

## Retrieval of Atmospheric Trace Gases Variability with Satellite Advanced IR sounders

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### Introduction

The new generation space-borne IR-sounders on board current or future environmental satellites (AIRS/Aqua, IASI/MetOp, CrIS/NPOESS, IRFS/Meteor) should provide high spectral resolution ( $0.5\text{-}1.0\text{ cm}^{-1}$ ) radiance measurements of continuous or quasi-continuous coverage from  $3.7$  ( $5.0$ ) to  $15.5\text{ }\mu\text{m}$  allowing to extract valuable information about tropospheric variations of trace gases (TG), namely  $\text{CH}_4$ ,  $\text{N}_2\text{O}$ ,  $\text{CO}$  (under clear sky conditions). Besides, some capabilities should exist for detecting variations of atmospheric carbon dioxide.

This paper describes the approaches developed for the inversion of advanced IR-sounders data and retrieval of  $\text{CH}_4$ ,  $\text{N}_2\text{O}$ ,  $\text{CO}$ , and  $\text{CO}_2$  columnar amounts (CAs). The next section presents brief overview of the retrieval procedures for above first three TG CAs from IASI-Infrared Atmospheric Sounding Interferometer data (Phulpin et al., 2002). These procedures exploit the limited number of the IASI spectral channels and the preceding IASI-based retrievals for the temperature and humidity profiles, and the surface temperature. The simulation study shows that, given rather accurate estimates for listed interfering factors, and nominal IASI instrumental noise characteristics, the sought quantities (CAs of  $\text{CH}_4$ ,  $\text{N}_2\text{O}$ , and  $\text{CO}$ ) can be specified with rather high reliability, i.e. the respective IASI mission objectives (target accuracies) can be achieved. Nevertheless, possible enhancement of existing IASI data inversion technique and retrieval procedures for TG columns is discussed.

The capabilities and limitations to monitor atmospheric  $\text{CO}_2$  variations with advanced IR-sounders have been also investigated. With respect to the measurements of the AIRS-Advanced InfraRed Sounder (on board EOS Aqua spacecraft) the sensitivity studies have been performed, focused on the construction of  $\text{CO}_2$ -dedicated AIRS super-channels (linear combination of pre-selected individual channels) in order to separate the effects of temperature profile and concentration of carbon dioxide variations. The original method to retrieve  $\text{CO}_2$  CA has been developed and tested based on application the empirical and synthetic regression estimators. The validation exercise carried out with actual AIRS data for the area of boreal forests (Western Siberia, Novosibirsk region) and for several dates of year 2003 demonstrates that the retrieval of the  $\text{CO}_2$  CA is really possible. In concluding remarks we discuss the problems and future works to better assess the capabilities of advanced IR-sounders in providing estimates of  $\text{CO}_2$  variability.

### Methodological details of $\text{CH}_4$ , $\text{N}_2\text{O}$ , and $\text{CO}$ retrievals

This section describes the approach developed for the CA retrieval of atmospheric  $\text{CH}_4$ ,  $\text{N}_2\text{O}$ , and  $\text{CO}$  from IASI measurements. The results of verification retrieval experiments with synthetic IASI data are briefly discussed, see also (Uspensky et al., 2000, 2005 a, b, 2006 a).

IASI-based retrieval of the atmosphere trace gas columnar amounts are based on the procedures earlier developed and validated (against simulated IASI measurements) within the dedicated International Sounding Science Working Group (ISSWG) activities performed during 1998-2003. The proposed retrieval methods exploit the preceding IASI-based retrievals for the temperature, humidity and the surface temperature, which are considered as the interfering factors of relevant inverse problems. These supplementary retrievals could be provided using correspondent components of the Modular Prototype Processor (MPP), the integrated IASI data processing software recently developed and validated in frame of the above-mentioned ISSWG studies (Trotsenko et al., 2003).

The MPP is capable of self-contained execution of several procedures to retrieve the geophysical parameters from IASI level 1c data. The list of the retrieved parameters, the target accuracies achieved using the simulated IASI measurements (in terms of RMS - Root Mean Square error per pixel), as well as the interfering factors and their required accuracies to be a priori specified are summarized in Tabl.1. In turn Fig.1 illustrates the number and spectral location of the selected IASI channels utilized for all MPP retrieval procedures.

Table 1. Summary of MPP retrieval accuracies

| MPP retrieval parameters           | Achieved accuracy (RMS per pixel) | Interfering factors to be a priori specified | Required a priori accuracy for interfering factors |
|------------------------------------|-----------------------------------|--|--|
| Surface Skin Temperature (SST)     | $\leq 0.5 - 1.0$ K                | No   | -  |
| Temperature profile (TP)           | $\leq 1.0 - 2.$ K / km            | No   | -  |
| H2O total column                   | $\leq 10$ %                       | SST, TP                                      | $< 1$ K, $< 2$ K/ km                               |
| H2O mixing ratio profile (HP)      | $\leq 20-30$ % / 2km              | SST, TP                                      | $< 1$ K, $< 2$ K/ km                               |
| O3 total column (O3 CA)            | $\leq 10$ %                       | SST, TP                                      | $< 1$ K, $< 2$ K/ km                               |
| O3 partial column (0-20 km layer)  | $\leq 20$ %                       | SST, TP                                      | $< 1$ K, $< 2$ K/ km                               |
| O3 mixing ratio profile (20-40 km) | $\leq 10$ % / km                  | SST, TP                                      | $< 1$ K, $< 2$ K/ km                               |
| CH4 total column (CH4 CA)          | $\leq 5$ %                        | SST, TP, HP                                  | $< 1$ K, $< 2$ K/ km, $< 30\%/2$ km                |
| N2O total column                   | $\leq 10$ %                       | SST, TP, HP, CH4 CA                          | $< 1$ K, $< 2$ K/ km, $< 30\%/2$ km, $< 10\%$      |
| CO total column                    | $\leq 10$ %                       | SST, TP, HP, O3 CA                           | $< 1$ K, $< 2$ K/ km, $< 30\%/2$ km, $< 10\%$      |

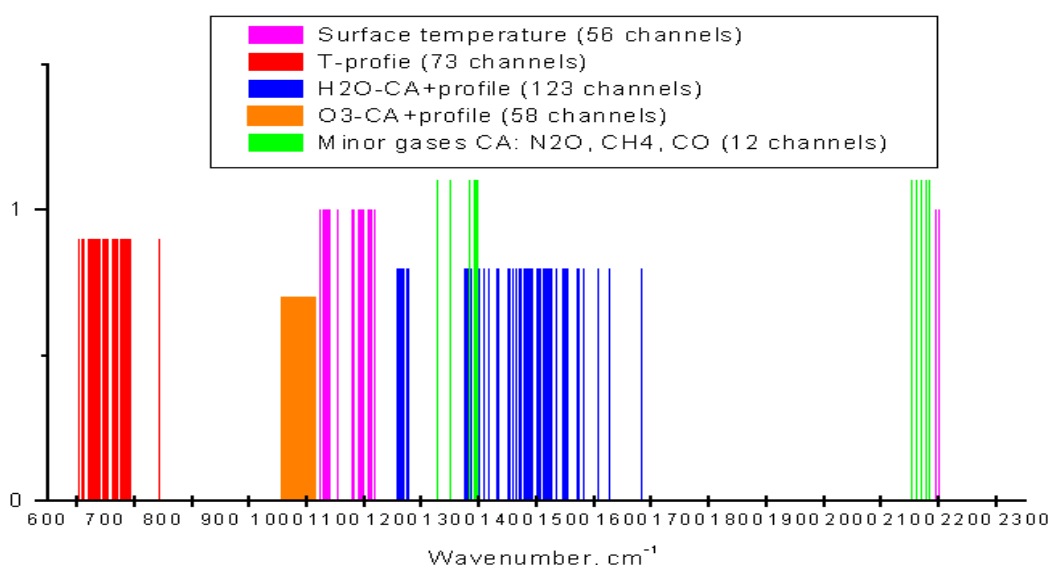


Figure 1. Selected sets of IASI channels applied in MPP retrievals

The MPP retrieval procedure for the TG columnar amounts is based upon the physical inversion method using limited number of the IASI spectral channels shown in Fig.1 (Uspensky et al., 2005 a, b). The first-guess estimates are provided on the basis of the climatological zonally and seasonally averaged data; the Gauss-Newton iteration algorithm is utilized for numerical solution of relevant non-linear inverse problem. The interfering factors, i.e. the temperature  $T(p)$  and the humidity  $q(p)$  profiles, where  $p$  is a pressure, and the surface skin temperature (SST) are taken into account using relevant preceding retrievals provided by correspondent MPP components, namely the regression type procedures for  $T(p)$  and  $q(p)$  (Trotsenko et al., 2003; Uspensky et al., 2003), and the physical multi-

window method for the case of SST (Trotsenko et al., 2003). All supplementary retrievals are also performed using pre-selected sub-sets of the dedicated IASI channels shown in Fig.1.

The verification retrieval experiments have been conducted using synthetic IASI data. Correspondent forward calculations have been carried out using specially developed fast radiative transfer model (FRTM), see, e.g. (Trotsenko et al., 2000). This model has been utilized for producing IASI measurements. Correspondent illustration of the retrieval experiments for the N<sub>2</sub>O case is presented in Fig.2, which shows the RMS retrieval errors as dependent on the atmosphere state implementations for different zones and seasons. In turn, Fig. 3 from (Uspensky et al., 2006 a) demonstrates the RMS retrieval accuracy achieved by relevant MPP procedure for the CH<sub>4</sub>. Below the summary of verification experiments is given, moreover the results are considered separately for methan, nitrous oxide, and carbon monoxide column retrievals.

#### CH<sub>4</sub> column amount retrieval

1. The CH<sub>4</sub> retrieval is carried out using 4 universal IASI channels (i.e. independent on the latitude/longitude zone and/or season): 1332.50, 1341.75, 1342.75, and 1346.75 cm<sup>-1</sup>.
2. The level of retrieval accuracy is at least better than 5 % (in terms of the RMS error) for all seasons and latitude/longitude zones, as well as rather wide range of the column variations (from -10% to +30%).
3. The above accuracy is achieved at moderate level of key interfering factors knowledge correspondent to the RMS accuracy (for the 1 km troposphere resolution) of 2K and 30% for the temperature and the water vapor, respectively.

#### N<sub>2</sub>O column amount retrieval

1. The N<sub>2</sub>O retrieval is performed using three IASI channels, namely, those centered at 1277.25, 1298.50, 1299.50 cm<sup>-1</sup>.
2. Absolutely robust and reliable N<sub>2</sub>O retrieval (within 4-9 % accuracy range) is available for all seasons and zones providing slightly better accuracy for the *a priori* T, q estimates, namely, 1.75 K and 25%, respectively as well as providing the prior estimate of CH<sub>4</sub> with the accuracy at least not worse than 5 %.

#### CO column amount retrieval

1. The CO retrieval is carried out using 5 universal IASI channels (i.e. independent on the latitude/longitude zone and/or season): 2103.25, 2111.50, 2119.75, 2127.75, 2131.75 cm<sup>-1</sup>.
2. The level of retrieval accuracy is at least better than 10 % for all seasons and latitude/longitude zones, moreover this accuracy is guaranteed only for rather wide range of the column variations (more than 10%).
3. The above accuracy is achieved at rather high level of key interfering factors knowledge correspondent to the RMS accuracy of 1.2K, 20% for the temperature and the water vapor and 10-15 % for ozone respectively.

Some concluding remarks to this section appear to be pertinent. We have developed rather efficient technique for the near real time retrieval of methan, nitrous oxide, and carbon monoxide CAs from clear sky IASI measurements and look forward to the availability of fully suitable data (actual IASI measurements) for operational testing. It is expected that the implementation of above technique will provide the CH<sub>4</sub>, N<sub>2</sub>O, and CO column estimates with target accuracies close to IASI mission objectives. However, the need exists to enhance the MPP retrieval procedures and to improve the reliability of output products in order to approach the accuracy levels required for a good representation of CH<sub>4</sub>, N<sub>2</sub>O, CO natural spatio-temporal variabilities (are set to 2-3%, 4-5%, and 10% respectively). Such option with respect to estimates of CH<sub>4</sub>, N<sub>2</sub>O columns exists, most likely, as recently reported in (Turquety et al., 2004), where IASI-based retrieval scheme using neural network technique has been proposed and evaluated.

Our methodological activities will be first of all focused on the development of the “integrated” two-stage retrieval schemes (involving the successive regression and physical inversion phases) for the case of T(p), q(p), and the ozone profile. Furthermore, in context of the trace gases retrieval the studies will be focused on the revised selection of dedicated IASI channels or super-channels in order to minimize the potential negative influence of the temperature profile uncertainties on the accuracy of trace gases retrieval.

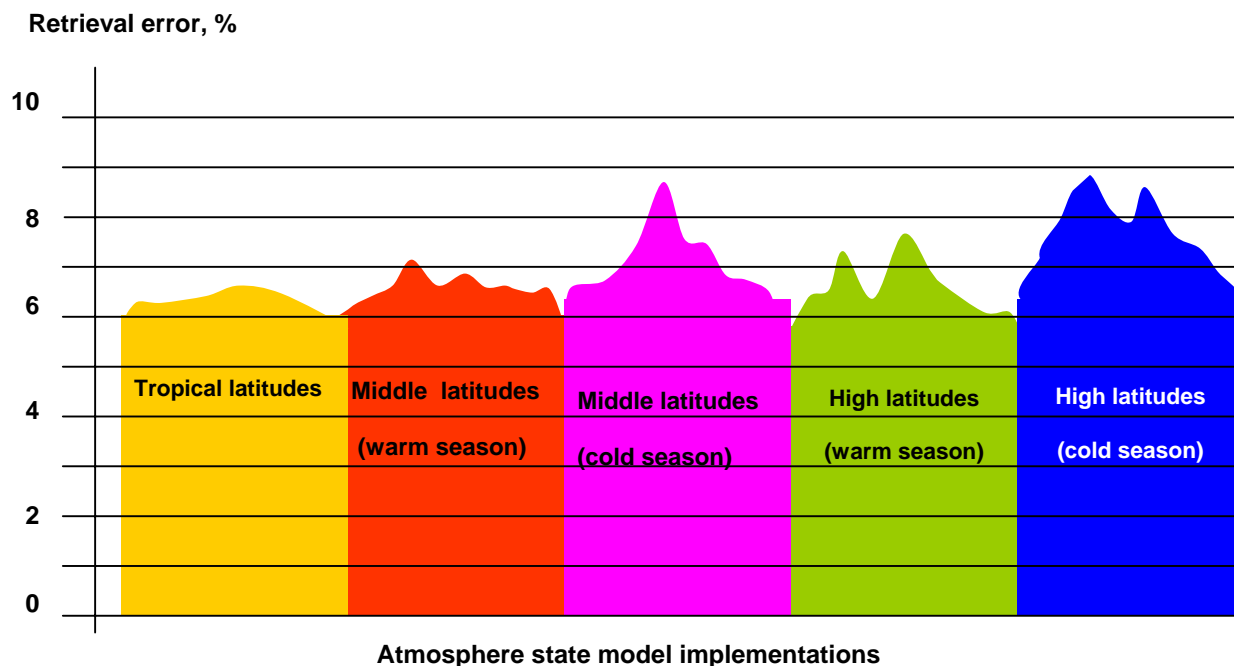


Figure 2. MPP retrieval accuracy for N<sub>2</sub>O columnar amount

### AIRS-based retrieval scheme for carbon dioxide column amounts

In this section we investigate the capabilities of high resolution thermal infrared measurements for detecting changes in CO<sub>2</sub> concentrations and estimating CO<sub>2</sub> column amounts, see also (Uspensky et al., 2005 a, 2006 b). The significant role of carbon dioxide in the carbon cycle and the energy balance of the Earth make it important to detect and to monitor its spatio-temporal concentration variability in the atmosphere. The current observing system for carbon dioxide has a significant gap as observations of CO<sub>2</sub> are mostly based on sparsely distributed surface measurements (approximately 100 sites around the world) as well as on even more sparse (but high quality) airborne in-situ observations. The only way to obtain respective global information on CO<sub>2</sub> is to develop the remote sensing techniques capable of retrieving CO<sub>2</sub> column amounts and profiles from satellite-based measurements.

The major objective of our study is developing and testing novel techniques suitable for the retrieval of CO<sub>2</sub> columnar amounts from AIRS/Aqua measurements. Several studies have already been addressed this issue, the overview of earlier proposed approaches can be found in (Uspensky et al., 2005 a, 2006 b). Here we will outline briefly focal points of performed studies, paying attention to the analysis and inversion of the AIRS data. Then we will address to the proposed methodology for estimating CO<sub>2</sub> columnar amount from AIRS data.

Preliminary feasibility studies (Chedin et al, 2003; Christi and Stephens, 2004) have demonstrated that IASI or AIRS data (matched with AMSU) can be used for estimating the CO<sub>2</sub> variations in the mid-and upper-tropospheric layers. Selection of AIRS channel subset in (Chedin et al., 2003) with well-known technique (Rodgers, 1996) demonstrates that around 50 AIRS channels are sufficient to extract most of the CO<sub>2</sub> information.

In (Barnet et al., 2004) the research algorithms have been developed for the retrieval of CO, CO<sub>2</sub>, and CH<sub>4</sub> with precision of 15%, 0.5% and 1% respectively from synthetic AIRS data. The AIRS data were simulated using Fast Radiative Transfer Model (FRTM) SARTA (Stand alone AIRS Radiative Transfer Algorithm), see (Strow et al., 2003). The sensitivity studies were carried out on the base of the "signal-to-noise ratio" (S/N) analysis.

The original procedure of AIRS channels selection for CO<sub>2</sub> and other trace gases retrieval is proposed in (Crevoisier et al., 2003) based on the study of the sensitivities of AIRS channels to variations of the different atmospheric components. As a result, the subset of 40-50 channels (within 15 and 4,3 μm bands) has been selected providing the retrieval of CO<sub>2</sub> in conditions of tropical, temperate and polar air masses. The results of above studies have been utilized in (Crevoisier et al., 2004) for the analysis of real AIRS data and retrieval the mid-tropospheric CO<sub>2</sub> concentration in the tropics (20°S ÷ 20°N). The retrieval method makes use of data in 8 AIRS channels located in the 15 μm spectral band as well as MW measurements in 3 AMSU-A channels. A mean precision of the method (comparing monthly averaged values) is about 2.5 ppmv.

The approach to build efficient CO<sub>2</sub> column (Q<sub>CA</sub>) retrieval methodology includes, as usually, following stages:

- collecting a dataset with representative samples of atmospheric state vectors and AIRS measurements— these may be real or simulated;
- analysis of the satellite data information content with respect to CO<sub>2</sub> perturbations( sensitivity studies), and selection of dedicated AIRS channel subsets;
- development, testing, and validating the procedure for retrieval carbon dioxide CA.

To generate a simulation dataset, one needs a representative sample of atmospheric state vectors that include the associated CO<sub>2</sub> column amounts Q<sub>CA</sub> and/or vertical profiles Q(p) of CO<sub>2</sub> mixing ratio. Various datasets can be utilized for compiling sample atmospheric state vectors, in particular, ECMWF or UKMO analysis data. As for CO<sub>2</sub> information, we used in our studies, along with two “typical” Q(p) profiles (mid- and high-latitudes), constant Q(p) profiles (Q<sub>CA</sub> in the range of 350-370 ppmv), and the results of airborne in-situ CO<sub>2</sub> observations (Arshinov et al., 2005; Zuev et al., 2005). Basing on detailed overview of spatio-temporal variability of atmospheric CO<sub>2</sub> concentration (Chedin et al., 2003; Christi et al., 2004) the variations of Q<sub>CA</sub> in the range 5-15 ppmv were chosen.

The modified version of FRTM SARTA has been implemented at SRC “Planeta” on a WINDOWS platform and than has been used for modeling AIRS measurements and for conducting sensitivity studies. Our techniques of satellite data sensitivity analysis and selection of dedicated channel subset (Trotsenko et al., 2003) has much in common with those from (Crevoisier et al., 2003; Barnett et al., 2004). The results of relevant studies can be partly summarized as follows (Uspensky et al., 2005 a, 2006 b):

- total column carbon dioxide changes of 10 ppmv from 370 ppmv (assuming a fixed temperature and humidity profile) produce changes in the CO<sub>2</sub> absorption bands of about 0.4Kt 13.9μm and 0.6K at 4.4μm (well outside of instrument noise);
- accounting for vertical distributions Q(p) of CO<sub>2</sub> versus assuming a constant Q<sub>CA</sub> ≡ 370 ppmv (T(p) and q(p) are fixed) produces changes in the carbon dioxide LW and SW absorption bands of about 0.5K;
- the CO<sub>2</sub>-dedicated channels subset is found to be close to correspondent subset from (Crevoisier et al., 2003).

Retrieval of CO<sub>2</sub> column amount Q<sub>CA</sub> or vertical profiles Q(p) from advanced IR sounders data is problematic since the signals in IR channels sensitive to CO<sub>2</sub> variations are also sensitive to temperature profile T(p) variations as well as to presence of clouds. Moreover the temperature and cloud variations should be treated as the main interfering factors. Therefore to advance the remote sensing methodology for monitoring CO<sub>2</sub> concentration from advanced IR sounders data means separating these effects. In line with this two approaches are appears to be suitable for AIRS data inversion: concurrent retrieval of “full” state vectors (incorporating some parameters relating to CO<sub>2</sub> abundance) and self-dependent (or stand alone) retrieval of CO<sub>2</sub> abundance characteristics (using ancillary information, e. g. extracted from the same AIRS data). The evident advantage of the first approach is that it should provide the accuracy improvement for T(p),q(p) retrievals due to more accurate knowledge of CO<sub>2</sub>. The second approach has the advantage as more flexible and less complicated and therefore it has been selected for AIRS data inversion.

The implementation of second approach depends crucially on the appropriate selection of dedicated channels and than super-channels (i.e. linear combination of dedicated channels), that should help to separate effects of temperature and carbon dioxide variations. In other words it is necessary to specify channels and super-channels with identical (or almost identical) and strongly

differing response to  $T(p)$  and  $Q(p)$  variations respectively. In what follows the relevant channels are designated as temperature-(or T-) and  $CO_2$ -dedicated. Solving this problem is based on the generalization of approach proposed in (Aumann et al., 2005).

Below is given a brief mathematical background of proposed techniques. The procedure of building relevant super-channels comprises of several steps, namely:

1) Selection of T- and  $CO_2$  -dedicated channels with “similar” temperature Jacobians or weighting functions  $H_T$ ; signals in one T-and several  $CO_2$ -dedicated channels are designated as  $T_B(I)$  and  $T_B(II)$ ,  $T_B(III)$ ,... respectively (radiances are presented in terms of brightness temperature  $T_B$ ).

2) Specification of “synthetic” channel with signal  $T_B(\text{synth})$  as linear combination of two or more  $CO_2$ -dedicated channels (signals  $T_B(II)$ ,  $T_B(III)$ ,  $T_B(IV)$ ,...) and with temperature Jacobian, close to the Jacobian of T-dedicated channel. Signal in the synthetic channel is formed using least square fitting in order to improve match in the temperature Jacobian of T-dedicated and synthetic channels; more exactly,  $T_B(\text{synth}) = K_1 T_B(II) + K_2 T_B(III)$ , where  $K_1$ ,  $K_2$  are derived as solution of extremal problem::

$$\min J_W(K_1, K_2) = \sum_i [H_{T,I}(p_i) - H_{T,\text{synth}}(p_i)]^2, \quad H_{T,\text{synth}}(p) = K_1 H_{T,II}(p) + K_2 H_{T,III}(p).$$

3) Derivation of super-channel (SC) with signal  $T_B(\text{sc}) = T_B(I) - T_B(\text{synth})$ .

Due to similarity of temperature Jacobians  $H_{T,I}$  and  $H_{T,\text{synth}}$  the signals  $T_{B,j}(\text{sc})$  should have small sensitivity to variations  $\Delta T_j(p) = T_j(p) - T_0(p)$ , where  $T_0(p)$  is reference temperature profile(component of reference vector  $\mathbf{x}_0$ ). Indeed, the signal in the super-channel can be presented as:

$$T_B(\text{sc}) = T_{B,0}(\text{sc}) + \delta_T T_B(\text{sc}) + \delta_q T_B(\text{sc}) + \delta_{Oz} T_B(\text{sc}) + \delta_{Q_{CA}} T_B(\text{sc}) + \varepsilon, \quad (1)$$

where  $T_{B,0}(\text{sc})$  is modeled signal calculated for vector  $\mathbf{x}_0$ ;

$$\delta_T T_B(\text{sc}) = (H_{T,I} - H_{T,\text{synth}}) \Delta T, \quad \delta_q T_B(\text{sc}) = (H_{q,I} - H_{q,\text{synth}}) \Delta q,$$

$$\delta_{Oz} T_B(\text{sc}) = (H_{Oz,I} - H_{Oz,\text{synth}}) \Delta Oz, \quad \delta_{Q_{CA}} T_B(\text{sc}) = (H_{Q,I} - H_{Q,\text{synth}}) \Delta Q_{CA}.$$

Terms  $\delta_T T_B(\text{sc})$ ,  $\delta_q T_B(\text{sc})$ ,  $\delta_{Oz} T_B(\text{sc})$  from (1) present input of variations  $T(p)$  and other interfering factors into signal variations  $\Delta T_B(\text{sc}) = T_B(\text{sc}) - T_{B,0}(\text{sc})$ . Variations  $|\delta_{Q_{CA}} T_B(\text{sc})|$  should exceed notably variations  $|\delta_T T_B(\text{sc})|$  as well as should exceed the instrumental noise.

Basing on the super-channel specification, the computationally simple algorithm of AIRS data inversion and  $\Delta Q_{CA}$  retrieval has been proposed. Formulae (1) can be presented as follows:

$$\Delta T_B(\text{sc}) = k_1 + k_2 \Delta Q_{CA} + \varepsilon,$$

where  $k_1 = \delta_T T_B(\text{sc}) + \delta_q T_B(\text{sc}) + \delta_{Oz} T_B(\text{sc})$ ,  $k_2 = H_Q(\text{sc})$ , moreover the value of  $|k_1|$  should be small. Linear relationship between  $\Delta Q_{CA}$  and measurements (variations  $\Delta T_B(\text{sc})$ ) leads to the following formulae for regression estimator of  $\Delta Q_{CA}$ :

$$\Delta Q_{CA}(\text{regr}) = C_1 \Delta T_B(\text{sc}) + C_2, \quad (2)$$

where  $C_1$ ,  $C_2$  – const are regression coefficients.

In (Aumann et. al., 2005) the first step of above procedure (building of super-channel) has resulted the choice of one T-dedicated channel N 1917 at  $2229.6 \text{ cm}^{-1}$ , as well as two  $CO_2$  - dedicated channels N 2109 ( $2388.2 \text{ cm}^{-1}$ ) and N 2113 ( $2392.1 \text{ cm}^{-1}$ ). Fig. 3 demonstrates that temperature Jacobians of channel N 1917 and synthetic channel (calculated with SARTA for two various atmospheric state vectors) are close to each other. Based on this it seems reasonable to proceed with steps 2), 3) in order to derive consecutively the signals in the synthetic channel, and in the super-channel:  $T_B(\text{synth}) = K_1 T_B(2109) + K_2 T_B(2113)$ ,  $T_B(\text{sc}) = T_B(1917) - T_B(\text{synth})$ .

The values of regression coefficients  $K_1$ ,  $K_2$  depend, in general, on the state vector  $\mathbf{x}$  (mainly, on the temperature profile  $T(p)$ ) and may be found using training sample of calculated (with SARTA) temperature Jacobians in AIRS channels of interest. According to experiments performed the magnitudes of  $K_1$ ,  $K_2$  change from 0.516 and 0.426 (warm season- June) to 0.322 and 0.512 (cold season – November).

The super-channel introduction reduces significantly the effect of temperature variations. Using of corresponding  $K_1$ ,  $K_2$  (that relate to interested time period and region) provides the variations in  $T_B(\text{sc})$  about 0.05K due to  $T(p)$  uncertainties in the range  $\pm 2.5K$  and variations about 0.27K(outside of instrument noise) induced by  $Q_{CA}$  variations in the range  $\pm 10 \text{ ppmv}$ . Thus the temperature uncertainty effects can be suppressed for the signal in AIRS super-channel, moreover the signal

appears to be sensitive to  $Q_{CA}$  variations. This feature justifies practically the proposed algorithm (2) for AIRS data inversion and retrieval the  $\Delta Q_{CA}$  (with reduced requirements to accurate knowledge the true profile  $T(p)$  in sounding point).

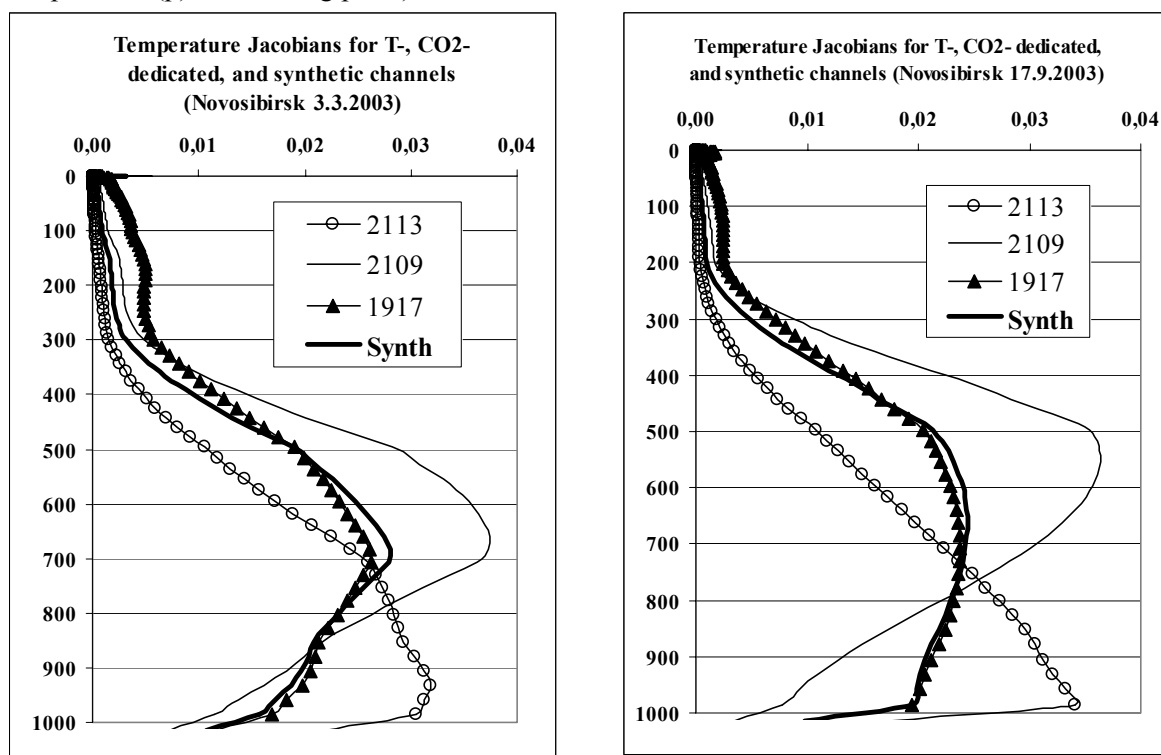


Fig 3 The temperature Jacobians for original (NN 1917, 2109, 2113) and synthetic channels

The value  $\Delta T_B$  (sc) is treated as predictor variable in the regression estimator (2), moreover  $T_B(sc)$  is generated from AIRS measured spectrum, and  $T_{B,0}(sc)$  is calculated with SARTA for known “full” atmospheric state vector (UKMO analysis data plus first guess carbon dioxide profile with  $Q_{CA} = Q_{CA}(ref)$ ).

There exist at least two approaches to build the regression estimator (2): to derive  $C_1$ ,  $C_2$  on the base of training sample with synthetic AIRS measurements (approach is designated as synthetic regression); to derive  $C_1$ ,  $C_2$  on the base of training sample with real AIRS measurements and collocated data on  $Q_{CA}$  (empirical regression). The advantage of the synthetic regression is evident, since anyone doesn't need to compile the training sample with real  $CO_2$  data. Unfortunately, the suitability of synthetic regression to real AIRS data is questionable. It depends on many factors (partially uncontrolled) and should be stated only via retrieval experiments. The empirical regression seems more suitable but its implementation depends crucially on ability of compiling representative training sample (in general it is rather difficult task due to very sparse  $CO_2$  observing system).

The formulation of regression algorithm (2) doesn't account for dependence on scanning angle. It is to some extent the simplification, but nevertheless the developed algorithm should work definitely for the clusters of sub-satellite footprints (pixels).

Developing and testing the retrieval procedure (2) has been carried out at first for the synthetic AIRS data over the area of boreal forests in Western Siberia. The UKMO (Bracknell) analysis data (January-December, 2003) have been utilized as input for SARTA calculations. For the regression estimator (2) and one month time period (June 2003) the regression coefficients  $C_1$  and  $C_2$  are found to be equal 35.9 and 0.14 respectively with correlation coefficient  $R^2 = 0.97$ . Note that coefficient  $C_2$  (which should account for possible biases) is close to zero. The second (undesirable) feature is rather large magnitude of  $C_1$ . This is caused evidently by relatively low sensitivity of signal (in  $CO_2$  – super-channel) to  $Q_{CA}$  perturbations. Large  $C_1$  values provide noticeable amplification of uncertainties in predictor variable  $\Delta T_B(sc)$  and may cause significant  $Q_{CA}$  retrieval errors. Therefore careful derivation of  $\Delta T_B(sc)$  is required involving possible filtering and averaging of original (real) AIRS cloud free data.

According to retrieval error statistics (experiments with independent sample of synthetic AIRS data -500 implementations for each of 5 magnitudes  $Q_{CA}$  given) the RMS error doesn't exceed 2.1 ppmv. Generally the accuracy of carbon dioxide CA retrievals from synthetic AIRS data is in the range 1.5-3.0 ppmv depending on adopted magnitudes of variations  $|\Delta T(p)|$ .

Validation of the AIRS-based CO<sub>2</sub> CA retrievals over Siberian boreal forests. In order to evaluate the efficiency of developed procedure (2) and to validate the retrievals against independent CO<sub>2</sub> observations, the series of retrieval experiments has been conducted for a sample of more than 15 granules of actual AIRS measurements. First of all we investigated the availability of independent ground-based (or airborne) CO<sub>2</sub> in-situ observations for the selected area of boreal forests and during the period of functioning AIRS/Aqua (end of 2002 and after). It was found to be suitable to use the results of airborne measurements that have been performed within the framework of a joint Japanese-Russian Project on the study of greenhouse gases in Siberian ecosystems, see e.g. (Arshinov et al., 2005). Regular measurements of the CO<sub>2</sub> concentration over the part of western Siberian forests have been carried out since 1997 till now with the use of an AN-30 flying laboratory. The region of airborne surveys (vicinity of Novosibirsk city) or Region Of Interest (ROI) is located at the right bank of the southern part of the Ob Reservoir. The airborne measurements cover the region 54° 08' -54° 33' N, 81° 51' -82° 40' E., moreover the boreal area consists 90% of coniferous trees. At the end of each month the ambient air is flask- sampled at heights of 0.5, 1.0, 1.5, 2.0, 3.0, 4.0, 5.5 and 7.0 km. As a result, the CO<sub>2</sub> profiles characterizing monthly variations of its vertical distribution have been specified. Further details can be found in cited paper of Arshinov et al.

Table 2 contains the monthly averaged magnitudes of  $Q_{CA}$  for the ROI (designated as Novos). and year 2003. Along with this analogous data are given for other Siberian region (vicinity of Surgut city) derived also from airborne observations.

Table 2. Monthly averaged CO<sub>2</sub> columns (ppmv) for two Siberian regions.

|        | Jan   | Feb   | March | Apr   | May   | June  | July  | Aug   | Sept  | Oct   | Nov   | Dec   |
|--------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| Novos  | 380.9 | 377.4 | 381.2 | 382.2 | 379.3 | 374.9 | 368.7 | 370.6 | 373.6 | 381.1 | 378.5 | 379.3 |
| Surgut | 378.7 | 379.6 | 380.2 | 381.0 | 379.3 | 375.8 | 369.0 | 368.2 | 372.0 | 375.2 | 376.2 | 379.0 |

At the first stage of our validation effort the testing of the SARTA code was performed by comparing modeled AIRS data with observed quantities for one case study – a granule of real AIRS data (N 208, June 25, 2003). This granule contains a subset of 120 cloud free footprints, covering the ROI. Radiances and brightness temperatures were calculated with SARTA using state vector  $\mathbf{x}$  (its components, namely, T- and q-profiles were extracted from the UKMO analysis) and compared with collocated AIRS-observations. The time window for match-up of satellite and UKMO analysis was about 6 hours; within a maximum distance of 160 km the AIRS footprints closest to the analysis grid point were used. Retrieved surface brightness temperature was used in the calculations. For each channel the sample of 120 cloud free observed  $T_B$  values (from 120 pixels within ROI) was compared with one calculated  $T_B^{calc}$ .

RMS differences between measured ( $T_B$ ) and calculated ( $T_B^{calc}$ ) brightness temperatures are found to be equal 0.463, 0.438, 0.679K for the channels NN 1917, 2109, 2113 respectively. Correspondent biases equal to - 0.081, 0.256, - 0.058K. The bias and RMS values look reasonable if to account for various types of error that may contribute to the differences between  $T_B$  and  $T_B^{calc}$ . These errors include:

- instrumental noise  $\epsilon_j$  (random errors);
- systematic instrument errors;
- forward-model errors (may include both systematic and random components, see (Strow et al., 2003);
- atmospheric model and sampling errors. In order to determine full state vector  $\mathbf{x}$ , the analysis data were complemented via extrapolation T-, q-profiles beyond 10 hPa and 400 hPa, as well as via



specification  $Q_{O_2}(p)$  and  $T_s, \epsilon_s$ . Along with this additional uncertainties (sampling errors) arise due to time and spatial windows between satellite and analysis data.

The above discussion enables to conclude that the SARTA code is rather efficient tool that can faithfully substitute LBL-codes for modeling AIRS measurements. Nevertheless further SARTA testing is needed to obtain representative error statistics.

Now we come directly to the description of the validation performance, which comprises of several steps:

Step 1 – collecting a dataset  $V$  with representative samples of real AIRS measurements and collocated atmospheric state vectors (including associated  $Q_{CA}$  values and/or profiles);

Step 2 – developing and testing the regression estimator (2) on the base of training/control samples extracted from dataset  $V$ ;

Step 3 – comparison the retrievals against airborne  $CO_2$  observations and assessment of the retrieval skill and application limits.

Below some comments and additional details are given relating to the accomplishment of steps 1-3.

Step 1: To compile dataset  $V$ , a set of real AIRS data, namely granules viewing pre-selected area (see above) and time period between January and December 2003 (for one-two dates of each month) have been downloaded from the website <http://daac.gsfc.nasa.gov>. The atmospheric T- and q-profiles for the same area and time period have been extracted, as already mentioned, from the UKMO analysis and complemented by results of airborne  $CO_2$  measurements.

Step 2, 3: Development and application of retrieval procedure (2) is based on the use of cloud free AIRS measurements. Therefore we need some tests to exclude cloud-contaminated data from AIRS-measured spectra while compiling dataset  $V$ . To perform cloud-screening, some well-known threshold procedures are usually applied to AIRS data in transparent channels, but in the framework of this study we preferred to utilize special multi-spectral data analysis toolkit (called HYDRA) that has been developed at CIMSS UW and is available at <http://www.ssec.wisc.edu/hydra/>. This toolkit enables to detect cloud contaminated data (on the base of analysis of surface and cloud features in transparent AIRS channels).

The efforts have been undertaken to compile representative training sample of collocated AIRS measurements and airborne  $CO_2$  observations for the ROI and 2003 year period. As already mentioned, we have downloaded more than 15 granules with real AIRS measurements for the ROI and time period between January and November 2003. The first experiments with real AIRS data inversion have demonstrated the necessity to build and to apply both the synthetic and empirical regression estimators (2), characteristic for several months.

Fig. 4 illustrates some results of testing the AIRS data inversion procedure (2) and validation the regression estimates  $Q_{CA}^{reg}$  against true (in-situ airborne) data. Here are plotted the curve characterizing monthly averaged behavior of  $Q_{CA}$  together with two various AIRS-based regression estimates  $Q_{CA}^{reg}$ . It should be reminded that  $Q_{CA}^{reg}$  are generated only for separate dates (when cloud free AIRS data were available for the ROI or “neighboring” area within respective granule) and are hardly be treated as consistent estimates of monthly averaged magnitudes  $Q_{CA}$ . Nevertheless, comparison of above values should provide some preliminary feasibility estimates for  $Q_{CA}$  retrievals. Due to very small size of the sample “retrieved - true values” as well as to different meaning of analyzed values (averaged or individual estimates) the retrieval precision estimates (the biases about 6-8 ppmv) look merely tentative. The extension of above studies is necessarily needed based on involving more real AIRS data, considering other ROIs as well as refinement the prototype inversion algorithm (2).

The results of validation exercise performance can be summarized as follows:

1) The proposed AIRS data inversion procedure enables to retrieve  $Q_{CA}$  variations over boreal forests that agree (at least qualitatively) with in situ airborne measurements. The decrease of carbon dioxide CA from March to July and the increase from July to November has been identified with a peak-to-peak variation of 8-10 ppmv that is also consistent with airborne measurements. A more detailed study is needed in order to assess the real accuracy level of retrievals.

2) Future work to better assess the capabilities of AIRS in providing  $CO_2$  information as well as to refine the proposed regression algorithm should accomplish the following:

a) Create a data set of CO<sub>2</sub> mixing ratio profiles (on the base of in situ airborne observations) representative of real variability for different regions over boreal forests complemented by collocated satellite measurements and data on respective atmospheric state vectors.

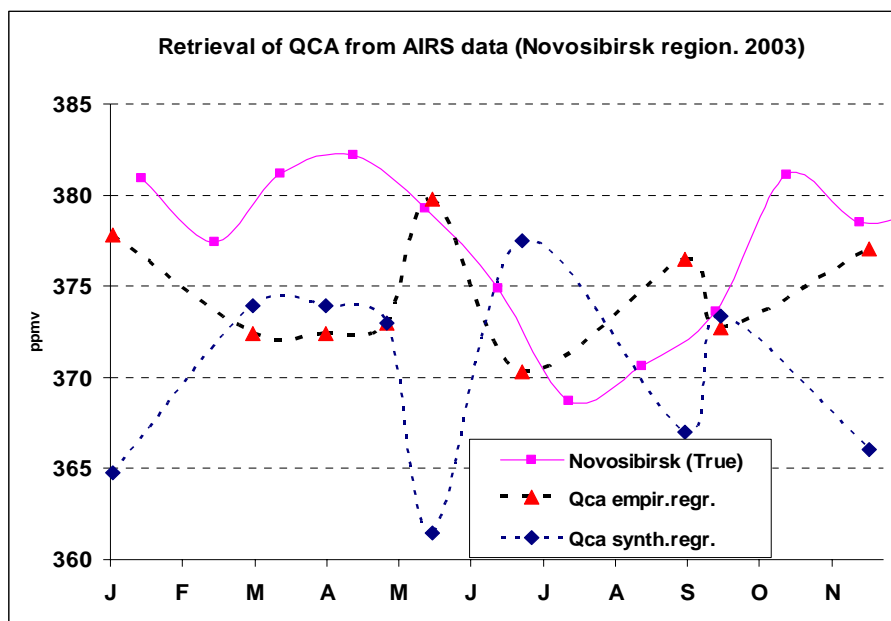


Fig. 5. The results of testing the AIRS data inversion procedure (2)

b) Build and test the empirical and the synthetic regression estimators (2).

c) Examine the behavior of retrieval errors as a function of regression type, season, geography, and the number of pixels to be averaged in space and time.

d) Refine the regression algorithm of CO<sub>2</sub> retrieval through more representative validation exercise, and utilize the regression estimator for Q<sub>CA</sub> as the first guess in the concurrent retrieval of “full” state vector.

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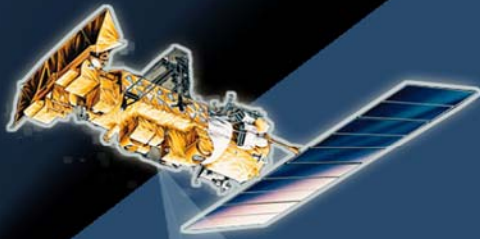
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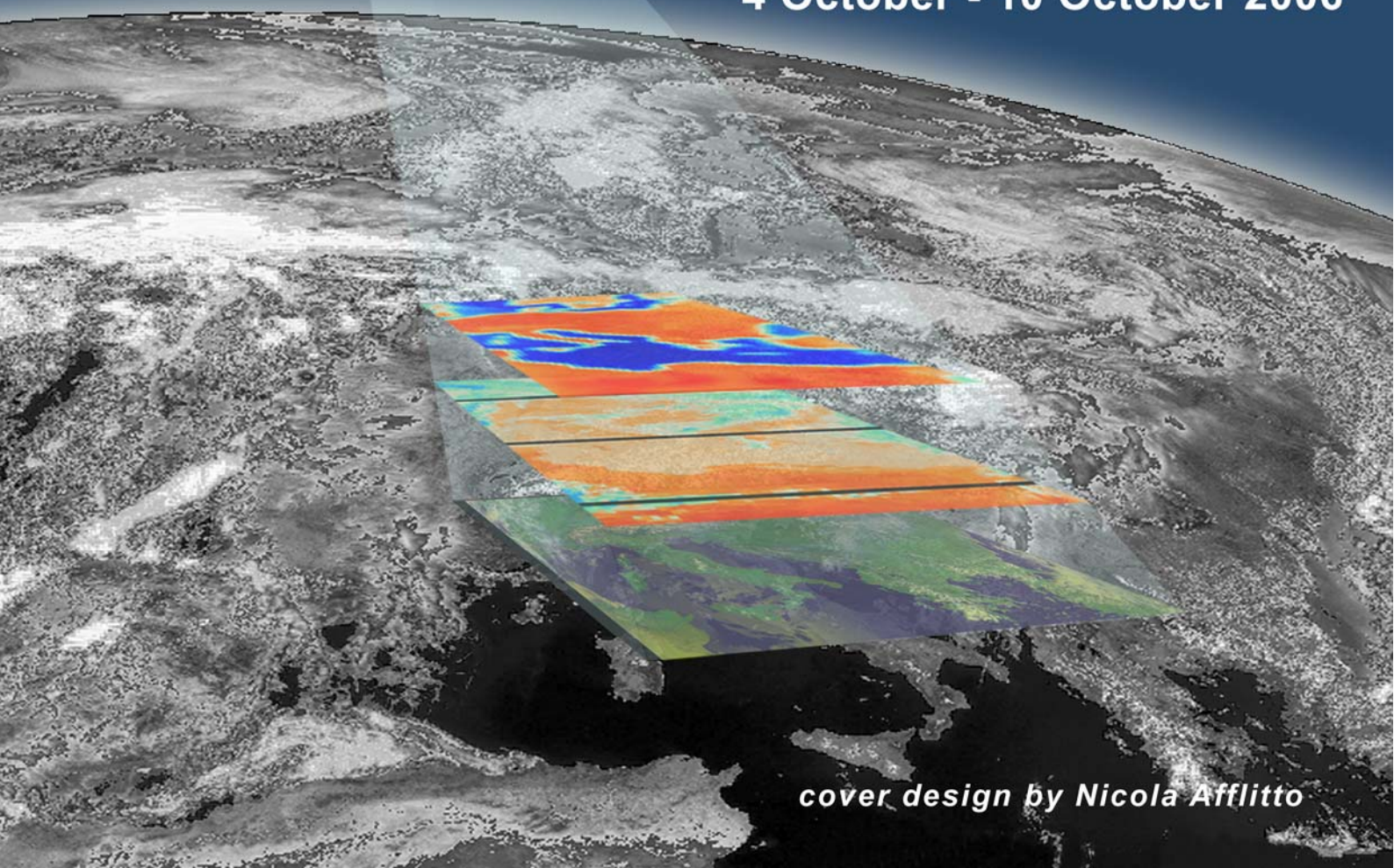
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