Sentinel-5 Precursor NO_2 and HCHO validation using NDACC and complementary FTIR and UV-Vis DOAS systems (NIDFORVal project)

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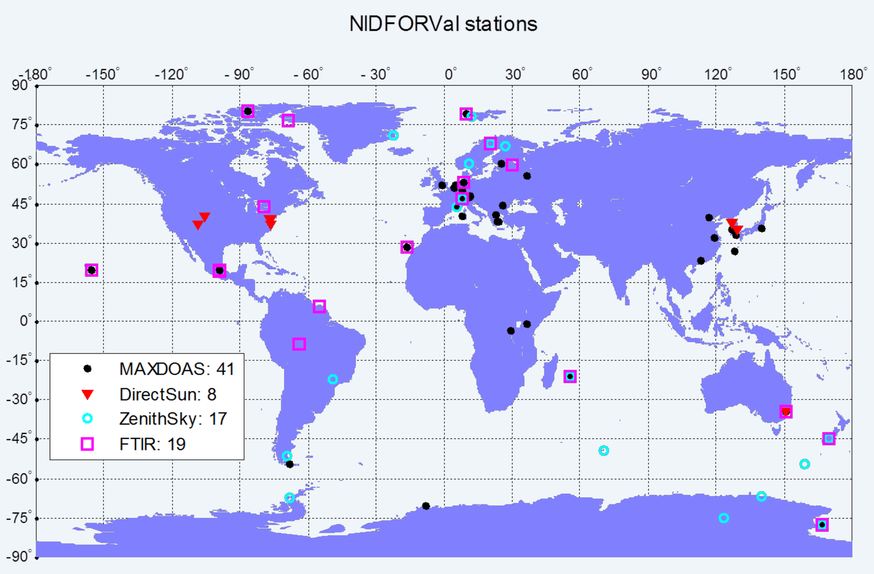
Objectives of the NIDFORVal project

- Use two **independent** techniques, Fourier Transform InfraRed (**FTIR**) and UV-Visible Differential Optical Absorption Spectroscopy (**DOAS**), to provide data that **fulfill the S5P validation requirements:**
  - **NO_2 total** columns from **DirectSun DOAS** measurements
  - **NO_2 stratospheric** columns from **FTIR** and **ZenithSky DOAS** measurements:
    Uncertainty requirement: systematic<10%; random= 0.5e15molec/cm^2
  - **NO_2 tropospheric** columns and profiles from **MAXDOAS** measurements:
    Uncertainty requirement: systematic=25-50%; random= 0.7e15molec/cm^2
  - **HCHO total** columns from **FTIR** and **MAXDOAS** measurements:
    Uncertainty requirement: systematic=40-80%; random= 1.2e16molec/cm^2
- **First task (WP1 and WP2):** provide **homogenized and characterized** FTIR and UV-Vis time-series (2016-2023) from **more than 80 instruments**, from NDACC (Network for the Detection of Atmospheric Composition Change) and complementary networks or recent infrastructures, **covering a wide range of latitude and pollution conditions**.



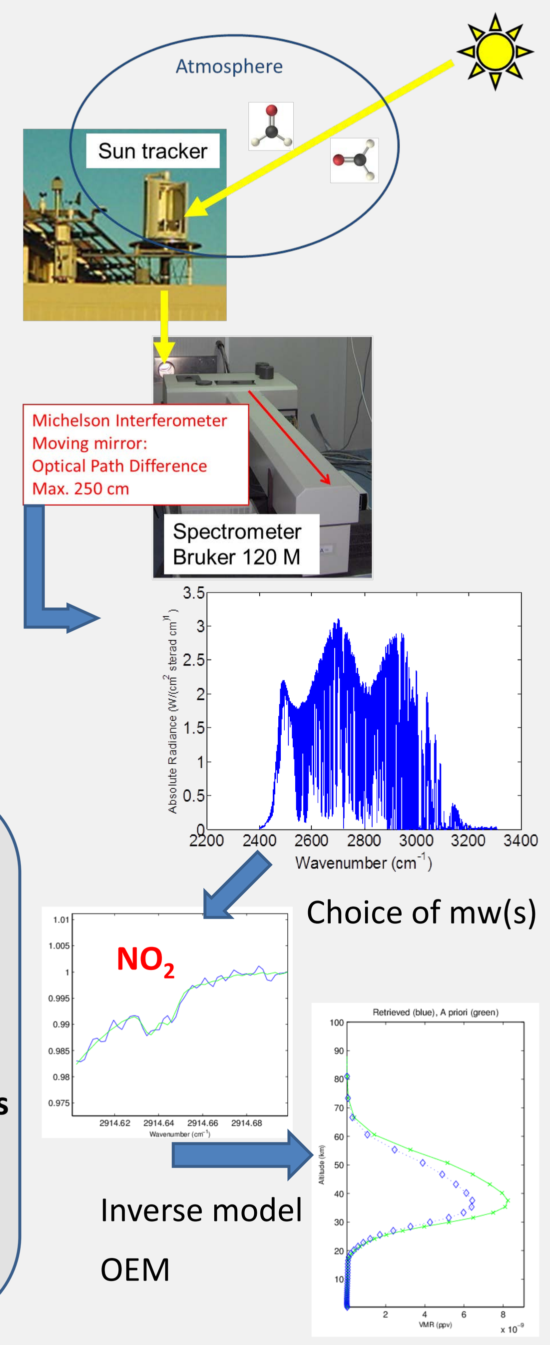
- **Second task: S5P validation in the rapid delivery Phase E1 (WP3), and in the routine Phase E2 (WP4).** The validation tools will be based on the expertise gained at BIRA during precursor projects (Multi-TASTE, O3M-SAF, NORS,…).

WP1: FTIR data harmonization and collection

- In NDACC: - FTIR spectra recorded in about 15 sites
  - species archived: O_3, HNO_3, HCl, HF, CO, N_2O, CH_4, HCN, C_2H_6 and $ClONO_2$.
- In NIDFORVal: define an **harmonized retrieval strategy for NO_2 and HCHO at NDACC and new FTIR stations:**

-Two codes used: SFIT4 (Pougatchev et al., 1995) and PROFITT (Hase, 2000), based on **Optimal Estimation** (Rodgers, 2000): **need a priori information**.

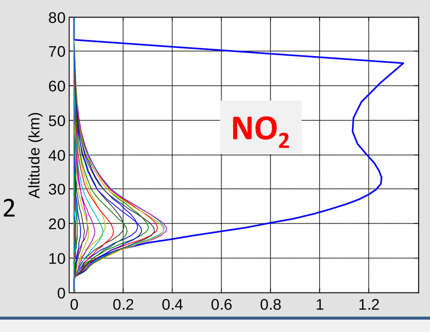
- Same spectroscopic database will be used.
- Pressure-temperature profiles from NCEP.
- **Important parameter in the retrieval strategy: the choice of spectral micro-windows (mw).** It will be based on previous successful studies.



NO_2: Kerzenmacher et al., 2008; Hendrick et al., 2012:

A common mw: 2914.6-2914.7 cm^{-1}: check if additional mws are suitable for humid sites. Degrees of freedom for signal **DOFS = 1-2; in the low-mid stratosphere.**

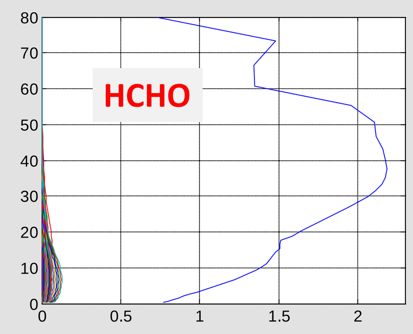
NO_2 FTIR uncertainties:
- systematic: 3-10%
- random: 0.3e15 molec/cm^2



HCHO: Vigouroux et al., 2009; Viatte et al., 2014; Franco et al., 2015:

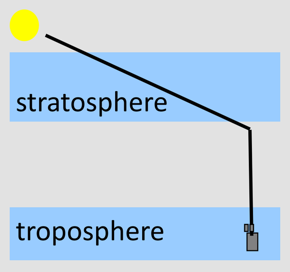
We will define the best set of mws. **DOFS = 1-1.5; in the troposphere.**

HCHO FTIR uncertainties: - systematic: 10-15%
- random: 0.5 - 1e15 molec/cm^2



WP2 UV-Vis DOAS data harmonization and collection

ZenithSky

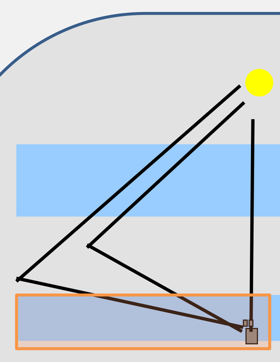


NDACC network since '90

Stratospheric NO_2 at twilight

- Effort in NDACC to harmonize VCD retrieval from twilight measurements:
  - common SCD retrieval settings
  - provided AMF LUTs
  - discussion on twilight reporting period (and effective SZA)
  - displacement of the effective air-mass location wrt to station coordinates to improve the overall homogeneity of the UV-Vis network (Van Roozendael and Hendrick, 2012; Hendrick et al., 2012).
- **NO_2 stratospheric columns uncertainty:**
  - Systematic: 11-15%;
  - Random: 0.6e15 molec/cm^2

MAXDOAS



National networks in the past decade

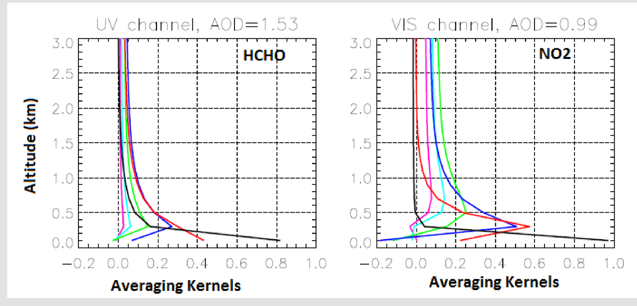
e.g., MADRAS (Kanaya et al., 2014), BIRA, BREDOM,Heidelberg, MPIC-Mainz networks, …

Tropospheric NO_2 and HCHO

- Effort to harmonize retrievals: Roscoe et al. 2010; Pinardi et al., 2013.
- Currently different methods used:
  - **Geometrical approach** (e.g. Honninger et al., 2004)
  - **Optimal estimation** (Friess et al., 2006)
  - **Parameterization**: vertical profile using analytical functions constrained by a few parameters (Irie et al., 2008)

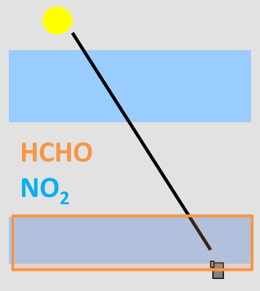
Recommendations will be formulated for NIDFORVal

- With inversion methods: **profiles in 0-4 km; DOFS=1.5-3**
→ tropospheric column + surface concentration + low resolution profile when possible.
- **Estimated tropospheric columns uncertainties:**
  - systematic <15% (NO_2); ~20% (HCHO);
  - random : ~30% (NO_2 and HCHO).



- **Optional Task: use a demonstration centralized processing system** (ESA CEOS-iCAL project, 2014-2016).

DirectSun



Pandora (NASA) network since a few years

Total NO_2

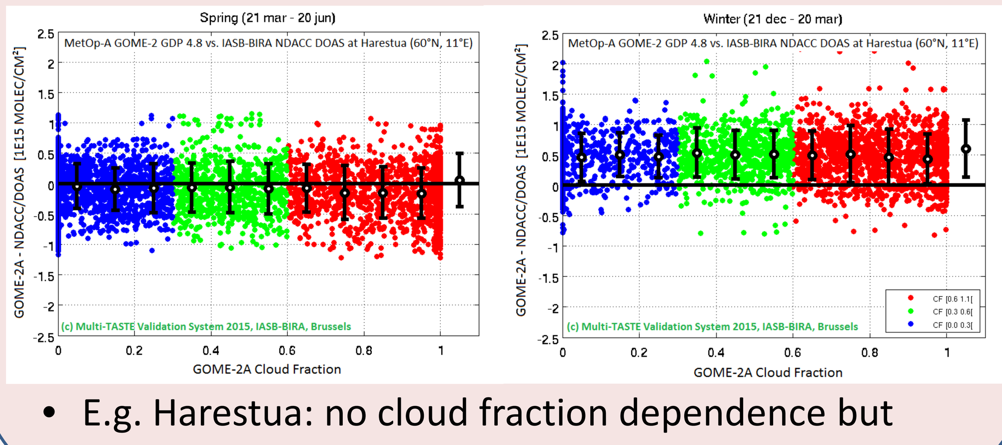
- DirectSun: sensitive to the whole column. Provides accurate total column measurements with a minimum of a-priori assumptions.
- Relies on research instruments and a set of PANDORA instruments (NASA and/or Pandonia network which are harmonized and quality controlled via centralized processing facilities).
- **NO_2 total columns uncertainty:**
  - Systematic: 10-15%
  - Random: ~2.8e14 molec/cm²

WP3 S5P Validation during Phase E1

- WP3 focuses in the analysis of the initial S5P data products based on a **subset of stations able to provide data in a rapid delivery mode.**
- WP3 will benefit from the strong expertise at BIRA in validation tools: Multi-TASTE (Hubert et al., 2015; Verhoelst et al., 2015), O3M-SAF CDOP (http://cdop.aeronomie.be/) and NORS (http://nors.aeronomie.be/) projects.

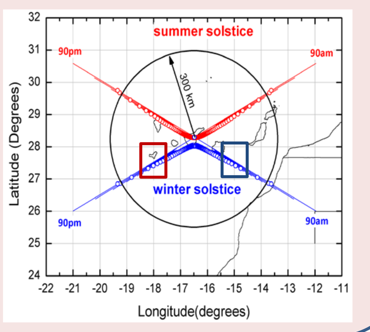
Validation of NO_2 GOME-2 with Zenith-Sky DOAS

- Multi-TASTE versatile validation system: importance of colocation and of photochemistry correction.
- Uncertainty on differences: few 1e14 molec/cm^2

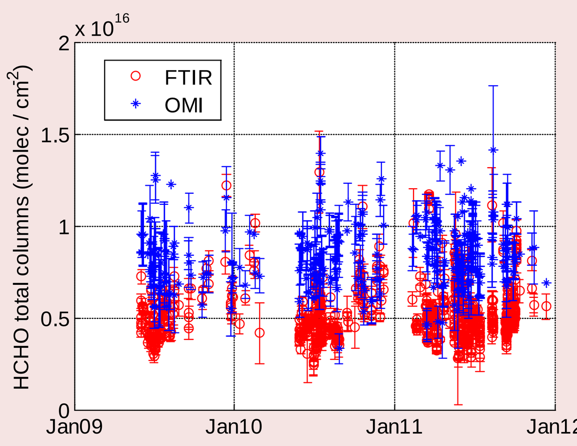


- E.g. Harestua: no cloud fraction dependence but **seasonal dependence.**

The colocation criteria takes into account the line of sight of ground-based data:



Validation of HCHO OMI with FTIR

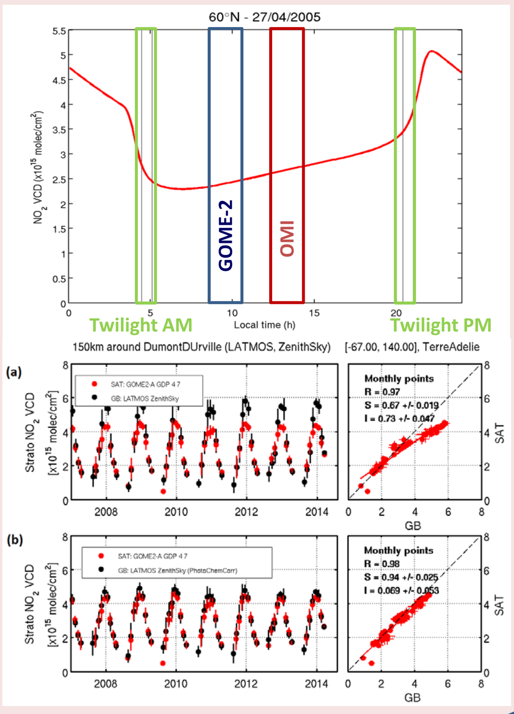


- Single FTIR data
- Mean of co-located OMI data at Reunion Island

- Bias= 48%
- Standard deviation=30%

Photochemical correction to take into account NO_2 diurnal cycle

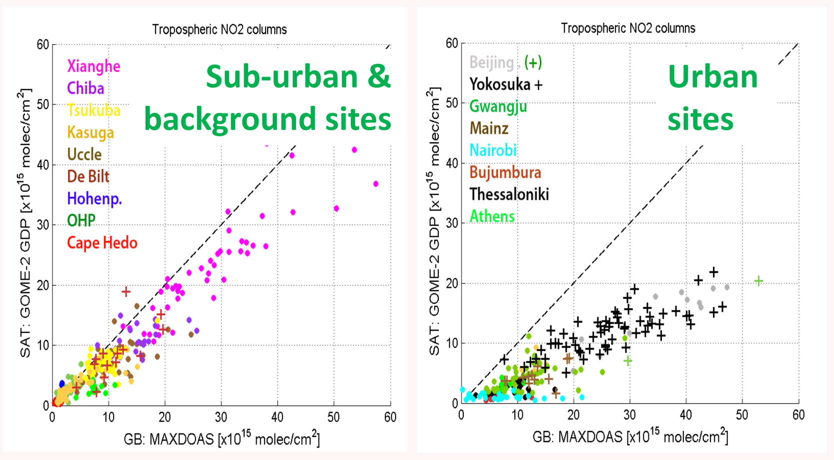
Ex: Zenith-Sky VCDs are photochemically converted to the satellite overpass SZA.



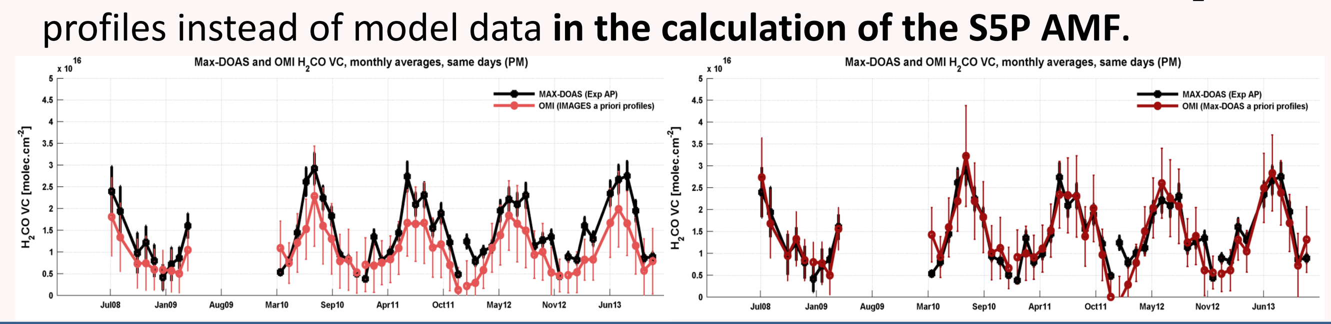
- At each station: **statistical bias and standard deviations of the differences** between S5P and correlative data will be compared to the uncertainties budget of the differences. The deliverable will be provided **6 months after the S5P launch.**

S5P Validation during Phase E2 (2016-2023)

- Validate the **seasonal cycles** and **the long-term stability** of S5P products by building tools for drift calculation based on previous projects (e.g. Hubert et al., 2015).
- **Perform FTIR / DOAS comparisons where both techniques are available**: quality control (Vigouroux et al., 2009; Franco et al., 2015; Hendrick et al., 2012) & use the different sensitivities of both techniques to explain differences in validation results.
- Study **representativeness of the sampled air masses for S5P 7x7km² resolution** : e.g. GOME-2 (40x80km²) tropospheric NO_2 validation with MAXDOAS urban/background sites.



- Study impact on S5P data of using **measured** NO_2 and HCHO profiles instead of model data **in the calculation of the S5P AMF.**



Xianghe station. (De Smedt et al., 2015)

International partners

FTIR (10)
IMK-ASF, KIT (Karlsruhe) – T. Blumenstock; IARC/AEMET (Spain) – O. García; UNAM (Mexico) – M. Grutter; UCAR (USA) – J. Hannigan; University of Wollongong (Australia) – N. Jones; University of Liège (Belgium) – E. Mahieu; Saint-Petersburg University (Russia) – M. Makarova; IUP-Bremen (Germany) – J. Notholt; NIWA (New-Zealand) – J. Robinson, D. Smale; University of Toronto (Canada) – K. Strong
UV-Vis DOAS (25)
AUTH (Greece) – A. Bais; LufBlick (Austria) – A. Cede; GIST (Korea) – J. Chong; BAS (UK) – S. Colwell; IUP-Heidelberg (Germany) – U. Friess; INTA (Spain) – M. Yela Gonzalez, O. Puentedura; DLR (Germany) – N. Hao; NASA (USA) – J. Herman; DWD (Germany) – R. Holla; FMI (Finland) – J. Hovila; Chiba University (Japan) – H. Irie; JAMSTEC (Japan) – Y. Kanaya ; IERSD-NOA (Greece) – S. Kazadzis; University of Leicester (UK) – R. Leigh; INOE (Romania) – A. Nemuc; LATMOS (France) – A. Pazmino, J.-P. Pommereau; KNMI (The Netherlands) – A. Piters; IAP/RAS (Russia) – O. Postylyakov; NIWA (New Zealand) – R. Querel; IUP-Bremen (Germany) – A. Richter, F. Wittrock; NILU (Norway) – K. Stebel; University of Toronto (Canada) – K. Strong; University of Colorado (USA), R. Volkamer; University of Wollongong (Australia) – S. Wilson; MPI-Mainz (Germany) – T. Wagner