Comparison of satellite and airborne measurements of the CO₂ concentration over Western Siberia

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The column mean concentration of carbon dioxide has been retrieved using WFM-DOAS algorithm, developed at Bremen University, Germany from data obtained with a SCIAMACHY spectrometer installed onboard Envisat satellite. The obtained data are compared with airborne measurements carried out in 2003 over two regions of Western Siberia, Surgut and Novosibirsk. The retrieved time behavior of CO_2 concentration during warm periods is in a good qualitative agreement with data of airborne sensing while being seriously underestimated in the presence of snow cover. Some possibilities of improving accuracy of the WFM-DOAS algorithm are discussed.

Introduction

From the very beginning of the industrial era, the volume concentration of carbon dioxide in the atmosphere has increased approximately from 280 to 380 ppmv. In view of the influence of CO_2 on climate, there is a need in monitoring its content on a planetary scale. In March 2002, European Space Agency (ESA) has launched a research satellite "Envisat" with a Scanning Imaging Absorption Spectrometer for Atmospheric Cartography (SCIAMACHY) installed aboard.^{1,2} One of the missions of the instrument is to determine the column mean concentration of the carbon dioxide in the atmosphere (XCO_2) . This is a new field of spaceborne monitoring, so it is yet difficult to judge the reliability of such measurements. The XCO_2 variations are small. For instance, the data from Ref. 3 indicate that depending on geographic region the amplitude of XCO₂ variations relative to the trend during one year is 7 to 10 ppmv that compares with the SCIAMACHY measurement errors.⁴

Development and adjustment of the methods for determining CO_2 concentration from satellite measurement data requires large amount of reference data on spatiotemporal variations of the carbon dioxide concentration in the Earth's atmosphere. Until recently, the source of these data has been the results calculated using the models of global carbon cycle,^{5,6} which, in their turn, are still far from being perfect. For instance, model results suggest that from the 6 to 7 billion tons (Gt) of carbon emitted yearly into the atmosphere with CO_2 as a result of anthropogenic activity, 3 Gt of carbon reside in the atmosphere, 2 Gt are adsorbed by the ocean, while it remains unknown what happens to the rest 1 to 2 Gt.

There is certain danger that adjustment of satellite algorithms of determination of CO_2 content in the

atmosphere using only calculated data will lead to vicious circle in the sense that model errors will cause concordant errors in the interpretation of satellite data which, in its turn, will complicate refinement of the carbon models themselves. This is especially important for northern latitudes where, as shown in Ref. 5, incomplete model account of uptake of the above-mentioned 1-2 Gt of carbon by boreal forests takes place.

In this regard, of great importance are new independent data of airborne measurements of CO_2 concentrations, obtained over Western Siberia,^{7–9} and usable for development and testing of satellite algorithms. The flights were conducted during one year over Surgut and Novosibirsk once a month; atmospheric air samples were collected at 8 heights in the range from 0.5 to 7 km.

In test runs of satellite algorithms of XCO₂ retrieval under different conditions, extremely useful is the information on the state of clouds and snow cover in the geographical regions under study. These data can be obtained from archive of ground-based observations at the stations of Russian meteorological service, freely accessible on the server "Weather of Russia".¹⁰

In the present paper we give a brief outline of the algorithm used for XCO_2 retrieval from SCIAMACHY data, and provide first results of its application to studies over Surgut and Novosibirsk (2003), for which the data of airborne measurements are also available.^{7–9}

1. Satellite spectrometer SCIAMACHY

The SCIAMACHY^{1,2} spectrometer is installed onboard an Envisat satellite. The satellite operates in

polar sun-synchronous orbit with the average orbit height about 800 km above the Earth's surface and with 10:00 LT equator-crossing time. The orbit is inclined at 98.6° with respect to equatorial plane. The complete survey of the Earth's surface takes 6 days. The satellite views the west regions of Siberia at approximately same time between 11:30 and 11:50 local solar time. The horizontal resolution of the measurements at nadir depends on orbit and spectral channel. On the average, it is 60 km across the footprint and 30 km along it on the earth's surface.

The SCIAMACHY device is a grating spectrometer. It sequentially performs nadir and limb measurements of spectra of reflected and scattered solar radiation in the wavelength range from 240 to 2400 nm. The instrument also measures the spectral atmospheric transmission when the sun and the moon appear over the earth's horizon. The spectral interval of SCIAMACHY is divided into 8 channels, whose characteristics are presented in Table 1, taken from Ref. 11.

Table 1. Characteristics of the channels of SCIAMACHY spectrometer¹¹

Channel number	Boundaries of the spectral channels, nm	Spectral resolution, nm	Material of detector	Temperature of detector, K	
1 (UV)	240-314	0.24	Si	200	
2 (UV)	309-405	0.26	Si	200	
3 (Vis)	394-620	0.44	Si	235	
4 (Vis)	604-805	0.48	Si	235	
5 (IR)	785-1050	0.54	Si	235	
6 (IR)	1000 - 1750	1.48	InGaAs	200	
7 (IR)	1940-2040	0.22	InGaAs	150	
8 (IR)	2265-2380	0.26	InGaAs	150	

The CO_2 content in the atmospheric column is retrieved from nadir measurements of upwelling solar radiation, obtained in the sixth spectrometer channel. This range contains the CO_2 absorption band centered at 1600 nm, which is relatively free of absorption by "interfering" gases (primarily water vapor). Simultaneously, measurements in the fourth channel are used to retrieve O_2 content (A-band centered at 760 nm). This makes it possible to calculate XCO_2 for column of dry air from the formula

$$XCO_2 = LCO_2/LO_2/w_{O_2},$$

where LCO₂ and LO₂ are the CO₂ and O₂ contents in atmospheric column; $w_{O_2} = 0.2095$ is the relative fraction of oxygen in dry air.

2. WFM-DOAS retrieval algorithm

To retrieve content of trace gas constituents (including CO_2) from data of SCIAMACHY spectrometer, the University of Bremen, Germany, has developed special Weighting Function Modified Differential Optical Absorption Spectroscopy (WFM-DOAS) algorithm.^{4,12} It is based on minimization of discrepancy of logarithms of calculated I_{mod} and measured I_{obs} brightness, normalized using extraterrestrial solar spectrum. The minimization is made by least squares method based on the following functional:

$$\sum_{i=1}^{n} \left[I_{\text{mod}}^{i}(V) - I_{\text{obs}}^{i} + P^{i}(a_{m}) \right]^{2} \to \min, \qquad (1)$$

where i = 1, ..., n are spectral channel numbers; V are all the column densities of all trace gases including CO_2 contributing to absorption within the spectral channel selected; $P^i(a_m)$ is the low-order fitting polynomial in I_{obs}^i with the constant coefficients a_m , m = 1-3.

For the efficient calculations of $I^i_{mod}(V)$ and determination of CO₂ from formula (1), a fast interpolation scheme, that uses reference values of $I^i_{mod}(V)$ for specified values of atmospheric optical parameters, was employed. More detailed description of the currently used version of WFM-DOAS retrieval algorithm can be found in Refs. 4, 12, and 13. Note that the minimum discrepancy (root mean square error), determined from (1), is used below as an indicator of the quality of the XCO₂ estimate.

Authors of the WFM-DOAS algorithm emphasized two aspects important in its application.⁴

First, in the process of retrieving the CO_2 concentration it is necessary (when possible) to sort out the cloud-containing pixels. For this, a special threshold algorithm has been developed as described in Ref. 4. It is based on measurement of atmospheric reflectivity (normalized intensity of outgoing radiation) using special auxiliary Polarization Measurement Device (PMD), a constituent part of SCIAMACHY. The spatial resolution of PMD is almost ten times higher than the resolution of SCIAMACHY itself, and the spectral range of the first channel PMD-1 is 320-380 nm. If a PMDderived reflectivity is higher than prescribed threshold value for any subpixel, the corresponding SCIAMACHY pixel is classified as cloudy.

Second, to eliminate obvious uncertainties in LCO_2 and LO_2 estimates, the operational version of WFM-DOAS algorithm of XCO_2 retrieval uses scaling factors, which do not depend on time and place of measurements. In this context, it is recommended in Ref. 4 to use, as yet, SCIAMCHY measurements only for analysis of spatiotemporal variations of CO_2 , while ignoring the absolute values of LCO_2 or XCO_2 estimates.

3. Determination of CO₂ concentration over Surgut and Novosibirsk

For a comparison with airborne observations^{7–9} we used XCO_2 retrievals based on SCIAMACHY measurements from April to October 2003. For better statistical representativeness, the extents of the territories, for which the satellite data analysis was performed, were increased in comparison with flight regions. Pixels were selected on areas bounded by

circles with radii 1000 km and centered at Surgut (61°24'N, 73°29'E) and Novosibirsk (more precisely, on the right bank of the southern part of Ob water storage basin, at approximately 54°N, 82°E).

To eliminate large errors due to instrument malfunctioning or incorrect performance of XCO_2 retrieval algorithm, we used pre-selection including simultaneous fulfillment of several one-sided or two-sided threshold criteria. Daily mean MCO_2 values of carbon dioxide concentration for each region were determined by the following formula

$$MCO_2 = \sum_k (XCO_2)_k P_k / \sum_k P_k$$
(2)

where k is the ordinal number of a pixel falling within the region under consideration; P_k is the indicator of selection, equal to unity if the XCO₂ estimate satisfies N = 8 for the given criteria, and to zero if at least one of the criteria is violated, that is,

$$P_k = \prod_{i=1}^N P_k^i.$$

Names of the criteria and the corresponding thresholds are presented in Table 2.

For the one-sided criteria, only one value is indicated. Table 2 also gives the probabilities of fulfillment of the conditions of individual criteria and their combinations calculated using observations over Novosibirsk (upper left number) and Surgut (lower right number) separately for all pixels and pixels classified as cloud-free according to PMD measurements.

The number of pixels, analyzed during Envisat satellite pass over the regions of Novosibirsk and Surgut in 2003 was about 80 000 and 100 000, respectively. Estimates of the daily mean concentrations of carbon dioxide MCO_2 for each satellite pass over the regions are presented in Fig. 1. Squares stand for MCO_2 values calculated for all pixels survived selection independent of the value of the cloud indicator, and circles for values calculated only for clear-sky pixels.

Solid curves are plotted according to results of integration of the vertical profiles of airborne XCO_2 measurements^{7,8} taking into account the exponential decrease of atmospheric pressure with height. For Surgut, these values were obtained according to measurement data of 1996 and recalculated for 2003 using interannual variability of the concentration.⁷

Similar recalculations have also been done for Novosibirsk taking into account that Arshinov et al.⁸ have presented the profiles averaged over 1997–2004.

Dashed lines show dates of the beginning and end of the period with snow cover. These days were determined from measurements of the depth of snow cover at meteorological stations located at the centers of the considered regions.¹⁰ The analyzed SCIAMACHY pixels may lie both to the north and to the south of these points at the distance up to 1000 km; therefore, for concrete pixels the indicated periods may differ by approximately a week from actual periods.

 CO_2 Analyzing the obtained results for concentrations, and taking into consideration the two above-indicated comments of the authors of the algorithm,⁴ we note that, under snow-free conditions, the results of MCO₂ retrieval using SCIAMACHY data qualitatively agree with airborne measurements. For the warm time of the year, the monthly MCO_2 variations are almost symmetric with minimum at the end of July. Maximum MCO₂ variability range, according to SCIAMACHY data, is from 12 to for both For 14 ppmv regions. airborne measurements, this range is 11-13 ppmv, i.e., it practically coincides with the satellite estimates. The absolute underestimation of satellite MCO_2 data, in comparison with airborne measurements, turned out to be identical for Novosibirsk and Surgut, being about 17 ppmv for June, as an example. This confirms the conclusion of Buchwitz et al.4 that it is possible, just by varying the scaling factors, to achieve the correspondence of satellite and actual (airborne, in this case) data.

ion er		Units (indicator)	Thresholds		Probability of fulfillment of criteria			
Criterion	Examined parameter		Lower boundary	Upper boundary	For all pixels	For cloud-free pixels only		(for all els)
1	Working direction of scanning	indicator		1.5	0.80 0.80	0.84 0.84	0.80	0.80
2	RMS discrepancy over spectrum	rel. units		0.007	0.86 0.79	0.98 0.85	0.68	0.63
3	LO_2	rel. units	0.50	1.02	0.83 0.77	0.85 0.74	0.59	0.54
4	Calculated LO ₂ error	%		2	0.76 0.79	0.96 0.98	0.47	0.47
5	LCO ₂	rel. units	0.50	1.08	0.78 0.75	1.00 0.93	0.45	0.45
6	Range of XCO ₂	ppmv	340	400	0.48 0.42	0.83 0.73	0.28	0.25
7	Calculated LCO ₂ error	%		8	0.50 0.55	0.90 0.93	0.22	0.24
8	Absence of clouds	Indicator		0.5	0.30 0.26	1.00 1.00	0.16	0.11

Table 2. Characteristics of criteria in determination of daily mean MCO₂ concentration

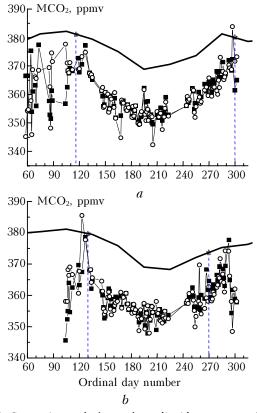


Fig. 1. Comparison of the carbon dioxide concentrations, retrieved using satellite and airborne measurements in the region of Novosibirsk (a) and Surgut (b) in 2003.

In the presence of snow cover, when values of solar zenith angle also increase, the performance of the WFM-DOAS algorithm is degraded. Values of the MCO₂ concentrations decrease in comparison with the concentrations in neighboring months when the snow is still or already absent. Seemingly, errors in determination of CO₂ concentration, caused by the presence of snow cover, are associated with the considerable differences in spectral behavior of albedo A of snow (Fig. 2) from neutral value of surface albedo A = 0.1, used in the WFM-DOAS algorithm⁴ during creation of reference database.

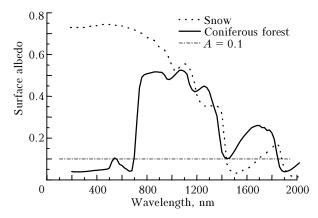


Fig. 2. Spectral albedo of different types of underlying surface (based on data from Refs. 14 and 15).

In particular, in the oxygen absorption band (760 nm) A of snow may reach 0.6–0.8, while in the CO₂ absorption band (1600 nm) $A \approx 0.03-0.06$.^{14,15} Note that the difference of the spectral behavior of surface albedo from the neutral one is also observed, though it is not that strong, for plants (Fig. 2, coniferous forest).

From analysis of the results it follows that the possibility of retrieving CO_2 concentration is influenced to a larger degree by snow than by clouds, because MCO₂, estimates with and without the account of pixels with clouds practically very little differ for both of the regions considered. More wavy character of the MCO₂ curves in Fig. 1 for clear pixels, seemingly, can be explained by the smaller bulk of statistical data used in averaging: as seen from Table 2, the number of clear pixels is a factor of 3 to 4 less than the number of pixels having survived at the remaining stages of selection.

In contrast to warning by Buchwitz et al.,⁴ the relatively weak influence of clouds on MCO₂ is caused by strong interrelation between LCO₂ and LO₂ estimates, whose correlation coefficients R lies in the range 0.92–0.96 for these two regions. However, even after exclusion of cloudy (according to PMD measurements) pixels, the correlation decreases insignificantly: R = 0.82-0.86. That high R values indicate that many cloudy pixels survive the existing selection, since under conditions of plain terrain only reflection from cloud top leads to approximately the same relative decrease of the lengths of scattering paths in two different, optically independent parts of the spectrum.

Indirectly (distance between meteorological stations and satellite pixel may reach a few hundred kilometers), overestimation of the number of clear pixels is also confirmed by the data of ground-based, visual observations of the state of the sky.¹⁰ Such observations are performed several times a day. The nearest time of observation, differing from the overpass time of Envisat satellite by less than 1 h, is 11:00 local solar time. In the majority of cases, the observers recorded the presence of clouds at this time. For instance, from the 106 days from April to October 2003, when satellite passed over Surgut, at all 9 meteorological stations, data from which were used for independent control of clouds in the region of aircraft flights, the clear sky was reported only 36 times out of all 954 observations. Note that only once (July 2, 2003), the absence of clouds was reported simultaneously for six of the nine meteorological stations. This statistics indicates that the relative number of clear pixels must not exceed 4% of the total number, which is 6 to 7 times less than the number selected from PMD data.

The presence of that small number of clear pixels can be explained by the fact that Envisat passes over Siberia at about solar noon. In the absence of stratiform clouds, the soil is already heated by this time, and there appear cumulus clouds which, because of the large size $(60\times30 \text{ km}^2)$ of SCIAMACHY pixels, will fall within SCIAMACHY field of view with high probability. Practically permanent presence of clouds will inevitably lead to underestimation of LCO_2 and LO_2 , whose values will be determined by cloud fraction and height of the cloud top. For the exact XCO_2 (or MCO_2) determination, it is necessary that these random underestimations, expressed in relative units, be not only correlated but also equal. In principle, taking into account that oxygen and carbon dioxide are well mixed in the atmosphere, the equality of relative LCO_2 and LO_2 variations during transition from clear-sky to cloudy conditions can be achieved through special selection of working channels in absorption bands of these gases. This in turn, will require a certain modification of the existing algorithm of retrieval of the carbon dioxide concentration.

Conclusion

The publication of results of *in situ* airborne measurements of the vertical profiles of carbon dioxide concentration,^{7–9} in combination with free access to archive of ground-based observations of Russian meteorological service, substantially simplifies the development and testing of satellite algorithms of determination of CO_2 concentration over Western Siberia. Obviously, only good agreement with the field measurement data may confirm the reliability of satellite measurements and algorithms used in their processing.

The paper presents the results of first uses of WFM-DOAS algorithm, oriented toward using the data of SCIAMACHY spectrometer, for two regions of Western Siberia. In the warm period of the year, the algorithm shows good qualitative agreement between time behavior of the CO_2 concentration determined with the data of airborne measurements both in the region of Novosibirsk and in the region of Surgut. The range of annual variability of monthly mean CO_2 concentrations, from satellite estimates (12–14 ppmv), practically coincides with the variability of airborne measurements (11–13 ppmv).

In cold period of the year, the satellite algorithm performs unstably and strongly underestimates CO₂ concentrations. Most likely, this is due to the presence of snow cover. The spectral albedo characteristics of snow in oxygen and carbon dioxide absorption bands drastically differ from spectrally neutral albedo A = 0.1, which was used in the reference database WFM-DOAS during retrievals from SCIAMACHY data. It should be expected that expansion of this database using data on the reflection spectra of real terrestrial surfaces and choosing concrete surface types as a function of pixel coordinates will make it possible to use the WFM-DOAS algorithm under these conditions as well. The presence of snow cover can be identified using ground-based meteorological information and from other satellite instruments, as well as using data of SCIAMACHY itself.

For West Siberian regions, the overpass time of the West European satellite Envisat is close to the local solar noon. In combination with large sizes of SCIAMACHY pixel, this leads to the fact that, with the probability higher than 95%, the instrument field of view will always contain either stratus or convective clouds. Simultaneous determination of the number of CO_2 and O_2 molecules in the atmospheric column between clouds and atmospheric top makes it possible to quantify the column mean CO_2 concentration under these conditions. To increase the accuracy and decrease cloud effect on the accuracy of the algorithm, the determination of CO_2 concentration should be performed in specially selected working channels of SCIAMACHY in oxygen and carbon dioxide absorption bands.

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