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Comparison of the Satellite and Ground-Based Measurements of the Hydrogen Fluoride Content in the Atmosphere

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Abstract—Satellite and ground-based measurements of the hydrogen fluoride (HF) total content (TC) are analyzed and compared. The HF profiles measured with an FTS device on the ACE satellite are used to calculate the TC and compare it with the ground-based measurements near St. Petersburg in 2009–2011. A comparison indicated that the seasonal variations in HF TC based on two independent measurements are in good qualitative agreement. Rare (nine) cases of direct comparison between two measurement types coordinated with respect to time (during the day) and site (no farther than 500 km) gave the following characteristics: the average difference is 8% and satellite data predominate over ground data; the standard deviation of a difference is 7%. In two cases of close measurement pairs (closer than 200 km), a comparison gave differences of 1 and 7%. The statistical characteristics of differences between two measurement types are in good agreement with the independent comparison of the ACE–FTS HF TC measurements with the NDACC network data.

Keywords: Fourier interferometer, total content, hydrogen fluoride, satellite-data validation, total content ground-based measurements

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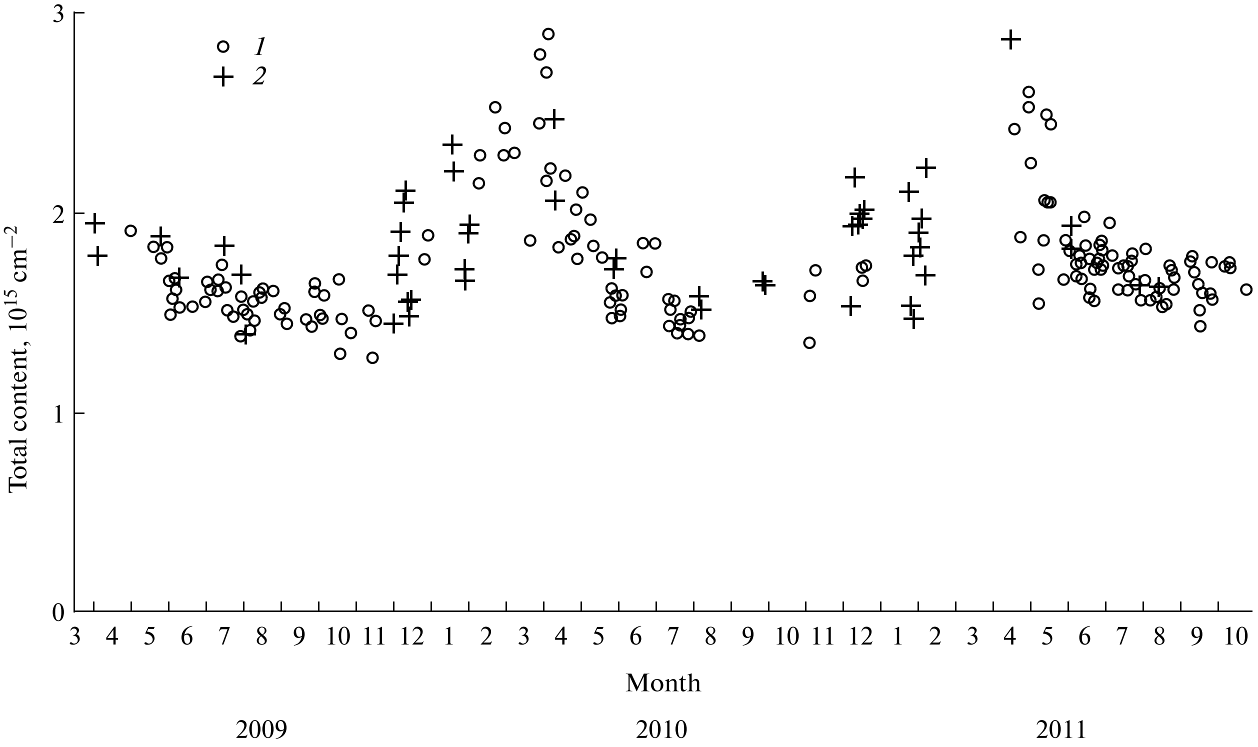
INTRODUCTION

The effect of the gas composition on the atmospheric characteristics, weather, and terrestrial climate, as well as the state of the ozonosphere, was considered during numerous satellite programs devoted to studying the atmospheric gas and aerosol composition using different methods (Timofeyev, 1989; WMO, 2003). The atmospheric chemistry experiment (ACE) with the Fourier IR spectrometer (ACE–FTS) has been one of the most important of these experiments in the last decade (Bernath, 2005). The device measures the direct solar radiation spectra during sunrises and sunsets with a high spectral resolution (0.02 cm^{-1}) in the 750–4400 cm^{-1} region, which makes it possible to determine the vertical profiles of the content of more than 30 gases (Mahieu et al., 2008). One important stage of satellite measurements consists of their validation using independent measurements, including ground-based ones. Such programs of the ACE–FTS data validation are described, e.g., in special issues of *Geophysical Research Letters* (*Geophys. Res. Lett.*, 2005, vol. 32, no. L15S01) and *Atmospheric Chemistry and Physics* (*Atmos. Chem. Phys. Discuss.*, 2008, vol. 8).

Since January 2009, the direct solar radiation spectra in the IR region have been measured on the ground with the spectral complex based on the Bruker IFS–125HR Fourier high-resolution spectrometer (Poberovskii, 2010) at the Atmospheric Physics Department, Faculty of Physics, St. Petersburg State University in Peterhof at a distance of 28 km west from the St. Petersburg center (59.88° N, 29.82° E). These measurements make it possible to determine the total contents (TCs) of many important climatically active gases (Poberovskii et al., 2010a). The same measurements are used to validate different satellite experiments. This work illustrates a comparison of the satellite and ground-based hydrogen fluoride (HF) TC measurements.

SATELLITE AND GROUND-BASED MEASUREMENTS

The sun occultation geometry of ACE–FTS observations makes it possible to measure about 30 solar radiation spectra per day. The spectra were measured in the sighting range varying from 150 km to the upper boundary of clouds with a vertical resolution of 3–4 km. The vertical step of measurements was 1.5–6 km for different geometry. During the first measurement-interpretation stage, the temperature and pressure vertical profiles were determined by analyzing absorption in the CO_2 lines. Absorption in the spectral windows, specially selected for each gas, was subsequently analyzed. These windows were selected in order to minimize the effect of interfering gases for altitudes from the lower mesosphere to the upper troposphere. The



The HF TC measurement from April 2009 to October 2011: (*1*) ground-based measurement in Peterhof; (*2*) ACE–FTS satellite measurements. The distance is no more than 500 km.

vertical profiles for the ratios of the studied gas mixtures, which were interpolated for the vertical grid with a 1-km step, were determined by analyzing solar spectrum successive measurements at different sighting altitudes. Information about the parameters of the molecular absorption fine structure from the well-known HITRAN databank was used when the measurements were analyzed. Thirteen spectral windows in the 1815–4143 cm^{-1} range were distinguished in order to determine HF TC (Batchelor et al., 2009). We emphasize that the sun occultation type of satellite measurements is characterized by a relatively small number of measurements per day and slow variations in the measurement latitude. The ACE–FTS measurements are performed at tropical, middle, and polar latitudes.

The first ground-based measurements of the HF content in Russia are analyzed in (Poberovskii et al., 2010b; Polyakov et al., 2011). Specifically, the satellite and ground-based measurements performed from April 2009 to April 2010 are preliminarily compared in (Polyakov et al., 2011). The present work used the ground-based measurements performed from April 2009 to October 2011.

The solar spectra measured on the ground had a spectral resolution of about 0.005 cm^{-1}, and the sig-

Statistical characteristics of the satellite and ground-based HF TC measurements and their differences

Distance, km	500	1000
Number of comparisons	9	43
Average SPbGU data, mole cm^2	1.62×10^{15}	1.70×10^{15}
Average ACE–FTS data	1.75×10^{15}	1.84×10^{15}
HF TC rmsd according to the SPbGU data, %	16	16
HF TC rmsd according to the ACE–FTS data, %	8	13
Average relative differences, %	The same	8
Rms relative differences,%	11	15
Relative rmsd (standard deviation) differences, %	7	13

nal-to-noise ratio, determined based on the zero signal hash, varied from 400 to 1600 and had a typical value about 1200. The SFIT2 program, which is used at the NDACC network stations, was used to interpret the measurements.

The 4038–4039 cm^{-1} spectral interval was used to determine HF TC. The data on the temperature profile in the atmosphere and (as an initial approximation) on the profile of the water vapor (an interfering gas) mixture ratio from the Aqua satellite level-3 data (AIRS and AMSU_A devices) (http://airs.jpl.nasa.gov/data_products/data_toc/) were also used to interpret ground-based measurements. We estimated that the random component of the TC determination error, based on the TC variability during the periods when the atmospheric states were stable and the device operated, is 1–2%. Note that different sources of the HF TC determination error were analyzed in (Schneider and Blumenstock, 2004). According to the estimates made in this work, the random component of the TC measurement error (at close signal-to-noise values) is 2.7%, and the HF line intensity specification error mainly contributes to the systematic error (4.3%). Similar estimates made in (Senten et al., 2008) indicated that the error total random component is 6% and the systematic error is ~5% (mainly due to the error of the HF absorption line intensity specification). Note that insignificant variations in errors estimated in different works are caused by different spectral intervals used and differences in the equipment characteristics, measurement conditions (solar zenith angles, etc.), and the states of the atmosphere during measurements.

RESULTS OF COMPARISON

The figure shows the daily average HF TC values according to the ground-based measurements and the values obtained by integrating the vertical profiles according to the ACE–FTS 2.2 data, measured in a circle with a radius of 500 km and centered in Peterhof. Note that the measurements performed with two devices very rarely coincide during a day (nine times); therefore, the figure demonstrates the results achieved using two devices during different periods and makes it possible to estimate only similarity in the time variations in the data obtained using two observation methods. The figure indicates that the measurements are in good qualitative and quantitative agreement. Both devices demonstrate HF TC minimums (the vernal–autumnal periods) and maximums (the winter–vernal periods) similar in values and duration and an increase in the HF content variations during the vernal–autumnal periods.

Analyzing a qualitative comparison of two measurement types, we will consider below differences in the results, subtracting the ground-based measurements from the satellite ones, and different statistical characteristics of these differences. Considering the relative difference, we will mean the ratio of a difference to the ground-based measurements. To avoid possible ambiguities, we will evidently indicate the used characteristics of the values and their differences. We will consider that $\bar{x}$ are the sampled average values, $\sqrt{\overline{x}^2}$ are the mean square values, and σ_x are the standard deviations (rms) of random value x represented by sampled values $\{x_i\}_{i=1,n}$

$$\bar{x} = \frac{1}{n}\sum_{i=1,n} x_i, \quad \sqrt{\overline{x}^2} = \sqrt{\frac{1}{n}\sum_{i=1,n} x_i^2},$$

$$\sigma_x = \sqrt{\frac{1}{n-1}\sum_{i=1,n}(x_i - \bar{x})^2}.$$

Common qualitative characteristics of comparisons are presented in the table.

According to the table, a comparison of the satellite and ground-based HF content measurements indicates that average differences in two measurement types are 8% for both disagreement criteria (500 and 1000 km) (in this case the ground-based measurements give smaller HF TC values); the mean square differences account for 11 and 15% for disagreements of 500 and 1000 km, respectively; and the standard deviation of differences are 7 and 13%, respectively.

The distance between two measurement types pronouncedly affects a comparison of the ground-based and satellite measurements of the HF content. When a disagreement is considerable (up to 1000 km), the mean square differences are close to the standard deviation of the HF content (natural variations) during the considered period (16%).

In two cases of comparisons (when the distance between two measurement types is smaller than 200 km), differences were 1 and 7%.

The HF content measurements were previously validated using version 2.2, when the HALOE device satellite data were compared with the balloon (FIRS-2 and Mark-IV) and Fourier spectrometer measurements at the NDACC network (six stations) (Mahieu et al., 2008). Two spatial disagreement criteria (1000 and 500 km) were used in comparisons (except for the Reunion Island tropical station, for which this disagreement was 1200 km). The time correlation was ±24 h.

Average differences for different stations were 6.54–13.9% and standard deviations were 7.42–10.88%. When comparisons of all ground stations were analyzed and the above criteria were used, the average relative difference and standard deviation were 7.4 and 11.4%, respectively. When the spatial disagreement was decreased to 200 km along the latitude, the average relative difference and standard deviation decreased to 2.8 and 8.7%, respectively.

A comparison performed in (Batchelor et al., 2009) indicated that the average and rms differences between the measurements performed in 2007 are considerable

(10.57 and 15.11%, respectively). In 2008 these values were 3.41 and 14.37%, respectively. When more rigid spatial–time criteria of the disagreement between the satellite and ground-based measurement were used, average differences decreased to 5.23 and 1.14% for the measurements performed in 2007 and 2008, respectively; at the same time, rms differences remained rather considerable: 8.88 and 16.81%, respectively.

The differences between the satellite and ground-based HF content measurements performed in Peterhof are in generally good agreement with the earlier comparisons (Mahieu et al., 2008; Batchelor et al., 2009). Taking into account the errors of two measurement types and the spatial–time variations in the HF content, we can state that the ACE–FTS device measures the HF TC with errors of ~5–10%.

CONCLUSIONS

The seasonal variations in the ground-based and satellite measurements are in good agreement. Both methods demonstrate that the seasonal variations in the HF TC are similar and this content variability increases during the winter–vernal period. Quantitative comparisons indicated that ACE–FTS measures the HF TC with errors no worse than 5–10% if the errors of two measurement types and the spatial–time variations in the HF content are taken into account.

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REFERENCES

AIRS data products. http://airs.jpl.nasa.gov/data_products/data_products_toc

Batchelor, R.L., Kolonjari, F., Lindenmaier, R., Mittermeier, R.L., Daffer, W., Fast, H., Manney, G., Strong, K., and Walker, K.A., Four Fourier transform spectrometers and the Arctic polar vortex: instrument intercomparison and ACE-FTS validation at Eureka during the IPY springs of 2007 and 2008, *Atm. Meas. Tech. Discuss.,* 2009, vol. 2, no. 6, pp. 2881–2917.

Bernath, P.F., McElroy, C.T., Abrams, M.C., Boone, C.D., Butler, M., Camy-Peyret, C., Carleer, M., Clerbaux, C., Coheur, P.F., Colin, R., DeCola, P., DeMazière, M., Drummond, J.R., Dufour, D., Evans, W.F.J., Fast, H., Fussen, D., Gilbert, K., Jennings, D.E., Llewellyn, E.J., Lowe, R.P., Mahieu, E., McConnell, J.C., McHugh, M., McLeod, S.D., Michaud, R., Midwinter, C., Nassar, R., Nichitiu, F., Nowlan, C., Rinsland, C.P., Rochon, Y.J., Rowlands, N., Semeniuk, K., Simon, P., Skelton, R., Sloan, J.J., Soucy, M.-A., Strong, K., Tremblay, P., Turnbull, D., Walker, K.A., Walkty, I., Wardle, D.A., Wehrle, V., Zander, R., and Zou, J., Atmospheric chemistry experiment (ACE): mission overview, *Geophys. Res. Lett.*, 2005, vol. 32, no. L15S01. doi 10.1029/2005GL022386

Mahieu, E., Duchatelet, P., Demoulin, P., Walker, K.A., Dupuy, E., Froidevaux, L., Randall, C., Catoire, V., Strong, K., Boone, C.D., Bernath, P.F., Blavier, J.-F., Blumenstock, T., Coffey, M., and Mazière, M., De Griffith, D., Hannigan, J., Hase, F., Jones, N., Jucks, K.W., Kagawa, A., Kasai, Y., Mebarki, Y., Mikuteit, S., Nassar, R., Notholt, J., Rinsland, C.P., Robert, C., Schrems, O., Senten, C., Smale, D., Taylor, J., Tétard, C., Toon, G.C., Warneke, T., Wood, S.W., Zander, R., and Servais, C., Validation of ACE-FTS v2.2 measurements of Cl, HF, CCl_3F and CCl_2S_2 using space-, balloon-, and ground-based instrument observation, *Atm. Chem. Phys.*, 2008, vol. 8, pp. 6199–6221.

Poberovskii, A.V., Makarova, M.V., Rakitin, A.V., Ionov, D.V., and Timofeev, Yu.M., Variability of the total column amounts of climate influencing gases obtained from ground-based high resolution spectroscope measurements, *Dokl., Earth Sci.*, 2010a, vol. 432, no. 1, pp. 656–659.

Poberovskii, A.V., Polyakov, A.V., and Timofeev, Yu.M., Measurements of the hydrogen fluoride total column amount in the atmosphere over the vicinity of St. Petersburg, *Izv., Atmos. Ocean. Phys.*, 2010b, no. 2, pp. 261–263.

Poberovskii, A.V., High-resolution ground measurements of the IR Spectra of solar radiation, *Atmos. Oceanic Opt.*, 2010c, vol. 23, no. 2, pp. 161–163.

Polyakov, A.V., Timofeev, Yu.M., Poberovskii, A.V., and Yagovkina, I.S., Seasonal variations in the total content of hydrogen fluoride in the atmosphere, *Izv., Atmos. Ocean. Phys.*, 2011, vol. 47, no. 6, pp. 760–765.

Schneider, M. and Blumenstock, T., Subtropical trace gas profiles determined by ground-based FTIR spectroscopy at Izana (28° N, 16° W): Five-year record, error analysis, and comparison with 3-D CTMs, *Atmos. Chem. Phys. Discuss.*, 2004, vol. 4, pp. 5261–5301.

Senten, C., De Mazière, M., Dils, B., Hermans, C., Kruglanski, M., Neefs, E., Scolas, F., Vandaele, A.C., Vanhaelewyn, G., Vigouroux, C., Carleer, M., Coheur, P.F., Fally, S., Barret, B., Baray, J.L., Delmas, R., Leveau, J., Metzger, J.M., Mahieu, E., Boone, C., Walker, K.A., Bernath, P.F., and Strong, K., Technical note: New ground-based FTIR measurements at Ile de la Réunion: observations, error analysis, and comparisons with independent data, *Atm. Chem. Phys.*, 2008, vol. 8, pp. 3483–3508.

Timofeev, Yu.M., Satellite methods for studying the gas composition of the atmosphere, *Izv. Akad. Nauk SSSR, Fiz. Atmos. Okeana*, 1989, vol. 25, no. 5, pp. 451–472.

WMO, The role of satellites in WMO programmes in the 2010s, *Tech. Doc. WMO/TD*, 2003, no. 117, p. 127.

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