

O3M SAF VALIDATION REPORT

Validated products:

Identifier	Name	Acronym
O3M-03	Near-Real-Time Ozone Profile	NOP
O3M-13	Offline Ozone Profile	OOP
O3M-38	Near-Real-Time High Resolution Ozone Profile	NOP/HR
O3M-39	Offline High Resolution Ozone Profile	OOP/HR



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Product Software Version: 1.25

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1General Introduction

This report contains validation results of the GOME-2/Metop ozone profile product retrieved by the Ozone Profile Retrieval Algorithm (OPERA) at KNMI. It covers the time period January 2007 until May 2011. Ozone profiles retrieved from reprocessed level-1b data were used in coarse resolation (CR) and in high resolution (HR).

Since this work was carried out in two different institutions, this document is split up into two separate parts. The first part contains the validation of the retrieved GOME-2 ozone profiles using balloon ozonesondes (chapter 2). This part will mainly validate the retrieved ozone profiles in the troposphere and the lower stratosphere. The second part shows the validation with lidars and microwave radiometers (chapter 3) describing the performance of GOME-2 retrieved ozone profiles in the entire stratosphere and in parts down into the troposphere. The outcome of both validation parts is summarized in the summary and conclusions section at the end of the report.

2Introduction

This report presents validation results for the O3M SAF GOME-2 ozone profile product. The validation was carried out using ozone profile measurements with balloon sounding data.

Ozonesondes are lightweight balloon-borne instruments which are able to make ozone measurements from the surface up to about 30 km, with much better vertical resolution than satellite data. In general also the precision and accuracy will be better, at least in the lower stratosphere and the troposphere. Another advantage is that ozone soundings can be performed at any time and at any meteorological condition.

The precision of ozonesondes varies with altitude and depends on the type of sonde used. Table 1 below shows indicative precision (in percent) of the Electrochemical Concentration Cell (ECC), Brewer-Mast (B-M) and the Japanese KC79 ozonesondes, at different pressure levels of the sounding (taken from the O3MSAF Science Plan).

Pressure level (hPa)	ECC	B-M	KC79
10	2	10	4
40	2	4	3
100	4	6	10
400	6	16	6
900	7	14	12

Table 1: Precision of different types of ozonesondes at different pressure levels

It is shown from Table 1 that the profiles from ozonesondes are most reliable around the 40 hPa level, which is around the ozone maximum. The error bar of profiles from ozonesondes increases rapidly at levels above the 10 hPa level, which is around 31 km altitude. For this validation report, only the station of Hohenpeissenberg is using B-M sondes, all the other 31 stations under consideration (Table 3) use ECC sondes, while KC-79 sondes have been used

until respectively September 2009 for Tateno-Tsukuba and Sapporo and November 2008 for Naha.

2.1Dataset description

GOME-2 ozone data used in this validation report is from the beginning of January 2007 up to the end of August 2009. GOME-2 ozone data was made available by KNMI at pre-selected sites. These sites correspond to sites where ozone soundings are performed on a regular basis. In order to have a more global view on the performance of the ozone profile product, we used about 25 stations, introducing the SHADOZ-network (Thompson *et al., 2003a,* Thompson *et al., 2003b,* <u>http://croc.gsfc.nasa.gov/shadoz/</u>) for the Tropical stations. For the other stations, data was made available by the World Ozone and Ultraviolet Data Center (WOUDC). (<u>http://www.woudc.org</u>) and the NILU's Atmospheric Database for Interactive Retrieval (NADIR) at Norsk Institutt for Luftforskning (NILU) (<u>http://www.nilu.no/nadir/</u>).

Latitude belts from North to South:

- 1. Polar stations North: green (67N 90 N)
- 2. Mid-Latitude stations North: black (30 N 67 N)
- 3. Tropical stations: Red (30 N 30 S)
- 4. Mid-Latitude stations South: grey (30 S 70 S)
- 5. Polar stations South: orange (70 S 90 S)





The algorithm version used for this retrieval of GOME-2 is mentioned in the general introduction of this report.

Ozonesonde data are generally made available by the organization carrying out observations after a delay in order to leave time for necessary verification and correction of the data quality. Nevertheless, some organizations make their ozone profile data readily available for validation purposes.

In this report, data has been split up into two time periods in order to report the previous periods with the reprocessed dataset. The two different time periods are:

- 01/01/2007 31/12/2010
- 01/01/2007 31/05/2011

The first time period is used to apply the general statistics and to exclude the seasonal behaviour effect, the second one is to show the time series until May 2011, for which a considerable amount of observational data is available.

A validation is performed in function of latitude belts. Figure 1 and Table 3 show an overview of the stations used in this validation report. The number of coincidences is summarized in the table below:

 Table 2: Overview of number of coincidences at different station locations for the time period 2007 –

 2011 for coarse resolution and high resolution pixels

Latitude band	Nr of coincidences CR-pixels	Nr of coincidences HR-pixels
Polar North (90-67)	26891	21975
Mid-Latitudes North (30-67)	29211	24425
Tropics (+30 – 30)	6629	5390
Mid-Latitudes South (-30-70)	4241	3474
Polar South (-70 -90)	3124	2776

Table 3: Overview of the stations taken into account with the numbers of sondes used in the analysis and the last day, a sonde was available for the intercomparison

STATION	Longitude	Latitude	Nr of sondes	Last day available ozonesonde
ALAJUELA	9.98	-84.21	111	23/10/2009
ALERT	82.50	-62.33	218	18/05/2011
ASCENSION	-7.98	-14.42	131	24/08/2010
BROADMEADOWS	-37.69	144.95	171	25/08/2010
CHURCHIL	58.74	-94.07	183	26/05/2011
DAVIS	-68.58	77.97	97	25/08/2010
DEBILT	52.10	5.18	238	30/05/2011
EUREKA	80.00	-85.56	353	25/05/2011
HOHENPEISSENBERG	47.80	11.02	496	30/05/2011
IRENE	-25.90	28.22	19	28/02/2008
JAVA	-7.50	112.60	62	30/03/2011
KELOWNA	49.67	-119.40	255	25/05/2011
KUALA_LUMPUR	2.73	101.70	73	01/02/2010
LAUDER	-45.05	169.68	86	18/12/2008
LERWICK	60.14	-1.19	198	25/05/2011
MACQUARIE_ISL	-54.50	158.94	161	24/08/2010
NAHA	26.20	127.68	156	18/05/2011

NAIROBI	-1.27	36.80	156	13/04/2011	
NATAL	-5.42	-35.38	146	03/03/2011	
NEUMEYER	-70.39	-8.15	274	29/05/2011	
NY-ALESUND	78.93	11.95	301	25/05/2011	
PARAMARIBO	5.81	-55.21	141	30/12/2010	
PAYERNE	46.82	6.95	597	31/12/2010	
SAMOA	-14.23	-170.56	105	19/08/2010	
SAN_CRISTOBAL	-0.92	-89.60	61	23/10/2008	
SAPPORO	43.06	141.33	155	26/05/2011	
SODANKYLA	67.37	26.63	310	25/05/2011	
TATENO-TSUKUBA	36.10	140.10	186	25/05/2011	
UCCLE	50.80	4.35	630	30/05/2011	
USHUAIA	-54.85	-68.31	88	18/05/2011	
WALLOPS_ISL	37.84	-75.48	224	31/05/2011	

2.2Comparison procedure

2.2.1Co-location criteria

The selection criteria, taken into account are two fold:

- The geographic distance between the GOME-2 pixel center and the sounding station location for the coarse resolution (CR) pixels is 300 km, for the high resolution (HR) pixels, this distance is reduced towards 100 km.
- The time difference between the pixel sensing time and the sounding launch time is the second criterion and is fixed at ten hours of time difference. Each sounding that is correlated with a GOME-2 overpass is generally correlated with several GOME-2 pixels if the orbit falls within the 300 km (resp 100 km for the HR pixels) circle around the sounding station. This means that a single ozone profile is compared to more than one GOME-2 measurement.

2.3Ozone sounding pre-processing

GOME-2 ozone profiles are given as partial ozone columns on 40 varying pressure levels, calculated by the Ozone Profile Retrieval Algorithm (OPERA) developed by KNMI. Ozone partial columns are expressed in Dobson Units.

Ozonesondes measure the ozone concentration along the ascent with a much higher vertical resolution than GOME-2. Ozonesondes have a typical vertical resolution of 100m while GOME-2 profiles consist 40 layers between the ground and 0.01hPa. Ozonesondes give the ozone concentration in partial pressure. The integration requires some interpolation, as GOME-2 levels never match exactly ozonesonde layers. This interpolation causes negligible errors given the high vertical resolution of ozonesonde profiles.

For the comparison, ozonesonde profiles are integrated between the GOME-2 pressure levels of the GOME-2 profile being compared. This means when a single ozonesonde profile is compared to different GOME-2 profiles, the actual reference ozone values are not the same given that the GOME-2 level boundaries vary from one measurement to another. This integrated ozonesondes data will be further referred in this report as X_{sonde} .

However, GOME-2 levels are relatively thick and GOME-2 layers boundaries show small variations compared to the layer thickness. So, the same layer always falls around the same altitude. The altitude of those layers can be considered as "fixed' and an "*averaged layer altitude (or pressure)*" is used for making graphs.

In this report, the validation of the GOME-2 profiles is calculated by using the averaging kernels (AVK) of the GOME-2 profile. The motivation to apply the AVK is to "smooth" the ozone soundings towards the resolution of the satellite, to look at the GOME-2 profiles with "the eyes" from the satellite. Equation (1) shows how the kernels have been applied.

$$X_{avk_sonde} = X_{apriori} + A (X_{raw sonde} - X_{apriori}) + error$$
(1)

Where A represents the averaging kernel, X_{avk_sonde} is the retrieved ozonesonde profile, X_{sonde} is the ozonesonde profile and $X_{apriori}$ is the apriori profile.

2.4Results

2.4.1Difference profiles

To calculate the relative difference profiles, we applied the following formulas:

For comparing the GOME-2 profile with the ozone sounding we apply:

$$(X_{\text{GOME-2}} - X_{\text{SONDE}}) / X_{\text{SONDE}}$$
(2)

Notify that X_{sonde} is integrated from ozonesondes measurements.

The line in the comparison figures (Fig.3), corresponding to these comparisons is colored black.

For comparing the GOME-2 profile with the smoothed ozonesondes, further referred in this report as AVK ozonesondes, by applying the averaging kernels (1), we use the following equation:

$$(X_{\text{GOME-2}} - X_{\text{AVK-SONDE}}) / X_{\text{AVK-SONDE}}$$
(3)

The line in the comparison figures (Fig.3), corresponding to these comparisons is colored blue.

Figures 3 shows relative difference profiles between GOME-2 ozone profiles at the one hand and on the other hand ozonesonde-, and AVK ozonesonde profiles for the latitude belts, listed in Table 2 for respectively the coarse resolution pixels and the high resolution pixels. The error bars represent one standard deviation on the mean error.

Figure 3:Relative difference profiles between GOME-2 ozone profiles, ozonesondes (black) and smoothed ozonesondes (blue), according to equations 2 and 3 for different latitude belts for the time period 2007-2010, CR (left) and the time period 2007–2010, HR (right)



Figure 3(continued):Relative difference profiles between GOME-2 ozone profiles, ozonesondes (black) and smoothed ozonesondes (blue), according to equations 2 and 3 for different latitude belts for the time period 2007-2010, CR (left) and the time period 2007–2010, HR (right)



For the Northern polar stations, the difference plots show an underestimation until -13 % in the stratosphere and an overestimation until +65 % in the upper troposphere, lower stratosphere zone, further referred as the UTLS-zone in this report. For the lower troposphere, the relative difference is within 15 %. Applying the averaging kernels improves the comparison significantly (+25 % in the UTLS-zone). For the high resolution pixels, the relative differences at the Northern polar stations improved. Relative differences are within the target values when validated against the X_{AVK-sonde}. The statistics in the stratosphere show a lower standard deviation for the HR pixels.

For the Northern Mid-Latitude stations, GOME-2 performs excellent for altitudes between 20 km and 30 km. There is an overestimation present in the UTLS-zone until +35 % for the coarse resolution pixels and until +30 % for the high resolution pixels, validated against the ozonesondes. With the $X_{AVK-sonde}$, the overestimation is within 15 % and therefore within the target values.

For the Tropical stations, ozonesonde data from the SHADOZ-network has been used to validate the GOME-2 retrieved ozone profiles. In the troposphere, it is observed that the collocated GOME-2 ozone profiles are overestimating the X_{sonde} profiles. The relative differences are within 30 % for heights between 0 km and 15 km. The UTLS-zone is overestimated by + 45 %. Higher than 20 km the relative differences are respectively for the CR and HR pixels + 4.46 % and 3.30 % with a standard deviation of resp. 8.5 % and 9.3 %.

For the Southern Mid-Latitudes, the retrieved GOME-2 ozone profiles are close to the observations; relative differences are within the 15 % for stratosphere and troposphere. The UTLS-zone shows an overestimation until +25 % in the UTLS-zone. With the $X_{AVK-sonde}$ the relative difference is strongly reduced for both time series.

The most temptative results are obtained at the station of Neumayer in the Southern polar belt. The relative difference is within 20 % for the troposphere for both time series. There is an overestimation present for altitudes between 15 and 23 km and around the UTLS zone (up to +45 %). For the high resolution pixels, this overestimation in the stratosphere is also present between 18 km and 23 km in height. The statistics for the X_{AVK-sonde} show elevated relative differences at a height of 19 km. This can be explained by the occurrence of the ozone hole in polar spring: where very low ozone concentrations (X_{AVK-sonde}) are responsible for these elevated relative differences (Table 5). Nevertheless, the individual comparisons show that GOME-2 is able to retrieve these particular ozone profiles, but still overestimates the amount of ozone. Figure 4 is an example of an ozone profile retrieval at Neumayer station on the 3rd of December 2008 (operational version, coarse resolution). It is also shown that the a-priori profile for the South Pole is higher than the retrieved and measured ozone profile (Figure 5).



Figure 4: Ozone profile retrieval at Neymayer station during low ozone event (20081203)

To report the validation results of GOME-2 ozone profile product in a more condensed way, the statistics for the different output levels of GOME-2 are reduced to three layers: Troposphere, UTLS-zone (Upper Troposphere, Lower Stratosphere) and Stratosphere (up to an altitude of 30 km). Since it is impossible to address just one altitude to the tropopause height for the different belts, Table 4 gives an overview on how we define the ranges in height for the different belts for troposphere, UTLS-zone and stratosphere:

 Table 4: Definition of the ranges in km for Troposphere, UTLS and Stratosphere for the different belts.

	Troposphere	UTLS	Stratosphere
Polar Regions	< 6 km	6 km - 12 km	12 km - 30 km
Mid-Latitudes	< 8 km	8 km - 14 km	14 km - 30 km
Tropical Regions	< 12 km	12 km - 18 km	18 km - 30 km

Table 5 shows an overview of the obtained results for the time period January 2007 – December 2010:

Table5: Relative Differences (RD) and standard deviation (STDEV) are shown (in percent) on the accuracy of GOME-2 ozone profiles product for the troposphere, UTLS-zone and the stratosphere for the five different belts for the time period January 2007 – December 2010, coarse resolution (CR) and the time period January 2007 – December 2010, source exercise the time perio

	Trop	osphere	L	JTLS	Strat	osphere
2007-2010 (CR)	RD (%)	STDEV (%)	RD (%)	STDEV (%)	RD (%)	STDEV (%)
Northern Polar Regions	7.60	13.98	18.28	37.93	-7.44	12.42
Northern Mid-Latitudes	2.38	19.80	14.45	48.78	0.84	10.71
Tropical Regions	21.18	34.44	33.93	50.25	4.46	8.48
Southern Mid-Latitudes	-2.06	14.32	5.98	32.95	1.95	12.41
Southern Polar Regions	-11.13	15.18	-16.20	24.20	8.74	48.61
2007-2010 (HR)	RD (%)	STDEV (%)	RD (%)	STDEV (%)	RD (%)	STDEV (%)
Northern Polar Regions	2.25	10.30	3.48	24.93	-6.92	9.29
Northern Mid-Latitudes	2.14	20.40	10.05	46.38	-0.19	9.97
Tropical Regions	18.48	45.98	24.58	46.10	3.30	9.26
Southern Mid-Latitudes	-1.36	17.32	1.23	28.35	0.55	10.78
Southern Polar Regions	-5.53	17.73	-10.23	27.78	1.84	36.46

It should be emphasized that due to low ozone concentrations, two regions show elevated relative differences: the stratosphere in the Southern polar region and the troposphere in the Tropical region.

- For the Stratosphere in the Southern polar region this is due to very low ozone concentrations observed with the ozonesondes during the ozone hole season. This results in elevated relative differences. They are however of no importance for the quality interpretation of the product, since the absolute differences for the stratosphere in the Southern polar region is on average -0.21 DU (standard deviation: 2.15 DU, for HR pixels), which is an acceptable value, comparable with other regions.
- For the troposphere in the Tropics, also low ozone concentrations are responsible for somewhat more elevated relative difference scores, although the target accuracy of 30 % is met. Also here, the absolute differences are small.

It can be concluded that besides the stratosphere in the Southern Polar region, the target values are met in the troposphere (30 %) and the stratosphere (15 %), not taking into account

the UTLS zone, which shows more elevated relative differences which cannot be appointed to the troposphere or the stratosphere.

Figure 5 gives an overview of the averaged ozone profiles for the GOME-2 retrieved ozone profiles, ozonesondes and AVK ozonesondes for the five latitude belts. It shows that in general GOME-2 matches quiet well, but underestimates the ozone concentrations in the upper stratosphere for the Northern Polar stations, overestimates the ozone profile in the lower stratosphere for the other latitude belts and overestimates for all the belts the UTLS-zone.

Taking all the results into consideration it can be concluded that the relative differences are not significantly different from 0 at the 2 sigma level. The biggest mean difference is detected for all the stations in the UTLS-zone, with an overall overestimation.

Notify that for the Polar stations and the Northern Mid-Latitude stations, the a-priori profile is in some cases much higher than the observed ozone concentrations by the soundings and retrieved ozone concentrations by GOME-2, which shows that the ozone retrieval algorithm is able to reconstruct profiles, which are significantly different from the a-priori profile.



Figure 5: Averaged profiles of GOME-2 profile (black), apriori profile (red), smoothed ozonesondes (blue) and ozonesondes (green) for the time period 2007-2010, CR (left) and for the time period 2007 – 2010, HR (right).

Figure 5 (continued): Averaged profiles of GOME-2 profile (black), apriori profile (red), smoothed ozonesondes (blue) and ozonesondes (green) for the time period 2007-2010, CR (left) and for the time period 2007 – 2010, HR (right).



2.5Behaviour at high latitudes

In the previous validation report (Delcloo and Kins, 2009), which reports about the operational coarse resolution ozone profile product, the results at Ny-Alesund and Eureka were significantly poorer than at the other stations. If we take into consideration the high resolution profiles, it is shown from Figure 6 that the averaged retrieved ozone profile for GOME-2 (black) still underestimates the observed ozone profile. The station under consideration is Ny-Alesund. The GOME-2 mean profile peaks in the lower stratosphere several kilometres below the ozone maximum, observed by the ozonesondes. For the other time periods (March 2008 – April 2008 and March 2009 – April 2009), a shift in the retrieved GOME-2 ozone profile is still present, but the smoothed AVK GOME-2 profile is much closer to the observations.



Figure 6: Averaged ozone profiles for NY-ALESUND for the time period March 2007 – April 2007 (left), compared with the time period March 2008 – April 2008 (middle) and the time period March 2009 – April 2009 (right.)

The poor comparisons at Ny-Alesund are correlated with high solar zenith angles (SZA) (possibly corresponding to the spring measurements) and the cloud top pressure as already reported in Delcloo and Kins, 2009. The SZA values for Ny-Alesund are varying between 90° in the beginning of March until 65 ° for the end of April. At 10 km and 12 km altitude, there seems to be a transition around a cloud top pressure of 700-800 hPa with all poor comparisons being concentrated at cloud top pressures lower than 700hPa. The same behaviour for the coarse resolution pixels was also observed at Eureka.

This behaviour could be related to a polarisation correction level 1b issue; for data from 2007 and 2008 for both data-sets R0 and R1 the polarisation correction is turned off at higher solar zenith angles (SZA). Since 7th of January 2009, a polarisation correction is applied at high solar zenith angles.

More recent results (March 2009 – April 2009) do not reveal this cloud top pressure dependency at Ny-Alesund anymore. This elucidates that the polarisation correction had an effect, but the averaged retrieved ozone profile is still shifted vertically downward for the coarse resolution pixels. There is also no dependency on CCF (cloud cover fraction) detectable to verify the polarization effect.

To summarize, for the high resolution pixels, as seen from Figure 6, the profiles significantly improved for the high latitude stations like Ny-Alesund and Eureka.

2.5.1Seasonal dependency

Figure 7a shows relative differences between GOME-2 and ozonesonde data for 6 altitude levels for the Northern Mid-Latitude stations. This graph shows if there is any seasonal dependency present in the GOME-2 dataset. At the Northern Mid-Latitude and Polar stations, there is during winter months and early spring an overestimation present in the UTLS-zone. For the rest of the season there are no significant tendencies present.

For the Tropical stations a systematic overestimation of ozone for the time period 2007 - 2010 is present in the UTLS-zone and lower stratosphere (Figure 7b).

Figure 7c shows the results for the high resolution pixels for the Mid-Latitude stations. It shows less seasonal undulations in the time series and also the standard deviation is smaller. The seasonal dependency is not as present as it is in the coarse resolution pixels.

Figure 7a: Seasonal dependency at different altitude levels for the Northern Mid-Latitude stations for the time period January 2007-December 2010(CR) (relative difference between GOME-2 and ozonesondes)





Figure 7b: Seasonal dependency at different altitude levels for the Tropical stations for the time period January 2007- December 2010(CR) (relative difference between GOME-2 and ozonesondes).



Figure 7c: Seasonal dependency at different altitude levels for the Northern Mid-Latitude stations for the time period January 2007- December 2010 (HR) (relative difference between GOME-2 and ozonesondes)

2.5.2Information content

Scatter plots in Figure 8 show the retrieved ozone partial columns as a function of the reference partial column measured by the ozonesondes. These plots show a measure of the amount of information actually present in the retrieved layer. This is done for 6 altitude layers for the Northern Mid-Latitude stations. To show the influence of applying the averaging kernels it is shown from Figure 9 that the slope values are improved (closer to 1) while the intercept values are closer to 0.

The interpretation of "better results" should be taken with care. Applying the kernels using equation 1 is a way to smooth the ozone profile towards a comparable vertical resolution of the retrieved ozone profile. High resolution effects like filaments present for example in secondary ozone maxima are mostly not seen by GOME-2 which results in sometimes large differences between observed and retrieved partial ozone columns.

The regression line in the scatter plots show that GOME-2 loses sensitivity in the lower troposphere and around the UTLS-zone (Figure 8).



Figure 8: Scatter plot at 6 different altitude levels for the stations at Northern Mid-Latitudes for the HR pixels (2007-2010)



Figure 9: Scatter plot at 6 different altitude levels for the stations at Northern Mid-Latitudes, applying the AVK for the HR pixels (2007-2010)

Another way to describe the information content delivered by the GOME-2 ozone profiles is to plot the correlation and slope between the ozonesonde profiles, $X_{AVK-sonde}$ profiles on the one hand and the GOME-2 ozone retrieved profiles on the other hand.

The correlation plot in Figure 10 shows the ability of GOME-2 to catch the day-to-day variation for the different altitude levels while the slope shows the sensitivity of GOME-2 at the particular altitude levels.

For the Northern Mid-Latitude stations, correlation between the ozone sounding concentrations and the retrieved GOME-2 ozone concentrations are between 0.35 and 0.8. When applying the AVK, the correlation is better.

The slope shows the lowest values in the lower UTLS-zone. For the Southern Mid-Latitude stations the results are comparable with correlations between 0.3 and 0.9. Very low correlations are also here present in the lower UTLS-zone.

For the Northern Polar Latitude belt correlations between 0.35 and 0.9 are found.

For the Tropical stations, correlations are found between 0.4 and 0.8.

Figure 10: Slope and correlation between retrieved ozone partial columns (DU) on the one hand and observed ozone partial columns (DU) (black) and smoothed ozone partial columns (DU) (blue) on the other hand for the HR pixels





2.6East-West Dependency

To verify any dependency on the East West direction of the scan, time series are plotted in function of these three different orientations of the sensor, which is connected to the parameter "IndexInScan" in the hdf5 files. When comparing the three different time series (Figures 11a, 11b and 11c), it is shown that the East pixels result in the retrieval of ozone profiles, containing more ozone compared with the ozone profiles, retrieved respectively from the Center pixels and the West pixels of the scan. In this example, some time series for the Northern Mid-Latitude stations are shown. It also shows that for the East pixels, the standard deviation is slightly higher for the different altitudes under consideration.

Figure 11a: Time dependency for the HR-pixels for the time period January 2007 – May 2011 for the pixels sensing the East side of the swap.





Figure 11b: Time dependency for the HR-pixels for the time period January 2007 – May 2011 for the pixels sensing the Center of the swap.



Figure 11c: Time dependency for the HR-pixels for the time period January 2007 – May 2011 for the pixels sensing the West side of the swap.

3. Validation of ozone profiles with lidar and microwave instruments

3.1 Instruments

Lidars and microwave radiometers are the only ground based instruments available for validation purposes in the upper stratosphere. Together, their altitude range covers appr. 13 km to 60 km. However, a few lidar and microwave instruments exist, with an extended coverage down to the ground as in Ny Alesund and Table Mountain.

The Differential Absorption Lidar (DIAL) technique provides accurate vertical distributions of ozone in the altitude range 15km to 50km, depending on the individual lidar system. Lidar radiation is strongly extinguished by clouds and daylight extremely deteriorates the signal to noise ratio so that measurements are restricted to cloud free nights. Typically, 5-8 lidar measurements per month can be carried out. Depending on atmospheric conditions and lidar system efficiency, an ozone measurement higher up lasts several hours.

	li	dar	microway	ve radiometer
Height [km]	precision [%]	height resol. [km]	precision [%]	height resol. [km]
15	5	1.4		
20	5	1.2	3	10
25	3	1.0	3	10
30	3	1.8	3	10
35	3	4.2	3	14
40	5	7.2	3	14
45	15	8.6	3	20
50	55	8.6	3	20
50-70			3	20

Table3.1: Typical values for precision and height resolution of lidars
and microwave radiometers (Steinbrecht et al., 1999).

Microwave radiometers measure the thermal radiation of a pressure broadened ozone emission line. The line width depends on pressure and temperature and is used to determine the altitude of the emitting gas. The measurement height extends from approx. 20 km to 75 km. In contrast to lidars, microwave radiometers are not strongly weather dependent and measure during daylight hours. On average, microwave profiles are measured on about 20 days per month. The integration time of one microwave profile varies from approx. 30 minutes to 4-5 hours according to the individual instrument.

Precision and height resolution of lidar and microwave instruments at different atmospheric altitude levels are shown in Table 3.1.

3.2 Dataset description

GOME-2 ozone profiles were made available by KNMI at co-ordinates covering the lidar and microwave reference sites.

The ground based reference profiles are from two databases, the NDACC (Network for the Detection of Atmospheric Composition Change, <u>http://www.ndsc.ncep.noaa.gov/</u>) and the ESA campaign database located at NILU (Norwegian Institute for Air Research, http://nadir.nilu.no/cdb/). NDACC controls the quality of the contributing instruments by standard operation procedures, as well as instrument and algorithm intercomparisons, this guarantees continuous quality of the profiles.

Measurement results of lidar and microwave instruments have to go through an evaluation process and thorough quality checks, so that the ozone profiles are not available in near real time. A minimum of one month is necessary to process the profiles but most stations need three or more months. NDACC demands that ozone profiles are submitted at least once per year to their database.

Table 3.2 lists all ozone profiles available for comparison within this validation period. Some reference stations operate only from autumn to spring, others had longer interruptions.

Station (instrument)	Lat/lon	availability
Ny Alesund (µwave)	78.9/11.9	Mar 2007 - Apr 2007 Mar 2008 Oct 2008 – Aug 2009 Mar 2010 – Sep 2010 Mar 2011 – May 2011
Andoya (lidar)	69.3/16	Feb – Apr 2007 Jan – Apr 2008 Sep 2008 – Mar 2009 Oct 2009 – Apr 2010 Sep 2009 – Feb 2011
Hohenpeissenberg (lidar)	47.8/11.0	Jan 2007 – May 2011
Bern (µwave)	47.0/7.6	Jan 2007 – Jul 2008 Oct 2008 – Jul 2010
Payerne (µwave)	46.8/7.0	Jan 2007 – Mar 2009 Jun 2010 – May 2011
Haute Provence (lidar)	43.9/5.8	Jan 2007 – Dec 2010
Tsukuba (lidar)	36.1/140.1	Jan - Apr 2007 Aug 2007; Oct 2007– May 2008 Oct 2008 – Apr 2009 Jan 2010 – Feb 2010
Table Mountain (lidar)	34.4/-117.7	Jan 2007 – Dec 2009 Apr 2010 – Dec 2010
Mauna Loa (lidar)	19.5/-155.6	Jan 2007 – Dec 2010
MaunaLoa (µwave)	19.5/-155.6	Jan 2007 – Dec 2010
Lauder (lidar)	-45.0/169.7	Jan 007 – May 2011

3*Table 3.2:* Reference ozone profiles available for comparison

3. O3M_SAF: Validation of ozone profiles with lidar and microwave radiometers

Lauder (µwave)	-45.0/169.7	Jan 2007 – Dec 2009
Rio Gallegos (lidar)	-51.6/-69.3	Jan 2007 – Nov 2010
Dumont d'Urville (lidar)	-66.4/140.0	Mar 2008 – Sep 2010

3.3. Comparison procedure

3.3.1 Co-location criteria

Lidar and satellite profiles closest in time are compared with each other. Since lidar measurements are performed during the night, they are compared to GOME-2 profiles measured either the day after or before the lidar profile. This means that a maximum time difference of 20 hours is allowed.

Microwave radiometers measure during the daylight and most stations do several soundings during a day. So usually GOME-2 ozone profiles can be compared with microwave profiles measured during the hour of the satellite overpass, but a maximum time difference of 4 hours is also allowed.

Only in rare cases the satellite pixel covers the ground station. Spatial co-location is therefore a question of satellite pixel size, satellite track and number of available profiles for validation purposes. Too narrow co-location margins may yield statistically insignificant results, due to a small number of comparisons. Large co-location limits may cause erroneous validation conclusions. For coarse resolution GOME-2 ozone profiles a spatial co-location of ± 2 degrees in latitude and longitude from the ground station was used for validation. With HR profiles the number of co-located pixels increases when the same spatial criteria are applied. Thus three different co-location criteria for HR pixels were tested to decide whether the spatial co-location confines should be narrowed. Fig. 3.2a shows the number of colocation days at Andoya for CR pixels (CR 2deg) and for HR pixels with pixel centres within ± 1 degrees in latitude and longitude from the ground station (HR 1deg). Fig 3.2.b shows the number of co-located pixels at Andoya for CR pixels (CR 2deg), for HR pixels within the CR borders (HR CR), for HR pixels with pixel centre within ± 2 degrees in latitude and longitude from the ground station (HR 2deg), and for HR pixels with pixel centre within ± 1 degrees in latitude and longitude from the ground station (HR 1deg). In most months the number of HR 1deg pixels is about the same as for CR profiles but there are several months with no colocation when this strong co-location criterion is applied. HR CR confines add up to an extremely large number of co-locations whereas the number of HR 2deg pixels is between these two extremes.



Fig 3.2a (left): Number of co-location days at Andoya for CR pixels (CR_2deg / black) and for HR pixels with pixel centres within ± 1 degrees in latitude and longitude from the ground station (HR_1deg / blue). Fig 3.2.b (right): Number of co-located pixels at Andoya for CR co-location criterion (CR_2deg / black), for HR pixels within the CR borders (HR_CR / green)), for HR pixels with pixel centre within ± 2 degrees in latitude and longitude from the ground station (HR_2deg / red), and for HR pixels with pixel centre within ± 1 degrees in latitude and longitude from the ground station (HR_1deg / blue).

To test the influence of the various co-location criteria on validation results, mean relative difference profiles for the three HR co-locations were calculated. The results for Ny Alesund, Andoya and Hohenpeissenberg are show in fig. 3.3. The validation of GOME-2 CR profiles had revealed that at the high latitude stations the differences between satellite and reference profiles are larger than at lower latitude stations. Fig 3.3 shows only for Ny Alesund differing, albeit statistically not significant, comparison results in the lower (13-15km) and the upper (>50km) stratosphere. Based on these results all satellite pixels with pixel centres within a distance of 2 degrees in latitude and longitude from the ground station are used for high resolution GOME-2 ozone profile validation.

Table 3.3 lists the number of co-located pixels and comparison days for all reference stations when the given spatial co-location criterion is applied.



Fig 3.3: Mean relative difference profiles between GOME-2 high resolution profiles and reference instruments at ground stations Ny Alesund (left), Andoya (centre) and Hohenpeissenberg (right) for three different co-location criteria: HR_2deg (black) = HR pixels with pixel centre within ± 2 degrees in latitude and longitude from the ground station, HR_CR (green) = HR pixels within the CR borders, HR_1deg (red) = for HR pixels with pixel centre within ± 1 degrees in latitude and longitude from the ground station.

Station (instrument)	GOME-2 pixels	Comparison days
Ny Alesund (µwave)	6648	239
Andoya (lidar)	1351	60
Hohenpeissenberg (lidar)	21479	571
Bern (µwave)	28524	784
Payerne (µwave)	26731	746
Haute Provence (lidar)	15492	410
Tsukuba (lidar)	4148	59
Table Mountain (troposphere lidar)	14314	234
Table Mountain (stratosphere lidar)	14975	248
Mauna Loa (lidar)	20322	377
MaunaLoa (µwave)	37945	701
Lauder (lidar)	14732	244
Lauder (µwave)	18540	345
Rio Gallegos (lidar)	6008	171

Table 3.3: Numbers of matching GOME-2 pixels and comparison days available for the validation period

3.3.2 Pre-processing of the ozone profiles.

GOME-2, lidar and microwave ozone profiles all report their results in different units (see table 3.4) and on different altitude levels. To consider the different altitude resolution of the instruments, smoothing and interpolation must be applied prior to comparisons. The smoothing procedure is applied to the data sets with the higher resolution, which in our case are the reference instruments. There are different approaches to perform the smoothing. Froidevaux et al. (2008) compared several smoothing approaches and concluded that their difference is small except in the range of large ozone values or sharp gradients. Here two different smoothing approaches are used. One method is the application of the GOME-2 averaging kernels to each single reference profile,

$$Z=X_{ap} + A * (X_{ref} - X_{ap})$$
(1)

where Z is the smoothed reference profile, X_{ap} is the a priori profile, X_{ref} is the reference profile and A is the averaging kernel matrix. The layers below and above the reference altitude are filled with the a priori profile.

In the second method, the reference profiles are also linearly interpolated to the GOME-2 altitude levels and then ozone partial columns are summarized for the GOME-2 layers. Reference ozone profiles are always cut off when their error attains 15%.

Since algorithm developers prefer comparisons with reference profiles smoothed with averaging kernel but most scientific users favour comparisons without averaging kernel smoothing, results of both profile versions are presented in this report.

Instrument	ozone unit	altitude unit
GOME-2	DU/layer	hPa
Lidar	molecules/cm ³	km
Microwave radiometer	ppmv	km

Table 3.4: Ozone and altitude units of GOME-2, lidar and microwave profiles

For each individual pair of co-located GOME-2 pixels and reference ozone profiles absolute and relative differences are calculated. These comparisons are mainly used to further check the suitability of the spatial co-location criteria and for the detection of outliers. In the following step average difference profiles of monthly, seasonal and yearly mean differences and for the average difference profiles of the entire measurement period are calculated.

3.4. Results

We present absolute and relative differences between GOME-2 profiles and reference instruments.

To calculate the absolute difference profiles, we applied the following formulas:

For comparing the GOME-2 profile with the reference we apply:

abs. diff
$$[DU/layer] = X_{GOME-2} - X_{reference}$$
 (2)

For comparing the GOME-2 a priori profiles with the reference profiles, we apply:

abs. diff_{apriori} [DU/layer] =
$$X_{apriori} - X_{reference}$$
 (3)

For comparing the GOME-2 profile with the smoothed reference profiles by applying the averaging kernels (AVK) (1), we apply:

abs. diff_{AVK} [DU/layer] =
$$X_{GOME-2} - X_{AVK-reference}$$
 (4)

To calculate the relative difference profiles, we applied the following formulas:

For comparing the GOME-2 profile with the reference we apply:

rel. diff [%] = $(X_{\text{GOME-2}} - X_{\text{reference}})/X_{\text{reference}} * 100$ (5)

For comparing the GOME-2 apriori with the reference profiles, we apply:

rel. diff_{apriori} [%] = (X_{apriori}- X_{reference})/X_{reference} * 100 (6)

For comparing the GOME-2 profile with the smoothed reference profiles by applying the averaging kernels (1), we apply:

rel. diff_{AVK} [%] =
$$(X_{\text{GOME-2}} - X_{\text{AVK-reference}})/X_{\text{AVK-reference}} * 100$$
 (7)

3.4.1 Mean differences between GOME-2/Metop and co-located lidar and microwave ozone profiles

Figure 3.4 presents an overview of comparison results between GOME-2 and lidar resp. microwave radiometer ozone profiles for the entire comparison period and all stations. It shows mean relative and absolute difference profiles. In table 3.5 the mean relative and differences between GOME-2/Metop and reference ozone profiles are summarized, together with the results for coarse resolution GOME-2 profiles.

Mean relative differences at all stations are equal within their error bars. This allows us to conclude that the presented comparison results are independent from the reference instruments and are of general validity. Mean relative differences between GOME-2 profiles and reference instruments smoothed by integration over GOME-2 layers have a larger fluctuation range than results from reference instruments smoothed with GOME-2 averaging kernels. This demonstrates that avk smoothing compensates ozone profile concentration gradients more than layer integration. Relative differences with avk reference profiles meet the target value for the stratosphere of $\pm 15\%$ at all altitude layers also in the troposphere, with the exception of the two polar stations (Andova and Ny Alesund), where GOME-2 ozone is up to 50% higher than the reference at the UTLS layers. Between 30 km and 50 km altitude GOME-2 has a negative bias of up to 15%, above 40 km the negative bias somewhat exceeds the 15% limit when compared with lidar instruments. This might be due to the lower precision of the lidar instruments combined with a lower number of lidar measurements available at these altitudes. Comparison with reference profiles smoothed by integration over GOME-2 layers generally show the same characteristic differences but all variations are amplified and the relative differences exceed the target of $\pm 15\%$ in the lower stratosphere and between 35 km and 45 km at many stations. The absolute difference profiles show the peculiarity of the two polar stations, at the UTLS and around 20 km the GOME-2 absolute differences are clearly larger than at the other reference stations.



Fig.3.4: Mean relative and absolute differences between HR GOME-2/Metop and lidar resp. microwave instruments. Left: reference profiles smoothed by integration over GOME-2 layers, centre: reference profiles smoothed with GOME-2 averaging kernels (avk), right: absolute differences GOME-2 – reference_avk.

The evaluation of average CR and HR comparison results show that high resolution profiles have a smaller bias than coarse resolution profiles. Between 35 km and 50 km and for avk smoothed reference the reduction of the bias is larger than 40% and significant within the 1sigma error bars, above 50 km the bias is significantly reduced by more than 70%. Below 35 km the GOME-2 bias is also substantially reduced (> 30%) but since the standard deviation is higher at the lower altitudes this decrease in bias is not statistically significant. The standard deviation itself is smaller in HR profiles than in CR profiles, which indicates that the scatter of the comparison results is smaller in HR profiles. In the case of reference profiles but since the standard deviations are much higher than in avk reference this reduction in bias is not significant.

Table 3.5: Mean relative and absolute differences between HR and CR profiles from GOME-2/Metop and reference ozone profiles, standard deviation is 1sigma of the station mean.

	mean vol difference	maan val difforen oo	maan val difference	maan val diffavan aa
altitudo	COME 2 reference	COME 2 reference	COME 2 reference avk	COME 2 reference
[km]	HR [%]	CR [%]	HR [%]	CR[%]
3	3.23 ± 36.69	-0.04 ± 16.39	-2.58 ± 5.23	-26.59 ± 20.19
4	0.06 ± 12.71	-0.10 ± 21.85	0.88 ± 6.42	-7.76 ± 26.52
6	2.25 ± 13.10	-5.04 ± 35.91	1.74 ± 19.08	11.51 ±44.03
7	12.19 ± 42.48	26.02 ± 37.50	27.40 ± 39.38	39.18 ± 78.58
9	12.98 ± 16.59	16.45 ± 22.98	16.23 ± 23.48	26.26 ± 42.65
10	12.88 ± 12.40	-0.93 ± 27.73	9.59 ± 11.15	7.56 ± 18.13
12	-4.29 ± 24.15	-0.09 ± 18.32	4.67 ± 8.92	3.24 ± 15.74
13	-2.74 ± 16.79	-1.64 ± 21.57	5.99 ± 6.39	6.79 ± 10.17
15	-6.09 ± 22.13	8.25 ± 16.81	7.92 ± 8.76	20.97 ± 13.83
16	5.21 ± 16.74	11.32 ± 12.10	6.83 ± 12.91	24.38 ± 23.25
18	10.30 ± 9.01	8.56 ± 10.57	3.49 ± 10.52	16.35 ± 19.28
19	8.24 ± 8.46	4.94 ± 6.96	0.25 ± 5.63	10.72 ± 15.22
20	4.73 ± 5.58	3.32 ± 6.39	-0.29 ± 4.39	3.82 ± 11.24
22	3.17 ± 5.49	1.25 ± 6.05	-1.00 ± 3.84	-0.65 ± 8.21
23	0.90 ± 5.42	-0.56 ± 5.75	-1.49 ± 3.55	-3.28 ± 6.31
25	-0.94 ± 5.23	-2.68 ± 5.23	-1.90 ± 3.45	-5.35 ± 4.91
26	-2.98 ± 4.57	-3.47 ± 4.61	-2.53 ± 3.22	-5.45 ± 6.37
28	-3.92 ± 3.64	-3.49 ± 4.73	-3.64 ± 3.09	-3.69 ± 6.33
29	-4.05 ± 3.50	-3.57 ± 5.62	-4.27 ± 3.23	-3.62 ± 6.87
31	-4.13 ± 3.93	-4.06 ± 6.88	-5.08 ± 3.46	-6.00 ± 6.98
32	-4.56 ± 5.01	-6.54 ± 7.90	-5.90 ± 3.46	-8.52 ± 6.48
34	-7.02 ± 5.72	-9.17 ± 8.82	-7.03 ± 3.18	-12.65 ± 6.51
35	-9.25 ± 5.79	-13.13 ± 9.20	-9.08 ± 2.96	-16.70 ± 6.65
37	-12.53 ± 5.93	-17.73 ± 7.57	-10.94 ± 3.12	-21.60 ± 6.66
39	-15.63 ± 5.69	-23.72 ± 5.29	-13.28 ± 2.99	-26.87 ± 5.81
40	-17.92 ± 5.78	-27.40 ± 7.94	-14.59 ± 3.27	-26.76 ± 8.06
42	-20.38 ± 8.49	-27.87 ± 7.00	-16.02 ± 3.29	-32.49 ± 6.71
43	-23.09 ± 10.79	-30.61 ± 13.94	-16.25 ± 5.30	-28.82 ± 9.31
45	-22.83 ± 15.30	-19.98 ± 8.47	-15.60 ± 3.74	-24.97 ± 4.81
47	-26.30 ± 26.00	-16.42 ± 11.67	-19.17 ± 10.17	-29.00 ± 5.71
49	-4.20 ± 11.26	-12.73 ± 14.75	-11.16 ± 2.85	-25.45 ± 7.11
51	-0.18 ± 11.95	-13.15 ± 16.68	-9.53 ± 2.52	-33.00 ± 6.73
52	0.48 ± 11.43	-15.20 ± 17.28	-8.86 ± 2.67	-32.71 ± 7.73
54	-0.32 ± 10.38	-19.30 ± 17.64	-8.37 ± 2.75	-30.17 ± 10.80
56	-2.64 ± 9.10	-25.61 ± 18.76	-9.11 ± 4.27	-45.64 ± 11.51
58	-7.44 ± 8.75	-33.46 ± 19.02	-5.95 ± 4.70	-33.30 ± 12.40

3.4.2 Mean differences between GOME-2/Metop and co-located lidar and microwave ozone profiles grouped by latitude belts

The following figures (3.5 - 3.16) show the mean comparison results grouped by latitude belts to elaborate regional differences. In chapter 3.5.3 time series and seasonal differences in the different latitude belts are presented. The stations are grouped as follows:

Arctic (Andoya, Ny Alesund)	65 N - 80 N
Northern mid latitude (Hohenpeissenberg, Bern,	
Payerne, Haute Provence, Table Mountain, Tsukuba)	30 N - 55 N
Suptropics (Mauna Loa)	20 N
Southern mid latitude (Lauder, Rio Gallegos)	40 S – 55 S

It must be considered that the number of GOME-2 pixels compared, the number of stations for each latitude belt and the time period of the comparisons is different for the regions (see also tab 3.2/3.3) hence the statistical significance of each latitude belt's results varies. In the following figures mean ozone profiles, absolute and relative difference profiles, height resolved histograms of relative differences and scatter plots of reference versus GOME-2 ozone partial columns for each latitude belt are presented.

3.4.2.1 Arctic Belt

The overview figure 3.4 has already shown that the comparison results in the arctic differ from the other stations in the UTLS and the lower stratosphere. The ozone profiles in the left of figure 3.4 reveals that the GOME-2 ozone profile is shifted in altitude compared to the reference. The rise in ozone starts at lower heights, the ozone maximum in GOME-2 is at the same layer as in the reference and above the maximum, the satellite ozone decreases faster. In consequence the relative difference profiles show a large positive bias (GOME-2 higher than reference) of up to 50% in the UTLS and a negative bias above the ozone maximum. However, besides the UTLS, the relative differences are within the target limits of \pm 15% in both avk smoothed and integrated reference profiles. The error bars indicate higher scatter of individual comparisons in the UTLS and the upper stratosphere.



Fig. 3.5: Left: Mean ozone profiles from HR GOME-2 (red), reference instrument (blue) and, reference instrument smoothed with averaging kernels (green) at 65 deg – 80 deg North. Absolute differences (centre) and relative differences (right) GOME minus reference (black), Gome minus reference smoothed with averaging kernels (green). Horizontal error bars are 1 standard deviation from single pixel comparisons, vertical bars are GOME-2 layers. Vertical lines in right graph indicate ± 15 % target value for comparisons in the stratosphere, and figures on the right are numbers of GOME-2 pixels compared at each layer.

Figure 3.6 shows histograms of the frequency distribution of the relative differences between satellite and integrated reference ozone profiles (3.6a, left) and avk reference profiles (3.6b, right). The histograms approve the broad dispersion of the relative differences in the UTLS and the high stratosphere. In the UTLS (5-15km) the distribution has a broad maximum ranging over about 30% relative differences and a strong tail towards positive differences, in avk references the maximum is more confined but the tailing is also found. In the high stratosphere (above 45 km) the distribution widens again, the maximum shifts towards negative relative differences with a distinct tail in the direction of positive relative differences. The comparison with avk reference profiles shows several distribution maxima in the upper stratosphere.



Fig. 3.6a (left): Histograms of relative differences at several altitude layers at 65 deg – 80 deg north. Red bars indicate ± 15 % target value and ± 30 % threshold for comparisons in the stratosphere. Fig. 3.6b (right): Histograms of relative differences at several altitude layers between averaging kernel smoothed profiles and GOME-2 at 65 deg – 80 deg north.

Scatter plots are a third way to present the comparison results, fig 3.7a shows the results for integrated reference profiles and fig. 3.7b for avk reference profiles. Highly correlated profiles (correlation coefficient >0.9) are found for integrated profiles from 35- 55km altitude layers. At 35-40km the regression line is almost on the 1:1 line, at higher layers the regression line tilts against the 1:1 line. With higher reference ozone values the GOME-2 ozone becomes lower, independently from the absolute ozone values. From 1 km to 10 km and from 25 km to 35 km the correlation coefficient is higher than 0.8, though still good, but between 10 km and 20 km almost no correlation is found.

Scatter plots with avk reference are not significantly different with two striking exceptions, the lower troposphere (1 - 5km) and the upper stratosphere (>45 km). In the 1-5 km layer high GOME-2 ozone with low avk reference ozone are found, as well as high reference ozone with low GOME-2 in distinct lines. This is an indication that the averaging kernels do not adequately distribute the ozone between the layers. In the upper stratosphere the maximum number of correlated pixels is below the 1:1 line but a high amount of pixels is found close to the 1:1 line also. These are the tailing and the secondary maxima we see in the histogram plots.


Fig. 3.7a: Correlations between HR GOME-2 ozone and reference ozone at several altitude layers for at 65 deg – 80 deg North. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.7b: Correlations between HR GOME-2 ozone and avk reference ozone at several altitude layers for at 65 deg – 80 deg North. Red line is result of linear regression, black line is the 1:1 line.

3.4.2.2 Northern Mid Latitude Belt

Figure 3.8 shows mean ozone profiles and difference profiles for the northern mid latitude stations. The three ozone profiles (HR GOME-2, integrated reference and avk reference) are identical within their error bars up to 30 km, above that layer the GOME-2 ozone decreases somewhat faster than the reference. The relative differences are within the target of \pm 15% from troposphere to stratosphere. Comparisons with the integrated profiles show higher variation than avk reference comparisons. With integrated profiles a negative bias (GOME-2 lower than reference) is observed in the troposphere and between 38 km and 45 km, a positive bias is found in the UTLS, around 20 km and above 50 km. Comparisons with avk profiles reveal a smaller positive bias in the UTLS and about the same negative bias between 38 km

and 45 km. As in the arctic, there are large error bars from the troposphere up to 20 km and above 50 km.

Accodingly, the histogram plots (figs. 3.9a, 3.9b) show a wider distribution between 5 km and 15 km and above 45 km with a tailing towards positive relative differences for the integrated profiles. The distribution for the avk reference profiles is in all altitudes narrower and has no tailing.



Fig. 3.8: Left: Mean ozone profiles from HR GOME-2 (red), reference instrument (blue) and, reference instrument smoothed with averaging kernels (green) for northern mid latitudes. Absolute differences (centre) and relative differences (right) GOME minus reference (black), Gome minus reference smoothed with averaging kernels (green). Horizontal error bars are 1 standard deviation from single pixel comparisons, vertical bars are GOME-2 layers. Vertical lines in right graph indicate ± 15 % target value for comparisons in the stratosphere, and figures on the right are numbers of GOME-2 pixels compared at each layer.





Scatter plots are presented in figs 3.10a,b. Highly correlated profiles (correlation coefficient >0.9) are found for integrated profiles from 25- 50 km altitude layers. From 10 km to 20 km and from 50 km to 55 km the correlation coefficient is higher than 0.8, though still good, but poor correlation is found in the lower troposphere (3km - 5km) with R=0.65 and no correlation exist between 5 km and 10 km. As in the arctic, regression lines are tilted against the 1:1 line. With higher reference ozone values the GOME-2 ozone becomes lower, independently from the absolute ozone values.

Scatter plots with avk reference are highly correlated (R>0.9) from 10 km to 60 km, with exception of the 20 km to 25 km layers were the correlation coefficient is 0.81. Up to 30 km the regression lines are close to the 1:1 line and above they are tilted in the same way as for integrated profiles.



Fig. 3.10a: Correlations between HR GOME-2 ozone and reference ozone at several altitude layers for northern mid latitudes. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.10b: Correlations between HR GOME-2 ozone and avk reference ozone at several altitude layers for northern mid latitudes. Red line is result of linear regression, black line is the 1:1 line.

3.4.2.3 Subtropical Belt

Figure 3.11 shows mean ozone profiles and difference profiles for the subtropics. It must be kept in mind that there is only one reference station in the subtropics (Mauna Loa) with one lidar and one microwave radiometer, so that the results of this single station might not be representative for the whole subtropical belt. Up to 30 km the reference ozone profiles is somewhat lower than the HR GOME-2 and the avk reference profiles. Like in the northern mid latitudes, the GOME-2 ozone decreases faster than the reference above the ozone maximum.

The relative differences are within the target of $\pm 15\%$, from 20 km – 38km and above 48 km. Around 40 km, a negative bias of up to 25% is observed. Below 20 km avk reference and integrated reference have a significantly different bias, comparisons with avk profiles give a strong positive bias of up to 40% and comparisons with integrated profiles reveal a large negative bias of up to 60%. Comparisons with the integrated profiles show higher variation than avk reference comparisons below 25 km only. As in the arctic and the northern mid latitude, there are larger error bars below 20 km.

Despite the larger error bars below 20 km, the distribution shown in the histogram plots (figs 3.12a,b) is not as wide as at the latitudes shown previously and no tailing neither in positive nor negative direction is observed. However, the distribution from 15 km to 20 km is somewhat broader than at the other altitudes. The subtropics are a region with a substantially smaller ozone variability than the more northern or southern latitudes, thus this less scatter in the distribution of relative differences might be expected.



Fig. 3.11: Left: Mean ozone profiles from HR GOME-2 (red), reference instrument (blue) and, reference instrument smoothed with averaging kernels (green) for 20 deg north. Absolute differences (centre) and relative differences (right) GOME minus reference (black), Gome minus reference smoothed with averaging kernels (green). Horizontal error bars are 1 standard deviation from single pixel comparisons, vertical bars are GOME-2 layers. Vertical lines in right graph indicate ± 15 % target value for comparisons in the stratosphere, and figures on the right are numbers of GOME-2 pixels compared at each layer.



Fig. 3.12a (above): Histograms of relative differences at several altitude layers for 20 deg north. Red bars indicate ± 15 % target value and ± 30 % threshold for comparisons in the stratosphere. Fig. 3.12b (below): Histograms of relative differences at several altitude layers between averaging kernel smoothed profiles and GOME-2 at 20 deg North.

Scatter plots are presented in figs 3.13a,b. Highly correlated profiles (correlation coefficient >0.9) are evaluated for integrated profiles from 25 km - 60 km altitude layers and for avk reference from 20 km - 60 km. At 15 km - 20 km, the integrated profiles show a correlation coefficient of 0.74 and between 20 km and 25 km of 0.86, the avk reference has a correlation coefficient of 0.87 at the 10 km - 20 km layer. Thus no realy poor correlation is observed at this subtropical station. The regression linea are tilted against the 1:1 line above 30 km as at the other latitude belts. Above 30 km altitude the GOME-2 and the reference ozone is grouped in small packages, the reason for that is not yet clear.



Fig. 3.13a: Correlations between HR GOME-2 ozone and reference ozone at several altitude layers for 20deg north. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.13b: Correlations between HR GOME-2 ozone and avk reference ozone at several altitude layers for 20 deg north. Red line is result of linear regression, black line is the 1:1 line.

3.4.2.4 Southern Mid Latitude Belt

Figure 3.14 shows mean ozone profiles and difference profiles for the southern mid latitude stations. The three ozone profiles (HR GOME-2, integrated reference and avk reference) are identical within their error bars at all altitude layers. The relative differences however reveal a negative bias of up to 16 % with integrated and 15% with avk profiles around 45 km. At all other heights the relative differences are within the target of \pm 15% Also the variations in the relative and absolute difference profiles is not significantly different between avk reference and integrated reference. Like at the other latitudes, high error bars are found from the upper troposphere (~ 7km) into the lower stratosphere (~18km).

Accodingly, the histogram plots (figs. 3.15a, 3.15b) show a broad distribution between 5 km and 15 km, with two maxima at 10 km to 15 km layers. Above 15 km the distribution is quite narrow and no tailing is observed. The avk comparisons have a slightly more confined distribution than the integrated reference comparisons.



Fig. 3.14: Left: Mean ozone profiles from HR GOME-2 (red), reference instrument (blue) and, reference instrument smoothed with averaging kernels (green) for southern mid latitude belt. Absolute differences (centre) and relative differences (right) GOME minus reference (black), Gome minus reference smoothed with averaging kernels (green). Horizontal error bars are 1 standard deviation from single pixel comparison, vertical bars are GOME-2 layers. Vertical lines in right graph indicate ± 15 % target value for comparisons in the stratosphere, and figures on the right are numbers of GOME-2 pixels compared at each layer.



Fig. 3.15a (left): Histograms of relative differences at several altitude layers for 40 deg - 55 deg south. Red bars indicate ± 15 % target value and ± 30 % threshold for comparisons in the stratosphere. Fig. 3.15b (right): Histograms of relative differences at several altitude layers between averaging kernel smoothed profiles and GOME-2 at 40 deg - 55 deg south.

Scatter plots are presented in figs 3.16a,b. The correlation results are similar to those from the subtropical station. Highly correlated profiles (correlation coefficient >0.9) are evaluated for integrated profiles from 25 km - 60 km altitude layers and for avk reference from 20 km - 60 km. Below 10 km the correlation is poor in both the integrated and the avk reference. The regression line is tilted against the 1:1 line above 30 km as at the other latitude belts. In the upper stratosphere the GOME-2 and the reference ozone is grouped in small packages, like at the subtropical station. This points to a GOME-2 measurement or retrieval effect rather than a reference instrument's, but final conclusions are not yet possible.



Fig. 3.16a: Correlations between HR GOME-2 ozone and reference ozone at several altitude layers for southern mid latitude belt. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.16b: Correlations between HR GOME-2 ozone and avk reference ozone at several altitude layers for southern mid latitude belt. Red line is result of linear regression, black line is the 1:1 line.

3.4.3 Seasonal mean differences between GOME-2/Metop and colocated lidar and microwave ozone profiles and time series grouped by latitude belts

The following figures (3.17 - 3.26) show the time series and seasonal mean comparison results grouped by latitude belts to elaborate seasonal differences and degradation of the GOME-2 instrument. The results are again grouped by latitudes as in chapter 3.4.2.

3.4.3.1 Arctic Belt

Time series from the arctic belt are not presented, since the measurements were restricted to the late winter and spring most of the time (see table 3.2), and only since recently Ny Alesund provides microwave data all year round. Figure 3.17 shows mean relative difference profiles

for spring, summer, autumn and winter. The numbers of pixels compared on the right of each plot shows that the most reference profiles are available for spring followed by summer, winter and autumn have less comparisons, thus the significance of these seasons results is lower than for the two other seasons. In winter only a few comparisons above 40 km and below 9 km were possible due to lack of data, so that winter results are only valid from 10 km - 40 km. Besides these restrictions, relative difference profiles are different during the seasons. The spring profile is almost the same as the average relative profile of the entire time period, which is not surprising since the number of profiles compared in spring is larger than the total of the other three seasons.

The relative difference profiles in spring show a large positive bias (GOME-2 higher than reference) of up to 50% in the UTLS and a negative bias above the ozone maximum. However, besides the UTLS, the relative differences are within the target limits of \pm 15% in both avk smoothed and integrated reference profiles. In summer the larger difference between avk reference and integrated profile comparisons is striking, although not significant within the 1 sigma error bars. Comparisons with avk profiles have a negative bias in the UTLS and also above 37km, when integrated profile comparisons have almost no bias. In autumn the bias in the UTLS is negative by up to 50% and in the higher stratosphere (>45 km) an increasing negative bias is found. In winter a slightly negative bias above 10 km is observed and almost no bias up to 40 km height.



Fig. 3.17: Seasonal mean relative difference profiles from left to right: spring, summer, autumn and winter. HR GOME-2 minus reference in black, Gome minus reference smoothed with averaging kernels in green. Horizontal error bars are 1 standard deviation from single pixel comparisons. Vertical lines indicate ± 15 % target value for comparisons in the stratosphere, and figures on the right of each plot are numbers of GOME-2 pixels compared at each layer and season.

Scatter plots for comparisons with avk smoothed reference profiles are presented in figures 3.17a,b for the four seasons. Again, the scatter plots from spring are not significantly different from the mean over all seasons. In the lower troposphere (1 km - 5 km) high GOME-2 ozone with low avk reference ozone are found, as well as high reference ozone with low GOME-2 in

distinct lines. This pattern is not found in the other seasons, but regarding the lower number of comparisons, it cannot yet definitely concluded whether this pattern is really a seasonal effect. In the 10 km to 20 km layers we find no correlation in summer and autumn, in spring the correlation is poor (R=0.57 resp. 0.62), but in winter the correlation is good at these altitudes (R>08). The tilting against the 1:1 line is found in all seasons, with higher reference ozone values the GOME-2 ozone becomes lower, independently from the absolute ozone values. In summer the GOME-2 and the avk reference ozone is grouped in small packages, as in the subtropics and southern mid latitudes, described above. This grouping is observed between 25 km and 50 km.



Fig. 3.17°a: Correlations between HR GOME-2 ozone and avk reference ozone in spring (above) and summer(below) at several altitude layers for polar regions. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.17°a: Correlations between HR GOME-2 ozone and avk reference ozone in autumn (above) and winter (below) at several altitude layers for polar regions. Red line is result of linear regression, black line is the 1:1 line.

3.4.3.2 Northern Mid Latitude Belt

Time series from the northern mid latitude stations are presented in fig. 3.18. The plots reveal mainly three effects.

First is a seasonal variation of relative differences. Comparisons with integrated profiles show a small seasonal variation from 20 km to 25 km, with a neagtive bias in winter and a positive bias in spring, summer and autumn. In 35 km to 40 km this bias is inverted and above 50km a positive bias in summer and negative bias in winter is observed in the years 2007-2009 only. Comparisons with avk smoothed profiles in the 20 km - 25 m and the 35 km - 40 km layers have the same seasonal variation, whereas the seasonal pattern above 50 km is not observed.

The second observation is an increasing negative bias with time, most certainly due to degradation of the GOME-2 instrument. The degradation signs started early (end 2008) in the higher layers (>40 km), since 2010 the degradation became clear at lower altitudes, too. From the start of the measurements in 2007 till 2011 the negative bias with both integrated and avk profiles increased by 15%. At the lower layers (~20 km) the bias increased by approx. 5% with integrated profiles and 3% with avk smoothed profiles.

Third point to mention is the higher scatter with integrated profiles below 20 km and above 45 km which becomes obvious in the error bars.

The seasonal mean profiles are identical within their error bars from 20 km to 40 km in all seasons. Higher above larger seasonal variations are found for integrated reference profiles. In spring and summer a mean negative bias of 23 % resp. 26 % is observed at 40 km, and a positive bias of 8 % resp. 11 % at 53 km height. In autumn and winter the mean negative bias is about 10 % and the mean positive bias 2-3 % smaller than in summer and spring. The maximum of the positive bias is shifted towards lower altitudes by 2 km - 3 km. Below 20 km a positive bias with maximum at 17 km is observed in all seasons it is highest in spring and summer and lowest in winter (spring 17 %, summer 17 %, autumn 14 %, winter 11%). Below that maximum the relative difference profiles are different during the course of the year. In spring and winter a secondary positive bias maximum is observed between 10 km and 11 km, in spring this bias is 37 % and in winter 16 %, whereas in summer at the same altitude a maximum negative bias (11 %) is found, during autumn a positive bias of up to 23 % is observed at 8 km. Taking the error bars into account, all these findings are statistically not significant and are just indicators that there are variations in and around the UTLS which are on average not reflected by the GOME-2 retrieval algorithm. Since the UTLS and the lower stratosphere are layers with high variations of ozone concentrations, the task to get the satellite ozone in individual profiles correctly is most demanding. The comparisons with avk smoothed reference profiles give much better results demonstrating that the averaging kernels distribute the ozone between the layers quite well. However, from spring to autumn a positive bias is found with avk smoothed profiles. This bias is 10 % in all seasons but shifts in height from 10 km in spring, to 12 km in summer and 14 km in autumn, thus reflecting the migration of the tropopause height within the year. In winter the avk relative differences meander between 0 5 % and 5%.



Fig.3.18: Time series of monthly mean relative differences between HR GOME-2/Metop and reference ozone profiles at several altitude layers for northern mid latitude stations. Comparisons with integrated reference profiles (above) and avk smoothed reference profiles (below) are shown. Error bars are 1 standard deviation from the monthly means. Black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.



Fig. 3.19: Seasonal mean relative difference profiles from left to right: spring, summer, autumn and winter. HR GOME-2 minus reference in black, Gome minus reference smoothed with averaging kernels in green. Horizontal error bars are 1 standard deviation from single pixel comparisons. Vertical lines indicate ± 15 % target value for comparisons in the stratosphere, and figures on the right of each plot are numbers of GOME-2 pixels compared at each layer and season.

Scatter plots are presented in figs 3.20a-d for comparisons with averging kernel smoothed reference profiles. The results are summarized in table 3.6.

	R>0.9	R>0.9	R>0.8	R>0.8	R=0.5-0.8	R=0.5-0.8	R<0.5	R<0.5
	Integr. Ref.	Avk ref	Integr. Ref	Avk ref	Integr. Ref	Avk ref	Integr. Ref	Avk ref
	[km]	[km]	[km]	[km]	[km]	[km]	[km]	[km]
Spring	25-45	15-20	15-20	10-15	4-5	3-10	5-10	<5
		25-60	45-55	20-25	20-25			
Summer	30-50	15-20	15-20	10-15		5-10	<10	
		25-60	25-30			20-25	20-25	
			50-55					
Autumn	15-20	10-20	10-15		4-5	5-10	5-10	
	25-50	25-60	50-55		20-25	20-25		
winter	25-45	10-20	10-20	20-25	4-5	5-10	5-10	
		25-55	45-55		20-25	20-25		

Tab 3.6: Altitude of correlations between GOME-2 and integrated reference resp. avk reference profiles at northern mid latitude stations, grouped by seasons and correlation coefficient ranges.

Avk reference profiles generally have a larger altitude range of high correlations (R>0.9) than integrated profiles. In summer the correlation is somewhat inferior than during the other seasons. Striking is the 20 km to 25 km range, where correlations at all seasons and for both, integrated and avk reference are worse than in the surrounding layers. Poorest correlations are found from 5 km - 10 km, whereas in the lower troposphere the correlations are slightly better.

The regression line is close to the 1:1 line at 15 km – 35 km, with exception of the 20 km- 25 km layers, from spring through to autumn and at 30 km- 35 km and 50 km- 55 km in winter for integrated reference comparisons. For comparisons with avk reference the regression line is close to the 1:1 line from 15 km - 35 km in spring, from 15 km – 20 and 25 km- 35km in summer, and from 15 km – 20 km and 25 km – 30 km in autumn and from 10 km - 30 km in. At all other layers the regression line is tilted towards the 1:1 line.

Grouping of GOME-2 and avk reference ozone is found between 35 km and 40 km and above 50 km in spring, in summer above 30 km and in autumn from 35 km onwards, in winter the grouping is vague and found only above 50 km. For comparisons with integrated profiles the grouping is not as distinct as for avk profiles, vague groping is observed in spring above 50 km and in winter between 40km and 45 km and above 50 km, in summer and autumn the grouping effect can be seen clearly above 30 km resp. above 35 km. This seasonal dependency of the grouping effect might be a hint that temperature can play a role in this case, which should be further investigated.



Fig. 3.20°a: Correlations between HR GOME-2 ozone and avk reference ozone in spring at several altitude layers for northern mid latitude belt. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.20°b: Correlations between HR GOME-2 ozone and avk reference ozone in summer at several altitude layers for northern mid latitude belt. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.20°c: Correlations between HR GOME-2 ozone and avk reference ozone in autumn at several altitude layers for northern mid latitude belt. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.20°d: Correlations between HR GOME-2 ozone and avk reference ozone in winter at several altitude layers for northern mid latitude belt. Red line is result of linear regression, black line is the 1:1 line.

3.4.3.3 Subtropics

Time series from the northern mid latitude stations are presented in fig. 3.21. Seasonal variation of relative differences are small and can be found with integrated reference profiles only between 16 km and 25 km. In winter the bias is by 5 % - 15 % lower than in the other seasons.

Degradation signs appear as increasingly negative bias. The degradation started early (end 2008) in the higher layers (>40 km). Below 30 km height, signs of GOME-2 degradation cannot be seen, yet. From the start of the measurements in January 2007 till December 2011 the negative bias with both integrated and avk profiles increased by 15% above 44 km. High error bars are found in both, integrated and avk reference comparisons in the 16 km to 19 km height range.

The seasonal mean profiles (fig 3.22) also show not much variation. All have a bulge of negative bias from 38 km to 50 km with maximum around 40 km. The maximum relative difference for integrated profiles is around -20 % in all seasons, for avk smoothed profiles the resp. value is -17 %. At 19 km altitude a maximum positive bias is found, which value varies with season, it is largest in spring and summer with ~30 % for avk reference and 20 % for integrated profiles and smallest in winter with 11 % for integrated and 9 % for avk reference profiles.

Scatter plots are presented in figs 3.23a-d for comparisons with averging kernel smoothed profiles. The results are summarized in table 3.7.

Tab 3.7: Altitude of correlations between GOME-2 and integrated reference resp. avk reference profiles at subtropical station, grouped by seasons and correlation coefficient ranges.

	R>0.9	R>0.9	R>0.8	R>0.8	R=0.5-0.8	R=0.5-0.8	R<0.5	R<0.5
	Integr. Ref.	Avk ref	Integr. Ref	Avk ref	Integr. Ref	Avk ref	Integr. Ref	Avk ref
	[km]	[km]	[km]	[km]	[km]	[km]	[km]	[km]
Spring	25-60	20-60	20-25	15-20	15-20			
Summer	20-60	16-60			16-20			
Autumn	20-59	17-59			17-20			
winter	30-58	25-58	25-30	18-25	18-25			

Correlation coefficients are better in the subtropics than the mid latitude stations. Reason for that is most certainly the lower variability of ozone concentrations throughout the year in the subtropics. On average the avk reference profiles have a larger altitude range of high correlations (R>0.9) than integrated profiles and both versions of reference profiles have better correlations in summer and autumn than in winter. Poor correlations (R= 0.5-0.7) are only observed for integrated profiles below 20 km in spring through to summer and below 25 km in winter. The regression line is close to the 1:1 line at 25 km – 35 km in winter for avk reference comparisons and at 25 km – 30 km in all other cases.

Grouping of GOME-2 and avk reference ozone is found above 35 km in spring and winter, above 30 km in autumn and from 16km – 20 km and above 25 km in summer for integrated profiles. For avk comparisons a very distinct grouping is observed at all altitudes in summer and autumn. In spring it occurs from 15 km to 20 and above 30 km and in winter above 35 km. As stated in chapter 3.4.3.2, this seasonal variation, together with the observations at other latitude belts, indicate that temperature can play a role in this case.





Fig.3.21: Time series of monthly mean relative differences between HR GOME-2/Metop and reference ozone profiles at several altitude layers for subtropical station. Comparisons with integrated reference profiles (above) and avk smoothed reference profiles (below) are shown. Error bars are 1 standard deviation from the monthly means. Black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.



Fig. 3.22: Seasonal mean relative difference profiles from left to right: spring, summer, autumn and winter. HR GOME-2 minus reference in black, Gome minus reference smoothed with averaging kernels in green. Horizontal error bars are 1 standard deviation from single pixel comparisons. Vertical lines indicate ± 15 % target value for comparisons in the stratosphere, and figures on the right of each plot are numbers of GOME-2 pixels compared at each layer and season.



Fig. 3.23°a: Correlations between HR GOME-2 ozone and avk reference ozone in spring at several altitude layers subtropical station. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.23°b: Correlations between HR GOME-2 ozone and avk reference ozone in summer at several altitude layers subtropical station. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.23°c: Correlations between HR GOME-2 ozone and avk reference ozone in autumn at several altitude layers subtropical station. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.23°d: Correlations between HR GOME-2 ozone and avk reference ozone in winter at several altitude layers subtropical station. Red line is result of linear regression, black line is the 1:1 line.

3.4.3.4 Southern Mid Latitude Belt

Time series from the southern mid latitude stations are presented in fig. 3.24 and sesonal mean profiles in fig 3.25.

A seasonal variation of relative differences, similar to the northern mid latitude stations is observed. Comparisons with integrated profiles show a small seasonal variation in from 20 km to 25 km with a negative bias in winter and a positive bias in summer. In 35 km to 40 km this bias is inverted, best seen in the avk reference comparisons.

Above the lidar range at 45 km, the time series end in Dec 2009, at that time the microwave measurements at Lauder terminated. It is not yet clear whether they will be restarted. So only the onset of the degradation at the end of year 2008 is documented. From the start of the measurements in 2007 till 2011 the negative bias with both integrated and avk profiles increased by 10% at 40 km altitude. At the lower layers (~35 km) the bias increased by approx. 5% with integrated profiles and 3% with avk smoothed profiles since the year 2010.

The seasonal mean profiles all have a negative bias between 35 km and 50 km., although their values and the maximum heights differ slightly between seasons. In spring and autumn the maximum bias is -18 % at 44 resp. 43 km altitude, in summer the relative differences have their maximum at 42 km with -20% and in winter the corresponding values are 43 km and -19%. For comparisons with avk smoothed reference profiles, the altitude of the maximum bias are the same but the values are somewhat lower, with -15 % in spring to autumn and -14% in winter. These differences are statistically not significant within the 1 sigma error bars. At 20 km - 35 km altitude, no bias is found during spring and winter, in summer the relative differences go from positive deviation (8%) around 20 km to negative deviation (-7%) at 35 km. In autumn a small negative mean bias of -5% is observed. Largest differences between seasons as well as between integrated and avk smoothed profiles are found below 20 km. Integrated profiles show a negative bias maximum of -23 % at 8 km, in summer a change from positive bias of 12 % at 8 km to a negative bias of -23 % at 11 km is observed. This pattern is inverted in autumn when a negative bias of -25 % at 8 km and a positive bias of 12 % at 13 km is found. In winter a clear positive bias with maximum value of 46 % at 8km is observed. Averaging kernel smoothed profiles below 20 km follow the same patterns in winter and spring, in winter the maximum bias is 14% lower and in spring it is 7 % higher for the avk profiles. In summer and autumn avk comparison differences below 20 km are \pm 0%. These findings demonstrate once more that the GOME-2 retrieval has difficulties to get the ozone values correctly in the UTLS with its high ozone variability.

Scatter plots are presented in figs 3.26a-d for comparisons with averging kernel smoothed profiles. The results are summarized in table 3.8.

Avk reference profiles generally have a larger altitude range of high correlations (R>0.9) than integrated profiles. The correlations are best in winter and lower in summer. As in the northern mid latitude belt the correlations in the 20 km to 25 km range are worse than in the surrounding layers in all seasons and for both integrated and avk reference. At mid latitude stations this altitude is the range of the ozone maximum, so this finding may be a hint that the ozone maximum especially in summer and autumn is not correctly matched by the GOME-2 retrieval. Poor correlations are found from 5 km - 10 km for integrated profile comparisons. For comparisons with integrated profiles the regression line is close to the 1:1 line at 25 km - 35 km in spring and at 15km – 20 km in autumn only. For comparisons with avk profiles the regression line meets the 1:1 line in spring at 20 km – 35 km, in summer at 15km – 20 km, in autumn at 15km – 20 km and 25 km - 30 km and in winter at 15 km – 25 km and 35 km – 40 km.



Fig.3.24: Time series of monthly mean relative differences between HR GOME-2/Metop and reference ozone profiles at several altitude layers for subtropical station. Comparisons with integrated reference profiles (above) and avk smoothed reference profiles (below) are shown. Error bars are 1 standard deviation from the monthly means. Black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere



Fig. 3.25: Seasonal mean relative difference profiles from left to right: spring, summer, autumn and winter. HR GOME-2 minus reference in black, Gome minus reference smoothed with averaging kernels in green. Horizontal error bars are 1 standard deviation from single pixel comparisons. Vertical lines indicate ± 15 % target value for comparisons in the stratosphere, and figures on the right of each plot are numbers of GOME-2 pixels compared at each layer and season.

Grouping of GOME-2 and avk reference ozone is found above 55 km in spring, in summer at 15 km to 20 km and above 30 km, in autumn above 50 km and in winter the grouping is vague only and found above 35 km. For comparisons with integrated profiles the grouping is not as distinct as for avk profiles, vague groping is observed in spring above 55 km and in winter between 35 km and 40 km, in summer and autumn the grouping effect can be seen more clearly above 30 km resp. above 50 km.

	R>0.9	R>0.9	R>0.8	R>0.8	R=0.5-0.8	R=0.5-0.8	R<0.5	R<0.5
	Integr. Ref.	Avk ref	Integr. Ref	Avk ref	Integr. Ref	Avk ref	Integr. Ref	Avk ref
	[km]	[km]	[km]	[km]	[km]	[km]	[km]	[km]
Spring	25-59	15-12	15-20	10-15	10-15	5-10	5-10	
		25-55		20-25	20-25			
Summer	15-20	15-20	25-30		10-15	10-15	6-10	6-10
	30-60	25-60					20-25	20-25
Autumn	25-59	15-20	15-20	10-15	10-15	7-10	7-10	
		25-59			20-25	20-25		
winter	25-59	15-59	15-25	6-15	7-15			

Tab 3.8: Altitude of correlations between GOME-2 and integrated reference resp. avk reference profiles at southern mid latitude stations, grouped by seasons and correlation coefficient ranges.



Fig. 3.26°a: Correlations between HR GOME-2 ozone and avk reference ozone in spring at several altitude layers in southern mid latitudes. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.26 b: Correlations between HR GOME-2 ozone and avk reference ozone in summer at several altitude layers in southern mid latitudes. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.26°c: Correlations between HR GOME-2 ozone and avk reference ozone in autumn at several altitude layers in southern mid latitudes. Red line is result of linear regression, black line is the 1:1 line.



Fig. 3.26°d: Correlations between HR GOME-2 ozone and avk reference ozone in winter at several altitude layers in southern mid latitudes. Red line is result of linear regression, black line is the 1:1 line.

3.4.4 Correlations with different parameters

Correlations of relative differences with parameters which might influence the GOME-2 ozone profile measurements were calculated. Among them are parameters which go into the GOME-2 retrieval, such as cloud fraction, cloud pressure, cloud albedo, surface albedo and solar zenith angle, or may originate from the satellite instrument like the scan angle or may be caused by the reference instrument like the averaging time of the lidars. For all the mentioned parameters correlations with relative difference were calculated. No correlations were found with the exceptions of solar zenith angle and scan angle, but also for these two parameters the correlations are weak and may only give a hint to the retrieval development group to keep an eye on these two parameters when improving the retrieval. They certainly cannot explain the described variations in the different altitude belts and altitude layers.

In the following figures (3.27 - 3.34) we present correlations with solar zenith angle at GOME-2 pixel centre (SZA_F) and scan angle (indscan) for the four latitude belts comparisons with averaging kernel smoothing.

Since the METOP satellite overpasses the ground based stations at approximately the same time throughout the year, the solar zenith angle changes in the course of the year. Influences of solar zenith angle on the GOME-2 retrieval should reflect in seasonal variations of relative differences. On the other hand, when seasonal variations have their source in other parameters then some kind of correlation with sza should be found as well. Thus a correlation with solar zenith angle does not automatically denote a substantial influence of this parameter on the GOME-2 retrieval. Additional factors must be checked.

In chapter 3.4.3 it has been shown that all latitude belts have largest variations in the course of the year below 20 km and above 40km altitude. These variations are smallest at the subtropical stations and increase towards the poles. Correlations with solar zenith angle also reveal this high variability below 20 km and above 40 km, as well as the higher scatter away from the equator. Apart from that, no correlation of any significance is observed with solar zenith angle.

Correlations of relative differences with GOME-2 scan angle are also not significant, only at the subtropical stations above 40 km a weak correlation, with correlation coefficients between 0.6 - 0.7 is observed, indicating higher relative differences in the eastern pixels and lower relative differences in the western pixels. The results in the southern and northern mid latitude belt show a tendency towards the same pattern, but with lower correlation. In the polar regions above 40 km the centre pixels seem to give somewhat better results (no negative or positive bias).



Fig. 3.27: Averaging kernel smoothed relative differences at arctic stations as function of solar zenith angle at GOME-2 pixel centre. Red line is result of linear regression, black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.



Fig. 3.28: Averaging kernel smoothed relative differences at northern mid latitude stations as function of solar zenith angle at GOME-2 pixel centre. Red line is result of linear regression, black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.


Fig. 3.29: Averaging kernel smoothed relative differences at subtropical station as function of solar zenith angle at GOME-2 pixel centre. Red line is result of linear regression, black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.



Fig. 3.30: Averaging kernel smoothed relative differences at southern mid latitude stations as function of solar zenith angle at GOME-2 pixel centre. Red line is result of linear regression, black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.



Fig. 3.31: Averaging kernel smoothed relative differences at arctic stations as function of GOME-2 scan angle. Numbers 1-8 are eastern pixels, 9-16 are centre pixels and 17-24 are western pixels. Red line is result of linear regression, black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.



Fig. 3.32: Averaging kernel smoothed relative differences at northern mid latitude stations as function of GOME-2 scan angle. Numbers 1-8 are eastern pixels, 9-16 are centre pixels and 17-24 are western pixels. Red line is result of linear regression, black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.



Fig. 3.33: Averaging kernel smoothed relative differences at subtropical station as function of GOME-2 scan angle. Numbers 1-8 are eastern pixels, 9-16 are centre pixels and 17-24 are western pixels. Red line is result of linear regression, black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.



Fig. 3.34: Averaging kernel smoothed relative differences at southern mid latitude stations as function of GOME-2 scan angle. Numbers 1-8 are eastern pixels, 9-16 are centre pixels and 17-24 are western pixels. Red line is result of linear regression, black horizontal lines indicate ± 15 % target value for comparisons in the stratosphere.

3.4.5 Comparison with other satellite instruments

For scientific research, such as ozone change evaluations, it is necessary to know how the ozone profiles of GOME-2/Metop compare to other satellite instruments. A literature survey was performed to compare validation results from other satellite instruments with the results presented here. The outcome is presented in table 3.9. The HR GOME-2 validation results compare well with other satellite instruments at all altitude levels. In the upper stratosphere the validation results show a higher variability within the satellite instruments and for each satellite instruments itself.

Satellite/compared to	Altitude 18km - 38km	Altitude 45-55km
GOME-2/lidar	-2% - ± 6%	-11% ± 13%
SageII/lidar	+2% - +8% ± 3-5%	+2% - +8% ± 3-5%
Sciamachy/lidar+µwave	-5%20% ± 10-15%	-25% ±15%
Gomos/sonde+lidar+µwave	-2.5% ± 14%	-2.5% ± 14%
Mipas/sonde+lidar+µwave	$\pm 5\% \pm 10\%$	±15% ± 20%
ACE-Maestro sunrise /lidar+SAGEIII	5-15%	5-15%
ACE-Maestro sunset /lidar+SAGEIII	5-10%	20-30%
Aura-MLS/aircraft lidar+SAGEII	±5%	+8%

Tab. 3.9: Mean relative differences and standard deviations of different satellite instruments compared to ozone sonde, lidar and µwave ozone measurements at different altitudes.

4. Summary and conclusions

This study contains global validation results of about 4.5 years of GOME-2 retrieved ozone profile data.

The *threshold* accuracies for the GOME-2 ozone profiles are 30% for the stratosphere and 70% for the troposphere. These targets are met for all the stations used in the analysis.

The *target* accuracies for the ozone profiles are respectively 30% in the troposphere and 15% in the stratosphere. This accuracy is reached for the HR pixels and at least partially in the stratosphere for the Southern polar station for the coarse resolution pixels.

GOME-2 HR- and CR ozone profiles give sensibly better results at Mid-Latitude stations than at the other latitude belts when compared to ozonesondes. Comparisons with lidar and microwave radiometers reveal best results from the subtropics to the mid latitude stations.

The mean relative difference between GOME-2 and $X_{AVK-sonde}$ as well as with avk_lidar and avk_microwave is in general within ±15 % in the troposphere (for heights below 7 km) and the stratosphere for heights between 15 and 60 km. For the Mid-Latitude belts there is an overestimation of about +15 % for the complete time period for heights between 10 km and 15 km, when compared with $X_{AVK-sonde}$, comparisons with lidars show a slightly lower overestimation of 7 %±8% at these layers. For heights between 20 km and 30 km the relative difference is close to zero and stable with a maximum standard deviation of about 10 %. Between 35 km and 50 km an increasing negative bias is observed when GOME-2 is compared to lidar and microwave instruments. It has its maximum around 45 km with -16% ± 5% for avk_reference, and -24% ± 16% for integrated reference profile comparisons. In the upper stratosphere (>50 km) the large bias of CR profiles (max. -45%±11%) is considerably reduced in the HR profiles to -9.3%±4% with avk profiles and 0% ±10% with integrated profiles.

For the Northern polar stations, GOME-2 underestimates until -15 % in the stratosphere and overestimates until +40 % in the UTLS-zone for the coarse pixels. For the lower troposphere, the relative difference is within 10 %. The relative difference between GOME-2 and the smoothed ozone profiles shows a better comparison in the UTLS-zone with an overestimation of about 30 %. When using the HR pixels, the profile has significantly improved, being within the 15 % error bound for the complete profile (0-30 km) when applying the averaging kernels. The stratosphere shows an underestimation of about -7 %, while the troposphere is showing an overestimation of about +2 %. The stratosphere. For the UTLS-zone the standard error is considerably larger.

The information content is lower in the troposphere, UTLS-zone and around the ozone maximum. It is lowest in summer and highest in winter at mid latitude and arctic stations. HR GOME-2 ozone profiles can be best recommended to users for Mid-Latitude stations from 25 km to 60 km, in the subtropics from 20 km – 60 km and in the Northern polar regions between 25 km and 45 km.

Also low ozone profiles have been successfully retrieved at Neumayer station. The algorithm has problems with the UTLS-zone and tends to overestimate the ozone in the lower stratosphere during winter- and early spring season. By using the high resolution pixels, the retrieved profiles improved significantly and all the target values are met for all stations when using the high resolution pixels, except for the tropical stations. This is related to the fact that small numbers are compared.

From the comparisons with other satellite validation results we may conclude that the HR GOME-2 ozone profiles are qualified for continuous monitoring of ozone changes.

5.Acknowledgement

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