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Derivation of the Carbon Dioxide Total Column in the Atmosphere from Satellite-Based Infrared Fourier-Transform Spectrometer IKFS–2 Measurements: Analysis and Application Experience

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Abstract—Based on retrospective comparison with the data of ground-based spectroscopic measurements carried out in Peterhof by St. Petersburg State University (SPbSU) and aircraft measurements carried out in the area of the Novosibirsk Reservoir by the Zuev Institute of Atmospheric Optics in 2019–2022, results of application of a new version of the regression technique for determining the total carbon dioxide XCO2 content (the mole fraction of atmospheric CO_2 in dry air) by measurements of the IKFS-2 infrared Fourier spectrometer of the Meteor-M No. 2 Russian meteorological satellite are analyzed. A description of changes made in the technique to improve the accuracy of satellite estimates is given. For example, to compensate for the influence of changes in IKFS-2 characteristics during a long flight on the XCO2 estimates, they are calibrated based on the results of ground measurements from the NOAA observatory at Mauna Loa volcano (the island of Hawai'i). After calibration and filtering of cloud scenes, the divergence of satellite estimates from ground and aircraft measurements is characterized by a mean square deviation of ~4 ppm or 1% of the total XCO2 content. To speed up the adaptation of the regression algorithm for XCO2 estimation to the IKFS-2 data, it is proposed to use on the new satellites XCO2 estimates from the TCCON ground-based network in addition to the contact measurements of CO_2 concentrations. Also, it is reasonable to use in the regressions the thickness of the cryodeposit on the IKFS-2 photodetector glass as another predictor characterizing the state of the instrument.

Keywords: carbon dioxide, regression, optical thickness, IKFS-2, ground-based measurements and transverse horizontal circulation

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INTRODUCTION

Changes in the concentration of atmospheric long-lived greenhouse gases have a significant impact on the Earth's climate. Among them, carbon dioxide is the most important greenhouse gas. The global concentration of atmospheric CO_2 has increased from 280 (in the pre-industrial era) to 419.9 million^{-1} by 2022 (WMO Bulletin, 2023). The World Meteorological Organization Bulletin (WMO Bulletin, 2023) indicates that the radiative forcing of long-lived greenhouse gases increased by 49% between 1990 and 2022, with CO_2 accounting for 78% of this increase. To improve our understanding of the natural and anthropogenic processes governing the atmospheric greenhouse effect, global data on the atmospheric CO_2 content with a good spatial and temporal resolution are needed, which can only be obtained through the development of satellite-based measurement techniques. They are based on the analysis of reflected and scattered solar radiation spectra recorded with near IR spectrometers (TANSO-FTS, OCO) or analysis of the spectra of outgoing thermal radiation recorded with IR hyperspectrometers (IASI, CrIS, TES, HIRAS, and IKFS-2 Fourier spectrometers and the AIRS diffraction spectrometer) (Uspenskii, 2022).

It should be noted that the IKFS-2 infrared Fourier spectrometer (Zavelevich, 2009) is currently the only serial satellite instrument in Russia that can be used for global monitoring of the carbon dioxide content in the atmosphere. It is installed on Russian polar-orbiting spacecrafts (SCs) of the Meteor-M series. In particular, the instrument successfully operated in orbit during the entire active lifetime of the

Meteor-M No. 2 spacecraft (2014–2023). Stability of IKFS-2 radiometric characteristics confirmed in a number of intercalibrations by foreign satellite instruments allowed us to develop a regression technique for estimating the volumetric content of carbon dioxide XCO2 in the Earth's atmosphere; the technique was presented in detail in (Golomolzin, 2022; Uspenskii, 2022). The predictors in the regression equation from (Golomolzin, 2022) are effective optical thicknesses calculated from measurements of the spectral intensity of the outgoing IR radiation in the IKFS-2 channels in the 11–14-μm range adjacent to the strong CO_2 absorption band centered at 15 μm. The reference values for the regression were XCO2 values calculated from high-accuracy measurements of carbon dioxide concentrations made in 2015–2016 on the high-altitude mast of the international ZOTTO observatory (the experimental site of the Sukachev Institute of Forest, Siberian Branch, Russian Academy of Sciences, approximately 22 km from the village of Zotino, on the left bank of the Yenisei River, Central Siberia), and published data of aircraft measurements (Arshinov, 2009) performed previously in the region of the Novosibirsk Reservoir. Additionally, XCO2 estimates obtained by results of ground-based measurements in 2015–2016 from the NOAA Observatory at Mauna Loa volcano (Hawai'i Island) were used.

The comparison of the XCO2 (IKFS) estimates in (Golomolzin, 2022) with the analogous estimates from the data of foreign CrIS and OCO satellite spectrometers over the Eurasian territory for 11 days in October 2021 showed a good agreement. The mean XCO2 (IKFS) values occupied intermediate values between estimates of analogs: 3.2 ppm above XCO2 (CrIS) and 1.2 ppm below XCO2 (OCO). Under clear sky conditions, for the IKFS-2 and OCO pixels coinciding in the location, the root-mean-square residual of the XCO2 estimates does not exceed 2 ppm.

However, when comparing (Nikitenko, 2024) with the XCO2 estimates obtained at SPbSU from ground-based measurements of solar radiation fluxes by the Bruker 125HR IR Fourier spectrometer (Peterhof, period of 2019–2022), a much larger amplitude of the annual variations of XCO2 (IKFS) and a significant underestimation of their values were revealed beginning from 2021. A similar picture was also observed when comparing with the published measurement data of the TANSO-FTS Fourier spectrometer of the Japanese GOSAT satellite in the area of the Finnish Sodankylä geophysical observatory (Taylor, 2022), the nearest TCCON network point to Peterhof. The results of comparisons of the SPbSU ground-based measurements and GOSAT estimates with median values of daily estimates from IKFS-2 data for its pixels within 250 km from Peterhof are discussed in (Nikitenko, 2024) and shown in Fig. 1.

In (Nikitenko, 2024), the first results of works on the improvement of the technique (Golomolzin,

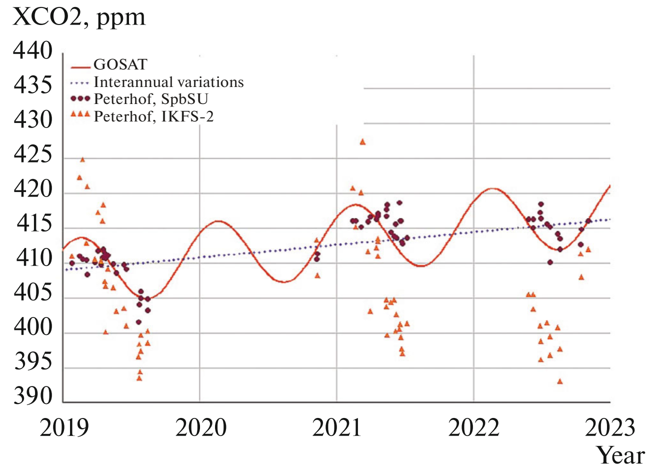

Fig. 1. Time variations of XCO2 values according to data of ground and satellite measurements near St. Petersburg for 2019–2022.

2022) are also presented. They are reduced to the refinement of the altitudinal variations of the CO_2 concentration from airborne measurements and additional calibration of XCO2 (IKFS) estimates from ground-based measurements of CO_2 concentrations at the NOAA observatory at Mauna Loa volcano (Hawai'i Island) in 2019–2022.

The work on further modification of the technique (Golomolzin, 2022) for XCO2 (IKFS) determination was continued and its results are reflected in this paper. In addition to comparisons with ground-based measurements of the SPbSU, it includes a description of a retrospective comparison of the results of the modified technique with contact airborne measurements of the IAO which were carried out for a number of years in the region of the Novosibirsk Reservoir. The performed comparisons with ground-based and airborne measurements of XCO2 in 2019–2022 taken as "truth" confirmed the effectiveness of the proposed modifications of the regression technique (Golomolzin, 2022) for XCO2 determination (IKFS-2) consisting in the formation of XCO2 reference values for the training sample based on a combination of contact measurements of concentrations on the high-altitude mast of the ZOTTO observatory, the NOAA observatory at Mauna Loa volcano, and airborne measurements of the IAO in Siberia.

In order to apply the data of specific IKFS-2 samples on new spacecrafts of the Meteor-M series (Uspenskii, 2021) in monitoring of the carbon dioxide content, it is reasonable to use a modified regression technique (Golomolzin, 2022). At the same time, the monitoring organization will require, generally speaking, prompt obtaining of regressions for each next satellite, since the measurements of specific IKFS-2 samples contain various kinds of systematic errors, including instrumental errors. In this connection, the

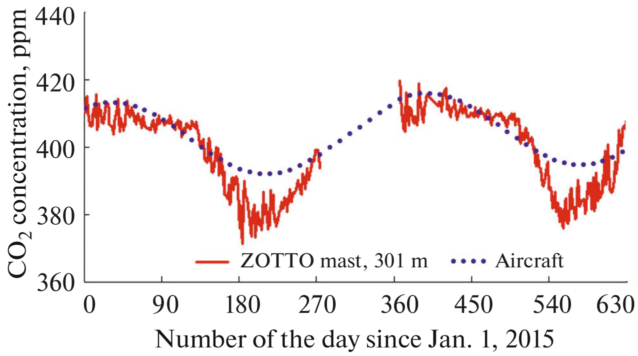

Fig. 2. Comparison of airborne measurements of the IAO with measurements of volumetric CO_2 concentrations at the high-altitude mast of the ZOTTO observatory.

paper discusses the inclusion of the cryodeposit thickness in the regression predictors for new IKFS-2. The change in the value of the thickness during the instrument operation due to the nonlinearity of the amplitude response of the photodetector may cause a bias in the XCO2 estimates. Note also that, to validate satellite XCO2 estimates and accelerate the obtaining of working regressions, data from the TCCON ground-based network can be used in addition to contact measurements (Wunch, 2011). For many locations in this network, XCO2 measurements are available within six months from the measurements.

In what follows, we analyze the reasons for the identified methodological errors of the regression technique (Golomolzin, 2022) and describe ways to reduce them.

REFINEMENT OF THE VERTICAL PROFILE OF THE CO_2 CONCENTRATION

As noted above, comparison of XCO2 (IKFS) estimates obtained from the original version of the technique (Golomolzin, 2022) with ground-based and satellite measurements for the period of 2019–2022 (see Fig. 1) showed a significant discrepancy in the annual variations of XCO2. The most probable cause is the chosen scheme of recalculating the CO_2 concentration profiles to the reference values of the total XCO2 content from measurements at the high-altitude mast of the ZOTTO observatory when obtaining the working regression.

We recall that in (Golomolzin, 2022) the calculations of reference XCO2 were carried out on days and hours when, according to the data of measurements at the mast, atmospheric mixing resulted in a uniform distribution of the CO_2 concentration in the surface layer of the atmosphere. The criterion for data selection was the coincidence (within ±1 ppm) of gas concentrations measured at all mast sites (between 4–301 m). When converted to the total XCO2 content in (Golomolzin, 2022), it was assumed that the constancy of the CO_2 volume concentration was maintained due to convective mixing of the atmosphere up to about 1.5 km (Belan, 1994). Between concentrations at this level and at 3 and 7 km, linear interpolation in altitude was used for the vertical profile (Arshinov, 2009) obtained from aircraft measurements in the corresponding month. At 7 km and above, the concentration was considered constant. The interannual variations in the data (Arshinov, 2009) were taken into account by introducing corrections to the airborne profile with respect to the concentration at a level of 0.5 km which, by virtue of the assumption, was taken to be equal to that measured at the ZOTTO mast. The XCO2 values calculated in this way were used to obtain reference XCO2 values for the date of flight of the Meteor-M No. 2 satellite by linear interpolation in time.

However, in the process of comparison with the approximation data of airborne measurements performed by the IAO directly in 2015–2016 (Antonovich, 2023), when the statistics for regression was collected (Golomolzin, 2022), it turned out that, for the warm period of the year, a significant difference between measurements of CO_2 concentrations at the ZOTTO mast and airborne measurements is observed even at an altitude of 500 m. As shown in Fig. 2, ground-based measurements yield lower values of concentrations as compared to airborne measurements (Antonovich, 2023), and the underestimation reaches about 15 ppm.

Proceeding from this, the vertical profile of volumetric CO_2 concentrations used to calculate XCO2 reference values was modified. Up to 300 m, it was determined by the concentration measured at the ZOTTO mast; between 300 m and 7 km, by linear interpolation in height of airborne IAO measurements; and above 7 km, by a constant concentration equal to the airborne concentration at 7 km.

It should be noted that the IKFS-2 measurements onboard the Meteor-M No. 2 satellite were carried out in the morning (~9 a.m. LT) and evening hours (~9 p.m.), when photosynthesis in the warm period was still/already unable to compensate carbon dioxide accumulation due to respiration of soil and vegetation. However, the reference values of XCO2 were not refined for the time of the satellite flyby. As shown by the performed estimation, the corrections made to account for the actual values of concentrations in the range of 0–300 m are random and do not exceed 1–2 ppm for most cases. This is significantly less than the spread of XCO2 estimates in individual pixels of IKFS-2, especially in the conditions of broken clouds, when it can reach 20 ppm.

For measurements in the NOAA observatory at Mauna Loa which were also used to obtain the working regression, the vertical profile of the CO_2 concentration was set to be constant and equal to the daily average value. The test carried out using the available profiles of airborne measurements (Vertical profiles of carbon dioxide, electronic resource) over the Moloka'i Island (Hawaii Archipelago) showed constancy of the volume concentration of CO_2 in height during the whole year; for this reason, no changes were made in the previously obtained values.

The refinement of the vertical profile of CO_2 concentration used for the determination of reference XCO2 in Central Siberia when obtaining the working regression made it possible to reduce the amplitude of annual variations in XCO2 (IKFS) estimates approximately to 10–12 ppm (Golomolzin, 2022), i.e., to values that correspond to ground-based (Bruker 125HR) and satellite (GOSAT) measurements near Peterhof.

TAKING INTO ACCOUNT CHANGES IN RADIOMETRIC CHARACTERISTICS OF IKFS-2

The decrease in the amplitude of annual variations in XCO2 estimates had no effect on the underestimation increasing with time in XCO2 (IKFS) estimates as compared to independent ground-based and satellite estimates. The time dependence of the mismatch of estimates means that there are some changes in the radiometric characteristics of IKFS-2—instrumental factors affecting the determination of XCO2 (IKFS) during the periods of obtaining the working regression and/or further regular measurements. During the entire active lifetime of the Meteor-M No. 2 spacecraft (2014–2023), the IKFS-2 Fourier spectrometer successfully operated in orbit and repeatedly participated in various intercalibration campaigns which confirmed the stability of its characteristics and high measurement accuracy. The error introduced into the measurements of spectral intensities (or brightness temperatures) of IR radiation by various factors is within the tolerances stipulated by the technical specification for the device; nevertheless, it can influence the error of XCO2 estimates.

As an example of such an influencing factor, Fig. 3 shows the time variations of IKFS-2 calibration in brightness temperatures over three spectral IR channels of the SEVIRI radiometer installed onboard the European geostationary satellites, Meteosat-10 (until 2018) and Meteosat-11 (starting from 2018). The calibrations were performed using synchronous registrations of IR outgoing radiation at the moment of the Meteor-M No. 2 satellite flyby of the area of the subsatellite standing point (0°) of the geostationary satellites in the Gulf of Guinea of the Atlantic Ocean. The SEVIRI radiometer, in turn, was periodically calibrated using the IASI Fourier spectrometer installed on the Metop-A and -B polar-orbiting satellites. Note that the GSICS (Global Space based Inter-Calibration System) special group at the World Meteorological Organization recognized the IASI Fourier spectrometer as an exemplary instrument for verifications (intercalibrations) of IR satellite instruments in orbit. The results of intercalibrations of SEVIRI brightness temperatures by IASI are clearly seen in the plot for the 13.4-μm channel in which the correction values go to zero after each calibration (Meteosat-11, 2018–2023). This indicates stability of the IKFS-2 performance in the spectral operating range of this channel. In contrast, the 12 μm-channel shows a change in the calibration correction from +0.1 (2019) to –0.1 K (2023) which is not compensated by IASI intercalibrations, i.e., it is a calibration change of IKFS-2 itself.

Additional distortions of the spectral dependence between measurements in individual channels of IKFS-2 can be introduced by ice cryodeposits. Figure 4 presents the time variations of the decreasing ice accretion rate on the mercury-cadmium-tellurium (MCT) photoresistor of IKFS-2 with an intrinsic temperature of about 80 K.

Cleaning of the photoresistor (defrosting) starts when the ice thickness $h = 1$ μm is reached. In 2015–2016, it was carried out approximately every ten days. The cleaning period increased with a decrease in the deposit accretion rate. In 2021, it reached 60 days and did not change further. The cryodeposit level in IKFS-2 is monitored by the NESR noise value in the center of the ice absorption band. The spectral (as a function of the wavenumber ν, cm^{-1}) transmittance of an ice film with different thickness h regard to the interference reflection at its boundaries (Hudgins, 1993) is shown in Fig. 5.

To the left of 950 cm^{-1}—in the spectral region involved for the determination of XCO2—the minimum transmittance for ice film thickness 1 μm is approximately 67%, while the transmittance at 900.1 cm^{-1}—the reference frequency that corresponds to the maximum atmospheric transparency and is used in the algorithm to determine atmospheric absorption spectral thicknesses—would be 80%. The use of internal calibration by the onboard calibration source in IKFS-2 measurements essentially levels out this difference but the presence of cryodeposits causes a shift of the operating point on the nonlinear amplitude response of the IKFS-2 MCT detector and the appearance of additional spectral distortions (Anokhin, 2011). The magnitudes of these distortions in the IKFS-2 channels are small but unknown and, due to the involvement of several channels in the working regression of measurements and its nonlinear nature, may cause a random error in the estimation of the XCO2 time trend. It should be taken into account that the rate of the cryodeposit increase immediately after cleaning is significantly higher (Mikhalchenko, 1988) than at the end of the working period when its thickness approaches the limiting value $h = 1$ μm. This leads to violation of homogeneity in measurement conditions when obtaining regression coefficients and using the regression for XCO2 estimates. For example, in 2015–2016, when cleanups were performed once every ten days, the fraction of time for IKFS-2 measurements with $h > 0.5$ μm

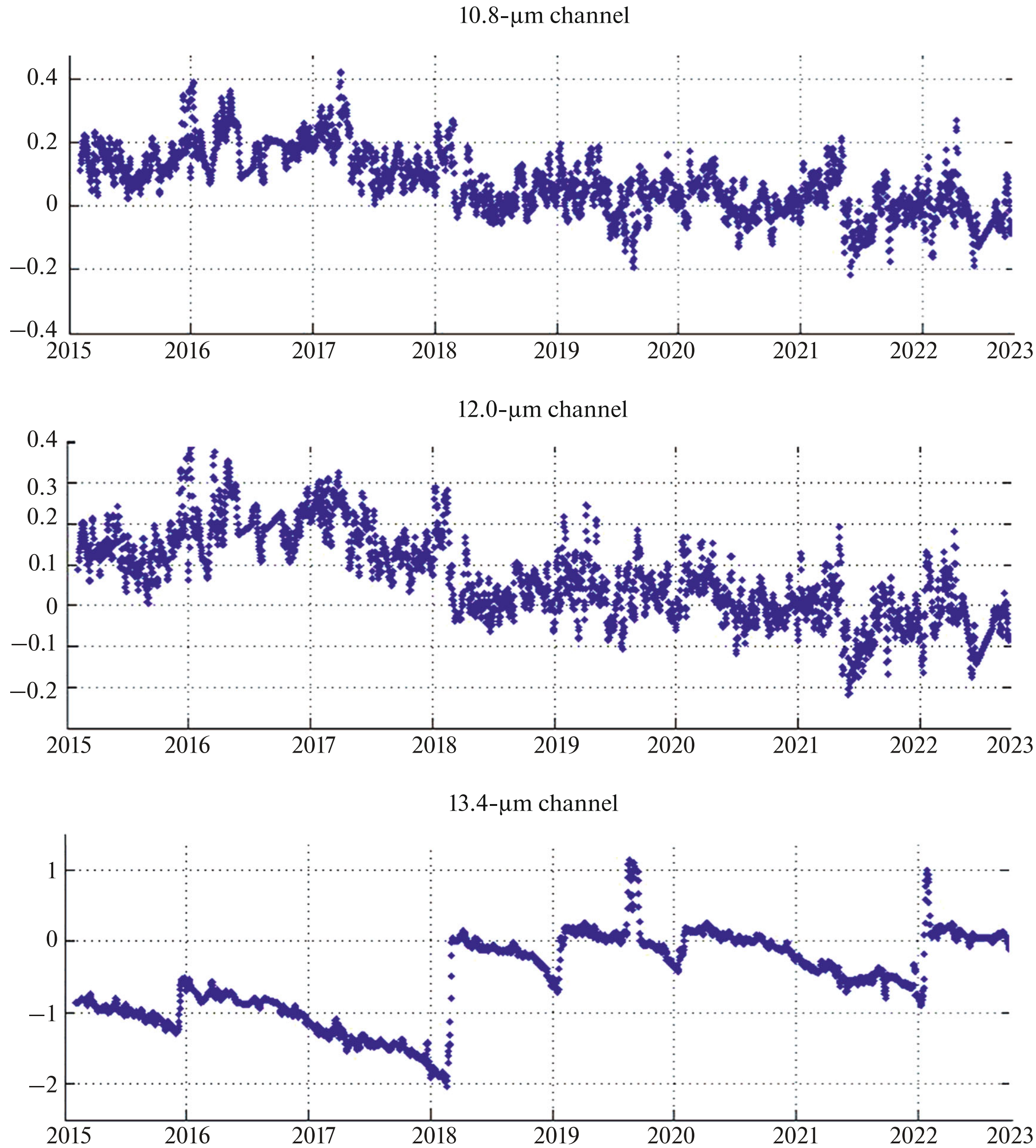

Fig. 3. Time variations of IKFS-2 calibration in brightness temperatures for the SEVIRI channels of the Meteosat-10 (before 2018) and Meteosat-11 (beginning from 2018) spacecrafts.

in obtaining the regression was about 7% less than for XCO2 estimates in 2019–2022, when the cleanup period was 60 days.

As follows from the above consideration, the correct determination of the interannual XCO2 trend is largely related to taking into account the condition of the device during the entire lifetime, including the period of measurements to obtain a working regression. Practical implementation of such consideration is possible by including the thickness of the cryodeposit available from the standard IKFS-2 output dataset as predictors of the regression. This should be done when determining XCO2 by data from the new satellites of the Meteor-M series, including Meteor-M No. 4 launched into a sun-synchronous orbit on February 29, 2024.

CALIBRATION OF XCO2 ESTIMATES FROM CONTACT MEASUREMENTS OF THE MAUNA LOA OBSERVATORY

It is impossible to take into account the possible temporal drift of some technical characteristics of IKFS-2 (for example, degradation of the onboard calibration source) when constructing the regression because the IKFS-2 output data do not contain relevant parameters suitable for inclusion in the predic-

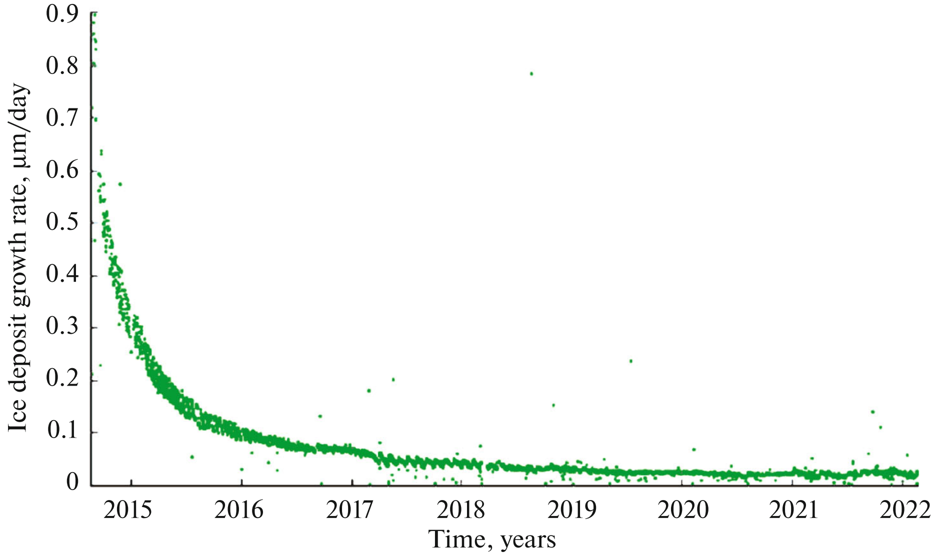

Fig. 4. Variation in the rate of increase in the cryodeposits on the photoresistor of the IKFS-2.

tors. It is also impossible to introduce any corrections based on the results of intercalibration during the flight: the stability of the radiometric characteristics of IKFS-2 is not worse than that of the IASI Fourier spectrometer mentioned above (Zavelevich, 2018).

As a consequence, it is reasonable to control and calibrate the XCO2 (IKFS) estimates themselves; for this purpose, some measurements should be selected as reference ones. The use of GOSAT or OCO-2 (Taylor, 2023) as reference estimates causes great difficulties in the spatial and temporal combination of different satellite data: foreign devices, compared to IKFS-2, have a significantly higher spatial resolution; in addition, GOSAT and OCO-2 measurements are almost completely absent over most of the Russian territory in winter.

The generally accepted reference data are results of contact measurements of CO_2 concentrations that have been conducted for more than 60 years at the Mauna Loa Observatory (Hawai'i) at an altitude of about 3400 m. As already noted, the vertical profile of the relative CO_2 concentration is almost constant (Vertical Profiles, electronic resource), so there is no difficulty in recalculating it to obtain XCO2 values. Figure 6 presents results of calibrating the XCO2 (IKFS) estimates from measurements at Mauna Loa. Hereinafter, their median values for IKFS-2 pixels falling within a 4° × 4°-square in latitude and longitude centered at the location of the reference data source were used as satellite estimates.

After calibration of the XCO2 (IKFS) estimates by Mauna Loa data, the root-mean-square discrepancy (rms) of the satellite and ground data is rms = 2.6 ppm and the correlation coefficient is $R = 0.67$. Additionally, to exclude in the XCO2 estimates errors due to cloud cover entering the IKFS-2 field of view, the condition $\eta < 1.05$, where η is the ratio of surface pressure to pressure at the height corresponding to the brightness temperature of a pixel in one of the atmospheric transparency microwindows, in the neighborhood of 11 μm, was used as a filtering criterion for cloud scenes. The threshold value $\eta = 1.05$ represents a compromise between an acceptable rms value and the number of IKFS-2 pixels included in the processing. The criterion $\eta < 1.05$, which was established empirically during the calibration by Mauna Loa data, was also used further when comparing IKFS-2 estimates with ground-based and airborne measurements in Peterhof and over the Novosibirsk Reservoir. This criterion was satisfied for approximately 20% of IKFS-2 measurements on the material of the analyzed samples.

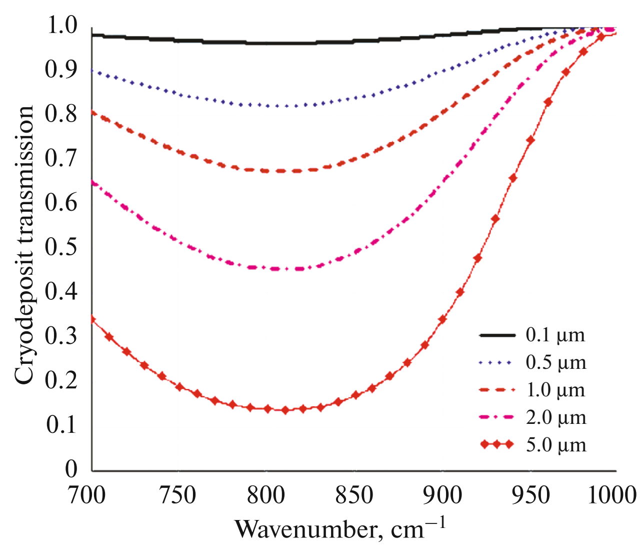

Fig. 5. Spectral transmission of cryodeposits.

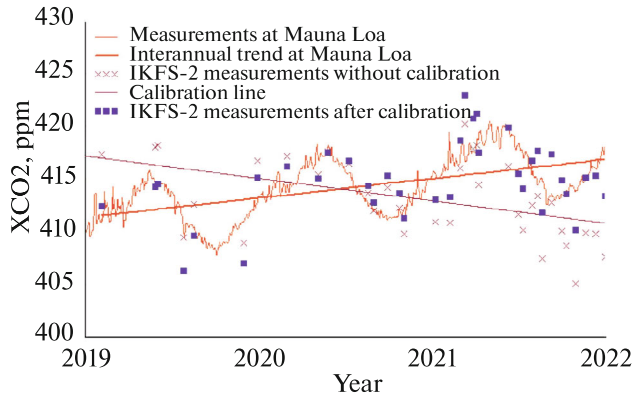

Fig. 6. Comparison of XCO2 estimates (IKFS) before and after calibration by data from Mauna Loa.

COMPARISON OF XCO2 (IKFS) ESTIMATES WITH DATA OF GROUND-BASED AND SATELLITE MEASUREMENTS NEAR PETERHOF

In (Nikitenko, 2024), the XCO2 estimates and the data from ground-based measurements of the Bruker 125HR Fourier spectrometer in Peterhof in 2019–2022 were compared for the first time. Additionally, the results of interpolation (up to 2020) and extrapolation (after 2020) of GOSAT (Taylor, 2022) estimates were involved from the region of the Finnish geophysical observatory Sodankylä, where one of the TCCON measurement network sites closest to Peterhof is located. In contrast to (Nikitenko, 2024), the results presented in Fig. 7 are obtained with filtering of cloud scenes according to the criterion $\eta < 1.05$ and applying a new linear function to correct the XCO2 values (IKFS) obtained by calibration of XCO2 estimates from Mauna Loa measurements.

The use of the η criterion resulted in the fact that days of IKFS-2 measurements not always coincide with days of the Bruker 125HR ground-based measurements, so the quantitative estimation of the accuracy of the satellite and ground-based XCO2 reconstructions is carried out by the method of double differences with respect to the GOSAT curve, which actually repeats measurements of the TCCON point in Sodankylä (the root-mean-square dsiscrepancy σ = 1.8 ppm; the correlation coefficient $R = 0.99$ (Taylor, 2022)). The mean bias Δ of the XCO2 (IKFS) estimates calculated in this way relative to the Bruker 125HR ground-based measurements was $\Delta = -0.86$ ppm. Correspondingly, for IKFS-2, the mean bias with the GOSAT curve values was $\Delta = -0.42$ ppm, the root-mean-square discrepancy rms = 3.4 ppm, the correlation coefficient $R = 0.80$; for Bruker 125HR, $\Delta = 0.44$ ppm, rms = 2.4 ppm, $R = 0.82$. In both comparisons, the standard deviations σ almost coincided with the rms values due to the smallness of the mean biases Δ.

COMPARISON OF XCO2 (IKFS) ESTIMATES WITH DATA OF AIRBORNE AND SATELLITE MEASUREMENTS NEAR THE NOVOSIBIRSK RESERVOIR

The results of retrospective comparison of XCO2 (IKFS) estimates obtained using the modified technique with airborne measurements of the IOA in the Novosibirsk Reservoir area are presented in Fig. 8. It also shows XCO2 (GOSAT) estimates, mainly for 2022.

Here, as before, results of measurements that are different in number and time are compared using the reference quasi-periodic curve—approximation of the annual and interannual variations of the total XCO2 content from airplane data. The vertical profiles of carbon dioxide concentrations of the IAO Optik labo-

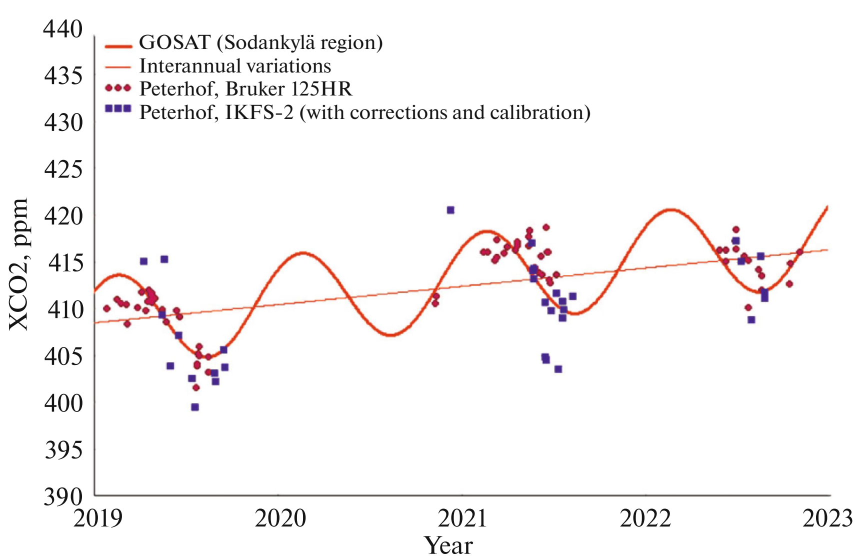

Fig. 7. Comparison of XCO2 estimates (IKFS) with satellite (Sodankylä region) and ground-based spectroscopic measurements of SPbSU (Bruker 125HR, Peterhof).

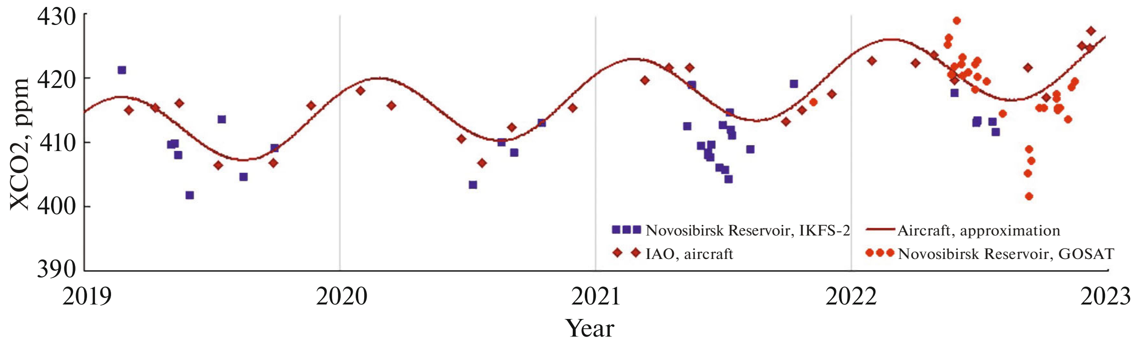

Fig. 8. Comparison of XCO2 estimates (IKFS) with results of airborne (IAO) and satellite (GOSAT) measurements in the region of the Novosibirsk Reservoir.

ratory airplane based on TU-134 (Anokhin, 2011) in the height range of 0–7 km served as the basis for calculations and approximation of the time variations of XCO2. In contrast to comparisons with the GOSAT data curve (Fig. 7) plotted from measurements over Sodankylä about 1000 km from Peterhof, the IAO airplane curve reflects data obtained directly in the vicinity of the Novosibirsk Reservoir near which the XCO2 (IKFS) estimates were obtained. In this connection, statistical characteristics of the accuracy of XCO2 estimates from GOSAT and IKFS-2 measurements are calculated relative to this quasi-periodic curve and presented in Table 1.

The reference curve is an approximation of airborne measurements. Naturally, it provides the best agreement with them as compared to satellite data. When comparing satellite data, the statistical characteristics are calculated for the entire time period of 2019–2022 under consideration. In addition, for GOSAT and IKFS-2, they were calculated only for time intervals when there were no large omissions of aircraft data. For example, the summer months of 2021 and 2022, when there were no aircraft flights, were not included in the calculation of statistical characteristics. As can be seen from the tables, the satellite estimates in this case give a better agreement and correlation with the airborne measurements for both devices.

CONCLUSIONS AND SUGGESTIONS

Comparison of estimates of total carbon dioxide XCO2 (IKFS) with estimates of XCO2 in the Peterhof area (2019–2022) using ground-based measurements of the Bruker 125HR IR Fourier spectrometer and Japanese GOSAT satellite revealed a large amplitude of the annual variations of XCO2 in the IKFS-2 estimates and their significant underestimation with time. As a consequence, the procedure for calculating the vertical profile of CO_2 concentration and the reference XCO2 values used in the regression was refined in the previously developed regression technique. In addition, in order to correctly determine the interannual variations of XCO2, the obtained estimates were calibrated using reference data—contact measurements of XCO2 at Mauna Loa.

The modification of the regression technique allowed us to significantly reduce the discrepancies with ground and satellite data. The average bias of XCO2 (IKFS) estimates with respect to ground-based Bruker 125HR measurements in Peterhof and airplane measurements in the Novosibirsk Reservoir area does not exceed 1 and 2 ppm, respectively. The standard deviation of XCO2 (IKFS) estimates from the data of ground-based and airborne measurements is approximately 4 ppm with the correlation coefficient $R \approx$ 0.7–0.8. Comparison with the data of long-term airborne measurements of the IAO in Siberia showed the

Table 1. Statistical characteristics of deviations in XCO2 estimates from the approximations of the XCO2 behavior according to long-term airborne measurements of the IAO

Data source	Δ, ppm	rms, ppm	σ, ppm	*R*	Number
Aircraft	–0.56	2.4	2.4	0.90	27
GOSAT (full period)	–1.24	5.7	5.6	0.61	31
GOSAT (taking into account aircraft data omissions)	–4.25	6.4	4.8	0.81	18
IKFS-2 (full period)	–3.75	5.6	4.1	0.56	36
IKFS-2 (taking into account aircraft data omissions)	–1.7	4.4	4.1	0.74	19

Table 2. TCCON stations for validation of IKFS-2 estimates of XCO2

Station	Latitude	Longitude	Altitude above the sea level, m
East Trout Lake (United States)	54.35 N	104.99 W	501.8
Park Falls (United States)	45.94 N	90.27 W	442.0
Sodankylä (Finland)	67.37 N	26.63 W	188.0
Harwell (United Kingdom)	51.57 N	1.32 W	142.0
Izaña, Tenerife (Spain)	28.31 N	16.50 E	2367.0

closeness of statistical characteristics of deviations in XCO2 (IKFS) and XCO2 (GOSAT) estimates.

Proceeding from this, it is reasonable to retain the former regression approach to determination of XCO2 by the IKFS-2 data. To obtain a working regression, it is recommended to use reference contact measurements of carbon dioxide concentrations at the high-altitude mast of the ZOTTO Observatory, at Mauna Loa volcano (NOAA Observatory), and airborne measurements of the IAO; as for the latter, for a more accurate determination of the vertical profile of CO_2 concentration, it is desirable to conduct them in Central Siberia, in the area of the ZOTTO Observatory.

To take into account the possible influence of cryodeposits on the accuracy of XCO2 estimation, their thickness should be included in the predictors of the working regressions obtained for new satellites of the Meteor-M series.

The systematic error in XSO2 estimates due to the state of the satellite radiometer and possible changes in its characteristics is difficult or impossible to take into account in the regression algorithm. The correct determination of the interannual variation of XSO2 requires calibration of the obtained estimates by reference measurements. The simplest way of this calibration is to use contact measurements at Mauna Loa without any use of a priori and model information.

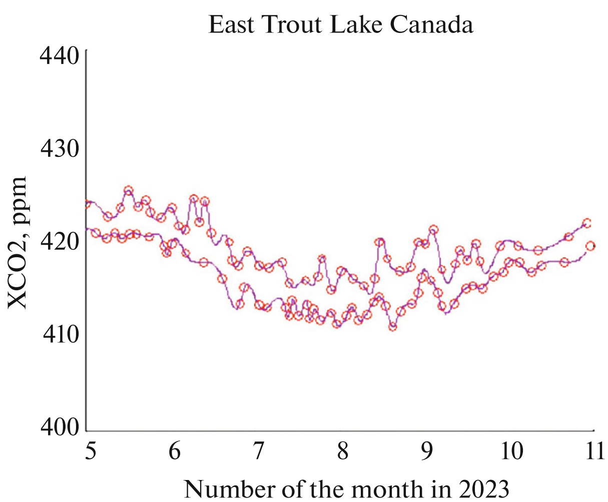

Fig. 9. Time variations of maximum and minimum XCO2 according to data of the East Trout Lake TCCON station.

In order to validate the obtained estimates, as well as to accelerate obtaining working regressions by contact measurements, it is suitable to additionally use data from the TCCON ground network. The TCCON network currently contains 26 stations. The XCO2 measurement data from TCCON stations can be obtained promptly (with a time lag of several months from the measurement date (TCCON, 2024)). As an example, Fig. 9 shows variations of XCO2 values from East Trout Lake station data in 2023, beginning from May.

It is likely that data from five TCCON stations presented in Table 2 will be sufficient to validate the XCO2 estimates.

In summary, it should be noted that the XCO2 estimates on the TCCON network when using different versions of the XCO2 retrieval software suite are calibrated by airborne measurements. For example, the switch in this suite to new spectroscopic information on atmospheric gases in 2021 changed the value of the calibration factor by 2% (i.e., an increase in XCO2 by 8 ppm) (Roshe, 2021). As a consequence, the use of TCCON data should be auxiliary in obtaining a working regression for the new IKFS-2; it should not replace contact measurements of vertical profiles of CO_2 concentrations from airplanes and high-altitude masts.

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CONFLICT OF INTEREST

The authors of this work declare that they have no conflicts of interest.

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