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Intercomparison of Satellite and Ground-Based Ozone Total Column Measurements

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Abstract—Ozone total column (OTC) measurements made in 2009–2012 near St. Petersburg by a Fourier Transform Infrared (FTIR) spectrometer (Peterhof, St. Petersburg State University (SPbSU)), an M-124 filter ozonometer, and a Dobson spectrophotometer (Voeikovo, MGO), as well as measurements made by a spectrometer ozone monitoring instrument (OMI) (onboard the AURA satellite) have been analyzed and compared. Comparisons have been performed both between ensembles of ground-based measurement data, as well as between ground-based and satellite data. It has been shown that the standard deviation for all devices is 2.5–4.5%; here, the FTIR and Dobson instruments measuring the direct sun are in better agreement with OMI than the M-124 ozonometer measuring the zenith-scattered solar radiation as well. A seasonal cycle in discrepancy with amplitude of 1.5% has been detected between two series of OTC measurements made by M-124 and OMI instruments for a total of 850 days. In fall and winter, the ground-based measurements underestimate the OTC values in comparison with satellite data; in spring and summer, the situation is reversed: ground-based data overestimate the OTC values. Also, it has been revealed that FTIR measurements systematically overestimate the OTC values in comparison with other instruments: from 1.4% (for Dobson) to 3.4% (for OMI). Taking into account the spatial and temporal discrepancy of independent ensembles of measurements and an analysis of standard deviations between ground-based and satellite measurement data, the FTIR spectrometer (SPbSU) can be recommended for OTC satellite data validation.

Keywords: ozone total column, atmospheric remote sensing methods, Fourier spectroscopy, satellite measurements validation

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INTRODUCTION

Changes in the content of radiatively active and atmospheric ozone-depleting gases in the Earth's atmosphere and their influence on weather and climate of the planet constitute a key problem in modern physics and chemistry of the atmosphere. Therefore, constant monitoring of their content is critical for understanding the Earth's climate formation and forecasting its changes. A key role in the Earth's climate formation is played by atmospheric ozone. Being a greenhouse and toxic gas in the troposphere, ozone controls the thermal structure of the stratosphere and UV surface luminosity.

In 1997–2001, the total global ozone column was 3% less than its total column before the 1980s (WMO, 2003). The decrease in the ozone total column (OTC) depends on latitude: no significant reduction can be found in the tropics, unlike the decrease by 3–6% at latitudes from 30 to 60°, depending on the hemisphere. Current views suggest that the decrease in OTC is caused by an increased content of chlorine and bromine compounds (due to anthropogenic impact), the growth of which was recorded by local and remote (ground-based and satellite) measurements. The problem of preventing the destruction of the ozone layer has stimulated the creation and improvement of the integrated global monitoring of OTC, which is the most accessible for measurements and informative parameter of the ozone layer state (Perov and Khrgian, 1989).

Currently this system includes subsystems of ground-based and satellite measurements of OTC. The ground-based measurement network uses mainly Dobson, Brewer, and M-124 instruments. The satellite measurements of OTC are conducted by different methods: by interpreting the measurements of reflected and scattered solar radiation and outgoing thermal radiation in different spectral ranges (Timofeev, 2010).

One important problem is the intercalibration of different measurement systems or the validation of satellite measurements of OTC by comparison with standardized ground-based measurements.

GROUND-BASED AND SATELLITE MEASUREMENTS OF OTC

Since the early studies of the atmospheric ozone layer, many different types of ground-based instrumentation have been proposed for OTC measurements. As early as in the 1930s, Dobson spectrophotometers (Dobson, 1957) pioneered regular observations of OTC and to date have remained the most accurate instruments for measuring OTC. In the 1960s, M-83 filter ozonometers appeared and later were replaced by M-124 ozonometers (Gushchin and Sokolenko, 1987). Since the mid-1970s, automated Brewer spectrophotometers appeared (Brewer, 1973). The World Meteorological Organization (WMO) united most of the OTC observation stations into a world ozone network, and the abovementioned three types of instruments became its basis.

This paper analyzes ground-based measurements of OTC using two instruments of the Main Geophysical Observatory (MGO) at Voeikovo (59.95° N, 30.70° E): a Dobson spectrophotometer and an M-124 filter ozonometer, as well as measurements of spectra of direct solar radiation by a Bruker 125HR FTIR spectrometer of St. Petersburg State University (SPbSU) conducted in Peterhof (59.88° N, 29.82° E).

Dobson spectrophotometer no. 108 (MGO) serves as a reference instrument for the ozonometric network of the Federal Service for Hydrometeorology and Environmental Monitoring (Rosgidromet) and has been regularly (once every 4 years) tested in international comparisons with the WMO reference instrument. From 1984 to 2009, the discrepancy with the results of measurements on the WMO reference instrument was no more than 1%. Normally, direct sun observations are performed with an error of a single OTC measurement of no more than 2%.

M-124 filter ozonometers use UV optical filters with two spectral ranges of a width of around 20 nm and with maxima at wavelengths of 302 and 326 nm (Shalamyanskii, 1993). Long-term measurements using an M-124 ozonometer have shown that their error in a single measurement of OTC does not exceed 5–8% and the error in the daily average OTC value is 3–4%. OTC observations using M-124 ozonometer no. 403, which is a working instrument for the Voeikovo ozonometric station, have been conducted daily (eight sessions per day). On clear days, parallel observations by a Dobson spectrophotometer are conducted, and the maximum discrepancies with this instrument normally do not exceed 10 DU.

The specific features of the Bruker 125HR FTIR spectrometer used to measure the spectra of direct solar infrared radiation with high resolution in SPbSU were described in detail in (Poberovskii, 2010). A IR-method designed as such to obtain data on OTC from measured spectra was considered in (Virolainen et al., 2011), which also described the potential shortcomings of this method. The measurements in stable atmospheric conditions yield an error of a single measurement of OTC of around 2–3%.

The satellite Ozone Monitoring Instrument (OMI) (Levelt et al., 2006) continues the series of horizontally scanning spectrometers for nadir measurements of outgoing (reflected and scattered) radiation in different spectral ranges, such as TOMS, GOME, and SCIAMACHY. The OMI operates onboard the American satellite AURA launched in 2004 to near-polar sun-synchronous orbit. The instrument measures spectra of outgoing radiation in the 270–500 nm range with a resolution of ~0.4 nm. The scanning mechanism of OMI makes it possible to conduct daily global mapping of the OTC field with a spatial resolution at a nadir of approximately 13 × 24 km^2. To extend the series of long-term measurements using Total Ozone Mapping Spectrometer (TOMS) satellite data (this program was launched in 1978), the OMI measurement data are interpreted using TOMS algorithm version 8. The stated error in OTC measurements using this algorithm is less than 2% (Bhartia, 2002).

ANALYSIS OF GROUND-BASED OTC MEASUREMENTS

This paper interprets IR measurement data with the help of the PROFFIT software package (Haze et al., 2004) developed at the University of Karlsruhe (Germany) and used at a number of stations of the international Network for the Detection of Atmospheric Composition Change (NDACC). For each day of spectrometric measurements, meteorological data (pressure and temperature profiles) obtained with the help of the automatic e-mail service of the NASA Goddard Space Cen- 1
ter (http://www.nasa.gov/centers/goddard/missions/ 1
index.html), as well as a priori data on the profiles of atmospheric parameters derived from the Whole Atmosphere Community Climate Model (WACCM) (http://www.cesm.ucar.edu/working_groups/WACCM/), was specified.

Table 1 demonstrates general data on FTIR as well as the characteristics of measurements and specific features of the solution of the inverse problem of OTC determination (spectral channels, resolution, relevant gases, and input parameters). For all available spectral measurements of solar radiation in the ozone absorption band of 9.6 μm (a total of 1190 spectra), we obtained OTC data in the St. Petersburg area for 189 days from April 2009 to March 2012 inclusively. For each of the days, data on individual measurements were summed and averaged. The number of spectra measured on different days varies from 1 to 18.

The results of comparisons of OTC measurements using all the three ground-based methods are demonstrated in Table 2. It should be noted that the number of comparisons differs for individual pairs of methods due to different numbers of pairwise measurements. The comparisons were made at the level of daily aver-

Table 1. Characteristics of FTIR measurements and specific features of their interpretation

Parameter	Characteristics
Spectroscopy	HITRAN 2008
Temperature profiles $T(p)$	Diurnal profiles NCEP NCEP
Interpreting package	PROFFIT 9.6
Spectral ranges, cm^{-1}	991.25-993.80 1001.47-1003.04 1005.00-1006.90 1007.35-1009.00 1011.15-1013.55
Climatology (a priori profiles)	WACCM (the same for all seasons)
Relevant gases	H_2O, CO_2, C_2H_4, O_3 (668), O_3 (686)
Instrument	Bruker 125HR FTIR spectrometer
Spectral resolution, cm^{-1}	~0.005
Measurement points	Peterhof--St. Petersburg (59.88° N, 29.82° E)
Measurement period	04.2009–03.2012 (189 days)

Table 2. Comparison of ground-based measurements by Dobson, FTIR, and M-124 instruments

Pairs of compared instruments	Number of comparisons	Mean square error, DU (%)	Mean error, DU (%)	Standard deviation from mean error, DU (%)	Correlation coefficient
Dobson–M-124	78	8.8 (2.6)	1.9 (0.6)	8.7 (2.5)	0.97 ± 0.01
FTIR–Dobson	74	12.8 (3.7)	5.0 (1.4)	11.9 (3.4)	0.95 ± 0.01
FTIR–M-124	186	16.6 (4.8)	9.8 (2.8)	13.5 (3.9)	0.96 ± 0.01

age values and calculations of the following three error parameters:

(*) mean square error: $S = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(x_i - y_i)^2}$;

(*) mean error:

$$M = \frac{1}{N}\sum_{i=1}^{N}(x_i - y_i); \qquad (1)$$

(*) standard deviation from the mean error: $\sigma = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(x_i - y_i - M)^2}$.

In calculating the percentile errors, the absolute values in Dobson units given in Table 2 referred to ensemble-averaged OTC measurements by the first of the pair of instruments listed in column 1. Analyzing Table 2, one can see that the best agreement is observed between measurements by Dobson and M-124 instruments. The systematic differences are only 1.9 DU, or 0.6%; the mean square error is 8.8 DU, or 2.6%; and the standard deviation from the mean error is 8.7 DU, or 2.5%. These small differences are explained by the fact that both instruments measure OTC at the same point and the M-124 instrument is calibrated by Dobson spectrophotometer measurements. A comparison of OTC-measured values between FTIR and Dobson instruments revealed a mean error of 5.0 DU (1.4%), a mean square error of 12.8 DU (3.7%), and a standard deviation from the mean error of 11.9 DU (3.4%). In this case, FTIR gives higher values of OTC in comparison with the Dobson instrument. One partial explanation of errors is the differences of measurement points (approximately 50 km). The comparison between FTIR and M-124 measurements shows that the systematic error increased to 9.8 DU (2.8%), the mean square error increases to 16.6 DU (4.8%), and the standard deviation from the mean error increased up to 13.5 DU (3.9%). The increased errors are caused by both the differences in measurement points and the lower accuracy of measurement by M-124. In this case, all the three instruments are characterized by high correlations between pairwise measurements (with a correlation coefficient of 0.95–0.97).

It can be clearly seen from the table that the FTIR measurements overestimate the OTC value in comparison with measurements by other ground-based instruments. A similar effect was detected previously in comparisons of UV-measurements by Dobson and Brewer instruments with FTIR (Viatte et al., 2011) and can be explained by the inconsistency between

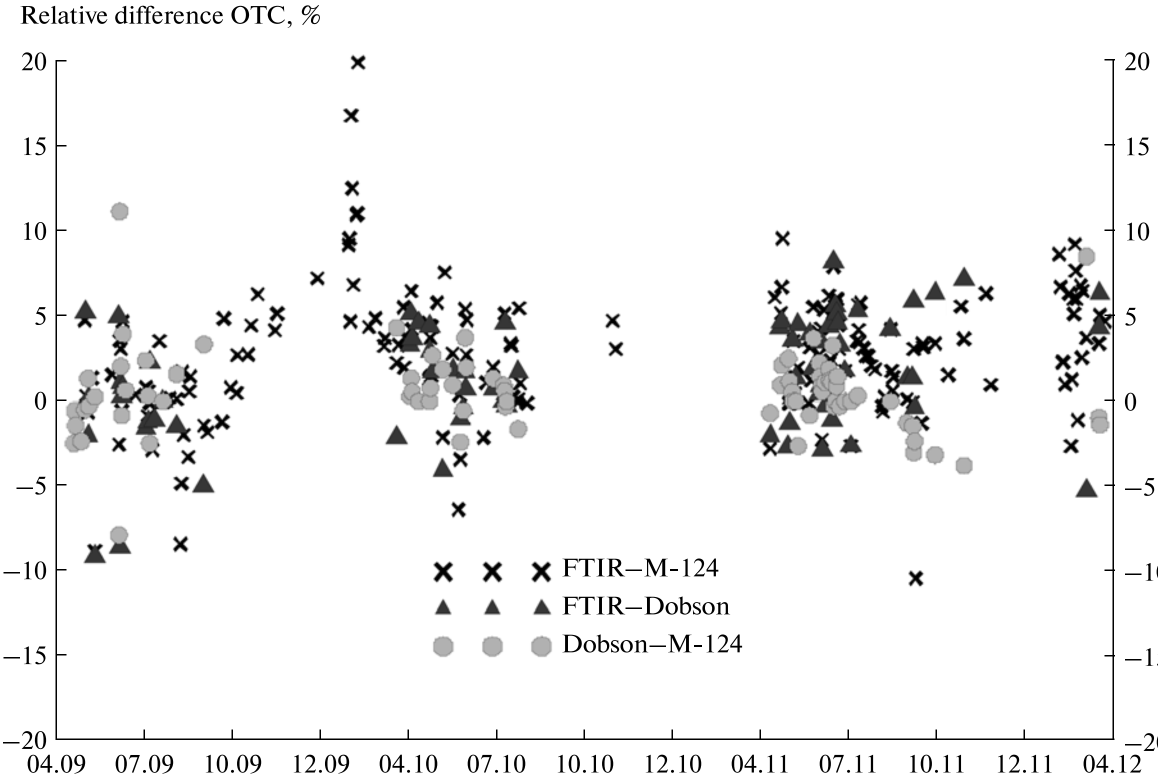

Fig. 1. Seasonal variation in errors of OTC data obtained with different ground-based instruments.

quantitative characteristics of molecular ozone absorption in the UV and IR spectral ranges.

The statistical data presented above refer to the entire observation period. It is interesting to consider the specific features of the temporal variation of comparison results. Figure 1 shows the seasonal variation of the relative error in OTC data obtained using different ground-based instruments. The data are for shown for those days when pairwise measurements by different instruments were available. It can be seen from Table 2 that this number is 186 days for the pair of FTIR and M-124, 74 days for the pair of FTIR and Dobson, and 78 days for the pair of Dobson and M-124. It can be seen from the figure that the main days for comparisons fall on summer, because the measurements by Dobson and FTIR instruments are conducted in sunny cloudless days.

Analyzing Fig. 1, one can note that, during the entire measurement period (three years), the systematic error between Dobson and M-124 measurements remained the same and the OTC measurements by the Dobson instrument exceed those by M-124 approximately by 0.6% (see Table 2). At the same time, the average error between FTIR and other instruments increases. The difference between FTIR and other instruments in 2009 was almost vanishing for the Dobson instrument and around 2% for M-124, whereas this difference by 2012 increased to 3.5% (on average 1.4% and 2.8%, respectively; see Table 2). This increase in the systematic difference can be associated with both a change in the FTIR operating mode and specific features of the sample for comparison. For example, the sample incorporated almost no joint measurements by different instruments from the fall 2010–spring 2011 and 2011/2012 winter periods. The scattering in the FTIR–M-124 difference in Fig. 1 exceeding 10% in January 2010 was apparently caused by specific features of measurements by M-124 at that time because, as will be shown hereafter, similar errors during this period can be found also in comparisons between M-124 and OMI data.

Figure 2 shows correlations between OTC values obtained by different ground-based instruments for the entire period of comparisons. The left panel indicates the correlations between FTIR and M-124 and the right panel indicates the correlations between FTIR and Dobson. Also, each of the figures includes a straight line marking a linear approximation of comparison results. The slope of this line is 0.96 for the FTIR–Dobson pair and 0.91 for the FTIR–M-124 pair. It can be seen that the previously detected systematic overestimation of data measured by FTIR in comparison with M-124 is observed usually for high OTC values. Several individual scatters in the average values of OTC may have a random character. The FTIR–Dobson pair reveals no such apparent pattern. Thus, the systematic error in measurements by FTIR

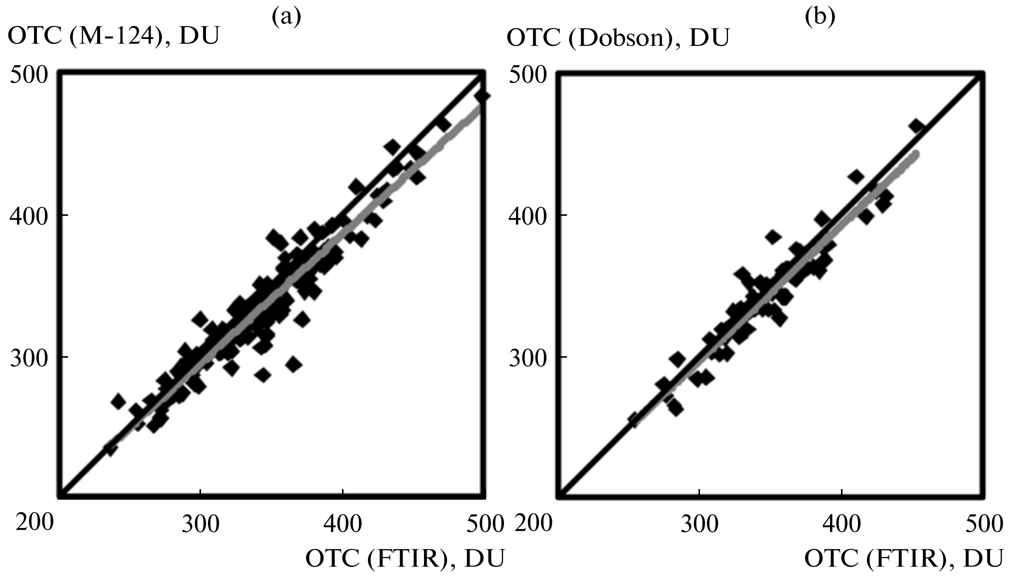

Fig. 2. Correlation between OTC values obtained in 2009–2012 by (a) FTIR and M-124 instruments and (b) FTIR and a Dobson spectrophotometer.

and M-124 instruments can result from less accurate measurements by the M-124 instrument.

In general, the results of OTC comparisons between FTIR (Peterhof, SPbSU) and data of independent ground-based measurements in Voeikovo make it possible to conclude that interferometric measurements are in better agreement with the Dobson instrument than with M-124. Taking into account the resulting estimates for the consistency between these two instruments and the fact that Dobson is a reference instrument for OTC measurements, one can recommend using FTIR for validating satellite measurements.

COMPARISON BETWEEN GROUND-BASED AND SATELLITE MEASUREMENTS OF OTC

The first results of extensive comparisons of ground-based measurements of OTC by Dobson and Brewer instruments and OMI satellite data are presented in (Balis et al., 2007). These results revealed a good agreement between ground-based and satellite measurements (within 1%) when TOMS algorithms are used for comparisons with 18 instruments measuring OTC in Europe, Canada, Japan, the United States, and Antarctica. McPeters et al. (2008) compared the measurements by OMI with 76 ground-based stations of OTC measurements by Dobson and Brewer instruments operating in the Northern Hemisphere. These comparisons showed that the satellite measurements yield higher values than the ground-based measurements by 0.4% on average. Buchard et al. (2008) revealed that the difference between OMI and ground-based measurements conducted at two French stations is in the range of 5%. Ialongo et al. (2008) compared OTC data measured by OMI with ground-based measurements conducted in Rome to reveal a good agreement for a variety of measurement conditions with systematic differences of 1.8%. A comparison of OMI data with ground-based measurements by a Brewer instrument at five Spanish stations showed generally a very good agreement; however, satellite values of OTC were higher approximately by 2%. The maximum values of errors reached 5% with a considerable seasonal variation (Anton et al., 2009).

In the present paper, we compare ground-based measurements of OTC made by FTIR (Peterhof), and M-124 and Dobson (MGO, Voeikovo station) instruments with data from OMI satellite measurements. As was mentioned above, the OMI data were interpreted using the TOMS algorithm version 8. This algorithm uses measurement data on outgoing radiation in several spectral UV-bands (~310–360 nm) with a resolution of around 1 nm. The technique is based on the regression approach: using a radiation model, the field of outgoing radiation is precalculated for different values observation conditions and different parameters of the atmosphere and underlying surface. Then the measurement results are used to determine the OTC magnitude corresponding to this radiation (McPeters et al., 1998). The OMI measurement data were taken from the open-access database available at http://avdc.gsfc.nasa.gov/index.php?site=1593048672&id=28 for the St. Petersburg station.

We compared ground-based and satellite data for 2009–2012, when the FTIR instrument was operating in Peterhof. Satellite measurements were used by averaging data obtained within 500 km of the place of ground-based measurements. Table 3 shows the statistical characteristics of ensembles of OTC measure-

Table 3. Comparison of ground-based measurements of OTC with OMI satellite data

Pairs of compared instruments	Number of comparisons	Mean square error, DU (%)	Mean error, DU (%)	Standard deviation from mean error, DU (%)	Correlation coefficient
Dobson–OMI	75	11.5 (3.3)	5.5 (1.6)	10.1 (2.9)	0.96 ± 0.01
M-124–OMI	850	14.8 (4.5)	–0.47 (–0.14)	14.8 (4.5)	0.96 ± 0.01
FTIR–OMI	178	15.5 (4.5)	11.8 (3.4)	10.0 (2.9)	0.98 ± 0.01

ments by ground-based instruments and by the OMI satellite instrument: the mean error, the mean square error, and the standard deviation from mean error (1). The ensembles vary in sample size, since we compared data of available pairwise measurements by different instruments. Here, as before, in calculating the percentile errors, the absolute values in Dobson units refer to ensemble-averaged OTC measurements by the first of the pair of instruments listed in column 1.

Analyzing the average error, one can see that the Dobson instrument systematically overestimates the TOC values as compared with OMI by approximately 5.5 DU (1.6%) and FTIR overestimates its values by around 11.8 DU (3.4%). M-124 has no systematic error with satellite data; however, these two instruments were compared for all seasons (850 days over 3 years), while the remaining ground-based instruments measured mainly in spring and summer. Here, it is interesting to note that the standard deviation from the mean error, which partially characterizes the measurement error by instruments, is the same for Dobson and FTIR in comparison with OMI and is equal to 10 DU (2.9%). For M-124, the standard deviation from the mean is 14.8 DU (4.5%), which means that the measurement error by the ground-based instrument is larger. The coefficient of correlation between ground-based and satellite measurements of OTC for all ensembles is 0.96 (M-124 and Dobson) and 0.98 (FTIR).

To understand the specific features of the systematic error of satellite and ground-based measurements, we analyze the seasonal variation of the relative error in M-124 and OMI data shown in Fig. 3. The data are shown for the period from April 2009 to April 2012. Additionally, the figure shows a straight line—a linear interpolation of the results—showing the trend in

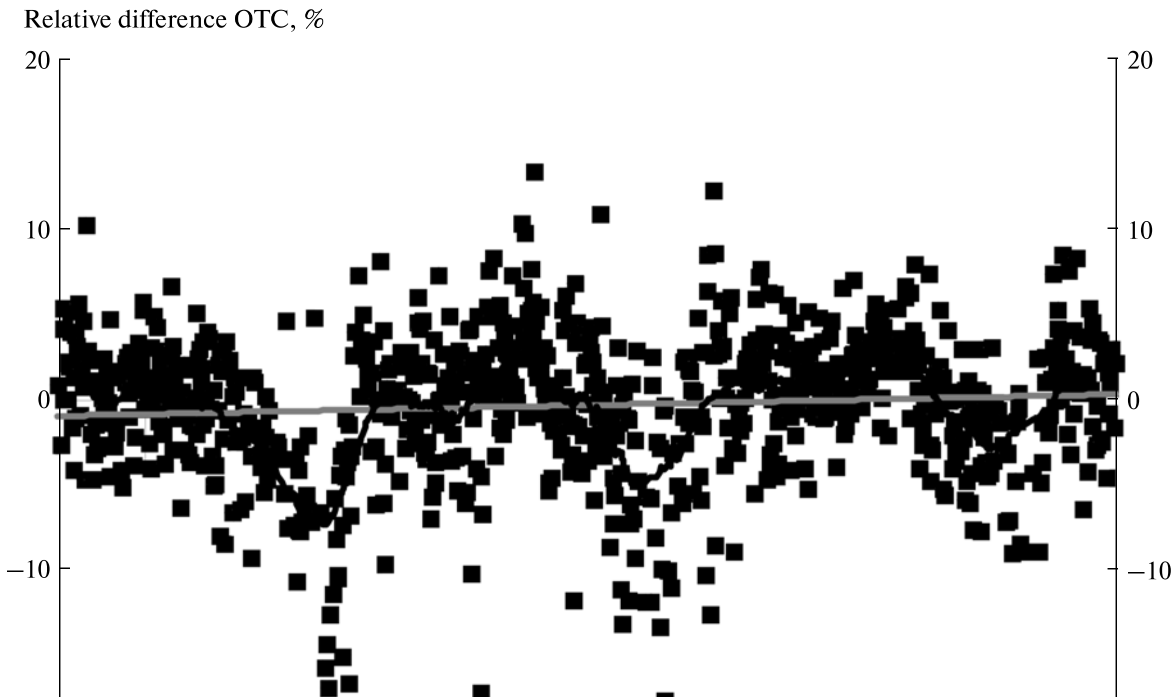

Fig. 3. Seasonal variation in errors of OTC data for M-124 and OMI.

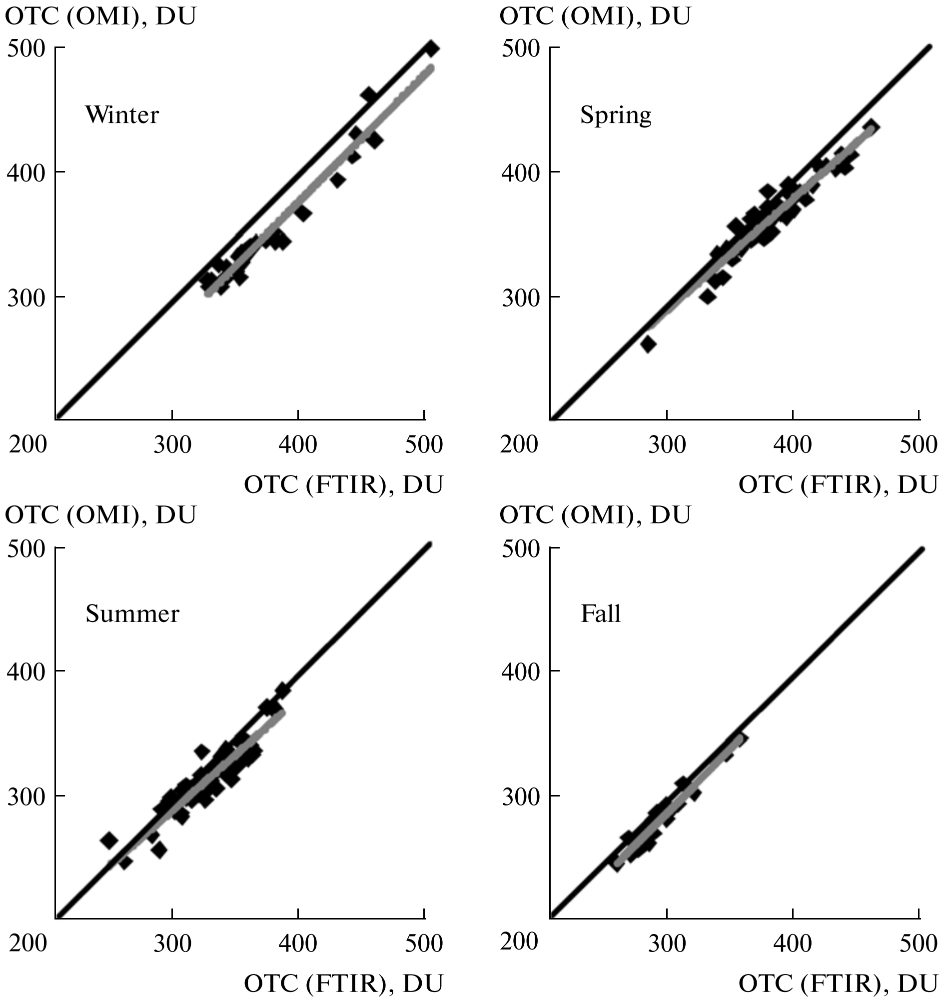

Fig. 4. Correlation between OTC values obtained by FTIR and OMI instruments for different seasons in 2009–2012.

errors over the period considered and a curve—the moving average—allowing one to track the seasonal variation in errors. Almost no systematic differences can be found over the entire period (the mean value varies from –0.9% in 2009 to 0.2% in 2012). At the same time, there is a pronounced seasonal variation in errors. In winter, the ground-based data are systematically lower than satellite data on OTC; in summer, the situation is the reverse: the M-124 data are higher than satellite data (up to 5 % in July–September). In general, a decrease of errors in winter with time is observed. Specifically, the average errors reached 7% in the 2009/2010 winter, 5% in the 2010/2011 winter, and 3% in the 2011/2012 winter. This may be due to both the different character of winters and the increased accuracy of measuring instruments.

Also, we analyzed the statistics both for the entire period of measurements and for seasons separately. For example, the mean error between M-124 and OMI (1) for fall and winter is –3.8 and –4.6 DU, respectively. For spring and summer, these values are 2.2 and 4.9 DU, respectively. All of these mean values are within ±1.5%. The standard deviation from the mean error for these two instruments is maximal in winter: up to 6.6% (22.4 DU). In the remaining seasons of the year, its value is 3.7–4.2% (11–13 DU). It can be concluded that the OTC measurement accuracy in winter is the lowest, which is likely associated with the use of M-124 in winter in the scattering mode and low angles of the Sun, leading to increased measurement errors.

Analyzing the same data for the FTIR–OMI pair, we can note that the mean error peaks in winter; the FTIR data on OTC exceed the OMI data by 5.5% (20 DU) on average. At the same time, no changes in the standard deviation from the mean are observed: its value is 2–3% for all seasons. This indicates that the FTIR instrument operates stably throughout the year. The systematic differences from satellite data in winter may be in part due to the fact that, at a low Sun, the OTC values are measured in different air masses for satellite and ground-based instruments. It should be noted that the correlations between ensembles for all seasons vary slightly, constituting 0.93–0.97.

In concluding the comparison between FTIR and OMI ensembles by seasons, we present Fig. 4, which shows correlations in OTC measurements for different seasons in 2009–2012. The figure clearly shows a systematic discrepancy in winter, some growth in systematic discrepancy in spring and summer at higher values of OTC, and minimum systematic and standard errors in fall between the two instruments.

CONCLUSIONS

In this paper we analyzed the ensembles of OTC measurements near St. Petersburg made with ground-based FTIR (Peterhof, SPbSU) and M-124 and Dobson (MGO, Voeikovo station) instruments, as well as with the OMI satellite instrument for the period from April 2009 to April 2012. Based on the study comparisons between OTC ensembles, the following results and conclusions were obtained:

(1) ground-based FTIR measurement data on OTC are in better agreement with data from the reference instrument—the Dobson spectrophotometer (mean difference of 1.4% and standard deviation from the mean of 3.4%)—than with M-124 data (mean difference of 2.8% and standard deviation from the mean of 3.9%);

(2) a seasonal cycle in discrepancy between two series of OTC measurements made by M-124 and OMI instruments (for 850 days) has been detected. In fall and winter, the ground-based instrument underestimates the OTC values in comparison with satellite data by an average of 1.5%; in spring and summer, the reverse (overestimation by 1.5%) occurs. The standard deviations from the mean are a maximum (up to 6.6%) in winter and 3.5–4% in other seasons. The growth of errors in winter is probably due to the increased measurement errors in winter;

(3) the comparison between FTIR and OMI data (178 measurement days) demonstrated a systematic overestimation of ground-based measurement data in comparison with satellite data, which is a maximum (5.5%) in winter and around 3% for the remaining seasons. The standard deviation from the mean for all seasons is stable and constitutes 2–3%;

(4) Taking into account the spatial and temporal discrepancy of independent ensembles of measurements and an analysis of standard deviations between ground-based and satellite measurement data, the FTIR spectrometer (SPbSU) can be recommended for OTC satellite data validation in the St. Petersburg area.

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