

Sentinel-5 Precursor NO₂ and HCHO validation using NDACC and complementary FTIR and UV-Vis DOAS systems (NIDFORVal project)

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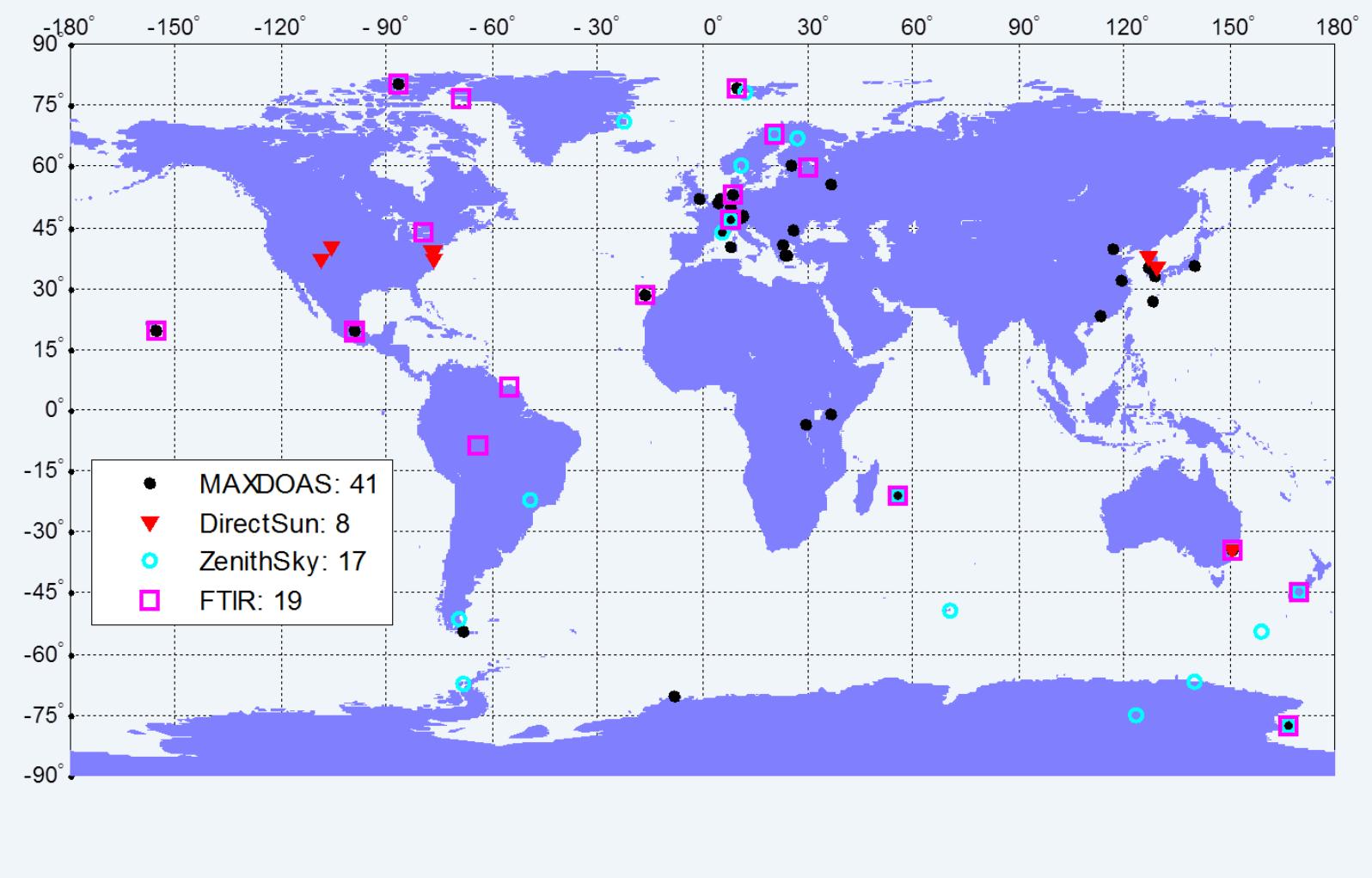


Objectives of the NIDFORVal project

- Use two **independent** techniques, Fourier Transform InfraRed (FTIR) and UV-Visible Differential Optical Absorption Spectroscopy (DOAS), to provide data that **fulfill the SSP validation requirements**:

- NO₂ total columns from **DirectSun DOAS** measurements
- NO₂ stratospheric columns from **FTIR** and **ZenithSky DOAS** measurements:
Uncertainty requirement: systematic<10%; random= 0.5e15molec/cm²
- NO₂ tropospheric columns and profiles from **MAXDOAS** measurements:
Uncertainty requirement: systematic=25-50%; random= 0.7e15molec/cm²
- HCHO total columns from **FTIR** and **MAXDOAS** measurements:
Uncertainty requirement: systematic=40-80%; random= 1.2e16molec/cm²

- 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:** SSP 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: O₃, HNO₃, HCl, HF, CO, N₂O, CH₄, HCN, C₂H₆ and ClONO₂.
- In NIDFORVal: define an **harmonized retrieval strategy** for NO₂ 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.

NO₂: 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**.

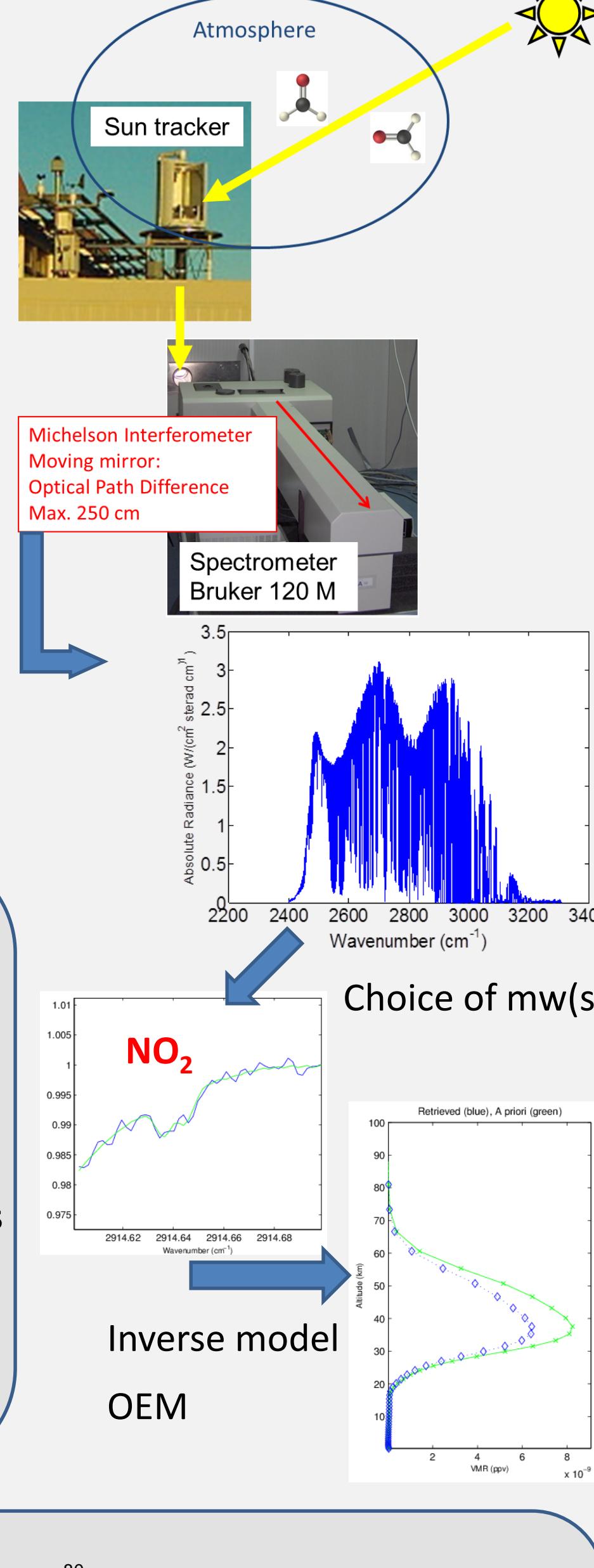
NO₂ FTIR uncertainties:

- systematic: 3-10%
- random: 0.3e15 molec/cm²

Averaging kernels at Reunion

Total column ak

Inverse model OEM

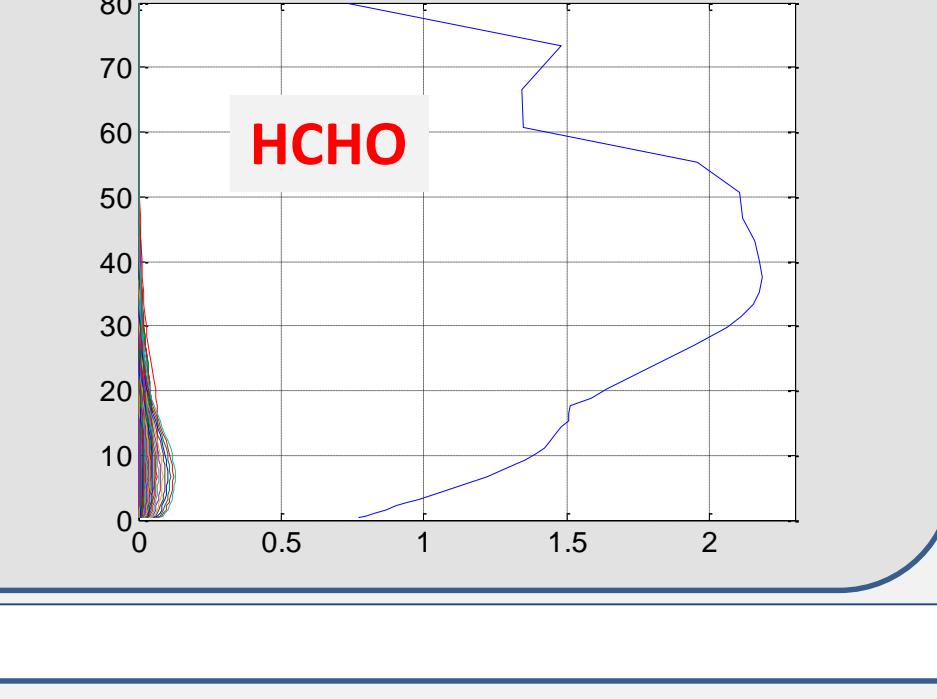


HCHO: Vigouroux et al., 2009; Viatte et al., 2014; Franco et al., 2015:

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/cm²



WP2 UV-Vis DOAS data harmonization and collection

ZenithSky



Stratospheric NO₂ 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).
- NO₂ stratospheric columns uncertainty:**
- Systematic: 11-15%;
- Random: 0.6e15 molec/cm²

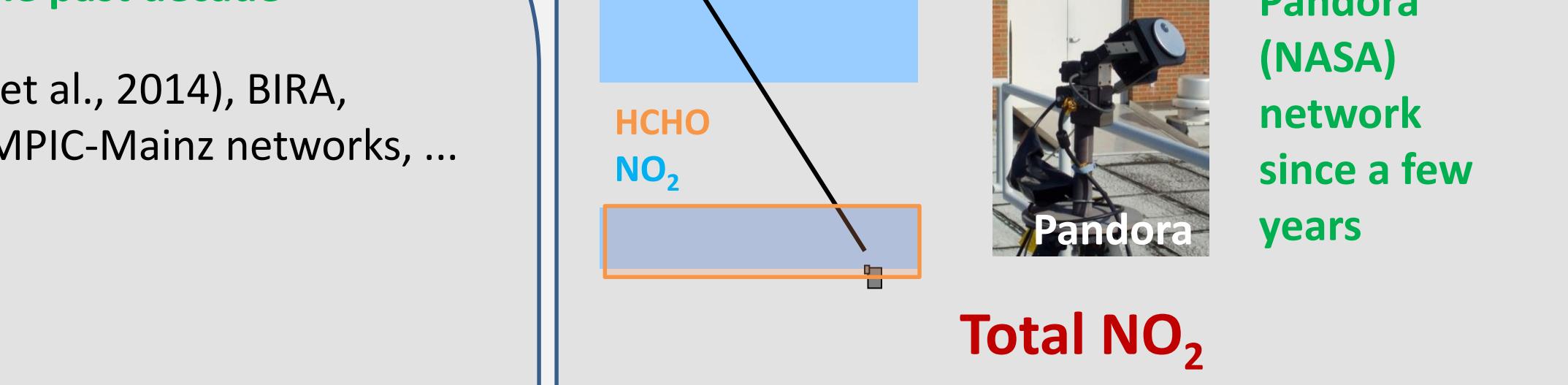
MAXDOAS



Tropospheric NO₂ 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)
- 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% (NO₂); ~20% (HCHO);
 - random : ~30% (NO₂ and HCHO).
- Optional Task:** use a demonstration centralized processing system (ESA CEOS-iCAL project, 2014-2016).

DirectSun



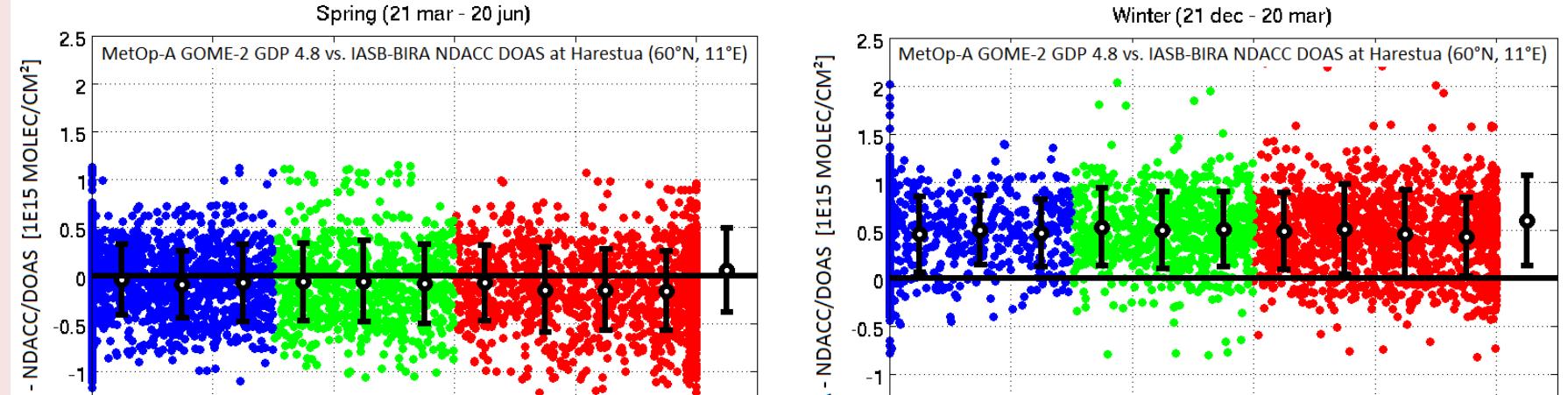
- Total NO₂**
 - DirectSun: sensitive to the whole column. Provides accurate total column measurements with a minimum of a-priori assumptions.
 - Relies on research instruments and a set of PANDORA instruments (NASA and/or Pandoria network which are harmonized and quality controlled via centralized processing facilities).
- NO₂ total columns uncertainty:**
 - Systematic: 10-15%
 - Random: ~2.8e14 molec/cm²

WP3 SSP Validation during Phase E1

- WP3 focuses in the analysis of the initial SSP 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; Verhoest et al., 2015), O3M-SAF CDOP (<http://cdop.aeronomie.be/>) and NORS (<http://nors.aeronomie.be/>) projects.

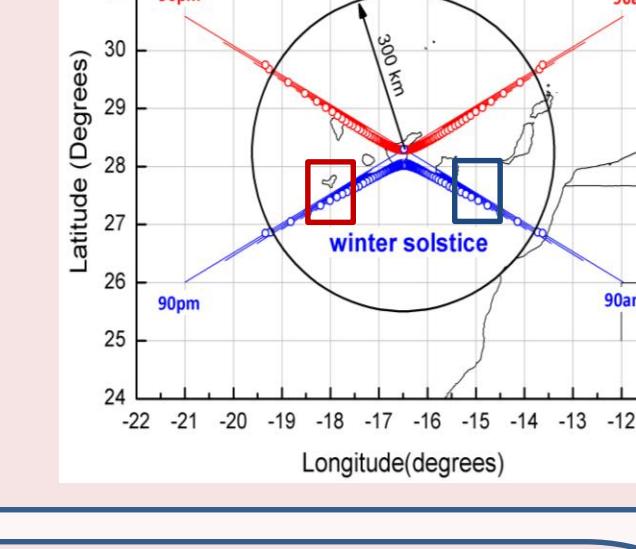
Validation of NO₂ GOME-2 with Zenith-Sky DOAS

- Multi-TASTE versatile validation system: importance of colocation and of photochemistry correction.
- Uncertainty on differences: few 1e14 molec/cm²



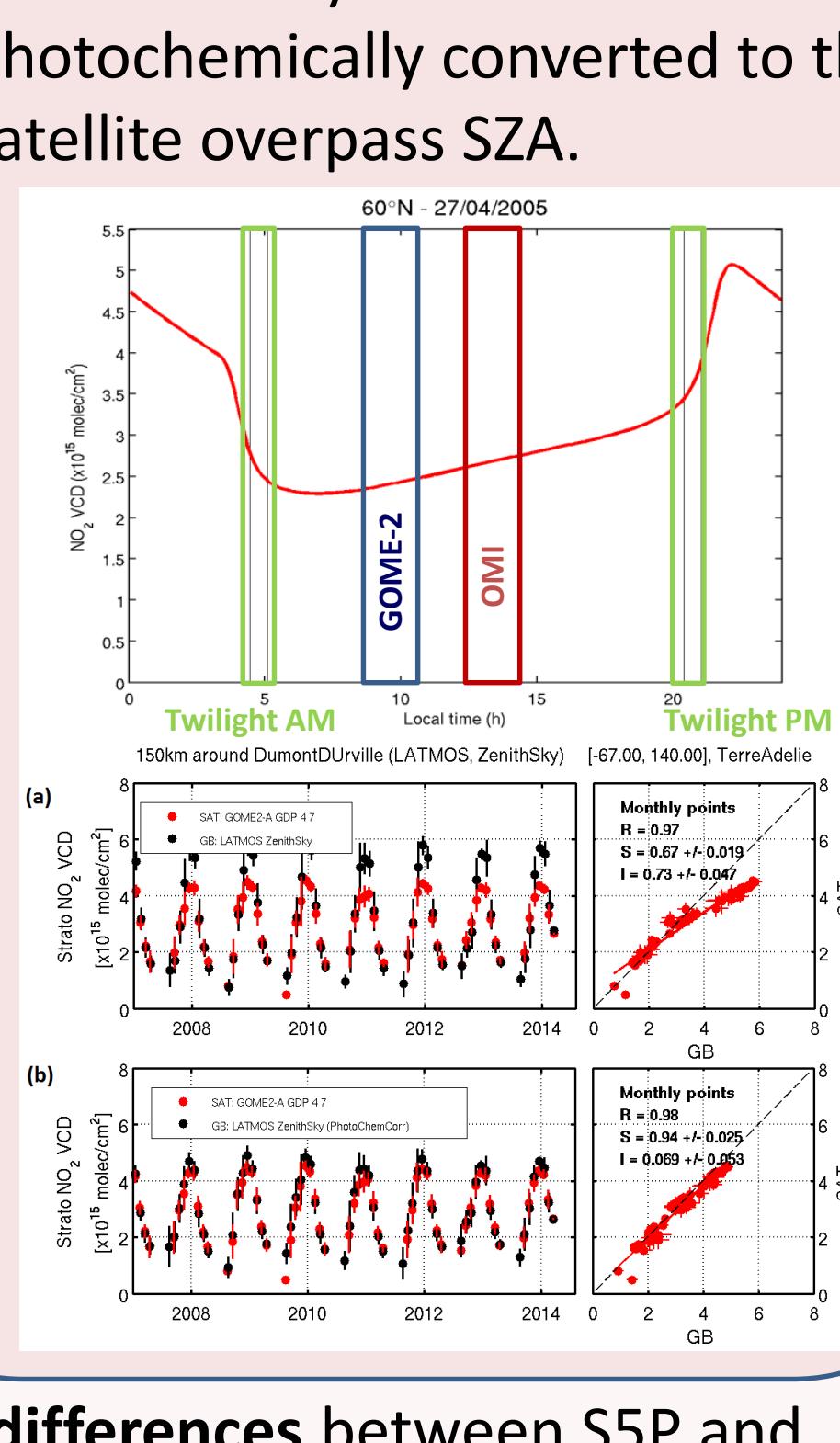
- E.g. Harestua: no cloud fraction dependence but seasonal dependence.

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



Photochemical correction to take into account NO₂ diurnal cycle

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



Validation of HCHO GOME-2 with FTIR

- Single FTIR data
- Mean of co-located GOME-2 data at Reunion Island

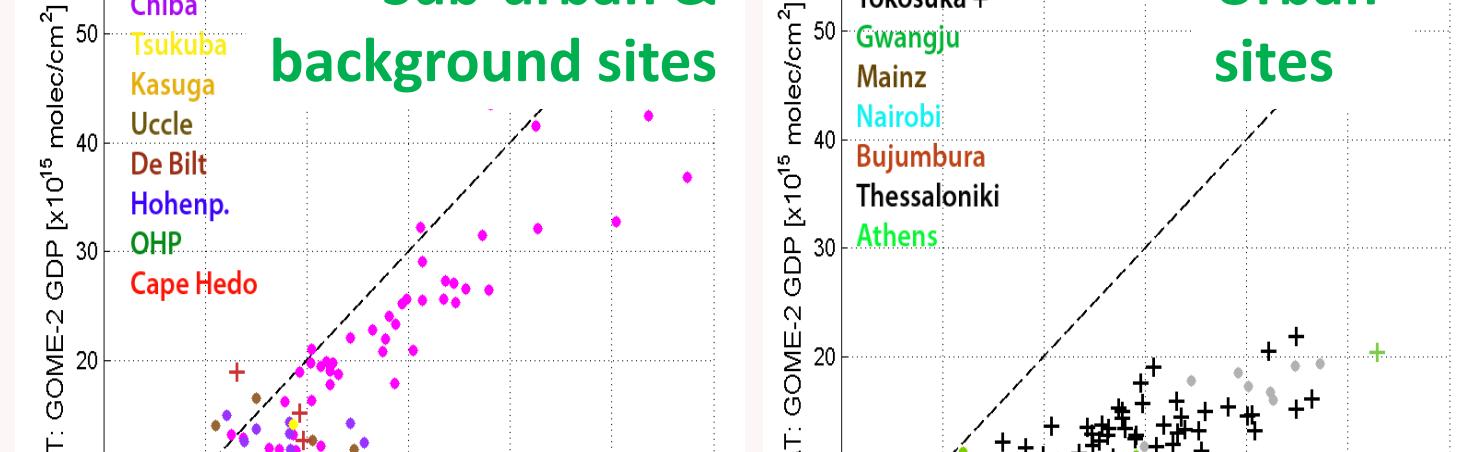
- Bias= 48%
- Standard deviation=30%

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

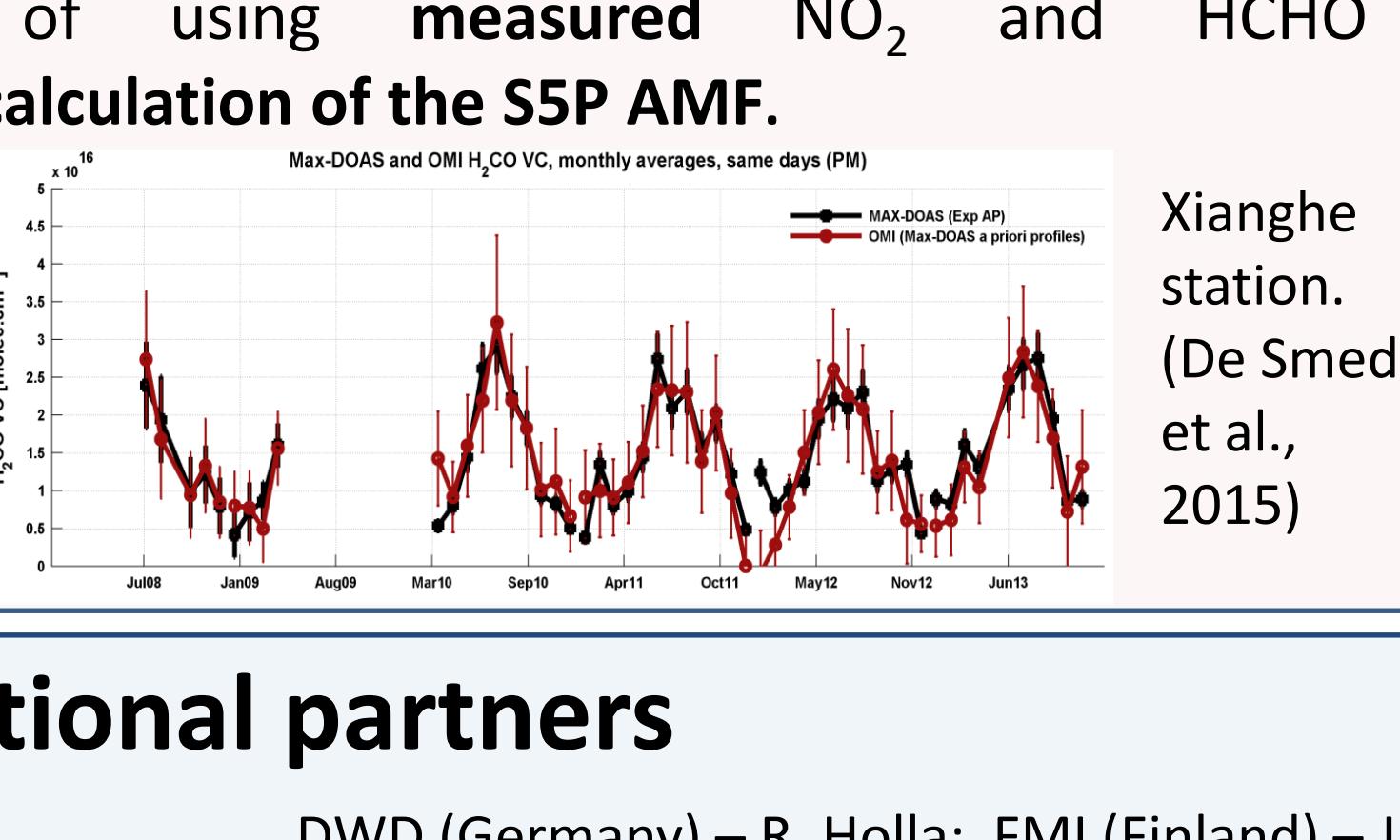
SSP Validation during Phase E2 (2016-2023)

- Validate the **seasonal cycles** and the **long-term stability** of SSP 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 SSP 7x7km² resolution :** e.g. GOME-2 (40x80km²) tropospheric NO₂ validation with MAXDOAS urban/background sites.



- Study impact on SSP data of using measured NO₂ and HCHO profiles instead of model data in the calculation of the SSP AMF.**



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 ; IERSO-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. Postolyakov; 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