

Overview of the progress achieved by the NDACC UV-vis Working Group during the NORS project

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BIRA

aeronomie.be

NORS/NDACC/GAW Workshop, 3-5 November 2014, Brussels, BE 1

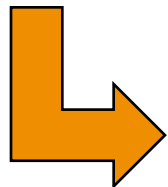


OUTLINE

- Harmonization of DOAS retrievals (O_3 , NO_2 , HCHO)
- Detection and characterization of clouds using DOAS
- Spatial representativeness of DOAS measurements
- Data format homogeneisation

Harmonization of DOAS retrievals

« *Standardisation of retrieval settings and parameters* »



Ensure the consistency of the data sets provided to the NORS validation server

DOAS method based on two steps:

1. Spectral inversion giving the slant column densities (SCDs)
2. Vertical column and/or profile retrieval from SCDs:



Twilight zenith-sky:

Total O₃ and stratospheric NO₂ vertical columns



MAX-DOAS:

Tropospheric profiles (NO₂, HCHO, aerosols)

Harmonisation of spectral inversion: Ex. NO₂

	RECOMMENDED SETTINGS	COMMENTS
Fitting interval	425-490 nm	Settings adequate for simultaneous NO ₂ and O ₄ retrieval with MAXDOAS instruments. For UV instruments, the alternative 400-450 nm interval is recommended.
Wavelength calibration method	Calibration based on reference solar atlas	The Chance and Kurucz (2010) solar atlas is recommended as wavelength registration reference
Cross-sections		
NO ₂	Vandaele et al. (1998), 220 K	This reference is the one included in the HITRAN data base. For stratospheric NO ₂ columns, fine adjustment of temperature effects can eventually be performed in a post-processing step using a simple monthly zonal climatology of temperature profiles. For tropospheric NO ₂ columns, the temperature dependence of the NO ₂ cross sections should be taken into account, at least by selecting cross sections at the appropriate temperature or by adding a second (pseudo) cross sections set.
O ₃	Bogumil et al, (2003), 223 K	O ₃ absorption cross-sections measured with the SCIAMACHY flight-model instrument.
H ₂ O	Harder and Brault (1997)	
O ₄	Hermans et al. (2003)	
Ring effect correction method	Chance and Spurr (1997)	It is recommended to use of an effective Ring cross-section. A high resolution Ring effect cross-section source (generated after Chance and Spurr, 1997) is provided on the NDACC web site. Note that this approach neglects the impact of the Ring effect on the NO ₂ absorption itself (molecular Ring effect).
Polynomial term	Polynomial of order 3 to 5 maximum	
Intensity offset correction	Slope	The intensity offset parameter corrects for spectral stray-light effects and for the wavelength dependence of the probability of Raman scattering (Ring effect). One usually recommends a slope correction (linear).
Data filtering for clouds	Enhancement of O ₄ and/or H ₂ O absorption	Clouds have a small effect on stratospheric NO ₂ . However, it is recommended to remove measurements showing large enhancements of O ₄ and/or H ₂ O slant columns.

Harmonisation of spectral inversion: Ex. NO₂

	RECOMMENDED SETTINGS	COMMENTS
Fitting interval	<ul style="list-style-type: none"> • O₃ and NO₂: 	Settings adequate for simultaneous NO ₂ and O ₄ retrieval with MAXDOAS instruments. For UV instruments, the alternative 400-450 nm interval is recommended.
Wavelength calibration method	<ul style="list-style-type: none"> ➤ Recommendations + cross-sections data sets made available from the NDACC UVVIS WG website 	Recommended as wavelength registration
Cross-sections		
NO ₂	<ul style="list-style-type: none"> ➤ Hendrick et al., ACP (2011) for O₃ • HCHO: 	For stratospheric NO ₂ columns, performed in a post-processing step the profiles. For tropospheric NO ₂ columns, the temperature dependence of the NO ₂ cross sections should be taken into account, at least by selecting cross sections at the appropriate temperature or by adding a second (pseudo) cross sections set.
O ₃	<ul style="list-style-type: none"> ➤ Pinardi et al., AMT (2013) 	measured with the SCIAMACHY flight-model instrument.
H ₂ O	Harder and Braut (1997)	
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Harmonisation of total O₃ and stratospheric NO₂ vertical columns retrieval

$$VCD(\theta) = \frac{SCD(\theta)}{AMF(\theta)}$$

Recommended AMFs for the SCD → VCD conversion:

- Look-up tables of O₃ and NO₂ AMFs generated by BIRA and made available with extraction tools at <http://www.ndacc.org>

O₃

Parameter	Value
O ₃ profile	TOMS TV8: -Latitude: 85°S to 85°N step 10° -Month: 1 (Jan) to 12 (Dec) step 1 -Ozone column: 125 to 575 DU step 50 DU
Wavelength	440 to 580 nm step 35 nm
Surface albedo	0 and 1
Station altitude	0 and 4 km
SZA	10, 30, 50, 70, 80, 82.5, 85, 86, 87, 88, 89, 90, 91, and 92°

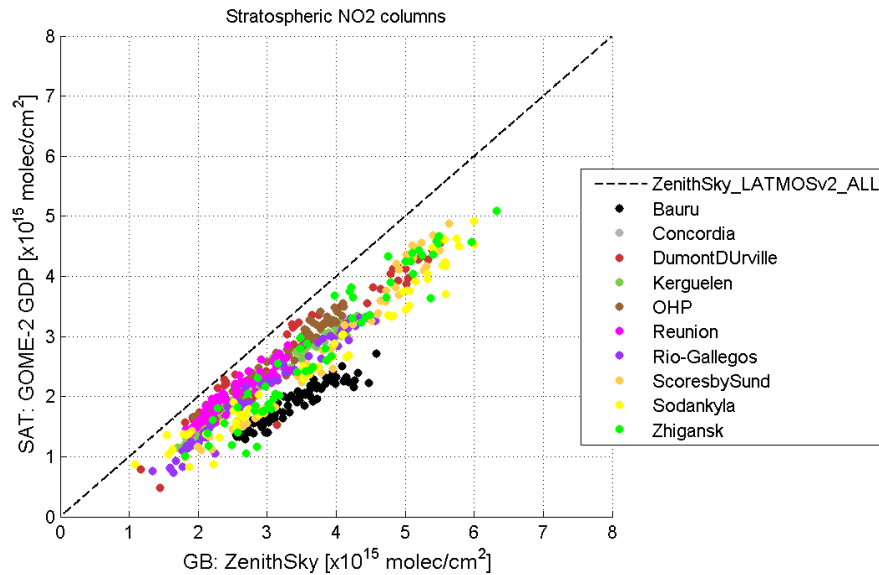
NO₂

Parameter	Value
NO ₂ profile	20-60km: HALOE, POAM-III (Lambert et al.'s climatology) -Latitude: 85°S to 85°N step 10° -Month: 1 (Jan) to 12 (Dec) step 1 -Sunrise and sunset 12-20km: SAOZ balloon climatology -Latitude: tropics, mid-, and high-latitudes -Resolved in seasons
Wavelength	350 to 550 nm step 40 nm
Surface albedo	0 and 1
Station altitude	0 and 4 km
SZA	10, 30, 50, 70, 80, 82.5, 85, 86, 87, 88, 89, 90, 91, and 92°

Stratospheric NO₂ VCD: SAOZ/GOME-2 comparison (2007-2014)

LATMOS/SAOZ V2

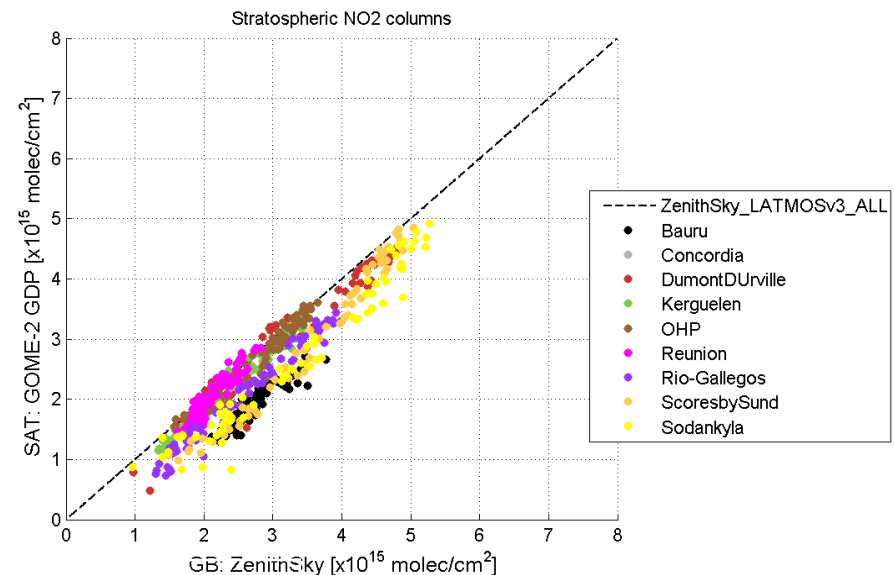
(single AMF based on yearly mean profiles for Tropics, Mid-latitudes or Polar regions)



V2

LATMOS/SAOZ V3

(new AMF climatology)



V3

Mean bias:

($\times 10^{15}$ molec/cm²)

SH -1.02 -0.34

NH -0.37 -0.44

Courtesy G. Pinardi

Method:

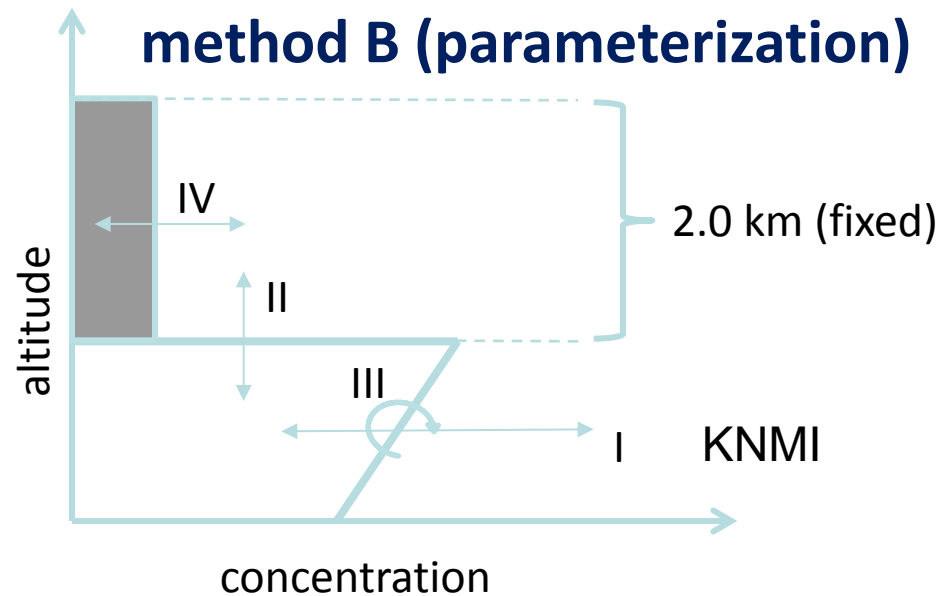
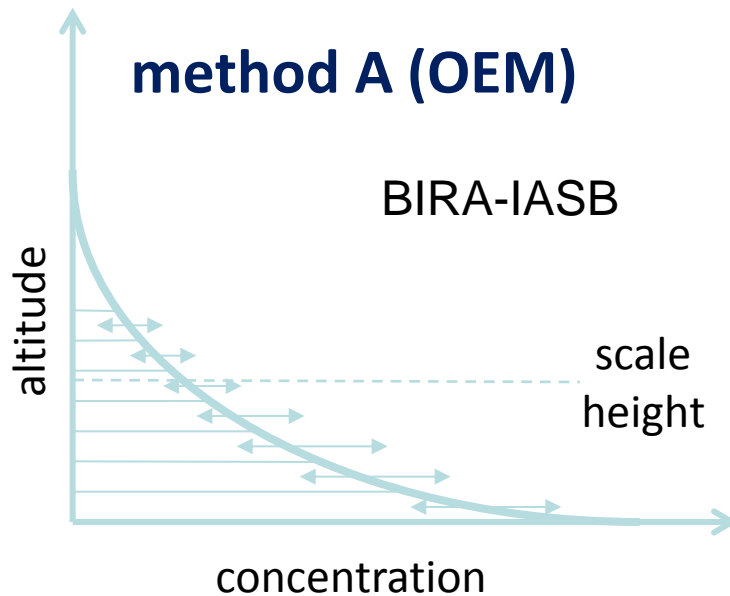
SAT extracted within 150km radius and mean value for every day

GB: AM VCD photochemically converted to SAT ovp time (considering the effective SZA of the air-masses) and corrected for different NO₂ xs T°

Compare only common days and then do monthly means of the daily comparisons

Performance of profiling methods: Optimal Estimation Method *versus* parameterization

Two alternative profile parameterizations:



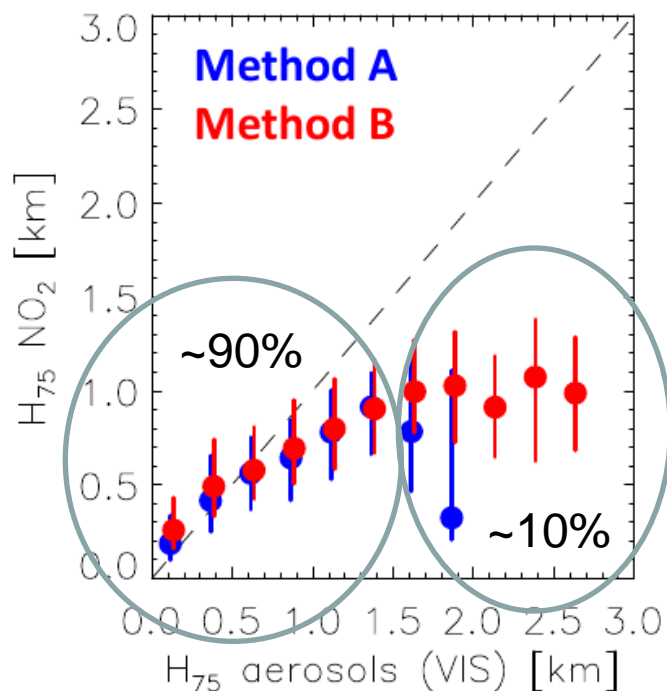
- 13 layers (0-4 km)
- On-line radiative transfer
- Exponentially decreasing a priori profile ($SH=\{0.5, 1.0, 1.5 \text{ km}\}$)

- 2-4 parameters defining profile shape
- Least Squares Fit + ensemble approach (50 runs)
- Forward simulations: Look-up table
- No a priori information

OEM versus parameterization: Application to MAX-DOAS observations at Xianghe

H_{75} : Height below which 75% of the tropospheric column resides

NO_2 and aerosols (visible)



- Method B has a larger dynamical range (higher H_{75} values can be retrieved) than method A
- In contrast, method A is found to be generally more robust/stable
- Quite good agreement between the two methods in the visible, especially for 90% of the data set where method B finds aerosol profiles below 1.5 km ($H_{75} < 1.5 \text{ km}$)
- Important study for future improvements of MAX-DOAS retrieval algorithms

How to detect clouds from MAX-DOAS observations ?

MAX-DOAS trace gas retrievals can be strongly affected by clouds (and aerosols)

- Clouds are bright

=> use **measured radiance**

- Clouds are white

=> use **colour index ($CI = I_{\lambda, \text{low}} / I_{\lambda, \text{high}}$)**

- Clouds change atmospheric radiative transfer

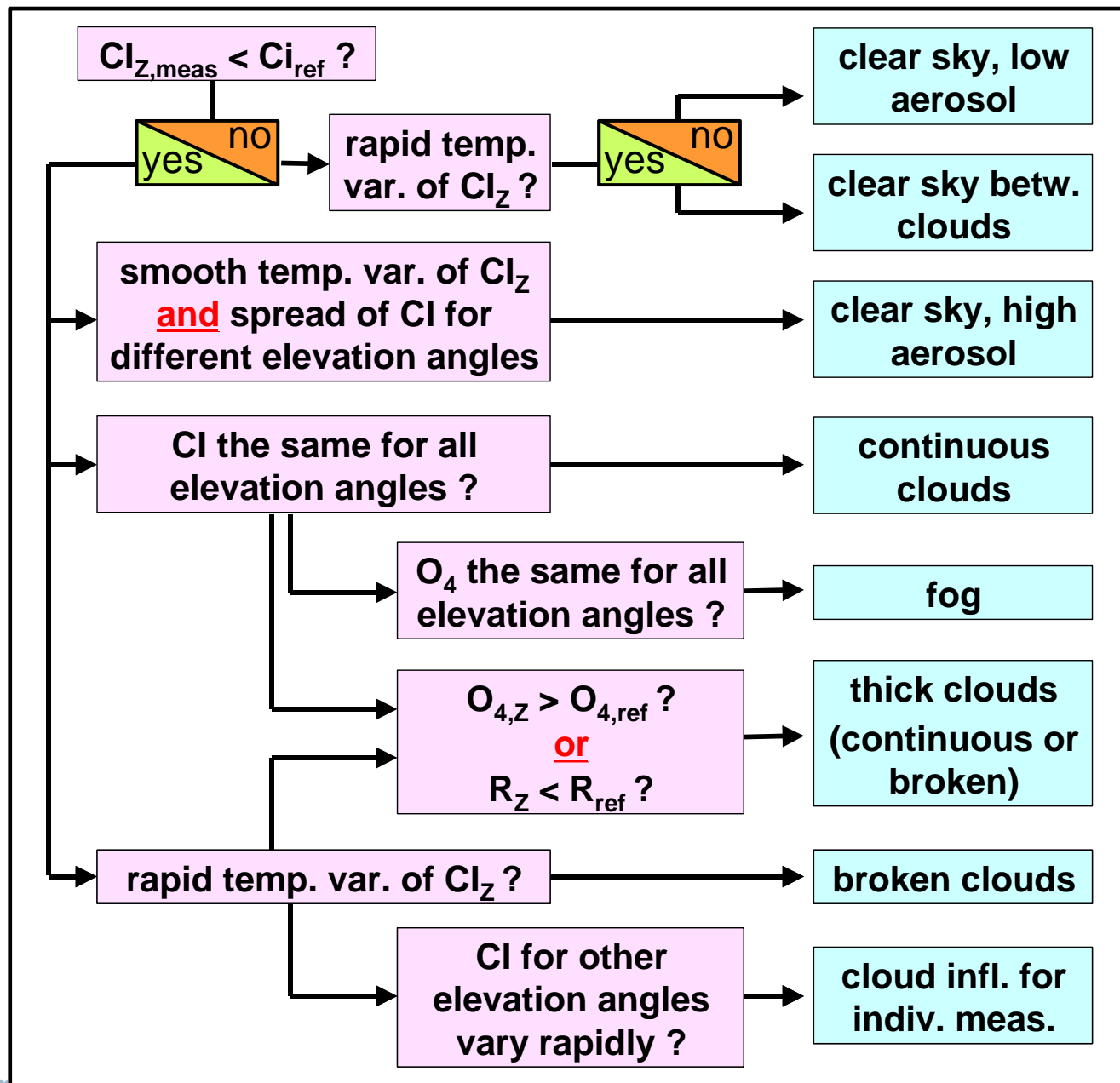
=> use **O₄ absorption and Ring effect**



© T. Vlemmix

MPIC/Mainz cloud screening method

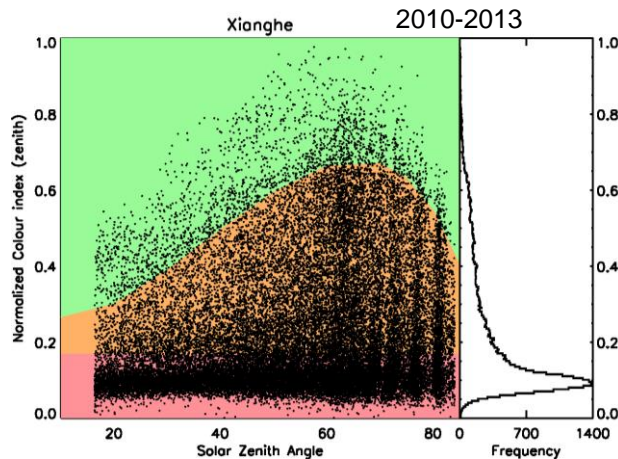
Cloud
classification
scheme



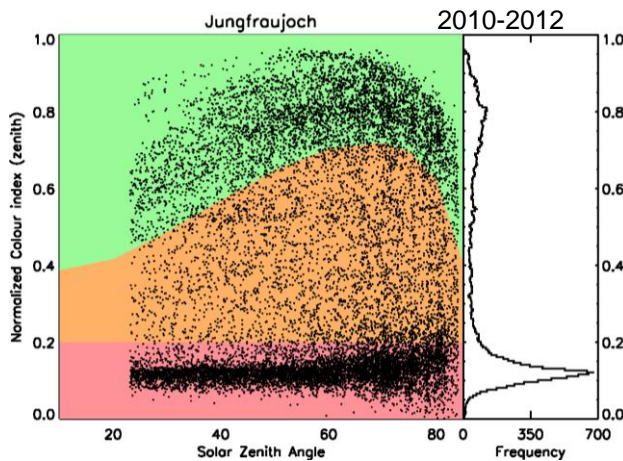
Wagner et al.,
AMT, 2013

BIRA cloud screening method (1)

Cloud screening flag (zenith only)



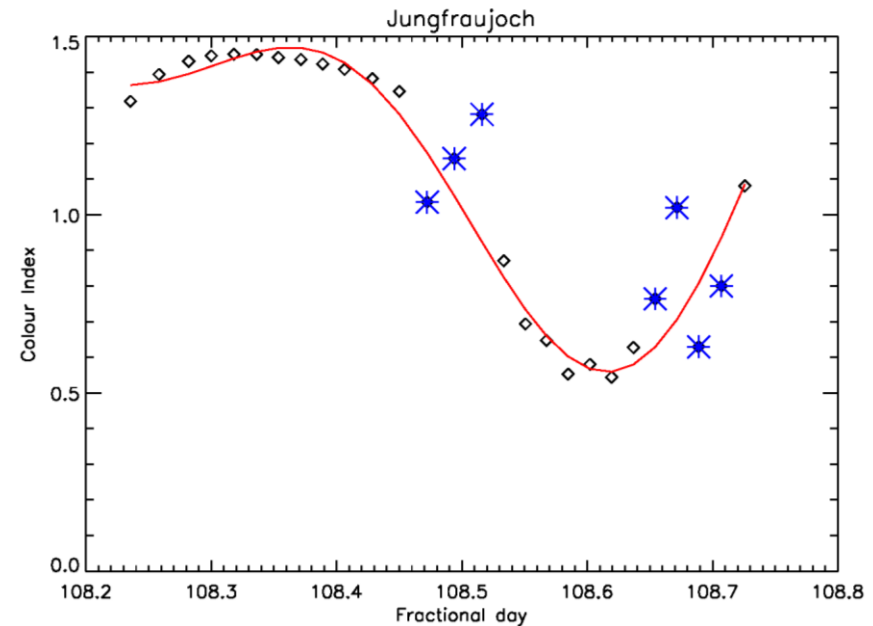
$$CI = \frac{I_{405nm}}{I_{670nm}}$$



$$CI = \frac{I_{405nm}}{I_{550nm}}$$

- Use of CI simulations to define different sky regimes: clear sky, intermediate, fully cloudy

Broken cloud flag (zenith only)

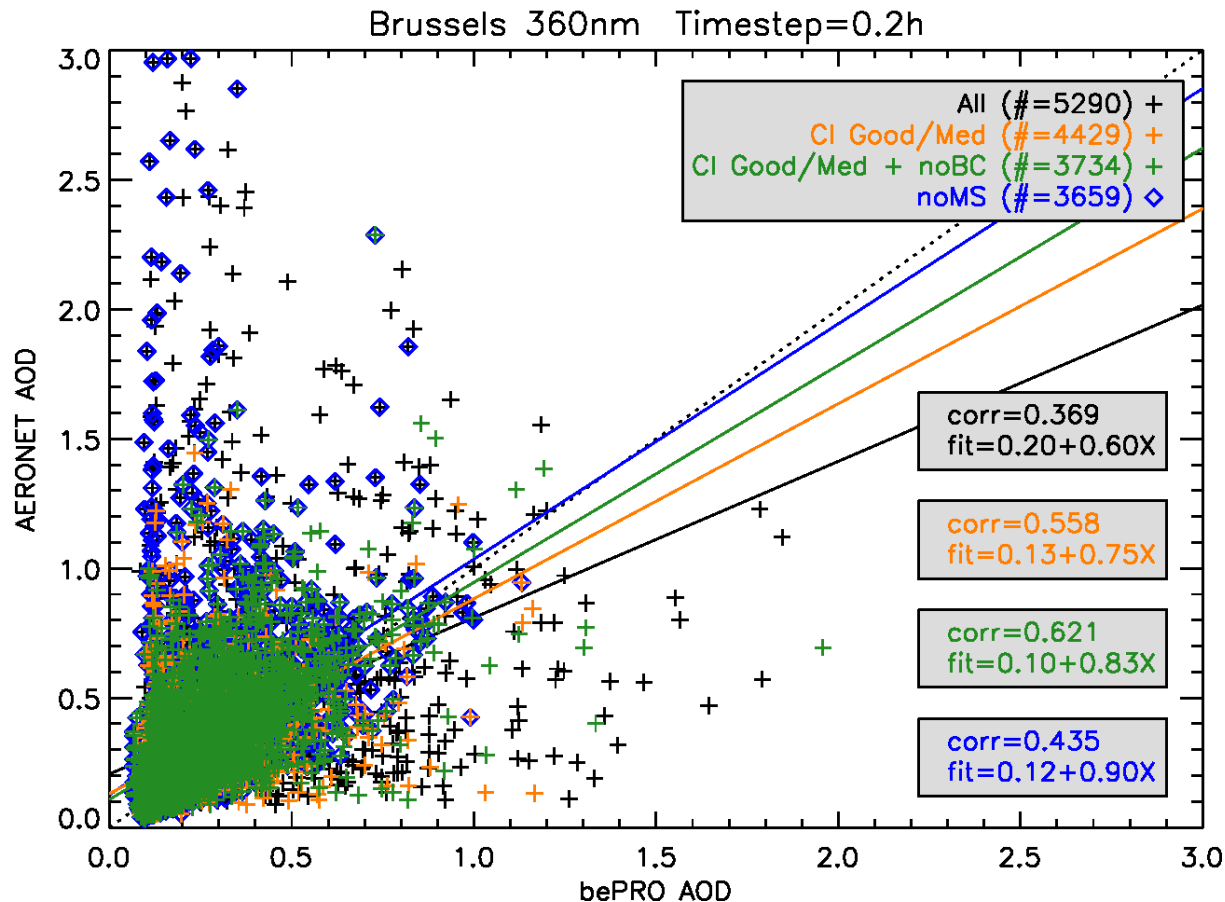


- Fitting of a double-sine function
- Outliers: presence of broken clouds

Gielen et al., AMT, 2014

BIRA cloud screening method (2)

Comparison MAX-DOAS/AERONET_v1.0



Gielen et al., AMT, 2014

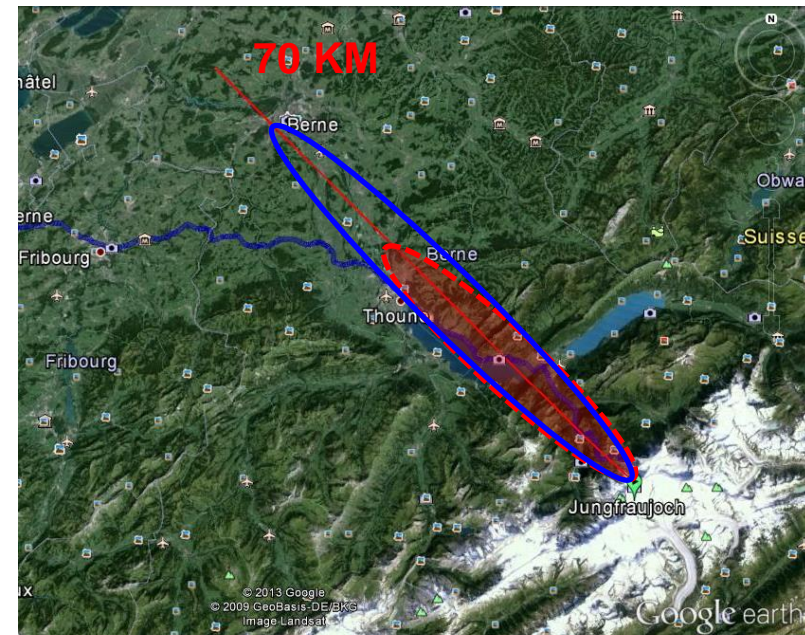
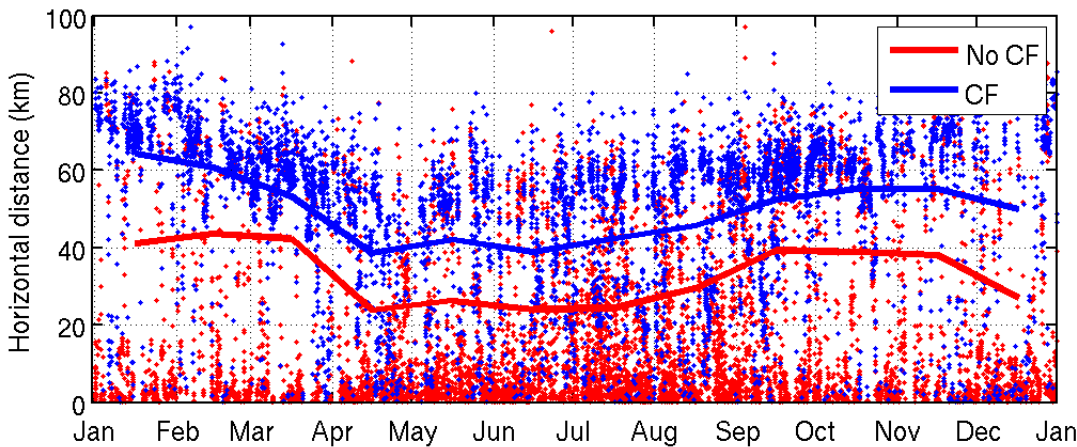
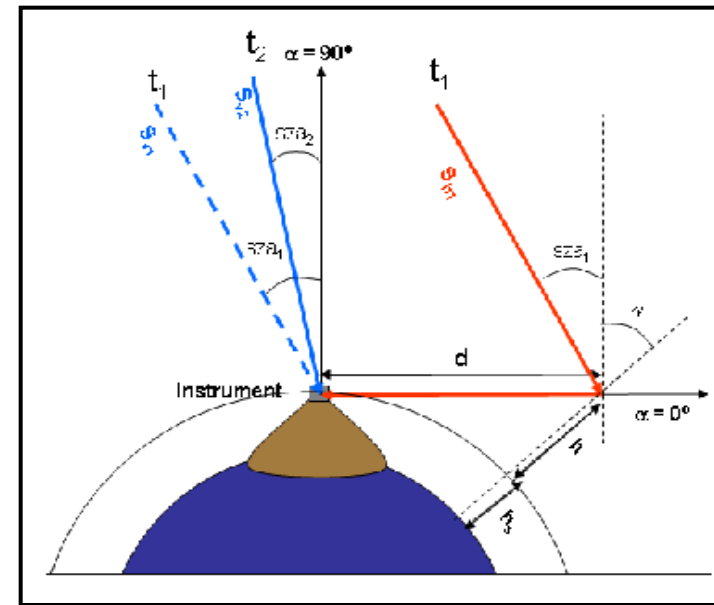
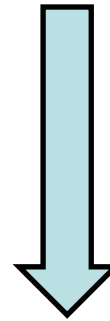
Horizontal representativeness: MAX-DOAS

Modified geometrical approach:

$$d = \frac{SCD_{O_4}(\alpha=0^\circ, SZA1, t_1) - SCD_{O_4}(\alpha=90^\circ, SZA2, t_2)f}{[O_4]_{station}}$$

Gomez et al., AMT, 2014

Application to Jungfrauoch (477 nm)

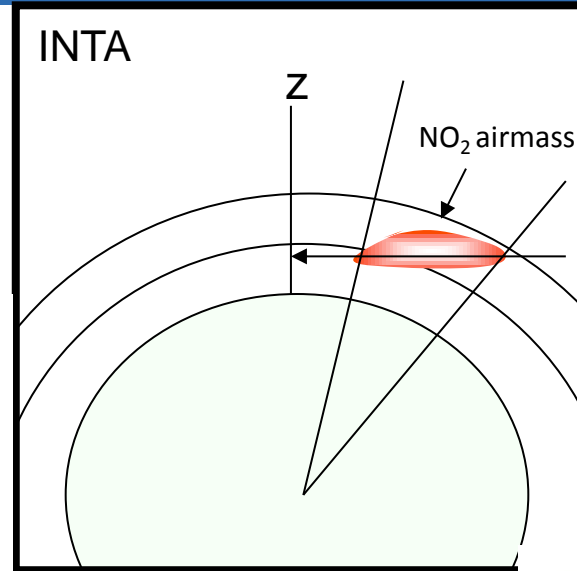


- From all scans: $d \sim 25-45 \text{ km}$
- From cloud-filtered scans (CF): $d \sim 40-65 \text{ km}$

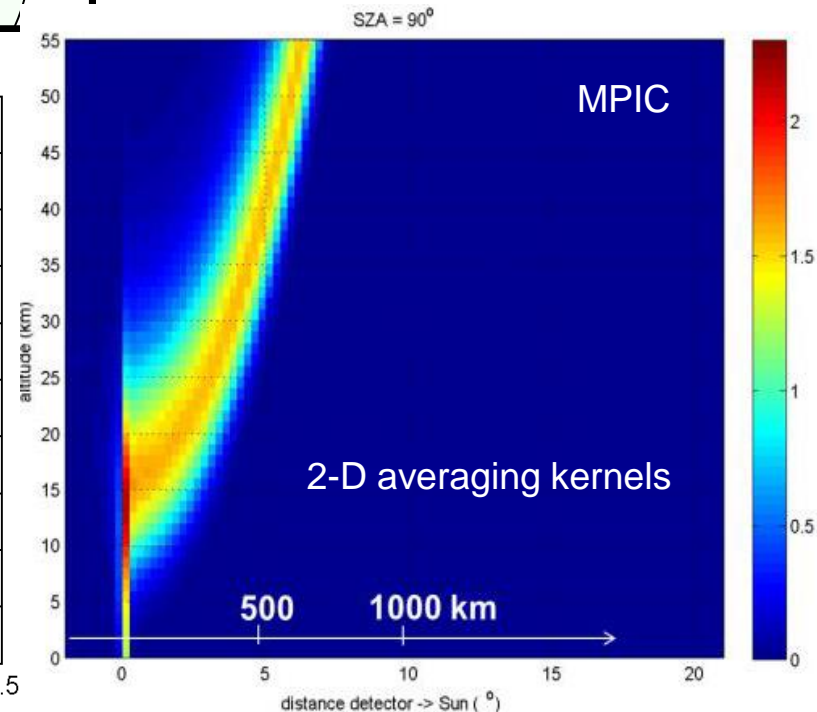
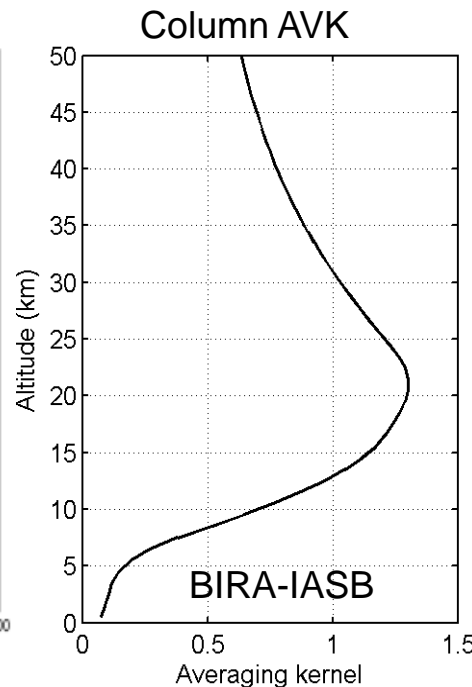
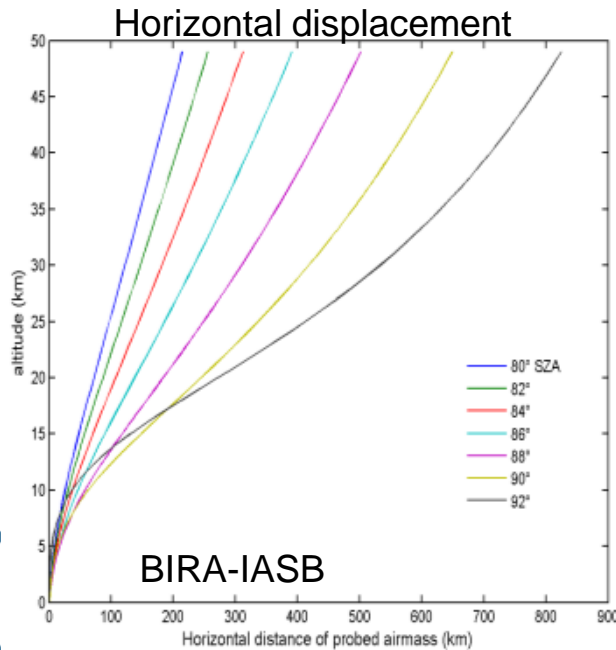
See also talks by Richter et al. and Remmers et al. tomorrow

Horizontal representativeness: twilight zenith

$$d(i) = \frac{\sum_{z,i=0}^{top-atmosphere} x(z,i) * WF(z)}{\sum_{z,i=0}^{top-atmosphere} WF(z)}$$



*Richter, A., et al., NORS
Deliverable D4.4, 2013*

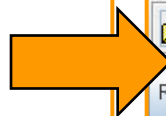


UV-vis data format homogeneization

From NASA-AMES to GEOMS hdf

data_1994_2013.dat HA1304.uv

```
1 56 1010
2 VAN ROOZENDAEL, M.
3 Belgian Institute for Space Aeronomy
4 UV-VIS spectrometer
5 THESEO
6 1 1
7 2013 04 03 2013 04 04
8 0
9 julian day of the current year
10 20
11 1e+013 1e+014 1e+013 0.01 1e+016 1e+017 1e+016 0.01 .001 .001
12 1e+013 1e+014 1e+013 0.01 1e+016 1e+017 1e+016 0.01 .001 .001
13 9999 9999 9999 9999 9999 9999 9999 9999 9999
14 9999 9999 9999 9999 9999 9999 9999 9999 9999
15 NO2 vertical column density (465 nm); molecules/cm**2 Morning
16 NO2 column density, slant path (465 nm); molecules/cm**2 Morning
17 NO2 vertical column error bar (465 nm); molecules/cm**2 Morning
18 Air mass factor for NO2 (465 nm) Morning
19 O3 vertical column density (510 nm); molecules/cm**2 Morning
20 O3 column density, slant path (510 nm); molecules/cm**2 Morning
21 O3 vertical column error bar (510 nm); molecules/cm**2 Morning
22 Air mass factor for O3 (510 nm) Morning
23 colour index: F550/F350 at 90. Morning normalised
24 colour index: F550/F350 at 93. Morning normalised
25 NO2 vertical column density (465 nm); molecules/cm**2 Evening
26 NO2 column density, slant path (465 nm); molecules/cm**2 Evening
27 NO2 vertical column error bar (465 nm); molecules/cm**2 Evening
28 Air mass factor for NO2 (465 nm) Evening
29 O3 vertical column density (510 nm); molecules/cm**2 Evening
30 O3 column density, slant path (510 nm); molecules/cm**2 Evening
31 O3 vertical column error bar (510 nm); molecules/cm**2 Evening
32 Air mass factor for O3 (510 nm) Evening
```



HDFView 2.9

File Window Tools Help

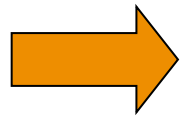
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- ANGLE VIEW_AZIMUTH
- ANGLE VIEW_ZENITH
- LATITUDE
- LONGITUDE
- CLOUD_CONDITIONS
- AEROSOL_OPTICAL_DEPTH.TROPOSPHERIC_INDEPENDENT
- AEROSOL_OPTICAL_DEPTH.TROPOSPHERIC_SCATTER.SOLAR.OFFAXIS
- NO2.MIXING.RATIO.VOLUME_SCATTER.SOLAR.OFFAXIS
- NO2.MIXING.RATIO.VOLUME_SCATTER.SOLAR.OFFAXIS_UNCERTAINTY.RANGE
- NO2.MIXING.RATIO.VOLUME_SCATTER.SOLAR.OFFAXIS_UNCERTAINTY.SYSTEM
- NO2.MIXING.RATIO.VOLUME_SCATTER.SOLAR.OFFAXIS_APRIORI
- NO2.MIXING.RATIO.VOLUME_SCATTER.SOLAR.OFFAXIS_AVK
- NO2.COLUMN.TROPOSPHERIC_SCATTER.SOLAR.OFFAXIS
- NO2.COLUMN.TROPOSPHERIC_SCATTER.SOLAR.OFFAXIS_UNCERTAINTY.RANGE
- NO2.COLUMN.TROPOSPHERIC_SCATTER.SOLAR.OFFAXIS_UNCERTAINTY.SYSTEM
- NO2.COLUMN.TROPOSPHERIC_SCATTER.SOLAR.OFFAXIS_APRIORI
- NO2.COLUMN.TROPOSPHERIC_SCATTER.SOLAR.OFFAXIS_AVK

Conclusions and perspectives

Significant progress have been achieved during NORs:

- **Data harmonization (recommended settings including ancillary data like e.g. cross-sections and AMF)**
- **Data quality assessment (cloud flagging, spatial representativeness)**
- **Data reporting (GEOMS hdf)**
- **Data delivery (daily submission to NORs RD database)**



This significantly improves the usability of UVVIS data for future satellite and model validation efforts (MACC-II/III, CAMS)

Thank you for your attention !