Comparison of ozone profiles by the Umkehr measurements taken at Belsk (52°N, 21°E) with the Aura Microwave Limb Sounder overpasses: 2004–2006

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[1] A comparison of ozone profile measurements by the Umkehr observations taken at Belsk (52°N, 21°E) by the Dobson spectrophotometer and collocated Earth Observing System (EOS) Microwave Limb Sounder (MLS) aboard the Aura platform during 2004–2006 site overpasses is presented. The MLS ozone vertical profiles from 1.5 and 2.2 retrieval algorithms and various Umkehr retrievals are considered. There is a good agreement between the ozone content in Umkehr layers. The mean difference $\sim \pm 5\%$, standard deviation of the relative differences $< 10\%$, and the correlation coefficient > 0.5 are found in the midstratosphere (Umkehr layers 5–7) and in the upper stratosphere (combined layers 8, 9, and 10). In the lower stratosphere (combined layers 2 and 3 and layer 4) the mean difference and/or standard deviation are larger but the correlation coefficient is still high (~ 0.8). Ozone content in Umkehr layers by integration of MLS version 1.5 and 2.2 ozone mixing ratio profiles behaves very similarly in the comparisons with the ground-based data.

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1. Introduction

[2] The understanding of mechanisms controlling the Earth atmosphere appears as the major reason for increasing efforts of the international scientific community during last decades. At present, our knowledge of characteristics of the gaseous composition of the atmosphere is built from different observation systems: airborne, balloon, ground-based, and satellite platforms. Because of the global perspective of the atmosphere monitoring, satellite system, which is based on remote measurements of the reflected and scattered solar and Earth radiation in various spectral ranges, is considered to be the most important component of the Earth observation system. The comparison of satellite data with independent well controlled ground-based data, collocated in space and time, is very promising for estimating the accuracy level of the satellite measurements.

[3] The Belsk Observatory (52°N, 21°E) being Central Geophysical Observatory of the Institute of Geophysics of the Polish Academy of Sciences has begun its activity in March 1963 with the measurements of the column amount of ozone (total ozone) and Umkehr ozone profile by the Dobson spectrophotometer and observations of various optical properties of the atmosphere (e.g., sunshine duration, global irradiance, etc.). During past decades of ozone and radiation measurements various efforts have been made to ascertain the data quality. Special attention has been paid to proper maintenance, calibration, modernization of instruments and the software used [e.g., *Dziewulska-Łosiowa et al.*, 1983; *Degórska et al.*, 1995; *Rajewska-Więch et al.*, 2006].

[4] The purpose of this study is a comparison of the ozone vertical profiles inferred from the Umkehr measurements taken at Belsk observatory with collocated satellite profiles derived from measurements by the Earth Observing System (EOS) Microwave Limb Sounder (MLS) instrument, which inspects thermal emissions lines from many trace gases at microwave wavelengths [*Schoeberl et al.* 2006; *Froidevaux et al.* 2006; *Livesey et al.*, 2006; *Waters et al.*, 2006]. The MLS data used for this comparison are taken from the Aura Validation Data Center (AVDC). The MLS ozone profile data are available from http://avdc.gsfc.nasa.gov/Data/Aura/index.html (free access). The satellite data taken prior to 1 January 2007 during the Belsk's overpasses are taken into account. In this paper we present results showing an agreement between ground-based and satellite ozone profile data.

2. Ozone Vertical Profile

[5] The ozone profiles derived from ground-based Umkehr measurements and Aura MLS observations are

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examined in this section. Various retrievals both for ground-based and satellite measurements are considered. The ozone content in selected layers in the stratosphere are compared. Standard statistical methods and Taylor diagram for visualization of the data differences are implemented to find an agreement between the ground-based and satellite data.

2.1. Umkehr Observations

[6] Umkehr observations are performed with ground-based spectrophotometers measuring the ratio of zenith-sky radiance at a UV wavelength pair, one strongly and other weakly absorbing. The wavelength pair radiances are measured from zenith sky under cloudless conditions for a set of discrete solar zenith angles (SZAs) changing from $60°-90°$ (standard Umkehr) or from $80°-90°$ (short Umkehr). Further, term "short Umkehr" is used to describe the Dobson Umkehr spectrophotometer observations using C-wavelength pair with the lowest SZA of $80°$ or results of the newest Umkehr retrieval (UMK04) applied to such measurements. The standard Umkehr retrieval UMK92 [*Mateer and DeLuisi*, 1992] partitions column ozone into 10 Umkehr layers that are divided into equal log-pressure vertical intervals, starting at the surface ($\sim$1013 hPa) and extending to layer 10 ($\sim$1 hPa to the top of the atmosphere). The ozone content above $\sim$10 km is reported in $\sim$5 km thick layers. Although the Umkehr retrieval yields ozone content in 10 layers, because of broad and strongly overlapping weighting functions, as well as finite measurement errors, the retrieval contains, at most, four linearly independent pieces of information. Measurement errors, smoothing errors, forward model errors, and inverse model errors were discussed by *SPARC* [1998] report. Recently, a new Umkehr retrieval (UMK04) has been proposed that features new a priori ozone profile information, updated forward model, and updated inverse model [*Petropavlovskikh et al.*, 2005]. They also suggested that ozone in layers 2 and 3 and in layers 8, 9, and 10 need to be combined prior to comparisons against other systems. Following their findings we analyze ozone content in standard layers 4–7, and in two thicker layers, layer 2+ (sum of layers 2 + 3) and 8+ (sum of layers 8, 9, and 10). Requirement of clear-sky conditions during the Umkehr measurements limits number of the ozone Umkehr profiles. Estimated measurement uncertainties for the Umkehr observations exhibit an altitude structure, i.e., 8% for 0 to 20 km integrated ozone, and $\sim$5% for 20–32 km [*Fioletov et al.*, 2006].

[7] Here we examine results of the Dobson spectrophotometer measurements taken at Belsk, Poland, for the period of 2004–2006. Ozone profiles retrieved by both UMK92 and UMK04 inversion procedure are taken into account. Three versions of UMK04 retrieval are analyzed: first, the retrieval that uses observations over traditional range of SZA—between $60°$ and $90°$; second, the retrieval that uses $70°$ SZA as a cut off; third, the so-called short Umkehr that uses $80°$ SZA as a cut off. Ozone profiles can be derived over Belsk only by the short-Umkehr version of UMK04 retrieval in periods of low Sun (late autumn and early winter).

2.2. MLS Observations

[8] Aura MLS instrument, using microwave emission to measure stratospheric temperature and constituents, has

begun its scheduled observations on 13 August 2004. It takes observations in several spectral bands. This paper uses "MLS standard product" for ozone retrieved from MLS radiance measurements near 240 GHz, providing the best overall precision for the widest vertical range [*Froidevaux et al.*, 2008]. Level 2 (geophysical products along the measurement track) version 1.5 (v1.5) and recent version 2.2 (v2.2) algorithm data have been examined in this study. MLS Level 2 data are stored in the Aura-specific implementation of the HDF-EOS (version 5) swath format. The file typically contains vertical profiles of the ozone mixing ratio and other geophysical parameters provided at nominal pressure levels. There are 37 levels between surface at 1000 hPa and top of the atmosphere at 10^{-5} hPa, among them 18 levels are above 1 hPa. Following recent recommendation of *Froidevaux et al.* [2008] we use MLS ozone mixing ratios from 215 to 0.02 hPa. Thus, we take into account the ozone mixing ratio at levels: 0.02, 0.05, 0.1, 0.15, 0.22, 0.32, 0.46, 0.68, 1.0, 1.47, 2.15, 3.16, 4.64, 6.81, 10.0, 14.7, 21.5, 31.6, 46.4, 68.1, 100, 147, and 215 hPa. To calculate ozone content in selected Umkehr layers, the ozone mixing ratios at the boundaries of Umkehr layers are calculated by interpolation of the mixing ratios from surrounding MLS pressure levels. Next the ozone mixing ratios are integrated over pressure levels (i.e., lower and upper boundary of Umkehr layer used in the Dobson Umkehr retrievals) to obtain layer ozone values. Umkehr layer has width $\sim$5 km but the MLS vertical resolution is $\sim$3 km, so a comparison between these methods cannot be straightforward. The Umkehr algorithm provides layer mean ozone values whereas MLS output is the ozone mixing ratio at many altitude levels not corresponding to the boundaries of the Umkehr layers. This could enlarge differences between the ozone profiles because ozone content in certain Umkehr layer derived from MLS data is additionally influenced by the ozone mixing ratio at levels below and above this layer. It is a result of the interpolation of the MLS mixing ratio to the Umkehr layer boundaries.

[9] In addition other fields in the swath help to screen the stratospheric MLS ozone profiles allowing to create a subset of the high-quality data appropriate for further comparison with the ground-based data. The criteria used for screening follow recommendations provided by *Livesey et al.* [2005] and *Froidevaux et al.* [2008] for MLS v1.5 and v2.2, respectively. *Froidevaux et al.* [2008] have found that MLS v2.2 yielded better agreement in comparisons with other satellite instruments, aircraft lidar, and balloon-borne remote and in situ sensors. For example, MLS v2.2 profile ozone values are on average within about 5% agreement with SAGE II coincident profiles in the stratosphere. Early validation studies of ozone profiles from MLS v1.5 algorithm revealed good overall agreement with other correlative ozone profiles in the stratosphere [e.g., *Froidevaux et al.*, 2006; *Hocke et al.*, 2007].

2.3. Collocation Criteria

[10] Ozone profiles are selected from MLS overpasses as being within plus or minus $2°$ of station latitude, $4°$ of station longitude. Total number of coincidental MLS v1.5 daily ozone profiles during the mid-2004 to late 2006 time period over Belsk is 518 but 188 profiles are available from MLS v2.2 retrieval. Because the Umkehr measurements
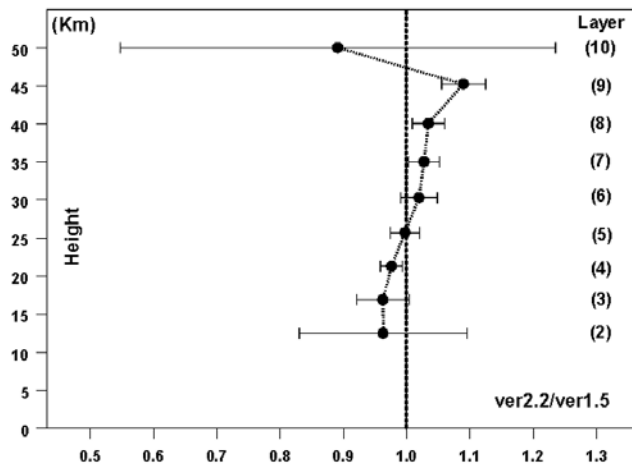
Figure 1. Mean ratio between the ozone content in Umkehr layer derived from MLS v2.2 and MLS v1.5 profiles during Belsk's overpasses in the period 2004−2006. The bar represents range: the mean value ± 1 standard deviation.

require cloudless conditions therefore, ∼100 daily profiles are available for comparison with MLS v1.5 and ∼40 profiles for MLS v2.2 over selected period of time. Figure 1 shows that the ratio between the ozone content in Umkehr layers derived from MLS v2.2 and MLS v1.5 profiles taken during 2004−2006 overpasses. The results for nine Umkehr layers, including all layers between layer 2 and 10 are shown. MLS v2.2 provides lower abundances in the lower stratosphere (up to Umkehr layer 4) and higher in the upper stratosphere (between layers 7 and 9). There were no acceptable satellite data to calculate the ozone content in layer 1 (i.e., 1000−250 hPa region representing mostly the troposphere). The Umkehr Dobson retrievals also do not yield reliable ozone content in this layer. The Belsk's pattern of the differences between the ozone content in Umkehr layers by integration of ver.2.2 and ver.1.5 MLS mixing ratios corresponds to that found in global comparisons of the ozone mixing ratio by ver.2.2 and ver.1.5 for selected levels [*Froidevaux at al.*, 2008]. They reported lower abundances of ozone by ver.2.2 near 100 hPa (in Umkehr layer 3), near zero change at 15−20 hPa (in Umkehr layer 5), and larger abundances near 1 hPa (in Umkehr Layer 9). The same pattern is seen in Figure 1.

2.4. Data Comparison: Standard Statistical Approach

[11] Standard statistical characteristics of the daily relative differences between the ozone content in Umkehr layers (ground-based minus satellite data in percent of ground-based value) are shown in Table 1, both for MLS v1.5 and v2.2. There is a good correspondence (bias ∼ ±5%, standard deviation <10%) in the layer ozone by two compared systems above layer 4. This also holds for layer 4 if only UMK92 retrieval is considered. In the lower stratosphere (layer 2+ and layer 4) we found an agreement between the Umkehr (UMK04 for layer 4) and MLS data; that is, the correlation coefficient is ∼0.9. However, bias or standard deviation are larger. MLS and Umkehr ozone profiles cannot fully describe ozone variability in the lower stratosphere because of appearance of laminae, which are very local phenomena, and it is not well reproduced by the ground-based and satellite retrievals.

[12] Figure 2 illustrates a correspondence between UMK92 and MLS v.1.5 ozone content in layers 4 and 8+. Figure 3 shows time series of the Umkehr ozone profile superimposed on MLS v.1.5 layer ozone. Knowing ozone

Table 1. Mean Value, Standard Deviation of the Relative Differences, Dobson Umkehr Minus MLS Layer Ozone in Percent of the Ground Value, and the Correlation Coefficient Between Dobson and MLS Data for Various MLS Retrievals and Dobson Umkehr Retrievals[a]

Umkehr Layer	MLS Ver.1.5 Bias SD Cor	MLS Ver.2.2 Bias SD Cor
	UMK92	
2 + 3	−6.47 14.61 0.92	−7.12 15.23 0.93
4	−5.32 6.71 0.86	−3.78 6.76 0.89
5	−5.73 10.05 0.62	−3.96 10.77 0.51
6	−6.72 10.22 0.70	−4.85 9.68 0.68
7	−1.72 7.87 0.60	−4.95 9.54 0.45
8 + 9 + 10	−0.38 7.81 0.66	−2.49 8.93 0.61
	UMK04 SZA$_{min}$ = 60°	
2 + 3	−11.6 17.34 0.92	−9.35 14.10 0.93
4	−16.8 12.78 0.85	−17.1 13.13 0.85
5	−3.57 9.25 0.73	−2.30 9.45 0.73
6	1.02 8.41 0.81	−2.13 8.13 0.82
7	−4.94 7.93 0.56	−7.64 9.36 0.44
8 + 9 + 10	−2.38 9.56 0.75	−4.64 10.85 0.65
	UMK04 SZA$_{min}$ = 70°	
2 + 3	−12.3 15.15 0.90	−9.64 16.10 0.91
4	−17.4 12.97 0.86	−17.7 12.60 0.86
5	−3.42 8.76 0.69	−2.46 9.39 0.73
6	0.81 8.61 0.80	2.15 8.24 0.81
7	−6.14 8.92 0.49	−8.10 9.38 0.73
8 + 9 + 10	−3.75 10.96 0.74	−5.89 11.46 0.66
	UMK04 SZA$_{min}$ = 80°	
2 + 3	−12.7 15.12 0.94	−10.3 11.33 0.96
4	−9.15 9.01 0.89	−9.56 9.33 0.91
5	−1.11 7.91 0.76	−0.71 8.77 0.78
6	1.28 8.15 0.82	2.44 7.87 0.84
7	0.91 6.99 0.69	−1.61 8.64 0.65
8 + 9 + 10	5.98 8.10 0.68	2.84 9.73 0.62

[a]Bias: mean value; SD: standard deviation; Cor: correlation coefficient. MLS Retrievals: v1.5 and v2.2. Standard UMK92 and UMK04 supposed different minimum SZA during the Umkehr observations.
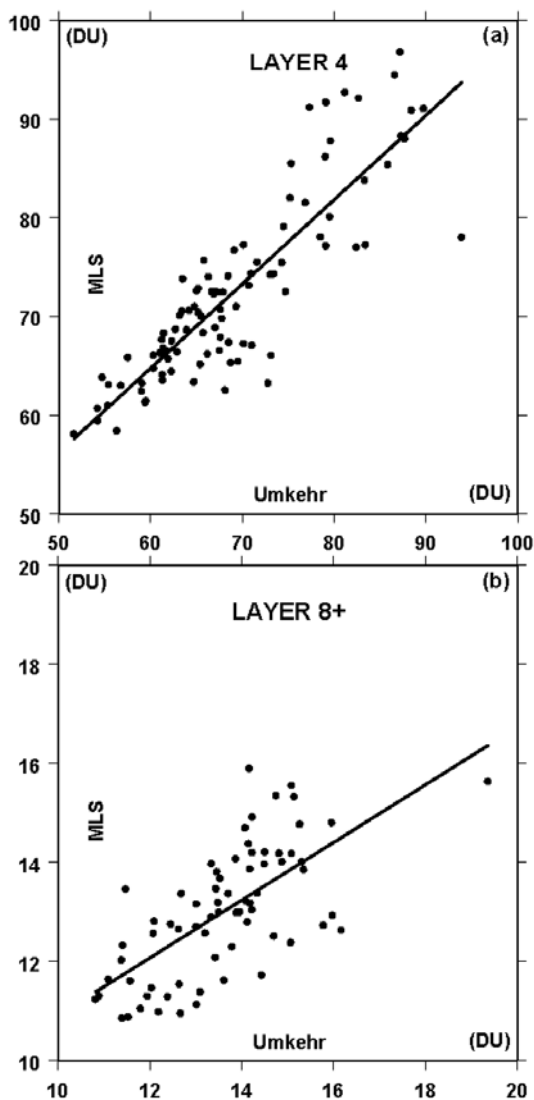
Figure 2. Scatterplot of MLS v1.5 layer ozone versus collocated Dobson Umkehr layer ozone based on UMK92 algorithm: (a) Umkehr layer 4; (b) Umkehr layer 8+.

Figure 3. Time series of MLS v1.5 (open circles) and the Dobson Umkehr layer ozone based on UMK92 algorithm (solid circles) for the period 2004–2006: (a) Umkehr layer 4; (b) Umkehr layer 8+.

variability in these layers is especially important for discussing the ozone recovery problem. Ozone in layer 4 (the lower stratosphere) and layer 8+ (the upper stratosphere) are mostly driven by the dynamical and by the chemical processes, respectively. Thus possible sources of the ozone variability can be easily delineated. Figures 2 and 3 corroborate a good agreement between the ground-based and satellite ozone profiles in some regions of the lower stratosphere and the upper stratosphere, in spite of that some of the MLS observations in the lower/middle stratosphere (up to ~50 hPa) and high stratosphere (above 1hPa) are "noisy" in nature. Upper boundary of precision range for individual MLS profiles exceeds 10% for these regions [see *Froidevaux et al.*, 2008, Table 2].

2.5. Data Comparison: Taylor Diagram

[13] Recently, a new statistical tool, Taylor diagram has been proposed for a visualization of correspondence between variou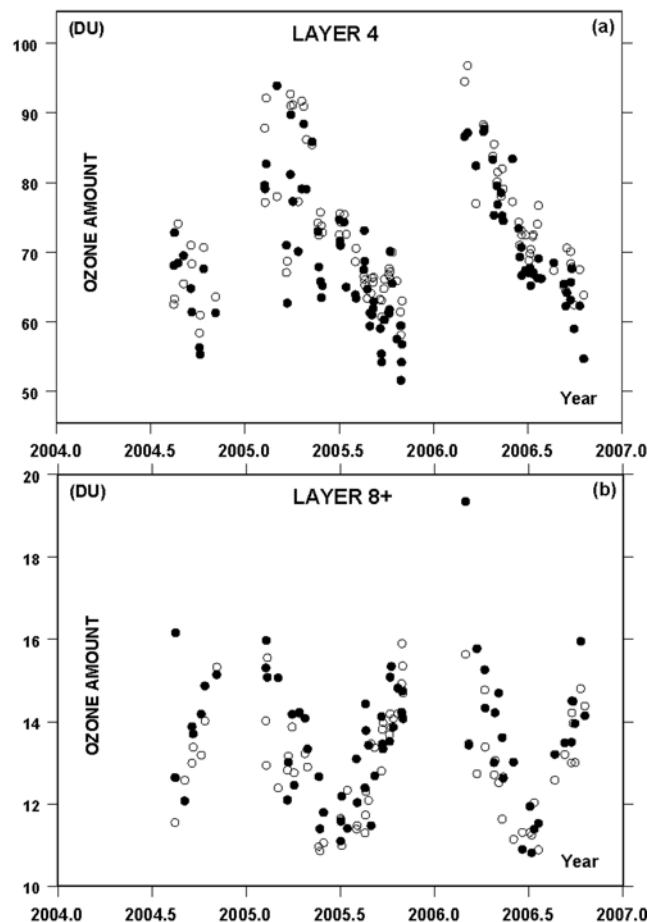s representations (or simulations) of a single variable [*Taylor*, 2001]. The level of agreement between various representations of data is inferred from location of a specific point on polar plot (Taylor diagram). The azimuth angle ϕ pertaining to this point is such that $\cos(\phi)$ is the

Table 2. Normalized Centered Pattern RMS Difference Between MLS Layer Ozone and the Dobson Umkehr Layer Ozone[a]

Layer	Ver.1.5 Ozone Mean 95% Range	Ver.2.2 Ozone Mean 95% Range
	UMK92	
2 + 3	0.54 (0.40 − 0.69)	0.41 (0.25 − 0.55)
4	0.52 (0.42 − 0.64)	0.42 (0.30 − 0.55)
5	1.03 (0.82 − 1.22)	1.06 (0.75 − 1.27)
6	0.92 (0.75 − 1.08)	0.90 (0.65 − 1.14)
7	0.80 (0.67 − 0.95)	0.92 (0.72 − 1.14)
8 + 9 + 10	0.76 (0.64 − 0.92)	0.87 (0.66 −1.25)
	UMK04 SZA_{min} = 80°	
2 + 3	0.58 (0.40 − 0.70)	0.45 (0.26 − 0.66)
4	0.47 (0.41 − 0.53)	0.42 (0.44 − 0.61)
5	0.80 (0.67 − 0.95)	0.80 (0.59 − 1.08)
6	0.70 (0.58 − 0.84)	0.63 (0.44 − 0.86)
7	0.73 (0.63 − 0.85)	0.76 (0.62 − 0.91)
8 + 9 + 10	0.79 (0.65 − 0.94)	0.87 (0.67 − 1.14)

[a]Mean: RMS difference. Results both for standard UMK92 and the short-Umkehr UMK04 retrieval are shown. The 95% confidence interval (95% range) of mean is in parentheses.
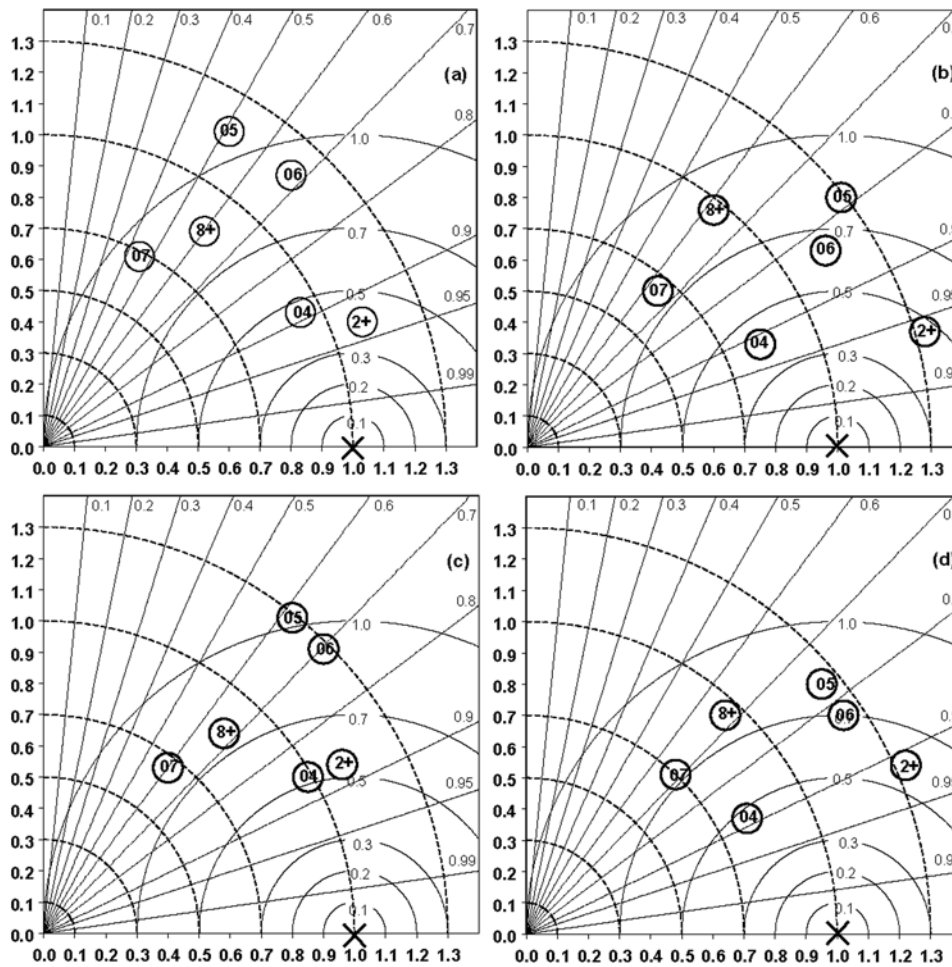
Figure 4. Taylor diagram for MLS layer ozone and collocated Dobson Umkehr data: (a) MLS v2.2 versus UMK92; (b) MLS v2.2 version versus short-Umkehr UMK04; (c) MLS v1.5 versus UMK92; (d) MLS v2.2 version versus short-Umkehr UMK04. Layer number is inside the circle.

correlation coefficient between two sources of the data (e.g., ground-based and the satellite data). A radius from the origin is given as the ratio of root mean square (RMS) of the first model values (here, ozone content in Umkehr layer by MLS) to RMS of the second model values (here, ozone content by UMK92 or UMK04). Full agreement between compared data sources is marked by point with coordinates ($\phi = 0$, radius = 1). Distance between points on Taylor diagram is equal to the centered pattern RMS difference, i.e., RMS of differences having the mean values subtracted from the compared samples. Thus, if we compare behavior of various models (such as ozone content in Umkehr layers by different retrievals) the best correspondence will be found for the point being the closest to the perfect agreement point ($\phi = 0$, radius = 1) [e.g., *Koepke et al.*, 2006; *Krzyścin and Rajewska-Więch*, 2007].

[14] Correspondence between the Umkehr and MLS data for all selected Umkehr layers is illustrated in Figure 4a (MLS v2.2 versus UMK92), Figure 4b (MLS v2.2 versus short-Umkehr UMK04), Figure 4c (MLS v1.5 versus UMK92), and Figure 4d (MLS v1.5 versus short-Umkehr UMK04). Taking into account distances between points on Taylor diagram and the point representing perfect agreement (cross sign in Figure 4) it appears that the Umkehr and MLS

layer ozone are in closer agreement in the lower stratosphere (layer 2+ and 4) than in other stratospheric levels. The lowest correspondence is for layer 5 and layer 8+ for UMK92 and the short-Umkehr UMK04 retrieval, respectively.

[15] The mean values are subtracted from the compared data. Thus Taylor diagram provides a measure of agreement in terms of the correlation coefficient combined with the ratio of the variability of the compared data sets. In spite of a large bias between the Umkehr and MLS layer ozone in the lower stratosphere (as shown in Table 1) it appears that the ground-based and satellite data are in reasonable agreement.

[16] A statistical test to find if differences between points' positions on Taylor diagram are statistical significant is not yet proposed. Here we apply the bootstrap methodology to estimate the significance of such differences. We construct a bootstrap sample of possible locations of the point on Taylor diagram. From all pairs of the Umkehr and MLS layer ozone values for selected Umkehr layer we randomly draw (with replacement) pairs and build an artificial sample having size of the compared original data sets. For each Umkehr layer, the procedure is repeated 1000 times. Table 2 shows 95% confidence range of the centered pattern RMS

difference between Umkehr Dobson layer ozone (by UMK92 and the short-Umkehr UMK04 retrievals) and MLS layer ozone (v1.5 and v2.2). The confidence range provides a measure of possible scatter of the point location on Taylor diagram relative to {0,1} point that is caused by uncertainties of the retrievals.

[17] An inspection of the values shown in Table 2 provides that UMK92 and the short-Umkehr UMK04 retrieval perform very similarly when compared with the satellite data. MLS v2.2 and v1.5 layer ozone behave almost in the same way in comparisons with the Dobson layer ozone. We cannot definitely decide which version of MLS agrees better with the ground-based data. The agreement between ground-based and satellite data (MLS v1.5) in layer 4 is better than that found in all higher layers because the 95% confidence ranges do not overlap.

3. Summary and Conclusions

[18] The Umkehr measurements of ozone vertical profile taken at Belsk observatory by the Dobson spectrophotometer are compared with Aura MLS measurements during the site overpasses in the period 2004–2006. The ozone mixing ratios obtained from MLS v1.5 and v.2.2 algorithm are integrated over layers corresponding to those used in the ground-based algorithms. Various retrievals for the ground-based Umkehr measurements are also examined: standard UMK92 and the newest UMK04 for assumed different minimum SZA during Umkehr observations (60°, 70°, and 80°).

[19] Standard statistical analyses are applied to the collocated pairs of the ground-based and satellite data. Parameters, such as bias, standard deviation, the correlation coefficient are calculated. Results of the comparison are visualized on scatterplots, time series plots, and Taylor diagram. The bootstrap technique is developed to find layer and retrieval yielding the best agreement between the ground-based and satellite data (in terms of the lowest value of the centered pattern RMS difference).

[20] There is an opinion that Dobson Umkehr measurements are too noisy to monitor short-term variability in atmospheric ozone but the technique is capable of monitoring long-term changes in monthly mean ozone [Petropavlovskikh et al., 2005]. However, a correspondence between individual profiles taken from the ground-based and satellite measurements is found in the stratosphere (between ∼250 hPa and ∼1 hPa). Mean differences in layer ozone are usually below 10%. In the midstratosphere and the upper stratosphere region (pressure <30 hPa, layers 5–8+), the mean difference is even smaller ∼5% and standard deviation of the relative differences are less than 10%. High correlation coefficient between the ground and MLS data exceeding 0.8 has been found for many Umkehr layers. Such high correlation is partially related to the Umkehr and MLS a priori profiles having in some layers large seasonal course that increases a correlation between two data sets. To estimate how seasonality affects the correlation coefficient, the mean seasonal course is subtracted from the daily data. Then, the correlation coefficients for remaining relative differences is calculated. We found lower correlation coefficients of about 0.5 but they are still statistically signifi-

cant. The performance of the Umkehr retrievals (UMK92 and UMK04 with the option to choose various minimum SZA during the measurements) are quite similar when compared against the same MLS retrieval version.

[21] The statistical methodology developed in the paper dealing with uncertainty of the point location on the Taylor diagram leads to conclusion that the short-Umkehr UMK04 retrieval provides high-quality ozone profile. This finding is very important for analyses of our historical ozone profile data. Many short-Umkehr measurements were made since the beginning of the Umkehr measurements at Belsk (March 1963). The measurements were not processed because up to now only standard UMK92 retrieval has been used for the ozone profile calculation that requires lower minimum SZA than typically found at Belsk during the late autumn/early winter subperiod of the year.

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