Chapitre 6

Geophysical validation of MIPAS ozone profile data and a new perspective on its error budget

Personal contribution to :
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Dans ce chapitre, nous présentons une validation géophysique des profils d'ozone inversés à partir des mesures de l'instrument MIPAS. L'apport le plus original est la prise en compte des caractéristiques de l'information sondée et l'estimation détaillée du bilan d'erreur complet lié à la comparaison des mesures MIPAS avec les mesures des instruments au sol. Nous y démontrons l'utilité des outils caractérisant la résolution horizontale de MIPAS développés au chapitre précédent dans un exercice de validation.

Ce travail a été réalisé dans le cadre du projet ProDEx CINAMON, dédié à la caractérisation, l'interprétation, l'application et la maturation des données d'Envisat liées à l'ozone. Il s'appuie sur diverses collaborations internationales financées par l'ESA dans le cadre du MIPAS Quality Working Group (QWG) et de son soutien observationnel TASTE (Technical Assistance to Envisat Validation by Soundings, Spectrometers and Radiometers). Ce dernier, financé initialement en complément au projet CINAMON pendant la phase de commission d'Envisat (2002-2003), fait depuis 2004 partie du programme d'exploitation régulier du satellite. Tandis que CINAMON développe les concepts et outils nécessaires, TASTE s'occupe des aspects plus opérationnels. L'objectif du projet TASTE est la validation à l'aide de mesures au sol des données atmosphériques inversées à partir des observations des trois instruments atmosphériques GOMOS, MIPAS et SCIAMACHY à bord d'Envisat. La première partie du projet concerne l'acquisition et la mise à disposition dans un délai temporel restreint des mesures indépendantes provenant d'une sélection de spectromètres, radiomètres et sondes basés au sol (spectromètres Dobson et Brewer, DOAS, FTIR, radiomètres M-124, ozonesondes et radiomètres micro-ondes). Une deuxième partie concerne la comparaison, avec ces mesures au sol, des colonnes totales (O_3, NO_2, CO, CH_4, HNO_3, N_2O, BrO et OClO) et des profils (O_3 et température) mesurés par les sondeurs atmosphériques d'Envisat. Le projet prévoit également la mise à disposition des résultats, leur valorisation par des publications et par des présentations lors de conférences dédiées et le soutien observationnel au QWG. Le projet TASTE s'est terminé en 2008 et le projet multi-TASTE assure la continuité du programme de validation à long terme des mesures ENVISAT tout en étendant les études à une plus large gamme de molécules et à d'autres satellites. A ce titre, il entre dans la stratégie de qualité des données établie par le Committee on Earth Observation Satellites (CEOS) pour le GEOSS.

Au cours des projets CINAMON et TASTE, nous avons étudié et comparé aux mesures sol différentes versions des algorithmes d'inversion du profil d'ozone pour GOMOS, MIPAS et SCIAMACHY. Nos résultats ont été successivement présentés aux conférences dédiées à la validation d'Envisat (ACVE 2 et 3, Frascati) et lors du Symposium Envisat and ERS 2004 (Salzburg). Ils ont permis l'amélioration progressive des algorithmes d'inversion. Les comptes-rendus de ces études ont notamment été publiés dans les actes de ces conférences [Blumenstock et al., 2004; De Clercq et al., 2004; De Clercq and Lambert, 2006a]. Le travail présenté ci-après concerne la validation géophysique de la dernière version des profils d'ozone MIPAS issus de la dernière version de l'algorithme opérationnel ESA IPF 4.61-4.62. Il entre dans le cadre d'un effort international et coordonné pour rassembler les résultats obtenus par différents groupes impliqués dans la validation des profils d'ozone MIPAS (validation à l'aide des mesures au sol, par ballon stratosphérique, par avion et satellitales) et obtenir une vue globale et harmonisée de la qualité des données MIPAS. Ces résultats comprenant la participation d'une vingtaine d'institutions internationales ont été publiés dans l'article coordonné Cortesi et al. [2007]. Une étude similaire a également été réalisée pour les profils de température MIPAS et est publiée dans Ridolfi et al. [2007].

Abstract

The Michelson Interferometer for Passive Atmospheric Sounding (MIPAS), on-board the European ENVIronmental SATellite (ENVISAT), was launched in 2002. From July 2002 to March 2004, the instrument has measured a continuous set of high resolution infrared spectra from which ozone profiles have been retrieved by the ESA IPF 4.61-4.62 processor. In this chapter, we report our contribution to a coordinated effort for the geophysical validation of MIPAS-ENVISAT operational ozone data. We compare MIPAS ozone profiles with independent measurements from ground-based networks of ozonesonde and lidar stations. In particular our analysis includes a complete assessment of the comparison error budget. We demonstrate that the error due to the difference in horizontal smoothing between MIPAS and ground-based data as well as the error due to the difference in geolocation are important contributions to the comparison error budget.

A clear indication of the validity of MIPAS O3 vertical profiles is obtained for most of the stratosphere, where the mean relative difference with the individual correlative data sets is always lower than ±10%. Furthermore, in the stratosphere (from 1 hPa to 30-40 hPa ; ≈ 23 to 48 km) these differences always fall within the combined systematic error and the standard deviation is fully consistent with the random error of the comparison. A lower quality of the agreement is generally observed in the lower stratosphere and upper troposphere, with biases up to 25% at 100 hPa (≈ 16 km).

6.1 Introduction

Ozone is one of the six atmospheric trace gases (H_2O, O_3, HNO_3, CH_4, N_2O and NO_2) that, along with temperature, constitute the set of target products of the Michelson Interferometer for Passive Atmospheric Sounding (MIPAS) [*Fischer and Oelhaf*, 1996] on-board the European ENVIronment SATellite (ENVISAT) and plays a pivotal role in the majority of the research areas covered by the scientific mission of the instrument [*Fischer et al.*, 2000]. The need for global and continuous monitoring of ozone total column and vertical distribution is primarily linked to its absorption properties in the ultraviolet, that prevent biologically harmful UV radiation from reaching the lower atmosphere and the Earth's surface, and to its impact as a radiatively active gas, that strongly influences the atmospheric heating rates. The former are, in fact, responsible for the protective action of the ozonosphere, that has been severely reduced by ozone depletion at high latitudes and whose recovery can be anticipated only by reliable projections which solve the existing uncertainties on the complex interactions between stratospheric gas-phase and heterogeneous chemistry and dynamics [*Solomon*, 1999; *von der Gathen et al.*, 1995]. The second is evident, first of all, throughout the mutual influence between natural variability and anthropogenic forcing on ozone concentration on one side and the alterations of the temperature profile on the other, that represents one of the most important feedbacks between atmospheric chemistry and climate [*Pyle et al.*, 2005].

A crucial step towards the exploitation of MIPAS O3 operational products in quantitative studies is, however, a thorough validation process, based on comparison with a comprehensive suite of correlative data sets and capable of deriving an overall assessment of the reliability and quality of MIPAS ozone measurements. The validation activity started three months after the ENVISAT launch (1 March 2002) with the calibration and validation experiments of the commissioning phase and continued during the 12 months of the main validation phase (1 September

2002 to 1 September 2003) and the first part of the long-term validation programme. Preliminary validation results achieved by the sub-groups of the ENVISAT Atmospheric Chemistry Validation Team (ACVT) contributing to the geophysical validation of MIPAS ozone profiles - i.e. the GBMCD (Ground-Based Measurements and Campaign Database), the ESABC (ENVISAT Stratospheric Aircraft and Balloon Campaigns) and the MASI (Model Assimilation and Satellite Intercomparison) sub-groups - were presented during the First and Second ENVISAT Validation Workshop (ACVE-1,2) and the 2004 ERS-ENVISAT symposium [*Lambert et al.*, 2003; *Soebijanta et al.*, 2003; *Blumenstock et al.*, 2004; *Cortesi et al.*, 2004; *Kerridge et al.*, 2004; *De Clercq et al.*, 2004]. Following the recommendations drawn after these validation exercises, the MIPAS ozone profile retrieval algorithm have been upgraded. The entire MIPAS data record acquired during the instrument nominal spectral resolution mission (July 2002 to 26 March 2004, see Section 6.2) was reprocessed in version IPF 4.61- 4.62. As a further and closing step, a coordinated effort was carried out to achieve a quantitative evaluation of the quality of MIPAS ozone data products, having both statistical strength and the widest spatial and temporal coverage, by merging individual results from a variety of independent reference measurements of proven quality (i.e. well characterized error budget). This analysis combines results of comparisons with ozone sonde, lidar and microwave measurements from individual ground-based stations and networks, with remote-sensing and in situ observations from balloon and aircraft field campaigns, as well as with profiles from concurrent satellite sensors, obtained by different teams. The final outcome of this activity was published by *Cortesi et al.* [2007] in the MIPAS Atmospheric Chemistry and Physics (ACP) special issue.

This chapter presents our personal contribution to the coordinated MIPAS ozone profile validation paper with a comprehensive intercomparison between MIPAS ozone measurements and correlative data obtained from extensive ground-based networks. In particular, the study includes an evaluation of the total error budget of the comparison and in particular of error contributions due to the difference in vertical and horizontal resolutions and to non-perfect collocation (Section 6.2). This work has been updated, since the paper publication, with recent results gained from the MIPAS horizontal resolution analysis presented in chapter 5 and published in *von Clarmann et al.* [2009]. Collocated measurements from ozonesondes and ground-based lidar of the Network for the Detection Atmospheric Composition Change (NDACC) were selected to carry out comparisons with MIPAS IPF 4.61 ozone profiles measured in 2003 (Section 6.3). Comparison of time series of ground-based and MIPAS ozone partial columns enables identifying groups of stations and time periods with a uniform pattern of ozone differences. The vertical and meridian structure of the differences is, then, investigated within the identified time periods (Section 6.4). The conclusion discusses the quality of MIPAS ozone retrieval with respect to the estimated comparison error bars (Section 6.5).

6.2 Ozone profile data sets

6.2.1 MIPAS

MIPAS is a middle infrared Fourier transform spectrometer operating on-board the ENVISAT platform and acquiring high resolution spectra of atmospheric limb emission in five spectral bands within the frequency range from 685 to 2410 cm^{-1} (14.6 to 4.15 μm) [*Fischer et al.*, 2008]. Launched on the sun-synchronous polar orbit of the satellite with an inclination of 98.55° and at an altitude of about 800 km, MIPAS performed quasi-continuous measurements at nominal spectral resolution (0.025cm^{-1} unapodized, corresponding to an interferometer maximum path difference equal to 20 cm) during a period of two years. In his standard observation mode, the instrument scanned 17 tangent altitudes for each limb sequence, viewing in the rearward direction along the orbit with a sampling rate of approximately 500 km along track and with a instantaneous field of view across track of about 30 km. The vertical scanning grid ranges between 6 km and 68 km, with steps of 3 km from 6 to 42 km, 5 km from 42 to 52 km, and 8 km from 52 to 68 km. MIPAS operation was temporarily halted at the end of March 2004 because of excessive anomalies observed in the interferometric drive unit and resumed in January 2005 in a new operation mode at reduced spectral resolution (0.0625 cm^{-1}) and on a finer vertical grid.

The data obtained during the instrument full spectral resolution mission, from 6 July 2002 to 26 March 2004, have been processed by using v4.61 and v4.62 of ESA level-1b and level-2 (based on an unconstrained non-linear least-square fit procedure) operational algorithms, as described in details in *Kleinert et al.* [2007] and in *Raspollini et al.* [2006] respectively, and provide a self-consistent set of quasi-continuous measurements for temperature and volume mixing ratio (VMR) of six target species. As the altitude registration still suffers from a pointing error, MIPAS profiles versus pressure scale should be considered. For the purposes of MIPAS ozone validation, the two versions of the ESA operational processor are substantially equivalent. Only v4.61 data is used for our comparisons with ground-based ozonesondes and lidars.

The total error budget on the ozone vertical distribution retrieved from individual MIPAS scans can be evaluated by combining the random contribution due to the mapping of the radiometric measurement noise into the retrieved profiles (expressed by the square root of the diagonal elements of the error variance-covariance matrix included in ESA level-2 data products) and the a priori estimates of systematic components [*Dudhia et al.*, 2002] derived from the analysis carried out at University of Oxford (see data available for five different atmospheric scenarios at http://www-atm.physics.ox.ac.uk/group/mipas/err). These systematic and the random components of the estimated error budget have an average value of about 6% and 5% respectively in the altitude interval between 20 km and 52 km.

6.2.2 Ground-based ozonesondes and lidars

Electrochemical concentration cell (ECC) ozone sondes are launched more or less regularly on board small meteorological balloons at a variety of stations from pole to pole. They yield the vertical distribution of ozone VMR from the ground up to burst point, the latter occurring typically around 30 km. Ozone VMR recorded at a typical vertical resolution of 100-150m is converted into ozone number density using pressure and temperature data recorded on-board the same balloon. Error on the ozone profile of ozone sonde depends on a large number of parameters. For ECC sonde important parameters are: the manufacturer of the sonde (SPC or EnSci), the percentage of the sensing solution used in the electrochemical cell and the type of correction applied for pump efficiency. Unfortunately, this information is not always given or well identified in the data files. However, as shown during the JOSIE (Jülich Ozone Sonde Intercomparison Experiment) chamber comparison [*Smit et al.*, 2007], if ozone sondes are operated in a specific way, a similar level of precision and accuracy is achievable from the different sonde types. Typical error estimates are systematic error from 3% (0-20 km) to 5% (20-35 km) and precision from 5% (0-20 km) to 7% (20-35 km).

Differential absorption ozone lidar (DIAL) systems provide the vertical distribution of night-time ozone number density at altitudes between 8-15 km and 45-50 km. Actual operation depends on the cloud cover and other measurement conditions. The typical integration time of an ozone measurement in the whole stratosphere is 4 h. Typical vertical resolution ranges from 300m up to 3 km depending on the altitude. The accuracy of the lidar ozone profile depends on the duration of the measurement and on the vertical resolution chosen to process the data. Individual errors bars are given in each ozone file. Typical accuracy estimates range from 3 to 7% from 15 to 40 km. At 40-45 km and above, due to the rapid decrease in signal to noise ratio, the error bars increase and significant bias reaching 10% may exist [*Godin et al.*, 1999; *Keckhut et al.*, 2004].

Most of ozone profilers perform network operation in the framework of international structures like the Network for the Detection of Atmospheric Composition Change (NDACC, http://www.ndacc.org, *Kurylo and Zander* [2001]), WMO's World Ozone and UV Data Center (WOUDC, http://www.woudc.org) , the Southern Hemisphere ADditional OZonesonde programme (SHADOZ, http://croc.gsfc.nasa.gov/shadoz *Thompson et al.* [2003]), major components of WMO's Global Atmospheric Watch programme (GAW). Prior to using data uploaded routinely to the WOUDC archive, their quality was investigated carefully on statistical and climatological grounds. MIPAS and reference data sets have been processed to select collocated profiles within a maximum spatial distance of 500 km and a maximum time difference of 6h. The selected comparison data set included ozone profiles from 39 ozonesonde stations and 8 lidar systems forming a robust set of independent and of well-known quality correlative measurements. Their complementary altitude ranges offer a ground to upper stratosphere access to the ozone vertical distribution and the variety of stations with different geolocation ensures a quasi pole to pole coverage. Stations and instruments contributing to the present study are listed in Tables 6.1 and 6.2.

6.3 Error budget of comparisons

MIPAS and ground-based instruments offer a different perception of atmospheric ozone. Such differences must be considered to interpret comparison results properly. To evaluate the comparison error budget, we took into account, along with the measurement and retrieval error of MIPAS and of the correlative instrument, the contributions associated with the vertical and horizontal smoothing differences and with the spatial separation of the two ozone profiles. Expanding Rodgers' theory and formalism [*Rodgers*, 1990], we considered, therefore, the following total comparison error covariance S.

$$\begin{aligned} S &= S_M + S_N + (A_{M,V} - A_{N,V}) S_V (A_{M,V} - A_{N,V})^T \\ &+ (A_{M,H} - A_{N,H}) S_H (A_{M,H} - A_{N,H})^T + S_{\Delta O_3} \end{aligned} \quad (6.1)$$

where:

S_M = MIPAS error (measurement, retrieval and retrieval parameters);
S_N = correlative instrument error (measurement, retrieval and retrieval parameters);
A_M = MIPAS averaging kernels, vertical (V) and horizontal (H);
A_N = correlative instrument averaging kernels, vertical (V) and horizontal (H);
S_V = atmospheric variability covariance (vertical);
S_H = atmospheric variability covariance (horizontal);
$S_{\Delta O3}$ = spatial distance error.

Table 6.1: List of ozonesonde stations contributing to MIPAS O_3 validation.

OZONESONDE

Station	*Location*	*Latitude*	*Longitude*	*Institute*
Alert	Canada	82.5	-62.33	MSC
Eureka	Canada	80.05	-86.42	MSC
Ny-Alesund	Svalbard	78.91	11.88	AWI
Thule	Greenland	76.51	-68.76	DMI
Resolute	Canada	74.72	-94.98	MSC
Scoresbysund	Greenland	70.48	-21.97	DMI
Esrange	Sweden	67.88	21.06	NIES
Sodankylä	Finland	67.37	26.67	FMI
Keflavik	Iceland	63.97	-22.6	INTA
Orlandet	Norway	63.42	9.24	NILU
Jokioinen	Finland	60.82	23.48	FMI
Churchill	Canada	58.75	-94.07	MSC
Edmonton	Canada	53.55	-114.1	MSC
Goose Bay	Canada	53.32	-60.38	MSC
Legionowo	Poland	52.4	20.97	IMGW
Debilt	Netherlands	52.1	5.18	KNMI
Valentia	Ireland	51.93	-10.25	ME
Uccle	Belgium	50.8	4.35	KMI
Praha	Czech Republic	50.02	14.45	CHMI
Hohenpeissenberg	Germany	47.8	11.02	DWD
Payerne	Swiss Alps	46.49	6.57	MCH
Tsukuba	Japan	36.05	140.13	JMA
Paramaribo	Surinam	5.81	-55.21	KNMI
San Cristobal	Galapagos	-0.92	-89.6	NOAA
Nairobi	Kenya	-1.27	36.8	MCH
Malindi	Kenya	-2.99	40.19	CRPSM
Natal	Brazil	-5.42	-35.38	INPE
Watukosek	Java	-7.5	112.6	JAXA
Ascension Island	Congo	-7.98	-14.42	NASA
Tutuila	Samoa	-14.23	-170.56	NOAA
Fiji	Fiji	-18.13	178.42	NOAA
Saint-Denis	Reunion	-21.06	55.47	CNRS
Irene	South Africa	-25.25	28.18	SAWS
Lauder	New Zealand	-45.03	169.68	NIWA
Marambio	Antarctica	-64.28	-56.72	INTA
Dumontd'Urville	Antarctica	-66.67	140.01	CNRS
Syowa	Antarctica	-69	39.58	JMA
Neumayer	Antarctica	-70.65	-8.25	AWI
Belgrano	Antarctica	-77.87	-34.63	INTA

Table 6.2: List of lidar stations contributing to MIPAS O_3 validation.

LIDAR				
Station	***Location***	***Latitude***	***Longitude***	***Institute***
Ny-Alesund	Svalbard	78.91	11.88	AWI
Andoya	Norway	69.28	16.02	NILU
Hohenpeissenberg	Germany	47.8	11.02	DWD
Haute Provence	French Alps	43.94	5.71	CNRS
Tsukuba	Japan	36.05	140.13	NIES
Table Mountain	California	34.23	-117.41	JPL
Mauna Loa	Hawaii	19.54	-155.58	JPL
Lauder	New Zealand	-45.03	169.68	RIVM

MIPAS and ground-based instrument error budgets are described in the literature and have been cited in section 6.2. Ideally, they are the error bars within comparison results (MIPAS/ground differences) should fit if the compared air masses were perfectly coincident. Smoothing and collocation differences increase the comparison error. This issue is illustrated in Figure 6.1 in the horizontal domain. The figure shows MIPAS spatial sampling of stratospheric ozone above Uccle in Belgium and Dumont d'Urville in Antarctica stations on top of a total ozone field derived from BASCOE assimilated data. Measurements around Dumont d'Urville are close to the border of the Antarctic ozone hole. The triangles and segments show the tangent points and horizontal resolution (Full Width at Half Maximum (FWHM) of ozone horizontal averaging kernels) of MIPAS measurement acquired during one month of operation (March 2003 at Uccle and November 2003 at Dumont d'Urville) in a 500 km radius around the stations. The figure illustrates for two examples the MIPAS horizontal perception of the atmospheric gradient and the ozone difference that might exist between the station and MIPAS tangent point geolocations. The horizontal smoothing error can be large when MIPAS line of sight (LOS) is parallel to a strong atmospheric gradient as for example at the bordure of the polar vortex but also where local inhomogeneities of the ozone field exist. Similarly, strong ozone differences may exist between the station and the MIPAS tangent point in such situations. In our study, we estimate separately errors due the difference in horizontal and vertical resolution and to difference in geolocation.

6.3.1 Vertical smoothing

MIPAS measurements' vertical resolution is of the order of 3 km. Generic vertical averaging kernels have been calculated by *Ceccherini* [2004] using a perturbation method. Ozonesondes and lidar have a different vertical perception of the ozone profile and have a slightly higher vertical resolution. This difference adds the so-called vertical smoothing error contribution to the comparison error budget. We estimate this effect using the vertical averaging kernels associated with the MIPAS retrieval of the ozone profile. First, the MIPAS averaging kernels are used to map the high resolution ground-based ozonesonde or lidar profile to the MIPAS low resolution perception. The a priori profile used in the MIPAS vertical averaging kernel estimation is also included as it may introduce an additional bias [*Ceccherini*, 2004]. Second, the smoothing difference error is estimated as the difference between the smoothed and original ground-based profiles:

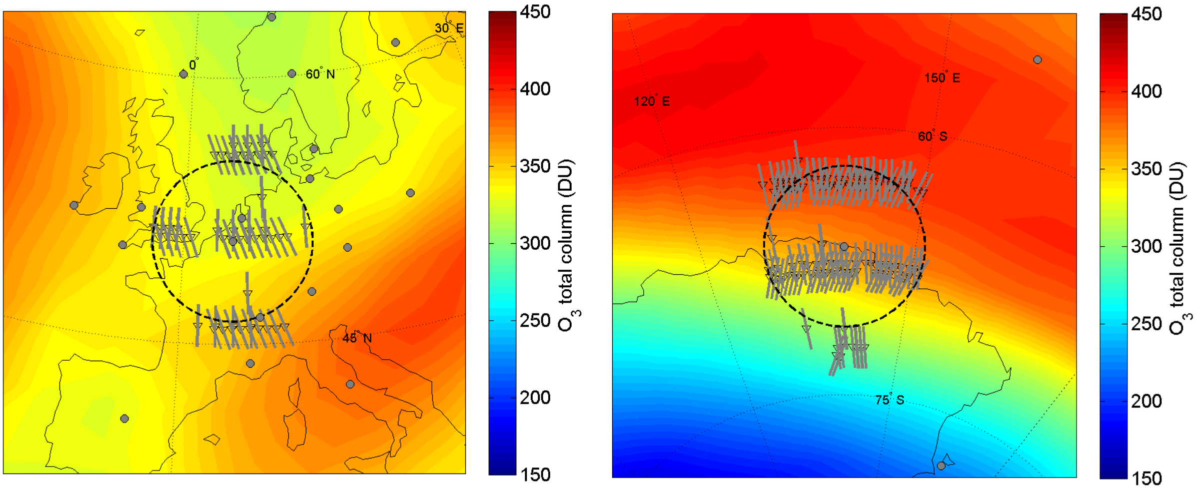


Figure 6.1: Spatial sampling of stratospheric ozone above Uccle in Belgium (left) and Dumont d'Urville in Antartica (right), achieved by Envisat MIPAS during one month of operation (March 2003 at Uccle and November 2003 at Dumont d'Urville) on top of a total ozone field derived from BASCOE assimilated data. Quasi-linear segments show, for tangent points within 500 km, the estimation of MIPAS horizontal resolution (FWHM of ozone horizontal averaging kernels) at 30 km altitude. Triangles locate tangent points of limb scans at 30 km. The dashed circle refers to the radius of 500 km around the stations. Grey dots identify nearby ozone-sounding stations.

$$\Delta_{x_V} = x_a^M + A_M \left(x_N - x_a^M \right) - x_N \tag{6.2}$$

where:

Δ_{x_V} = vertical smoothing error;

x_N = ozonesonde or lidar high resolution profile;

x_a^M = MIPAS a priori ozone profile used to compute the vertical averaging kernels.

Systematic bias is calculated as the mean value of Δ_{x_V} and random error as its 1σ standard deviation.

6.3.2 Horizontal smoothing

Similar to what happens in the vertical direction, MIPAS and ground-based instruments have a different horizontal resolution. While ground-based instrumentation captures only a portion of the air mass probed by MIPAS, MIPAS smoothes atmospheric inhomogeneities over several hundred kilometres. Horizontal averaging kernels for MIPAS one-dimensional retrievals have recently been calculated by *von Clarmann et al.* [2009] (see Chapter 5). Applying the same procedure than for the vertical smoothing error to estimate the horizontal smoothing error contribution would necessity a high resolution ozone field but, the usual latitude step of current models is of the order of 3-5°, which is equal or larger than the MIPAS horizontal resolution. The MIPAS uncertainties associated with horizontal smoothing are calculated rather as an estimate of the ozone gradient interfering with the MIPAS line of sight (LOS), that is, the horizontal component of atmospheric noise associated with the MIPAS measurement:

$$\Delta_{x_H} = abs(\vec{\nabla} X_{MEDIAN} \cdot \vec{1}_{ENVISAT}) |AK_H|_{FWHM} \tag{6.3}$$

where:

Δ_{x_H} = horizontal smoothing error (or horizontal component of atmospheric noise);

$\vec{\nabla} X_{MEDIAN}$ = ozone gradient at the median point of MIPAS horizontal averaging kernel;

$\vec{1}_{ENVISAT}$ = ENVISAT direction (MIPAS LOS is backward along track);

$|AK_H|_{FWHM}$ = Full width at half maximum of MIPAS horizontal averaging kernel.

Both parallel or anti-parallel gradient will result in the same random error contribution (estimated as the mean value of Δ_{x_H}). The ozone gradient is estimated from 4-dimensional ozone fields generated by the Belgian Assimilation System of Chemical Observations from ENVISAT (BASCOE, *Errera and Fonteyn* 2001; *Fonteyn et al.* 2003). BASCOE is a data assimilation system of stratospheric chemistry using the four-dimensional variational (4D-VAR) method. In the course of a run, BASCOE can ingest satellite observations. The resulting "assimilated field" is an estimate of the chemical composition of the stratosphere based both on the set of observations and on the physical laws describing the evolution of the system synthetized into the model. They are defined at 37 hybrid pressure levels from 0.1 hPa down to the surface. The horizontal resolution of BASCOE standard outputs is 3.75° in latitude by 5° in longitude. For our study we have used off-line version v3q33 of BASCOE fields. It is important to note that BASCOE absolute ozone fields have shown to compare reasonably to HALOE, CRISTA and MLS and, more important here, that relative fields are accurate [*Errera and Fonteyn*, 2001; *Fonteyn et al.*, 2003].

6.3.3 Spatial distance

Finally, to complete the comparison error budget, the ozone partial column difference induced by the spatial/temporal separation of the two ozone profiles can be estimated by:

$$\Delta_{O_3} = O_3(X_{MEDIAN}^{MIPAS}) - O_3(X_{STATION}) \tag{6.4}$$

where X_{MEDIAN}^{MIPAS} is the geolocation of the MIPAS tangent point (estimated as the geolocation of the median point of the horizontal averaging kernel), $X_{STATION}$ is the ground-based station geolocation and $O_3(X)$ the ozone volume mixing ration at the corresponding location and time estimated using BASCOE assimilated ozone fields. Systematic bias is calculated as the mean value of Δ_{O_3} and random error as its 1σ standard deviation.

6.4 Comparison results

6.4.1 Partial columns

The first segment of our study concentrated on the analysis of time series of the differences between MIPAS and ground-based ozone partial column data. The analysis included assessments of the different contributions to the total comparison error, as defined in the previous Section. Comparison results vary significantly between the lower stratosphere, where dynamics and chemistry interfere, with clear influences of tropospheric dynamics, and the higher stratosphere, where photochemistry dominates. Consequently, a classification based on regularities in the pattern of the O_3 partial column differences emerges: in the lower stratosphere (75-35 hPa; ≈18-23 km), results regroup around synoptic and regional systems and the systems linked to stratospheric transport; reaching into the middle stratosphere (35-15 hPa; ≈23-28 km), we move from large synoptic groups to a more zonal behaviour and we can extend the previously described synoptic systems to group more stations; in the middle and upper stratosphere (15-7 hPa and 7-3 hPa; ≈28-34 and 34-40 km), zonal symmetry becomes dominant and comparisons results follow this behaviour. Deviations from zonal symmetry nevertheless exist and must be taken into account.

A typical output of the comparison carried out for the aforementioned groups of measurement sites is displayed in Figures 6.2, 6.3 and 6.4 presenting, respectively the results obtained at Arctic, Western and Central Europe, and Equatorial stations. The plots show, as black dots, the percentage relative difference in ozone partial column (75-35 and 35-15 hPa at Arctic and Equatorial stations and 75-35, 35-15, 15-3 and 3-7 hPa at European stations) between MIPAS and correlative ozonesonde and lidar data over 2003, and smoothing and collocation errors (systematic in plain and random in dashed) estimated by the aforementioned methods. Grey rectangles identify monthly means (central line) and standard deviations of the differences. Red curves give the range of atmospheric variability smoothed by the MIPAS measurement, that is, an upper limit of the expected difference between MIPAS and ground-based ozone column data. Blue curves show the error contribution due to difference in geolocation between ground-based and MIPAS measurements.

Both horizontal smoothing and geolocation difference are important contribution to the comparison error budget reaching 5% on average (i.e. a value comparable to the instrument measurement error themselves) and even 20% in Antarctica during ozone hole. Although smaller, they correlate with the standard deviation of comparisons and reflects the atmospheric natural variability, being larger in winter at middle and high latitude stations. Their amplitude is also larger in the lower stratosphere influenced by the tropospheric dynamics than in the more zonal middle and upper stratosphere. Errors associated with vertical smoothing differences are smaller. Their effect could account for a small, constant offset in the comparisons. The sum of all these contributions including MIPAS and ground-based instrument measurement error (not shown) can be expected to account for the observed standard deviation of the comparisons, but not for systematic differences as those appearing in Figure 6.3 and 6.4 in the lower stratosphere in summer 2003.

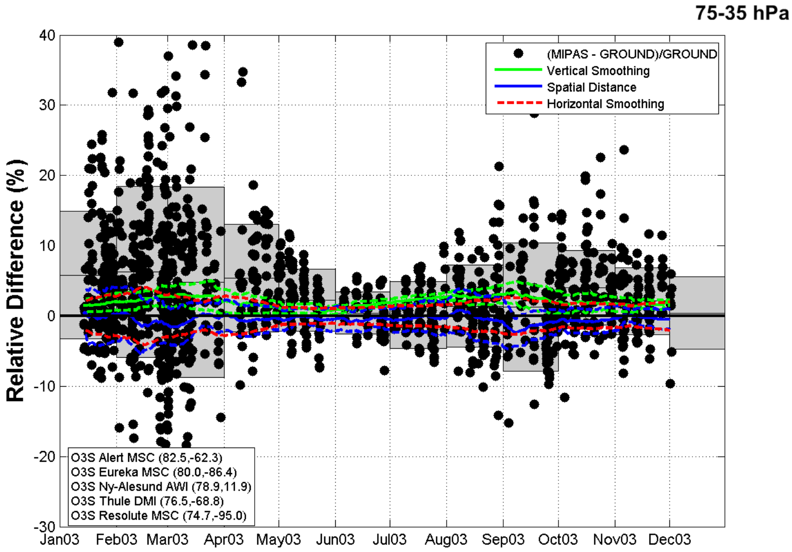
In most cases, comparison results can be interpreted by considering the different error contributions. However, in some cases, they cannot account fully for the difference noticed between MIPAS and correlative partial column data. MIPAS reports larger partial columns than the ground based-instruments:

- in the 75-35 hPa layer at stations from northern and southern mid latitudes, equator and tropics (Figure 6.3 and 6.4);
- at 35-15 hPa over stations at the equator, in the tropics 6.4, and in Antarctica during ozone hole event.

6.4.2 Vertical and meridian structure

The first step of our analysis was qualitative in getting an overall view of the agreement between MIPAS and WMO/GAW ground-based data, and also in determining time periods and groups of stations where comparison results are sufficiently consistent to allow the meaningful derivation of statistical values. As a second step of our analysis, we derived vertically resolved statistics of the comparisons between MIPAS v4.61 ozone profiles and correlative data. The comparisons have been performed at each individual station listed in Tables 6.1 and 6.2 and summary plots have been computed for stations belonging to the same synoptic system/zonal region and showing mostly identical comparison results. The groups are the same as above, except that in this case we have separated ozone sondes and lidar results to allow better discrimination of ground-based error contributions. At Arctic, Northern and Southern middle latitude sites, the results can be separated between 1 October to 31 March and 1 April to 30 September. At tropical and equatorial stations, the weak seasonal variation allows us to draw annual plots. At Antarctic stations results can be separated between "ozone hole" (that is, for 2003, 21 August to 15 October) and "normal ozone" periods (that is, for 2003, 16 October to 20 August).

Some examples of the results obtained for the relative differences of MIPAS O3 vertical profiles with ozone sonde and lidar data are shown in Figures 6.5, 6.6 and 6.7. Each plot shows, for each collocated pair of profiles, relative differences between MIPAS and correlative measurements (light grey lines). To eliminate vertical smoothing differences, high-resolution correlative measurements have been previously convoluted with MIPAS averaging kernels and biased by the first-guess profile, following the method proposed by Rodgers and Connor (2003). Black lines depict statistical values (mean and 1σ standard deviation) of the absolute or relative differences between MIPAS and ground-based data. Red lines depict the total systematic error of the comparison. The mean difference between MIPAS and ground station data should be compared to these lines. The total systematic error of the comparison is calculated as the quadratic sum of MIPAS and ozonesonde



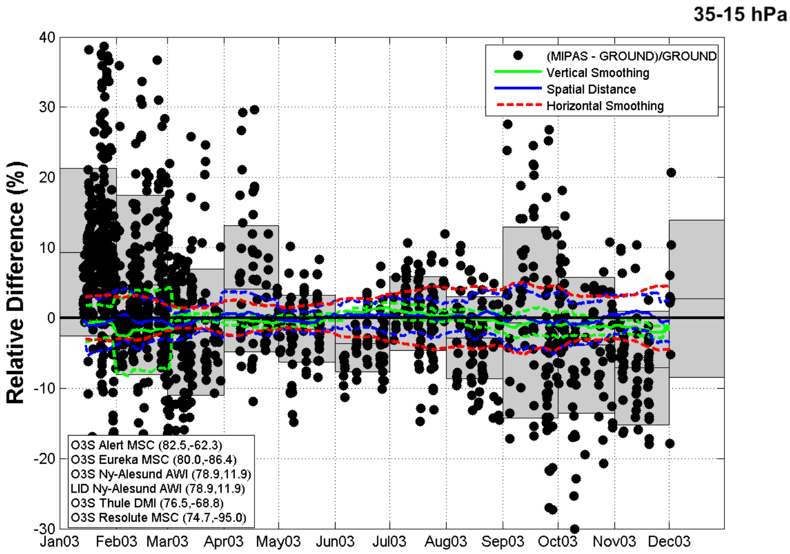
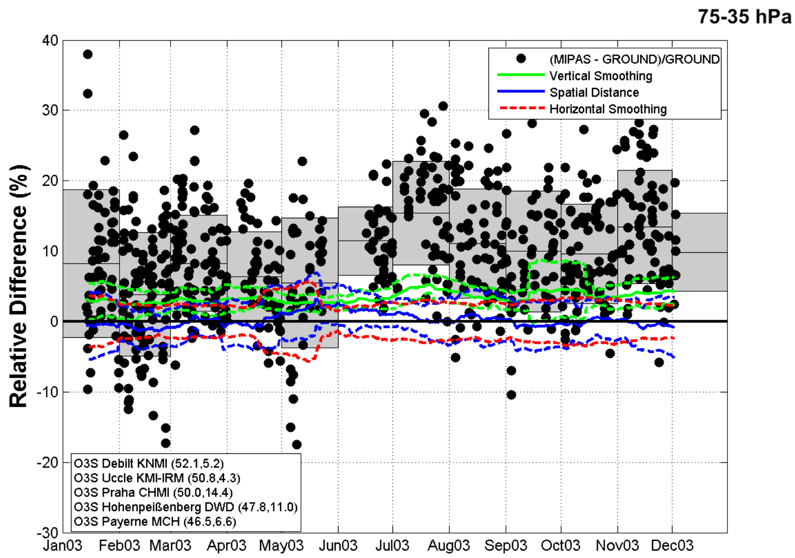
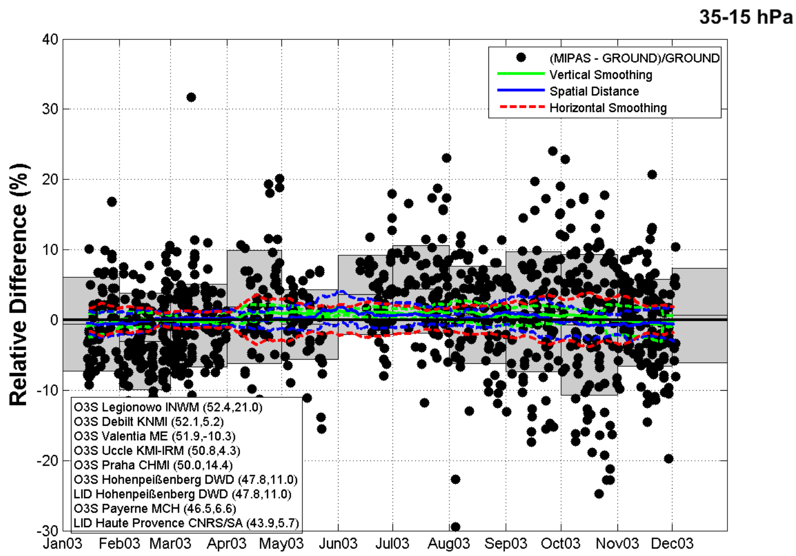


Figure 6.2: Time-series of the percentage relative difference in ozone partial column (75-35 and 35-15 hPa) between MIPAS and correlative ozonesonde data at five Arctic stations for 2003, and estimated smoothing and collocation errors (systematic in plain and random in dashed). Grey-shaded rectangles identify monthly means (central line) and standard deviation of the differences.


75-35 hPa
Relative Difference (%)
(MIPAS - GROUND)/GROUND
Vertical Smoothing
Spatial Distance
Horizontal Smoothing
O3S Debilt KNMI (52.1,5.2)
O3S Uccle KMI-IRM (50.8,4.3)
O3S Praha CHMI (50.0,14.4)
O3S Hohenpeißenberg DWD (47.8,11.0)
O3S Payerne MCH (46.5,6.6)
Jan03 Feb03 Mar03 Apr03 May03 Jun03 Jul03 Aug03 Sep03 Oct03 Nov03 Dec03


35-15 hPa
Relative Difference (%)
(MIPAS - GROUND)/GROUND
Vertical Smoothing
Spatial Distance
Horizontal Smoothing
O3S Legionowo INWM (52.4,21.0)
O3S Debilt KNMI (52.1,5.2)
O3S Valentia ME (51.9,-10.3)
O3S Uccle KMI-IRM (50.8,4.3)
O3S Praha CHMI (50.0,14.4)
O3S Hohenpeißenberg DWD (47.8,11.0)
LID Hohenpeißenberg DWD (47.8,11.0)
O3S Payerne MCH (46.5,6.6)
LID Haute Provence CNRS/SA (43.9,5.7)
Jan03 Feb03 Mar03 Apr03 May03 Jun03 Jul03 Aug03 Sep03 Oct03 Nov03 Dec03

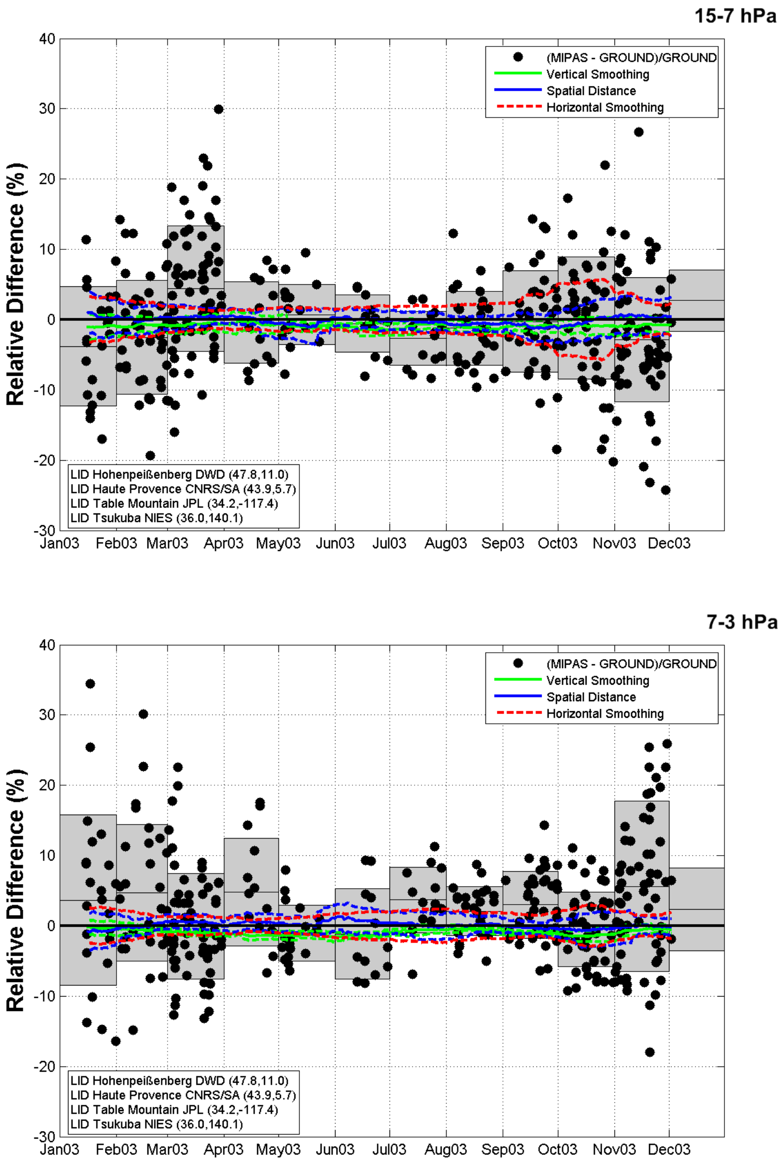
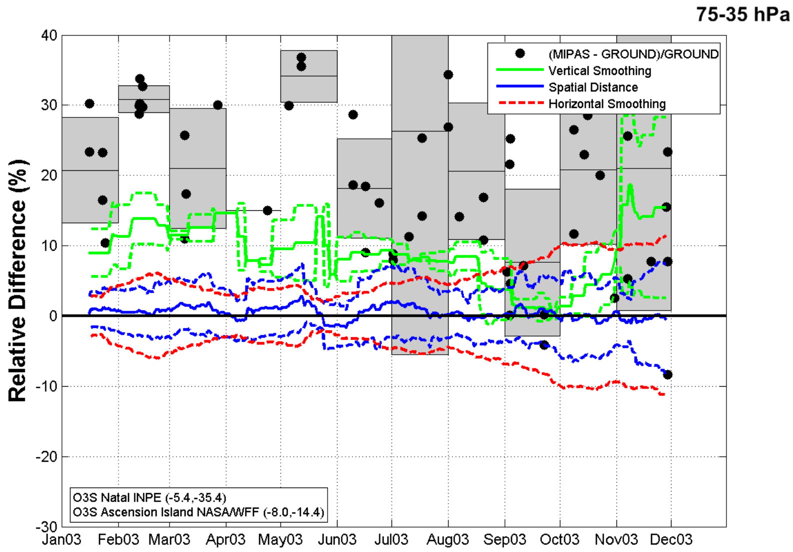


Figure 6.3: Time-series of the percentage relative difference in ozone partial column (75-35, 35-15, 15-7 and 7-3 hPa) between MIPAS and correlative ozonesonde and lidar data at Western and Central Europe stations for 2003, and estimated smoothing and collocation errors (systematic in plain and random in dashed). Grey-shaded rectangles identify monthly means (central line) and standard deviations of the differences.



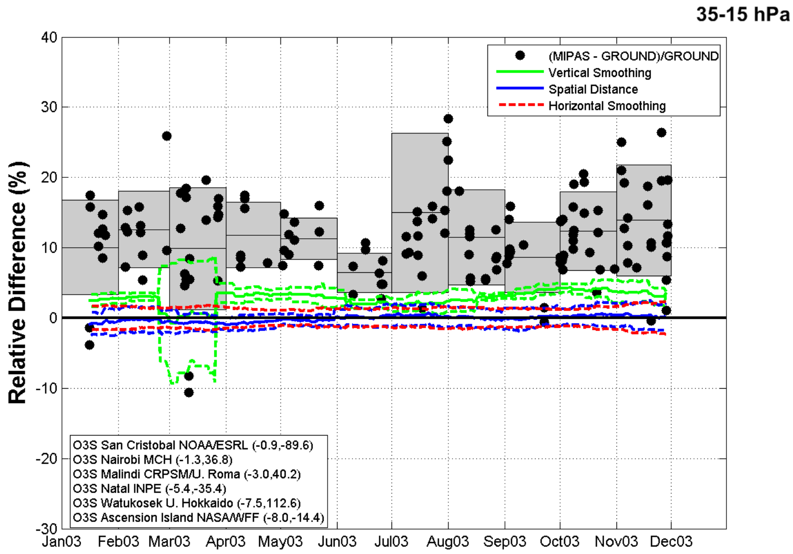


Figure 6.4: Time-series of the percentage relative difference in ozone partial column (75-35 and 35-15 hPa) between MIPAS and correlative ozonesonde data at Equatorial stations for 2003, and estimated smoothing and collocation errors (systematic in plain and random in dashed). Grey-shaded rectangles identify monthly means (central line) and standard deviations of the differences.

systematic error and the systematic bias due to non-perfect collocation (spatial/temporal distance, as explained in Section 6.3). The yellow block delimited by dashed red lines depicts the total random error of the comparison. This value should be compared with the standard deviation of the differences. This total random error of the comparison is calculated as the quadratic sum of MIPAS random error, ground-based random error, random contribution of spatial/temporal distance and LOS inhomogeneity. We should remark that low ozone concentrations lead to large relative difference although absolute differences are small. Then, mean and standard deviation of relative difference obtained below 12-15 km at middle and high latitudes, below 20 km at tropical and equatorial are not relevant.

These comparisons results confirms those obtained with the partial column time series analysis. As expected, the random error budget of the comparisons including contribution from horizontal smoothing and geolocation differences can fully account for $\pm 10\%$ standard deviation of the differences observed in the stratosphere. In general MIPAS ozone profiles show a good agreement with correlative data and the mean differences fall within the systematic error budget, except in a few cases. MIPAS reports larger ozone concentration by more than 20% than the ground based-instruments: (a) in the lower stratosphere at stations from Northern and Southern mid latitudes, Equator and Tropics; (b) in the middle stratosphere over stations at the Equator, in the Tropic of Capricorn, and in Antarctica during ozone hole events;

These validation results are summarised in Fig.6.8, that reports mean relative differences for the two considered time periods of 2003 versus latitude. Results for all stations have been averaged within bin of 5° of latitude. MIPAS overestimation of the ozone concentration in the lower stratosphere of the inter-tropical zone and during ozone hole reaches 20% to 25%. Below the tropopause the results are more scattered. For other geophysical states, the mean agreement between MIPAS and correlative instruments usually falls within the 10% level and often better.

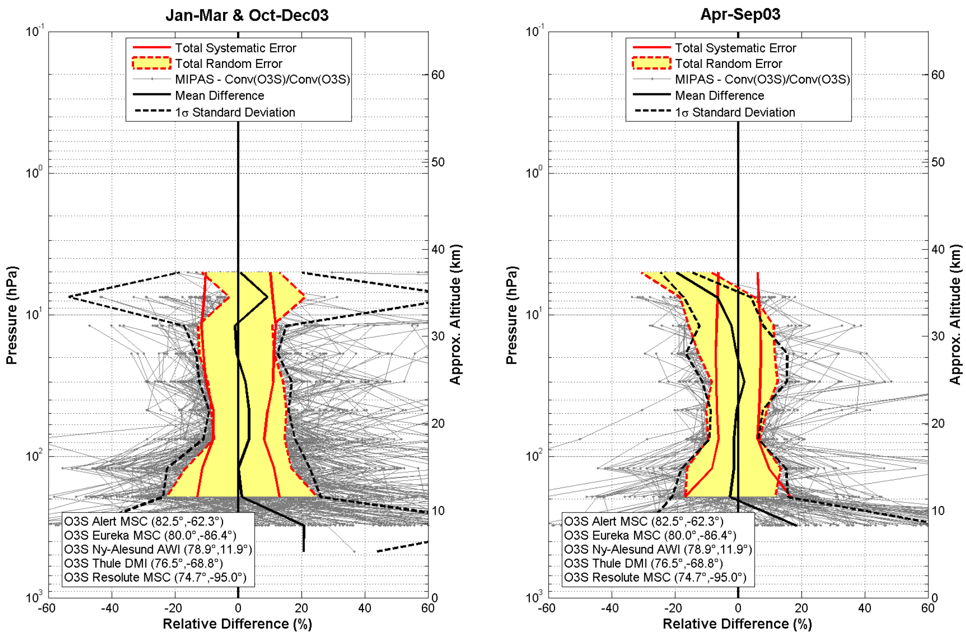


Figure 6.5: Vertically resolved statistics of the relative differences between MIPAS O3 data and ozonesonde measurements in the Arctic (see main text for explanations).

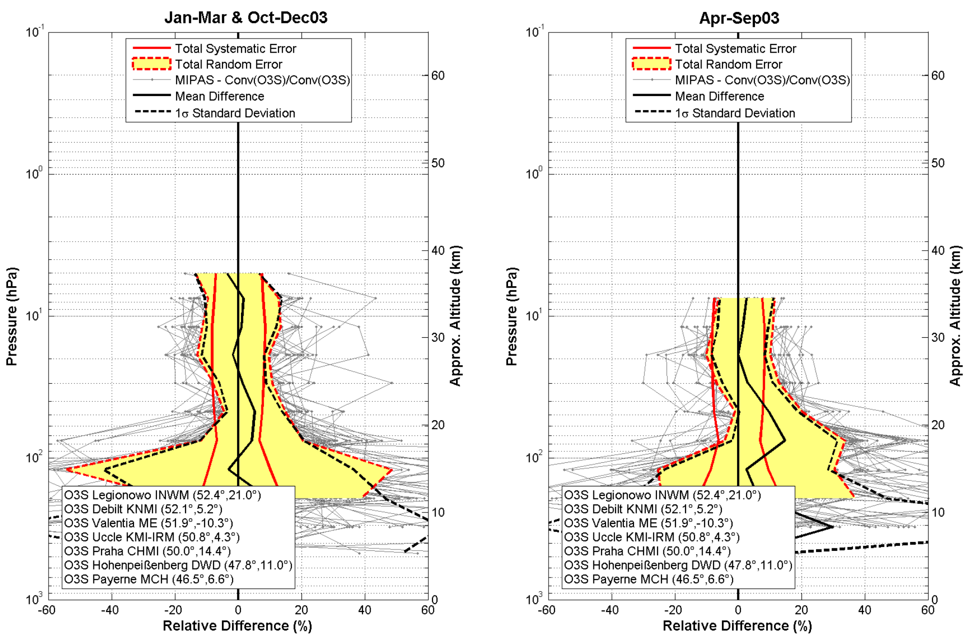


Figure 6.6: Same as Figure 6.5 but for ozonesonde measurements at Western and Central Europe stations.

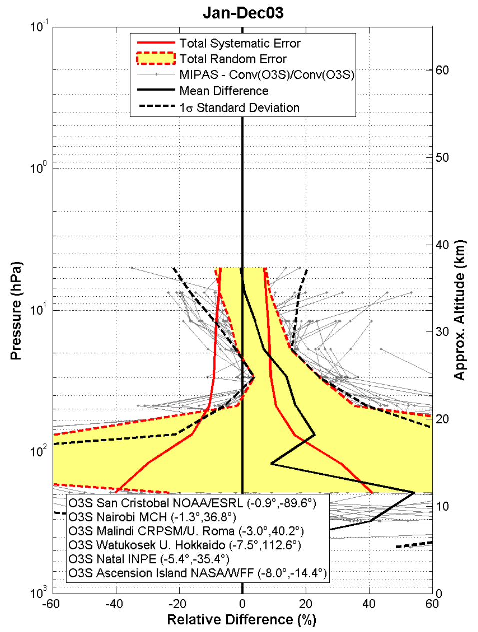


Figure 6.7: Same as Figure 6.5 but for ozonesonde measurements at Equatorial stations.

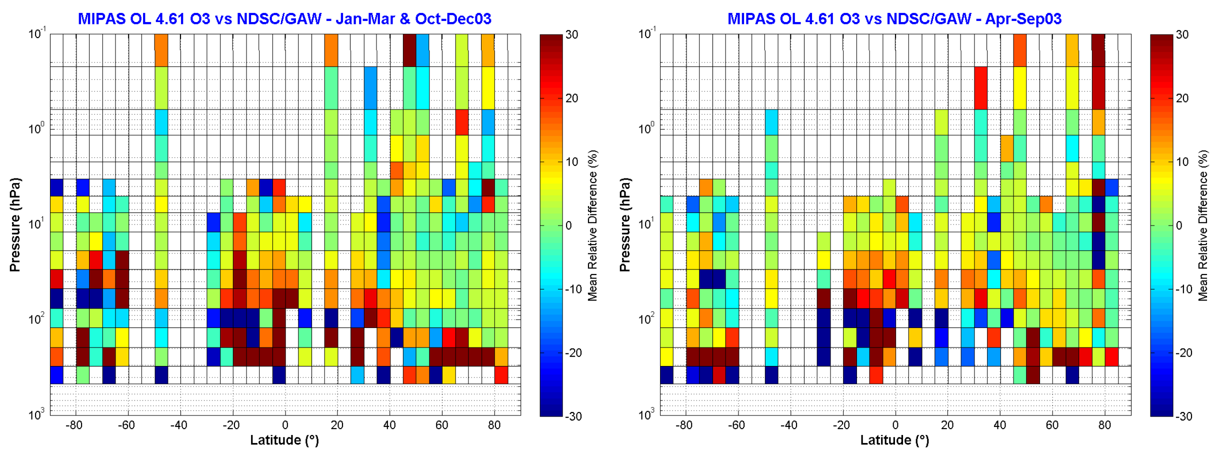


Figure 6.8: Mean relative difference between MIPAS and correlative ozone concentration versus pressure and latitude. Data from January to March and October to December 2003 (left) and from April to September 2003 (right).

6.5 Conclusion

In this paper, we have presented the results of an extensive analysis aimed at the validation of MIPAS-ENVISAT O_3 vertical profiles obtained in 2003 during the instrument full spectral resolution mission and retrieved using versions 4.61 of the ESA IPF operational processor.

The validation strategy was based on the synergistic use of independent correlative data sets provided by ground-based networks of ozonesonde stations and lidars. MIPAS ozone partial columns and vertical profiles have been confronted to collocated measurements from more than 40 ground-based stations. The different geolocations of the ground-based stations and the different altitude range covered by the two techniques enable pseudo-global investigations. As detailed documentation about operational retrievals and related errors is available both for MIPAS and ground-based data, we have been able to calculate the total error budget of the comparisons. Vertical smoothing, horizontal smoothing and geolocation difference contributions to the comparison error budget have been estimated experimentally.

Comparison results reflect dynamics and photochemistry influences. In the lower stratosphere, results regroup around the synoptic systems and in the higher stratosphere, dominating photochemistry yields a more zonal behaviour. Temporal analysis of the relative differences between MIPAS and correlative data helps to identify time periods were statistical analysis is relevant. Vertically-resolved statistics (mean and standard deviation) computed for these time periods have been compared to the systematic and random components of the comparison error budget. The standard deviation of the comparisons correlates well with the estimated random error. The analysis demonstrates that horizontal inhomogeneities captured by MIPAS air masses and geolocation difference represent important components of the comparison error budget. In general MIPAS/ground mean differences fit within the systematic error budget and are within 10% level, except in a few cases. MIPAS reports larger ozone values by 20 to 25% in the lower stratosphere of the inter-tropical zone and in Antarctica during the ozone hole. Below the tropopause more scattered results are obtained. Based on our results and similar conclusions obtained by other teams, *Cortesi et al.* [2007] attribute this issue to a residual cloud contamination of the MIPAS spectra.

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