CEOS Intercalibration of Ground-Based Spectrometers and Lidars

Minispectrometer Intercalibration and Satellite Validation

Report 6 :

Validation protocol

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Document Change Record

Issue	Date	Page	Observations
1	2013-11-08	All	First draft version
2	2013-11-15	5, 6, 10	Minor corrections and typos
3	2013-11-29	3	Minor addition

1 Introduction

This report is deliverable D6 of the project [RD01, RD02]. Section 2 examines results of previous comparisons between Pandora measurements and satellite retrievals. Section 3 shows an initial study comparing the reprocessed Pandora O_3 and NO_2 data at two stations with observations from SCIAMACHY. Section 4 presents our suggested validation strategy to be applied to the entire Pandora data base.

1.1 Reference Documents

No	Description
RD01	Inter-calibration of ground-based spectrometers and Lidars – Minispectrometer Intercalibration and Satellite Validation [Statement of Work], Issue 1, Revision 0, GMES-CLVL-EOPG-SW-13-0001, 15 January 2013.
RD02	Inter-calibration of ground-based spectrometers and Lidars – Minispectrometer Intercalibration and Satellite Validation [Proposal], Contract: 22202/09/I-EC, RFQ/3-12340/08/I-EC, 22 January 2013.
RD03	Inter-calibration of ground-based spectrometers and Lidars – Minispectrometer Intercalibration and Satellite Validation, Report 2: Recommendations for Inter-Calibration of minispectrometer networks, 25 September 2013.
RD04	Tzortziou M., J.R. Herman, A. Cede, C.P. Loughner, N. Abuhassan, and S. Naik, Spatial and temporal variability of ozone and nitrogen dioxide over a major urban estuarine ecosystem, J. Atmos. Chem., DOI 10.1007/s10874-013-9255-8, 2013.
RD05	Reed, A.J., et al., Effects of local meteorology and aerosols on ozone and nitrogen dioxide retrievals from OMI and pandora spectrometers in Maryland, USA during DISCOVER-AQ 2011, J Atmos Chem, DOI 10.1007/s10874-013-9254-9, 2013.
RD06	Tzortziou, M., J.R. Herman, A. Cede, and N. Abuhassan, High precision, absolute total column ozone measurements from the Pandora spectrometer system: Comparisons with data from a Brewer double monochromator and Aura OMI, J. Geophys. Res., 117 (D16303), doi:10.1029/2012JD017814, 2012.
RD07	Herman, J., A. Cede, E. Spinei, G. Mount, M. Tzortziou, and N. Abuhassan, NO2 column amounts from ground-based Pandora and MFDOAS spectrometers using the direct-sun DOAS technique: Intercomparisons and application to OMI validation, J. Geophys. Res., 114 (D13307), 10.1029/2009JD011848, 2009.
RD08	Inter-calibration of ground-based spectrometers and Lidars – Minispectrometer Intercalibration and Satellite Validation, Report 1: List of minispectrometers considered in this activity, 10 April 2013.

1.2 Definitions, Acronyms and Abbreviations

No	Description
DU	Dobson Units
ESA	European Space Agency
GSFC	Goddard Space Flight Center
Izana	Izana Atmoshperic Research Center
NO_2	Nitrogen Dioxide
O_3	Ozone
OMI	Ozone Monitoring Instrument
SCIAMACHY	SCanning Imaging Absorption SpectroMeter for Atmospheric CHartographY

2 Previous comparisons between Pandora data and satellite retrievals

Pandora data from a limited number of stations have been compared to OMI retrievals of O_3 and NO_2 previously [RD03 to RD07]. The following observations are made based on the analysis of those studies:

1. All studies used the OMI station overpass data available at `http://avdc.gsfc.nasa.gov/`.
2. All studies used the standard Pandora cloud filtering (O_3 uncertainty <5DU and NO_2 uncertainty <0.05DU).
3. For all studies the ground data are averaged in time for an interval centered at the OMI-overpass time. Since the satellite data provide a spatial average over its footprint, a temporal average for the ground data is considered more representative than a snapshot exactly at the overpass time. The length of interval used is 60min or 120min, except for the NO_2 comparison in RD3, where it is 20min.
4. All studies limited the OMI-data to those with cloud fraction smaller than 0.2. Allowing larger cloud fractions made the comparisons for both O_3 and NO_2 irrelevant.
5. The studies limited the OMI-data to those observations, where the center of the satellite pixel was within 20km [RD07], 50km [RD03, RD06], or 60km [RD04, RD05] from the ground location. This limitation has a moderate influence on the O_3 comparison, but a significant effect on the NO_2 comparison.
6. The correlation coefficients between satellite and ground data is typically above 0.9 for O_3, and much smaller for NO_2 (<0.7).
7. Since O_3 total columns are in general spatially homogeneous, differences between satellite and ground O_3 data (after applying proper filtering for clouds) are dominated by differences in instrument calibration and algorithm.
8. Since NO_2 total columns are in general spatially inhomogeneous, differences between satellite and ground NO_2 data (after applying proper filtering for clouds) are dominated by differences in the observed air mass from ground and space. The satellite scans air masses from an extended region, while the ground-based direct sun measurements scans air from a rather narrow cone extending from the instrument to the top of the atmosphere in the direction of the solar beam.
9. The differences ground NO_2 data minus satellite NO_2 data are typically positive for urban ground sites and negative for rural sites, where urban settlements are in close proximity.

3 Initial study comparing Pandora with SCIAMACHY

There is no official ESA-site available with preprocessed SCIAMACHY overpass data for a number of ground locations. This means the user would have to extract data from the level 2 files, which is very time-consuming. Alessandro Burini from ESA has agreed to perform such an extraction of overpass data for us (see section 4). In the meanwhile, for this initial study, we used preprocessed overpass data from the following sources:

For NO_2 and O_3 at station GSFC, latitude 38.99° north, longitude 76.83° west:
`http://www.temis.nl/airpollution/no2col/data/scia/overpass/Goddard_sciano2.dat`
`http://www.iup.uni-bremen.de/gome/wfdoas/overpass_scia/SC447GOD.dat`

For NO_2 station Izana, latitude 28.31° north, longitude 16.50° west:
`http://www.temis.nl/airpollution/no2col/data/scia/overpass/Izana_sciano2.dat`

Figures 1 and 2 show scatterplots of total columns from SCIAMACHY versus Pandora for NO_2 and O_3 from Pandoras 3 and 9 at GSFC, and for NO_2 from Pandora 101 at Izana. The ground-data are cloud filtered using the standard Pandora cloud filter and are averaged in time for an interval centered around the SCIAMACHY-overpass time. Based on the experience of RD03, we have chosen an interval is 60min for O_3 and 20min for NO_2. SCIAMACHY data are not filtered at all, which means they include all footprints up to a distance of 300km to the ground location. This is caused by a lack of proper entries for the filtering in the overpass data that were used (e.g. cloud fraction or exact footprint position missing for O_3). Nevertheless, an indirect cloud filter for SCIAMACHY is given with the Pandora cloud filter, since cloudy moments at the ground site are often coinciding with high cloud fraction in the satellite retrieval.

As expected the correlation between Pandora and SCIAMACHY total O_3 columns is very good (>0.95, figure 1), while for NO_2 columns it is much smaller (figure 2). The large point-to-point scatter for NO_2 can be explained by the large SCIAMACHY footprint in combination with the spatial inhomogeneity of NO_2.

Some statistics on the differences between Pandora and SCIAMACHY data are given in table 1. The agreement for O_3 can be considered excellent despite the unfiltered satellite data.

Table 1: Differences Pandora minus SCIAMACHY total columns, all numbers are in DU

Gas	Instrument	Location	Median	25-75 percentile range	10-90 percentile range
O_3	Pandora 3	GSFC	-4.2	-10 to +3	-15 to +10
O_3	Pandora 9	GSFC	+0.4	-5 to +6	-9 to +10
NO_2	Pandora 3	GSFC	0	-0.09 to +0.08	-0.18 to +0.15
NO_2	Pandora 9	GSFC	0	-0.10 to +0.10	-0.18 to +0.22
NO_2	Pandora 101	Izana	+0.07	+0.04 to +0.12	-0.01 to +0.12

For NO_2 columns at GSFC, the median difference is 0, which is excellent, but at first glance somewhat surprising. One might have expected higher values from ground than from space, since GSFC is located in an urban environment at the north-east side of Washington DC. However we must consider that the SCIAMACHY footprint is large and the center can be up to 300km away from the ground station. Therefore the satellite data can include even more polluted regions than GSFC, e.g. downtown Washington, Baltimore, or even Philadelphia.

The differences in NO_2 at Izana are significant. A more detailed analysis is needed to find the reason for this.

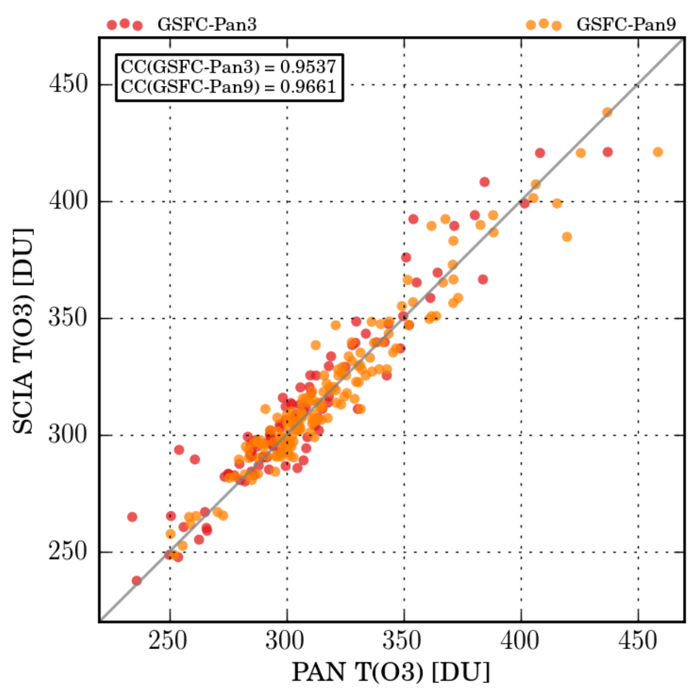

Figure 1: Scatterplot of SCIAMACHY total O_3 columns (SCIA T(O_3) versus Pandora total O_3 columns (PAN T(O_3)) for Pandora 3 (Pan 3) and Pandora 9 (Pan 9) at GSFC.

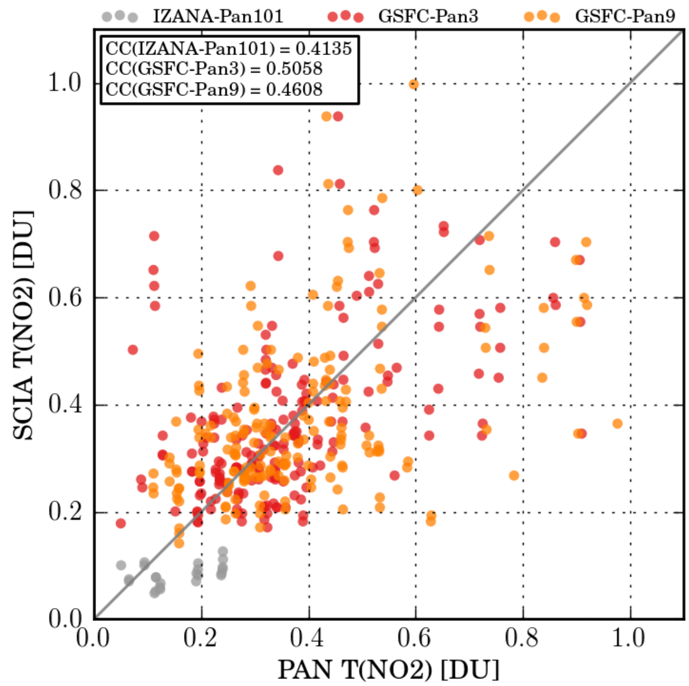

Figure 2: Scatterplot of SCIAMACHY total NO_2 columns (SCIA T(NO_2)) versus Pandora total NO_2 columns (PAN T(NO_2)) for Pandora 3 (Pan 3) and Pandora 9 (Pan 9) at GSFC and for Pandora 101 (Pan 101) at Izana.

4 Validation strategy

Based on our experience from past comparisons with satellite data [RD03 to RD07] and the study presented in section 3, we suggest the following strategy for the validation of SCIAMACHY total O_3 and NO_2 columns with the entire Pandora data base, reprocessed in the framework of this project:

1. Extract SCIAMACHY overpass files from the level 2 data for each station listed in table 1 of RD08. This effort will be carried out by Alessandro Burini from ESA and is scheduled to be finished by 22 November 2013. We discussed with Alessandro Burini the specific parameters to be extracted. In addition to the obvious choices (time, vertical column amount) the overpass data will also include the center and corner positions of the footprint, air mass factors, quality flags, and the cloud fraction.

2. We will develop software to filter both ground- and satellite-data for specific criteria, average the ground data around the SCIAMACHY overpass time, and then compare the two data sets.

3. We will analyze the sensitivity of the results to the following parameters:

   - Uncertainty limits used for Pandora cloud filter
   - Time period for the averaging of the ground data
   - Size and location of the satellite footprint
   - Cloud fraction

4. For NO_2 validation we plan to make two comparisons: one with the unchanged satellite data and another including a "climatological correction" to the satellite data. This correction will be based on time-averaged satellite data of total or tropospheric NO_2 columns at the highest possible resolution. The technique is illustrated and explained in figure 3, where we use monthly mean tropospheric NO_2 columns from OMI available at `http://www.temis.nl`. We would prefer to do this at an even higher resolution, but such data are not available. By adding the climatological correction we do not necessarily expect a higher correlation of the data, but we think it might help to understand

systematic difference between the data sets at some stations. It does not matter whether this correction is based on total or tropospheric column amounts, as only the difference between nearby locations is used. However, if we can only get a high resolution map from OMI data, then the different overpass times (∼9:30 and ∼14:30 local time for SCIAMACHY and OMI respectively) might influence the analysis.

5. The obtained results will be evaluated, interpreted, and presented in deliverable D7 of the project.

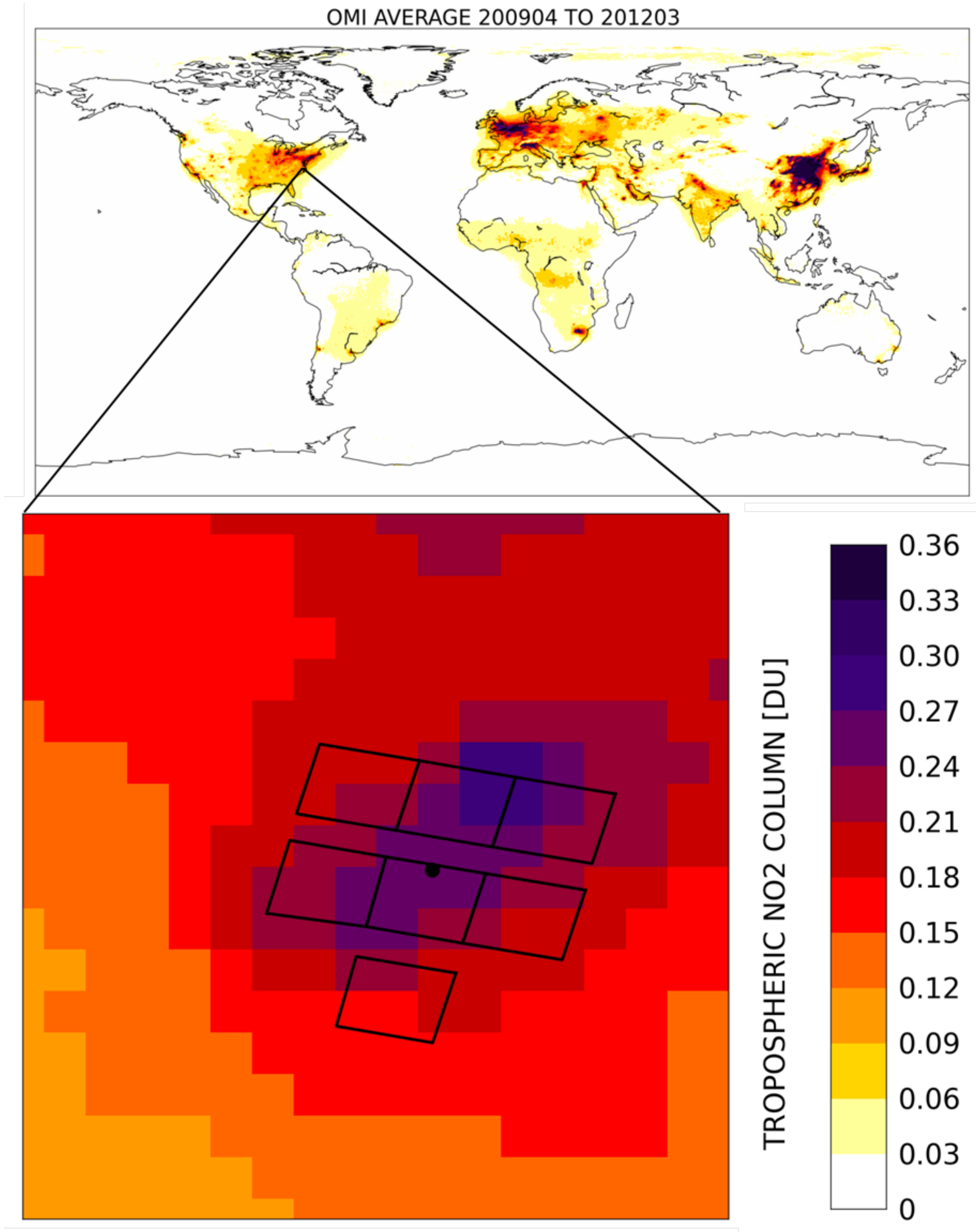

Figure 3: Top panel: Average over OMI monthly mean tropospheric NO_2 columns from April 2009 to March 2012 for the whole world in a cylindrical equidistant representation. Bottom panel: Zoom of the top panel in the region 78° to 76° longitude west and 38° to 40° latitude north. The black dot is the Pandora location at GSFC. Black squares are the closest SCIAMACHY footprints on 8 Nov 2011. Color bar is the same for both panels. The climatological correction will consist of adding to the measured satellite overpass value the difference between the value at the location and the averaged value over the SCIAMACHY footprint.