SUMMARY OF THE ATMOSPHERIC CHEMISTRY INSTRUMENT VALIDATION

Paul Snoeij(1), Peter Fletcher(2), Rob Koopman(3), Patrick Wursteisen(1), Tobias Wehr(1), Claus Zehner(3), Evert Attema(1)

(1) ESA-ESTEC, Keplerlaan 1, 2201 AZ Noordwijk, The Netherlands, Email: paul.snoeij@esa.int
(2) RSAC, Prospect Place, Mill Lane, Alton, Hampshire, GU35 2SX United Kingdom
(3) ESA-ESRIN, Via Galileo Galilei, Casella Postale 64, I-00044 Frascati, Italy

ABSTRACT

This paper summarizes the results of the validation of the Envisat atmospheric instruments as presented by the validation teams during the ACVE-2 workshop.

1. OVERVIEW

The second workshop on the Atmospheric Chemistry Validation of ENVISAT (ACVE-2) was held at ESA-ESRIN on 3-7 May 2004. This paper summarises validation work that has been carried out since the Envisat Validation workshop in December 2002, for the three ENVISAT atmospheric instruments: SCIAMACHY, MIPAS and GOMOS.

This summary has two parts: firstly, issues that are common to all three instruments are presented and then results relating to the individual instruments are discussed in more detail. The ACVE-2 provided an important opportunity for scientists involved in validation work to present their findings to a wider ACVT community and to ESA in particular. It is important to present to ESA the results of validation and to define validation requirements in the short term (the main validation phase is due for completion in 2004) and throughout mission life.

ACVE-2 was an undoubted success involving a total of 120 participants, 60 oral presentations and 50 posters. The number of atmospheric products reviewed was equally impressive: 11 from SCIAMACHY and 8 from both MIPAS and GOMOS.

Both SCIAMACHY and GOMOS continue to operate well. Unfortunately, MIPAS has been switched off since 26 March 2004, as a consequence of problems with non-redundant components of its interferometer, the. At the time of writing, work is underway to enable MIPAS to resume operations, by reconfiguring the interferometer to operate at 40.99% of its original spectral resolution. Preliminary assessments indicate that for several species, only a slight degradation of data quality is to be expected.

2. COMMON ISSUES

2.1 Introduction

The following sections summarise various issues that were raised in presentations and in subsequent discussion. They are not specific to any particular atmospheric chemistry instrument.

2.2 Validation Datasets

The provision of Envisat validation datasets for comparison with other measurements, and the timing of the reprocessing of data was discussed at length. In principle, it is desirable to have sufficient data to enable the comparison of measurements over a complete year, and thus be able to analyse seasonal effects. However, the amount of time dedicated to reprocessing data will always be linked to the implementation of new versions of processors. It takes several months to re-process data and this becomes wasted effort if a new version of a processor is implemented shortly after. The situation requires careful planning and ESA will continue to manage the resources available to it in the best manner possible. Generalising the procedure executed for the ACVE-2 It was clear, however, that a well-defined validation reference dataset should be reprocessed with priority after each processor upgrade, before reprocessing the whole mission.

It was acknowledged that the validation datasets contained outlier data that are unsuitable for inclusion in validation analysis. ESA has chosen to provide validation teams with a relatively weakly filtered dataset, as this facilitates characterisation of processor anomalies. The results of the ACVE-2 will support improved error characterisation, which subsequently helps to improve processing algorithms and data filtering in future processor versions.

2.3 Platform Pointing Accuracy

The extraction of species profiles from limb sounding instruments depends on the platform pointing direction being known to a high accuracy. Since December 2003, the pointing accuracy of Envisat has improved.
substantially, however, some latitudinal oscillation persists (Fig. 1), affecting all limb-sounding observations. Envisat now exceeds its design specification and achieves pointing accuracy around 1km, although a pointing accuracy within 150m has been suggested as a more appropriate scientific requirement.

![Residual latitudinal variation](image)

*Fig. 1 Residual latitudinal variation (Source: IMK)*

### 2.4 Coincidence of Envisat and Other Measurements

In many cases, products from Envisat are now closely matching measurements from other instruments; ground based, airborne and spaceborne. Analysis has also shown, perhaps not surprisingly, that some of the closest comparisons are achieved when measurements are made with a minimum of separation in terms of time and space. It is necessary, therefore, to develop procedures that provide, at the very least, statistical descriptions of the degree of coincidence between Envisat data and validation measurements. Providing hard and fast criteria for defining good or bad coincidences is not considered appropriate because it depends on the atmospheric situation. Large differences in time and space between validation measurements could be acceptable if the atmosphere was largely homogeneous or when accurate chemistry and transport modelling is applied.

In a related topic, it was clear that the presentation of validation measurements could be made more meaningful if averaging kernels were used also for the in-situ measurements. This would help overcome the situation where large differences in vertical resolution were evident between Envisat data and other measurements.

### 2.5 Communications

The complexities associated with Envisat validation, and the large numbers of scientists involved, mean that effective communication is extremely important and that there is always scope for improvement.

Requests have been made for increased documentation relating to changes to processor algorithms and initialisation files, and, in addition, that auxiliary data files should be suitably documented. Information on the status of the reprocessing of datasets was also needed.

By the same token, scientists do not always take full advantage of the documentation that is available, including on the Envisat website where, for example, auxiliary data files and monthly reports on the individual instruments are posted. Similarly, it is important for data users to read the disclaimers and take note of the product-quality flags associated with the released products.

### 2.6 Cross-comparison Between Envisat Instruments

Validation activities so far have involved products from Envisat instruments being compared with equivalent data from other instruments. Given that the validation of atmospheric instruments onboard Envisat has become more advanced, it is now considered appropriate to cross-compare products from SCIAMACHY, MIPAS and GOMOS. The need to monitor measurement coincidence in terms of time and space will continue to be important, given the different viewing methods and geometries involved.

### 3. SCIAMACHY VALIDATION RESULTS

#### 3.1 SCIAMACHY Level-1b Processing

IPF v5.01

Level-1b processing has undergone significant improvement and many of the issues that have yet to be tackled are, however, understood. Channels 7 and 8 are subject to icing problems, but even so there is good information in the non-operational CH4 and CO2 products, which are largely derived from data acquired from these channels. A stray-light signal in Channel 7 has also been identified and needs to be addressed so that the potential for results of high precision can be realised. Further work is required on Level-1b calibration including: reflectance, irradiance values, polarisation measurements and better handling of
Raman scattering effects. Limb reflectance has yet to be validated.

3.2 SCIAMACHY Column Products
IPF v5.01

The following products have been validated:

O3 The NRT product is providing agreement with other measurements in the order of 2-10%. Solar Zenith Angle dependence is in the order of 8-10%, with other dependencies related to total ozone amount and season and latitude. Non-operational products retrieved by different institutes indicate a worldwide bias of between 1-1.5%. A viewing angle dependence of 2% and cloud fraction dependence of 2-2.5% is also reported.

![Fig. 2 Validation of SCIAMACHY O3 with ground based measurements (Source ACVE-2: J-C. Lambert)](image)

NO2 As with O3 the NRT product is now greatly improved. For comparison sites in unpolluted areas, good agreements are found (differences being in the order of a few $10^{14}$ molec.cm$^{-2}$). Larger differences are found in polluted areas due to sensitivity to tropospheric conditions. Non-operational products are also shown to have good agreement.

BrO The NRT product has agreements in the order of ±20% for cases other than those involving small slant column densities. Non-operational BrO products give promising results when compared with GOME and ground based instruments.

The following SCIAMACHY products are all derived from non-operational processors:

OClO These are generally in good agreement with GOME. Including polarisation correction and eta and/or zeta spectra can make improvements.

CH4 Offsets of up to 5% are observed when cloud free pixels are compared.

CO Offsets of up to 40% are observed when cloud free pixels are compared.

N20 Offsets of up to 20% are observed when cloud free pixels are compared.

CO2 Initial results look reasonable.

H2O Results derived from visible channels provide at best, a small offset of around –10%.

3.3 SCIAMACHY Profile Products
IPF v5.01

The following profile products from the Offline processor have been validated:

O3 Bias from −8 to 12% is found when compared with ground-based data. The platform pointing errors may account for much of this variation.

NO2 Values from SCIAMACHY are ~50% higher than measurements from HALOE between 25 and 40 km.

The following profile products from the non-operational processors have been validated:

O3 Bias of −7 to 15% were found when compared with HALOE products.

NO2 Values are within 15% of HALOE at 22-33km and 10-35% lower than SAGE II (SAGE II values may be too high). Good agreement has been found with SAOZ (<15%) when a photochemical correction is applied.

BrO Initial comparisons have produced encouraging results, although the results deteriorate below 20km, suggesting a photochemical correction is needed.
3.4 SCIAMACHY Clouds and Aerosol
IPF v5.01

Cloud fraction products derived from the NRT processor show good, and in some cases very good, correlation with other measurements. Operational cloud top pressure products are generated from climatology in the current processor version and have therefore not been subject to validation.

The aerosol products have demonstrated that they are very sensitive to Level-1b processing in relation to the handling of polarisation factors. When an additional correction is applied, good comparisons are found with TOMS and MERIS measurements.

3.5 SCIAMACHY Conclusion

There has been a good improvement in the quality of SCIAMACHY products and many SCIAMACHY products are now available for research, both operational and non-operational. More validation is necessary to determine seasonal and other effects and to validate those products, such as SO2, that require special events (high pollution episodes) for comparisons to be made. Further work needs to be carried out on Level-1b processing, however, there is real confidence that tangible benefits will accrue from further investment in this area.

4. MIPAS Validation Results

4.1 MIPAS Level-1b Processing
IPF v4.61

MIPAS Level-1b processing is currently using version 4.61 of the software both for NRT and Offline products. Version 4.61 is working well and incorporates improvements relating to spectra oscillation anomalies, NESR reporting, the suppression of aliasing spikes and the inclusion of an ADC saturation flag. Version 3.2 of the level 1B auxiliary data files incorporates modifications to reduce forward/reverse oscillations in non-linear channels and the reduction of spectral calibration variation along the orbit.

A number of improvements to Level-1b processing have been identified. For processing software, these include: corrections of open anomalies, offset validation, improve ILS retrieval and spectral calibration. For the auxiliary data file suggestions are: improve non-linearity characterisation and ILS parameters.

Level 2 processing software has been modified to reject observations affected by clouds, and the level 2 processing configuration for Offline product generation has undergone a major change to extend the retrieval range of most species, and tighten the convergence criteria of the iterative retrieval. In addition, the retrievals benefit of a reduction in retrieval oscillations due to the improved non-linearity calibration of the level1B products.

4.2 MIPAS Operational Products
IPF v4.61

The following products have undergone validation:

- **O3**
  Comparisons show good quality from 20-55km, with no obvious biases and a precision of between 10-15%. In comparisons with HALOE data, systematic differences are found in the mesosphere.

- **H2O**
  Results from 15-30km are good and within the combined error bars. Validation indicated low bias in the lowermost stratosphere and high bias above 30km, in particular with regard to the hydrogen budget. Some oscillations in the results were observed in the upper stratosphere.

- **CH4, NO2**
  Only a limited amount of validation work has been carried out so far. A high bias is indicated in the lower stratosphere in the mid-latitudes. The presence of outliers in the N2O-CH4 correlation also needs to be investigated.

- **HNO3**
  Very good agreements have been found especially in cases where measurements are highly coincident. MIPAS peak values tend to be higher. In a specific case high biases are found with FTIR ground based column measurements, probably due to differences in the spectroscopic reference data used.

- **NO2**
  Strong diurnal variation in this species makes validation a challenging task and indeed there are deviations found between measurements from UV/VIS and IR ground based instruments. However, based on a limited number of comparisons involving model-based diurnal correction, reasonable agreement is found in the region 25-45km with evidence that the seasonal variation of this species is also captured by MIPAS.
Temperature

The results of validation suggest that the MIPAS data is generally of good quality. Maximum mean differences in the mesosphere/stratosphere are $\pm 6k$ (MIPAS/HALOE), in the upper stratosphere $\pm 4k$ (MIPAS/POAM III), and in the lower stratosphere $\pm 2.5k$ (MIPAS/POAM III). A precision of $2-4k$ is found in the stratosphere but these results may be affected by atmospheric variability.

4.3 MIPAS Conclusion

MIPAS operational products are generally of very good quality. The problem areas are well understood and include performance at lower altitudes, biases and remaining oscillations in the data. Whilst emphasis has been placed on the validation of the operational products, enormous potential exists for the more than 25 non-operational products, which have already undergone some initial validation. With the enforced modification to the way in which MIPAS operates, it is necessary to define the nominal and special modes for future operation, and appropriate validation strategies.

5. GOMOS

5.1 GOMOS Level-1b Processing

IPF v4.02 and GOPR6.0

The current version of the processor (4.02) contains important modification to the level 1 processing. Level 2 processing algorithms also required important improvements. These improvements could not be implemented into the operational processor in time for the ACVE-2 workshop. For that reason ESA has provided the validation teams with products generated by the prototype processor chain developed at ACRI. The main improvement concerns improving the retrieval of O3 from the secondary peak at 75-100km. The outstanding issue for Level 1 processing remains the bright limb mission.

5.2 GOMOS Level-2 Products

GOPR 6.0 prototype

The following products were validated:

O3

In the region 18-50km, a negative bias of up to 5% was observed when the results were compared with ground-based instruments. Associated with this analysis, an RMS of 10-15% was found at altitudes of 18-50km. For SAGE II comparisons, the equivalent value was 5-15% between $\sim 20-50$km. Above 50km, diurnal variation seems to account for deterioration in the agreements. Work involving assimilation models concluded that a precision of at least 5% has been achieved for about 60% of all GOMOS measurements. A recommendation to use ECMWF data to validate the O3 product up to the stratopause needs to be considered.

NO2

Quantities of NO2 from GOMOS products were compared with measurements from balloons, POAM and SAGE II. No bias was found in the region 20-35km for balloon data and 20-30km for satellite data. Below 20km and above 40km the NO2 products appear not reliable.

NO3

From the validation data available it was apparent that GOMOS recorded the about correct total stratospheric ($>20$km) amount of NO3 although the vertical structure was not well produced.

Temperature and Density

Following the removal of 25-50% of the high-resolution temperature profile (HRPT) data that had unrealistic values, analysis was performed against data from POAM III, SAOZ balloon and ground-based measurements. At less than 20km, measurements were within 10-12k, between 20-30km: 2-4k (best in the tropics) and from 25-32km: 15k. Agreement within 10k was observed between GOMOS and ground-based instruments at 38km. Again from ground-based instruments, a bias of $+5-10k$ was found at 25-32km, decreasing above this level. It is
pointed out that HRTP will always be difficult to validate due to collocation problems relating to atmospheric situations that can be relatively local and short lived. There was only one comparable measurement for density, which was acquired from the ozone lidar at ALOMAR and agreement was within 5-10%. It is recommended that ECMWF data be used for the more effective validation of temperature products.

Fig. 4 Correlation of air density between GOMOS and ECMWF (Source ACVE-2: ACRI)

H2O Only tentative validation has been carried out on this product, although comparisons with ELHYSA and sonde profiles suggest that it is of the correct magnitude. It was recommended that ground based passive microwave sounder data be incorporated in the validation datasets, after a larger number of GOMOS H2O retrievals show reasonable results.

Aerosol PSC has been detected, however, the GOMOS aerosol model has yet to be checked.

5.3 GOMOS Conclusion

GOMOS retrieval performance has improved considerably since December 2002. As expected the accuracy and precision of the products have been found, to very much depend on limb-illumination condition, stellar magnitude, stellar temperature and measurement obliquity. When selecting individual profiles for validation, therefore, it was important to select profiles with stars of magnitude and temperature appropriate to the retrieved species that is being validated. Product quality should therefore be established as a function of stellar parameters (star magnitude and temperature) and limb-illumination condition (bright limb, dark limb, twilight/straylight). The spectroscopy (cross-section data) used in the retrievals should be reconsidered, in particular in view of desired consistency with SCIAMACHY and GOME retrievals. It was also pointed out that the data products contain disclaimers on product quality and that the users should take note of them before using the data.

With regard to the retrieval of vertical structures, the discrepancy between the performance of the GOMOS and the LPCE algorithm (which appeared to produce better results) needs to be investigated, including selection of spectral windows for the retrievals.

6. Overall Conclusions and Recommendations

So far not all operational and non-operational products have been validated. For those which have been, and especially the core species such as Ozone which have been subject to ongoing validation, it has been determined that the Envisat products and validation measurements are now in closer agreement. These promising results are usually related to upgrades to the processors, which are in turn derived from a better understanding of the operation of the instruments in space. Participants in the course of the workshop made the following recommendations:

6.1 SCIAMACHY Recommendations

- Operational data processor (level 1b-2) should include a.s.a.p. known improvements from the scientific retrievals.
- Operational DOAS algorithms should be improved to be consistent with current and future GOME operational algorithms to create a consistent data set.
- The level 1b-2 processor should include possibilities to correct for spectral features and offsets in the nadir reflectance, similar to non-operational retrievals (until calibration issues are solved)
- There is an urgent need for improvements of level 0-1 processor regarding polarisation features in UV and calibration of the NIR channels (7&8)
- A well-defined validation reference set should be processed completely after with each processor upgrade, before reprocessing the complete mission.
- Reported product format problems should be taken into account (via PCR (Processor Change Requests)).
- Product user manuals should be written.
- Auxiliary files should be available and well documented.
6.2 MIPAS Recommendations

- A MIPAS-SAG type of group needs urgently to be established in order to
- Define the future nominal mode at reduced spectral resolution
- Decide on the operation scenario for special modes
- Recommend future validation needs
- In order to achieve progress in validation on a product by product basis dedicated small groups need to be formed and financially supported

6.3 GOMOS Recommendations

Future validation work:
- Ozone is primary mission goal and continued validation is recommended
- Include inter-comparisons with MIPAS/SCIA, ground-based MW (H2O), ECMWF (stratospheric temperatures)

Algorithms:
- Evaluate concurrent algorithms using the same GOMOS transmittances

Mission:
- Re-evaluate mission scenario (star selections), w.r.t. instrument capabilities and scientific objectives

GOMOS NO2,NO3:
- Discrepancy on vertical structure between algos (GOMOS and LPCE) to be investigated.
- Compare GOMOS data with larger data sets: MIPAS, SCIAMACHY (moon), and Sage III (moon) night time mandatory.

GOMOS O2
- Validate with ECMWF up to stratopause (50 km).
- Investigate spectroscopy (Camy-Peyret)
- If bias persists, then: establish bias distribution (season, latitude, altitude)
- Brute force correction with empirically determined bias

H2O from GOMOS
- Compare GOMOS with MIPAS
- Compare with 6 years data from MPAE Lindau radiometer.

7. Acknowledgment

The authors would like to thanks all the teams involved in the acquisition and analyses of the in-situ measurements, the Quality Working Groups and the teams involved in the Envisat data processing, the validation teams for the comparison of in-situ with Envisat data and the species coordinators, who had the difficult job to collect the information from the individual teams and to present a coherent result at the workshop.