scientific products:

- IFE Bremen, Stefan Noel, AMC-DOAS from channel 4 (see presentation)
- IFE Bremen, Michael Buchwitz, WFM-DOAS from channel 4 (1 day-comparison showed good agreement with AMC-DOAS product)
- MPI-Mainz - Rüdiger Lang , from channel 3/4, in cooperation with Ahilleas Maurellis from SRON (last validation results presented showed –20 to –25% offset compared to ECMWF and radiosondes)
- Uni-Heidelberg – Thomas Wagner, from channel 4 (good results for GOME and good comparison for 1 day between GOME and SCIAMACHY).

Assimilation of H_2O

Question: Is assimilation of SCIA H2O feasible?

Answer: Yes, GOME and SCIAMACHY would contribute mainly over land as independent source. GOME-2 would give a long-term perspective. ECMWF could be interested.

Slit-function change effect AMC-DOAS
A short discussion took place on the effect of slit-function change for the AMC-DOAS product. Validation of the AMC-DOAS product, retrieved using the old slit-function for the validation reference dataset, with correlative data from radiosondes and ATOVS showed a –10 to –15% offset. These results by KNMI were in agreement with previous validation results acquired from IUP-Bremen itself. They found a systematic offset between the SCIAMACHY measurements and ECMWF and SSM/I data of 10%, SCIAMACHY being lower.
The new version of the AMC-DOAS product, with a slit-function change was made available mid 2004. Comparisons performed by IUP-Bremen with ECMWF and SSM/I showed that the 10% offset was diminished for the day they analysed. When comparing the new version data for the validation reference dataset to radiosondes and ATOVS data, only an improvement of 1 to 2% was found.
It should be noted that the validation reference data set is based on different level 1 data than the products IUP-Bremen used in their comparisons. Furthermore IUP-Bremen only made comparisons on one day, on a global scale and for the validation reference set KNMI made comparisons on different days but on a limited number of locations.

Session VIII: aerosol

A talk was given by Jolanta **Kusmierczyk** about the retrieval of aerosol optical thickness (AOT) with SCIAMACHY and GOME. Validation of GOME AOT showed very good results. The retrieval will be applied to SCIAMACHY data in the near future.

Discussion on aerosol validation
The retrieval of aerosol properties largely depends on the accuracy of the reflectance. The operational Absorbing Aerosol Index (AAI) doesn't correct for the current systematic offset in the reflectance, so deviations of more than 100\% are seen. The scientific AAI from KNMI is retrieved with a reflectance correction parameter and compares well to the TOMS AAI. The scientific AOT product from IFE is also retrieved with radiometric correction parameters. First comparisons show consistency with ground-based measurements of BAER.

Good cloud-screening is necessary for accurate aerosol retrievals. The validation of aerosols should now be contined on a global scale. Validation with MERIS is a possibility that should be exploited.

Session IX: clouds

Alexander Khokanowski presented his retrieval method SACURA for cloud optical thickness, cloud top height, cloud cover, cloud albedo, liquid water path, thermodynamic phase, and average particle size. Preliminary validation was performed on a few of the products. Cloud-top-height compares well with AATSR, cloud optical thickness and reflection function correlate well with MERIS, although slightly underestimated. Cloud effective radius correlate well with MODIS, although slightly underestimated.

Discussion on cloud validation

The products currently available to the validation teams are the operational product (OCRA) and the KNMI product (FRESCO: effective cloud cover and cloud-top pressure). OCRA and FRESCO cloud cover agree well, apart from a viewing angle dependence in OCRA and an overestimation of FRESCO over desert areas. Both problems are understood and both algorithms are being upgraded to solve the problems. The cloud-top pressure of FRESCO is typically 100 hPa lower than ground-based measurements (also shown by **K.-H. Fricke**).
It is important to relate the validation results to the intended use. For cloud products used in DOAS retrievals the assumptions that go into the DOAS retrieval should be consistent with those for the clouds. So the sensitivity of the DOAS products to the specific properties of the cloud products should be investigated.

Session X: O_3 profiles

Yasjka Meijer, **Dorien Lolkema**, and **Arjo Segers** presented their plans for the validation of SCIAMACHY ozone profiles; Yasjka coordinates the ESA project EQUAL for the validation of ENVISAT operational ozone and temperature profiles with lidars, Dorien will use ozone sondes and lidars specifically for SCIAMACHY profiles (operational and scientific products) and Arjo will mainly use assimilation and models.

Discussion on ozone profile validation

Envisat pointing

It is clear that the Envisat pointing problem makes it difficult to do a proper validation of ozone profiles. The pointing should have been improved after December 2003, but this should still be checked. There is a clear requirement on the reprocessing of data with a corrected pointing (Paul Snoeij confirms that this is intended). Additional corrections probably remain necessary: currently it is preferred to have an altitude retrieval included in the profile retrieval.
Validation can contribute to the characterization of the altitude shifts. One should look for latitudinal, longitudinal and time variations.
A look-up table with correction is under development (Christian von Savigny).

Profile comparisons

Validation results are difficult to compare, a.o., because use of different quantities. The general agreement seems to be to use number density versus height (for SCIAMACHY), since these are the quantities retrieved. Other quantities like vmr and pressure are derived from that using temperature and pressure profiles, which are not always accurate.

Session XI: CO, CH4, CO2, and N2O columns

At present, 3 scientific algorithms are available for CO and CH_4 data, and actually one (WFM-DOAS) for N_2O and CO_2 data, namely:

- Iterative Maximum Likelihood Method (IMLM) (SRON),
- Weighting-Function Modified DOAS (WFM-DOAS) (Univ. Bremen) and
- Interactive Maximum A Posteriori method (IMAP) (Univ. Heidelberg).

The data products are total column amounts and mean volume mixing ratios expressed as the ratios of the column to the column of O_2 or CO_2.

Only the WFM-DOAS algorithm is presented in detail at this Workshop, by M. Buchwitz, Univ. Bremen – the other ones have been presented at previous workshops. **M. Buchwitz** presents the algorithm in brief, incl. the averaging kernels (contrasted to MOPITT kernels). He highlights some results for CO, CH4 and CO2, in comparison with MOPITT or model data. The improvement for CH4 between the v4.1 and v4.0 version – to deal with the degradation of the signal transmission due to buildup of the ice layer on the detectors - is demonstrated; but it is also shown that the latest v4.1 version not yet completely solves the problem. He provides some estimates of uncertainties (bias and precision) for the WFM-DOAS products – however not yet taking into account the latest results of validation – presented in the talk by Bart Dils (see below).

Discussion

It is pointed out that the actual cloud mask is a very conservative one, designed for greenhouse gas detection with very stringent requirements as to precision. It is based on the backscatter signal in the UV, and does not discriminate between ice and snow and clouds. The radiative transfer characteristics in the NIR need to be investigated better to see whether useful information about the molecular species like CO can be obtained below the clouds.

- Results over sea do exist, but are not shown because they are less reliable and because the actual focus is on getting accurate data over land. The remark is made that it may be worthwhile to look at sunglint data for which more reliable data may be obtained.
- The question arises why the April 2003 data for CO show lower CO than the MOPITT data; the answer is that this is not understood yet – low sampling frequency of the SCIAMACHY data for this period may be part of the explanation.

Validation results with ground-based FTIR network data covering the products from all three algorithms are presented (B. Dils, et al., BIRA-IASB). Other validation efforts using GB and ship-borne FTIR data have been presented in the GSVT session. **B. Dils** shows the network of ground-based FTIR data that are used for validation of the NIR products of SCIAMACHY (CO, CH4, N2O and CO2). The validation approach is explained, incl. some caveats. The validation uses individual data; no averaging is applied. The results seem to agree reasonably well with results from other validation efforts – see below.

Discussion:

- It is pointed out that SCIAMACHY takes a sample over the ground-based locations at a very specific moment of the day; therefore the scatter in the SCIAMACHY data should be compared somehow to the daily variability of the measured species at the ground-based location. But, in most cases, in the comparisons between SCIAMACHY and ground-based data, the ground-based data are daily mean values, and the daily variability at the sites is of the order of a few percent (to be verified).
- The question of how to deal with mountainous sites is raised. It is stressed again that the actual approach is quite crude and does not account for the inhomogeneity in the bottom altitude of the SCIAMACHY pixel, when it is over complex terrain like is the case close to the Jungfraujoch and Zugspitze.

It is planned to make comparisons between ground-based data and model data (e.g., TM3 and TM5) to better account for the ground-altitude.

General discussion on validation of nadir NIR products

From the presentations, it is clear that enormous progress in the data products quality has been achieved since the work on the NIR products has started. Also the amount of processed data available has increased a lot (about all the consolidated orbits of 2003). First order corrections for the dark current signal variations, dead/bad pixels and impacts of ice on the detector affecting signal transmission and line shape functions, have been implemented.

- *Qualitatively:* It has been clearly demonstrated that SCIAMACHY is able to detect source/sink areas of CO and CH_4 and CO_2
- *Quantitatively*: Precisions are getting close to the required ones:
    - Precision for CO ~ 30 % (compare to 10% req)
    - Precision for CH_4 ~ 5 % (compare to 1% req)
    - Precision for N_2O ~ 20 % (compare to <1% req)
    - Precision for CO2 ~ 5% ? (only limited validation up to now)

It is also clear that different validation approaches are complementary and should be pursued:

- Validations with ground-based (GB) FTIR network data (NDSC) suffer from limited coverage in time and space, but have the advantage of using high quality certified data. Mountainous sites are more difficult to deal with.
- Validation using model results (e.g., TM3) have the advantage of global coverage in time and space; What is missing bup to now are comparisons between model data and the GB FTIR network data. This is planned in a very near future.
- Validation using satellite data (e.g., MOPITT) also offers the advantage of global coverage. The problem here is that the correlative satellite data have their own limitations. For example MOPITT is less sensitive to the lower troposphere (with the sensitivity varying as a function of surface and atmospheric conditions), and has a positive bias in the lower troposphere.

The discussion focuses on:

1) Ways to improve the NIR data products. Is there a chance to achieve required precision? Or can requirements be relaxed using appropriate inverse modeling techniques?

It is argued that the retrieval residuals have not come down yet to the S/N ratio of the instrument (spectra) – therefore improvements are still feasible and it seems reason able to expect that one will achieve the required precision. For example using more CO lines in the retrieval is envisaged; it requires however a large effort because one has to eliminate all systematic errors across the spectrum.
At present inverse modeling analyses seem to indicate that the precisions as requested for the data products are necessary to be able to improve the emission databases. The question is however whether other approaches (e.g., dealing with monthly means, regional averages,…) cannot already provide useful advances.

2) The perspectives for operational implementation (at ESA)?

The opinions are that 1st a good L1 product has to be delivered from the operational processors 2nd that a high-quality product must be demonstrated before operational implementation.

Session XII: General discussion and summary

Some issues about the future of SCIAMACHY validation were addressed within this session.

Next workshops

There was a proposal to have dedicated workshops for groups of products (such as 'nadir NIR') after some improvements have been realized, with both retrieval and validation teams.

Integration of planned campaigns and projects

Funding for dedicated manpower for SCIAMACHY validation is sparse. Involve relevant projects in the SCIAMACHY validation effort (e.g. ACCENT-Troposat II).