Precursors_cci+

Challenges in assessing the quality of Climate Data Records for Precursors of Ozone and Aerosol Essential Climate Variables

Steven Compernolle, Jean-Christopher Lambert, Tijl Verhoelst, Corinne Vigouroux, Bavo Langerock, Gaia Pinardi, Mahesh Kumar Sha, Arno Keppens, Daan Hubert, Lieven Clarisse, Cathy Clerbaux, Thomas Danckaert, Isabelle De Smedt, Maya George, Isolde Glissenaar, Andreas Richter, Sora Seo, Nicolas Theys, Martin Van Damme, Pieter Valks, Folkert Boersma, Michel Van Roozendael, and Simon Pinnock

Precursors_cci+ Validation: Addressing ATMOS 2021 recommendations

This talk will be a lot about

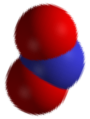
	Calibration and Validation
R36	On Cal/Val the audience requested support for ground-based observations that are crucial for any satellite product comparison activities. The following aspects should be addressed: • Make use of trans-national research infrastructures and data sets for multiple Cal/Val projects or campaigns. Foster collaboration across organisations to access facilities (mobile instrumentation and fixed observatories) and co-design activities such as measurements campaigns and training; • Coordinate between different ground-based networks to report uncertainties in a similar way, considering both random and systematic values; • Harmonise reference datasets from networks such as TCCON and MUSICA-NDACC; • Further advanced platforms that provide access to diverse data and advanced possibilities for using and visualising data in Cal/Val activities.

and touches also on

	Clouds
R31	The audience highlighted the importance of cloud height knowledge. The choice of cloud retrieval algorithm can have a considerable impact on trace gas retrievals, e.g., where a change of algorithm version number can lead to noticeable differences. Work on cloud retrieval algorithms deserves to be studied further.

Why is precursor validation important?

S5P\TROPOMI



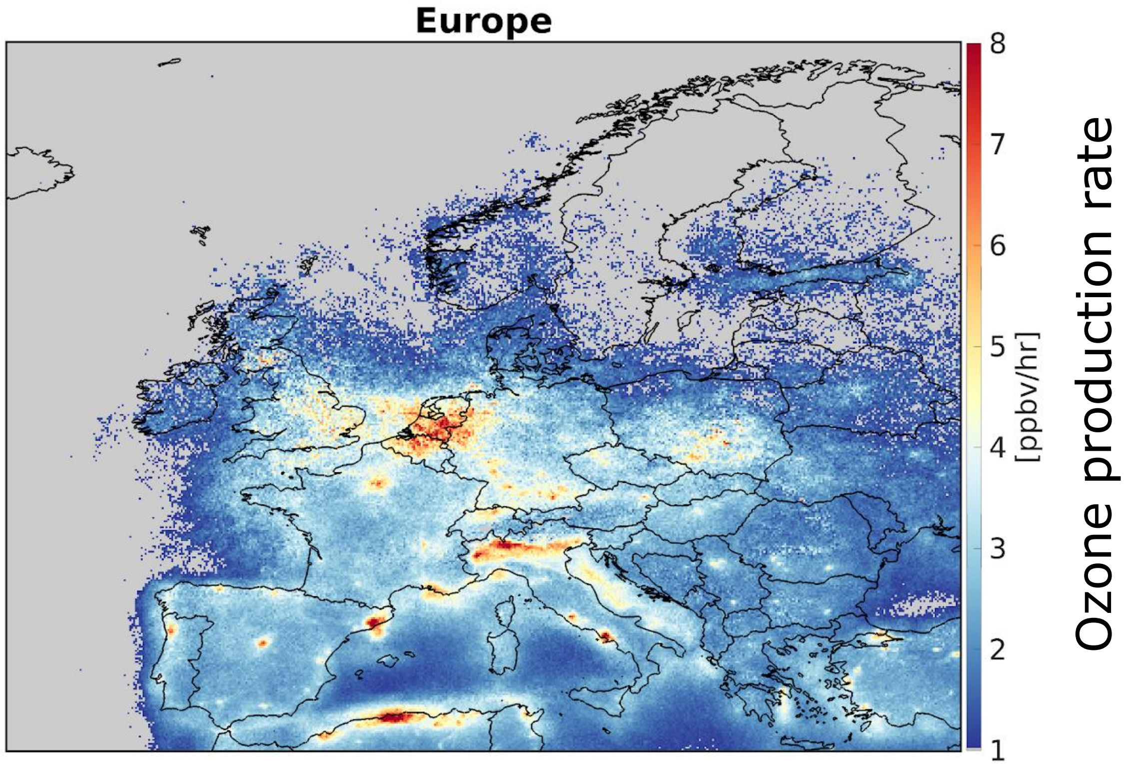
NO2

HCHO

Feasibility of robust estimates of ozone production rates using satellite observations across the globe

Amir H. Souri[1,2]*, Gonzalo Gonzalez Abad[3], Glenn Wolfe[1], Tijl Verhoelst[4], Corinne Vigouroux[4], Gaia Pinardi[4], Steven Compernolle[4], Bavo Langerock[4], Matthew S. Johnson[5], Bryan N. Duncan[1]

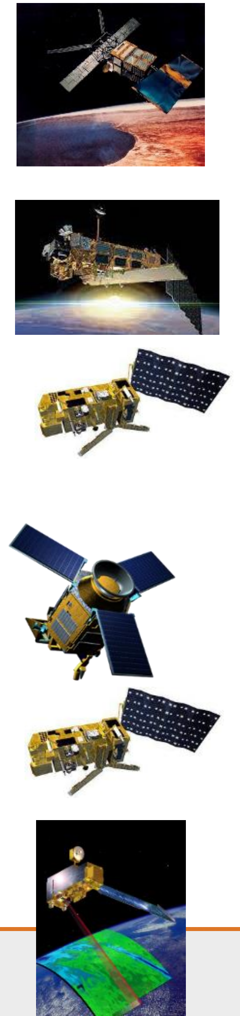
ACP, submitted. See also pres Amir at QOS 2024

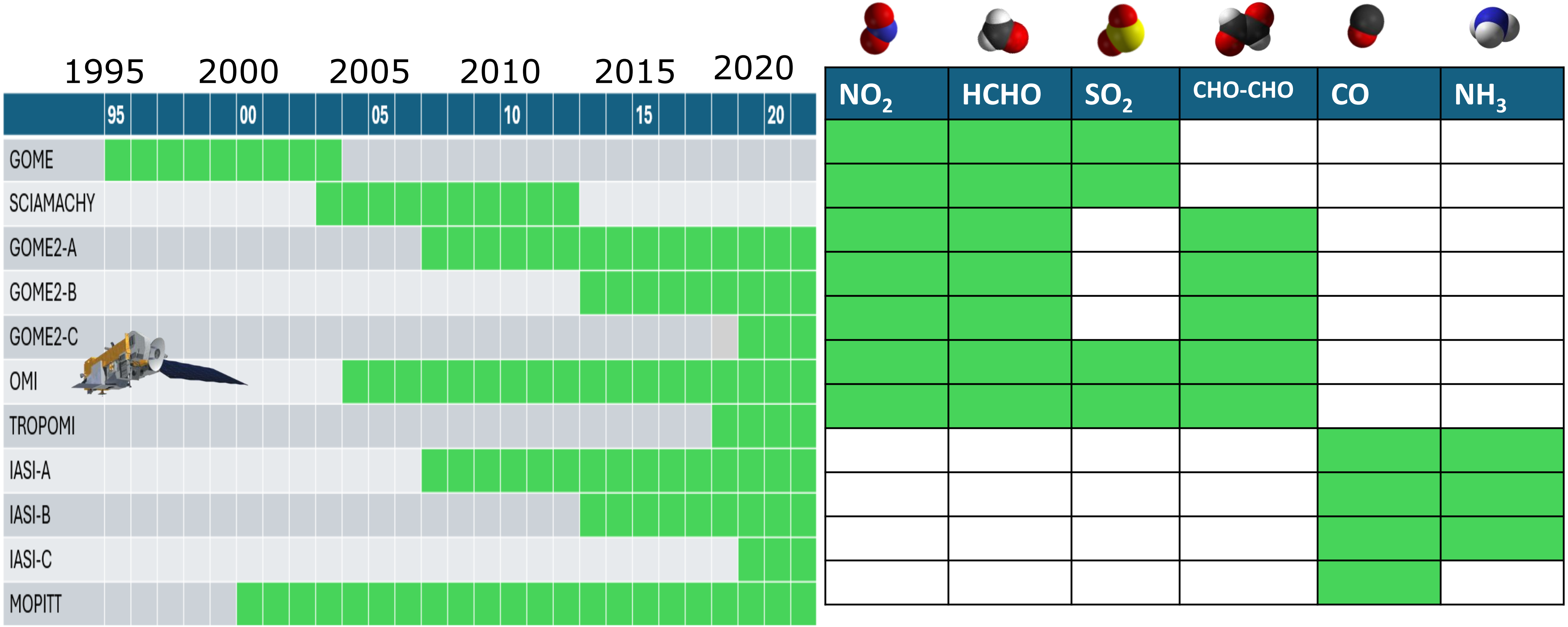


Bias correction + diagnostic uncertainty from validation

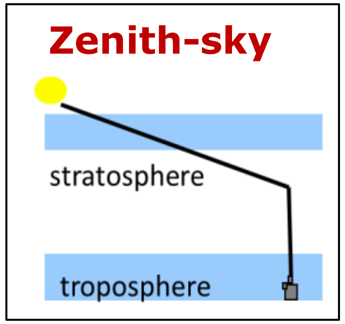
Precursors_cci+ Project (2022-2025)

Goal: harmonized multi-sensor L3 Climate Data Records for precursors of ozone and aerosol

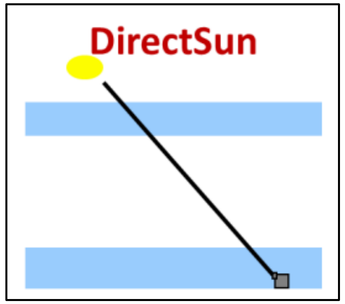




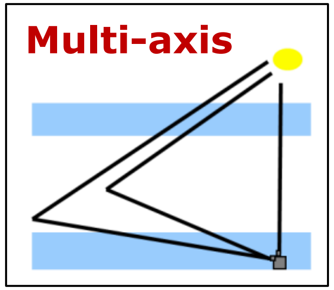
Ground-based Fiducial Reference Measurements



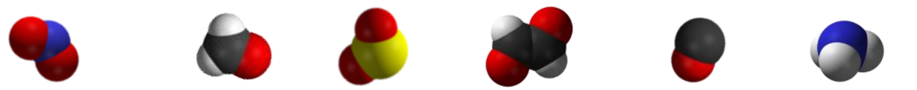
Zenith-sky DOAS:
stratospheric column



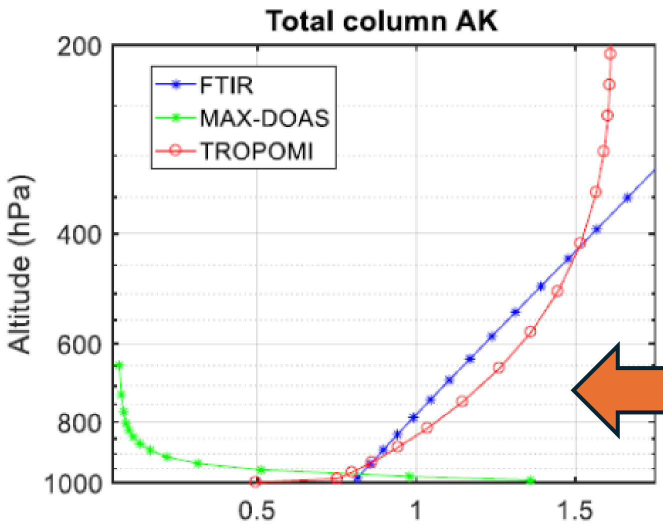
Direct Sun:
DOAS: total column
FTIR: column + profile



Multi-axis DOAS:
tropospheric column + profile



	NO_2	HCHO	SO_2	CHO-CHO	CO	NH_3
ZSL-DOAS	Strato					
Direct sun DOAS	Total					
Multi-Axis DOAS	Tropo					
FTIR						

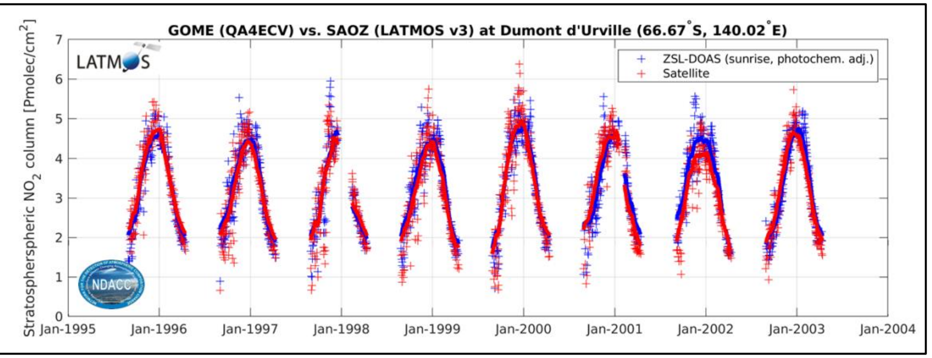


Complementarity of FRMs, e.g., vertical sensitivity

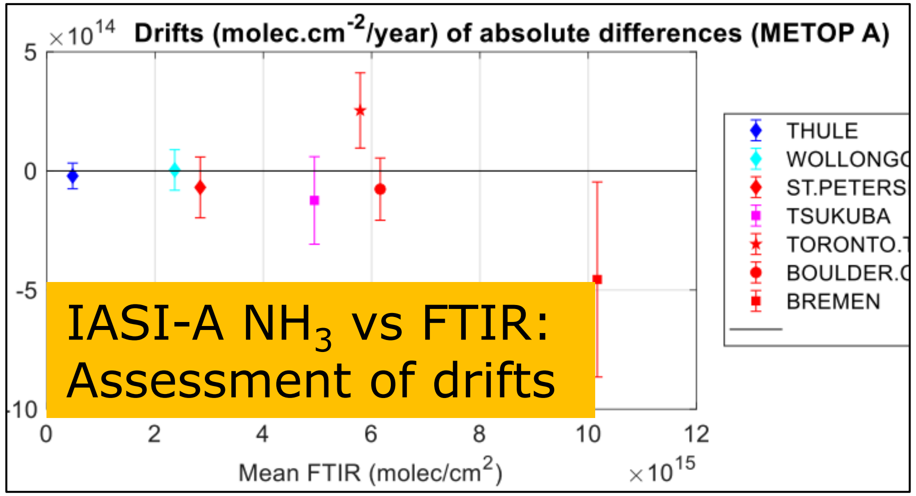
Ground-based data collected from networks

or obtained directly from instrument PIs

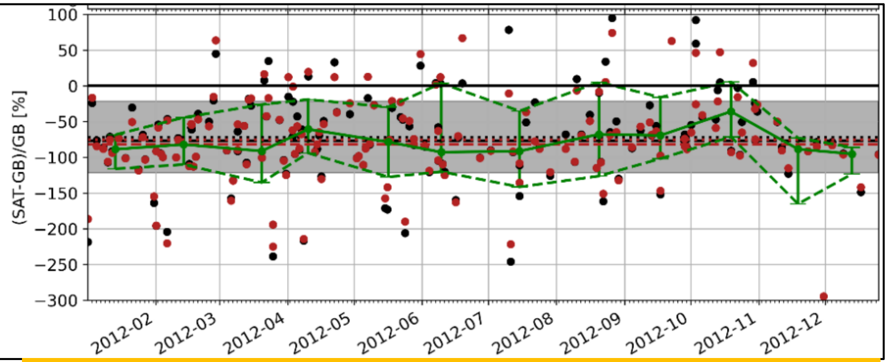
GOME NO_2 vs SAOZ @Dumont d'Urville since 1995



IASI-A NH_3 vs FTIR: Assessment of drifts



OMI SO_2 vs MAX-DOAS@Xianghe



More validation results in

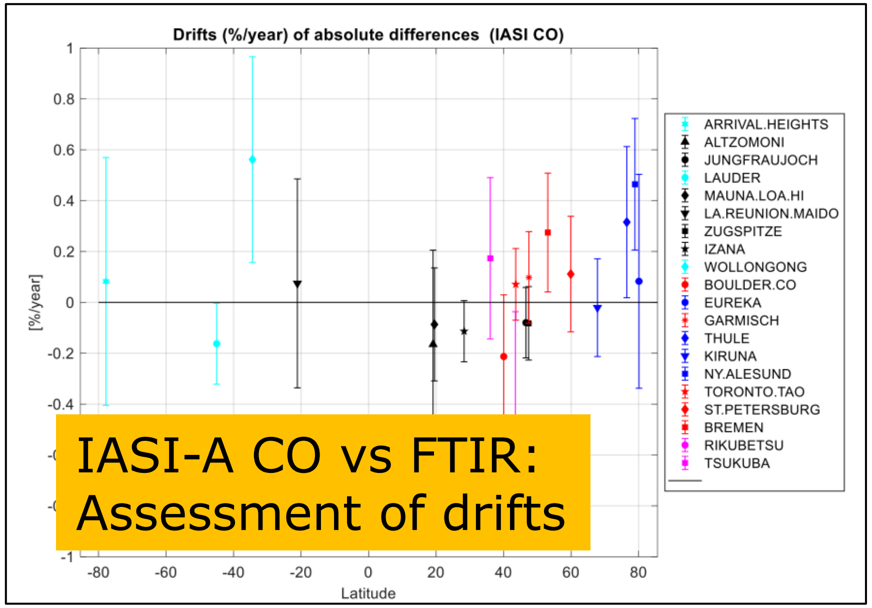
Precursors_cci+

ESA Climate Change Initiative (CCI)

esa

D4.1 Product Validation and Intercomparison Report

IASI-A CO vs FTIR: Assessment of drifts



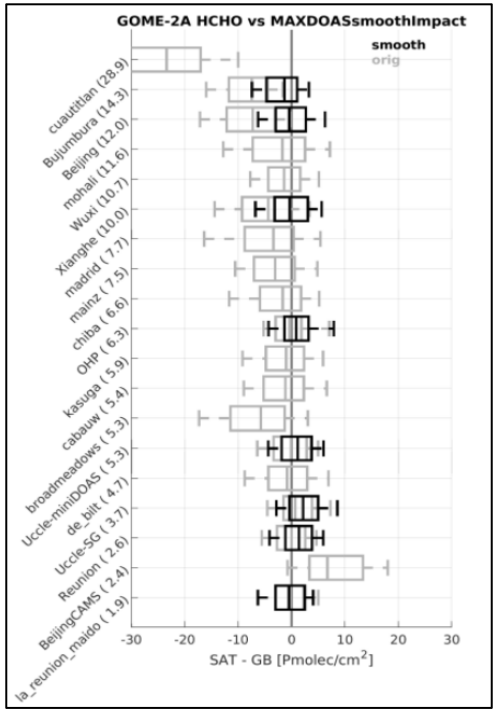
Compliance vs. user requirements (e.g., GCOS IP 2022)

Table 6-4. Compliance with GCOS requirements for HCHO L3 data.

Quantity	Requirements T|B|G	Compliance/evaluation		Remark
Horizontal resolution	100|30|10 km	L3: 0.2°x0.2° grid		The spatial resolution breakthrough requirement is achieved.
Temporal resolution	30days |1day|1h	L3: Monthly	L3: Daily	User requirements T or B are reached.
Bias	Not specified	Check summary in Table 6-3.		Bias is positive for clean sites; negative for polluted sites Bias and dispersion will be used in the next PVIR to validate random and systematic uncertainties.
Dispersion	Not specified	Check summary in Table 6-3		
Total uncertainty (1-sigma)	Absolute: 20e15|8e15|4e15 *molec/cm²	**Clean (< 2.5E15 molec/cm²):** Morning sat D: 4-4.4E15 molec.cm^{-2} (>250%) Afternoon sat M: 1.1-2.1E15 molec.cm^{-2} (>76-138%)		The "goal" is reached in absolute values for all conditions, and the "threshold" is reached in % for polluted conditions.

x>Threshold	Threshold≥x>Breakthrough	Breakthrough≥x>Goal	Goal≥x

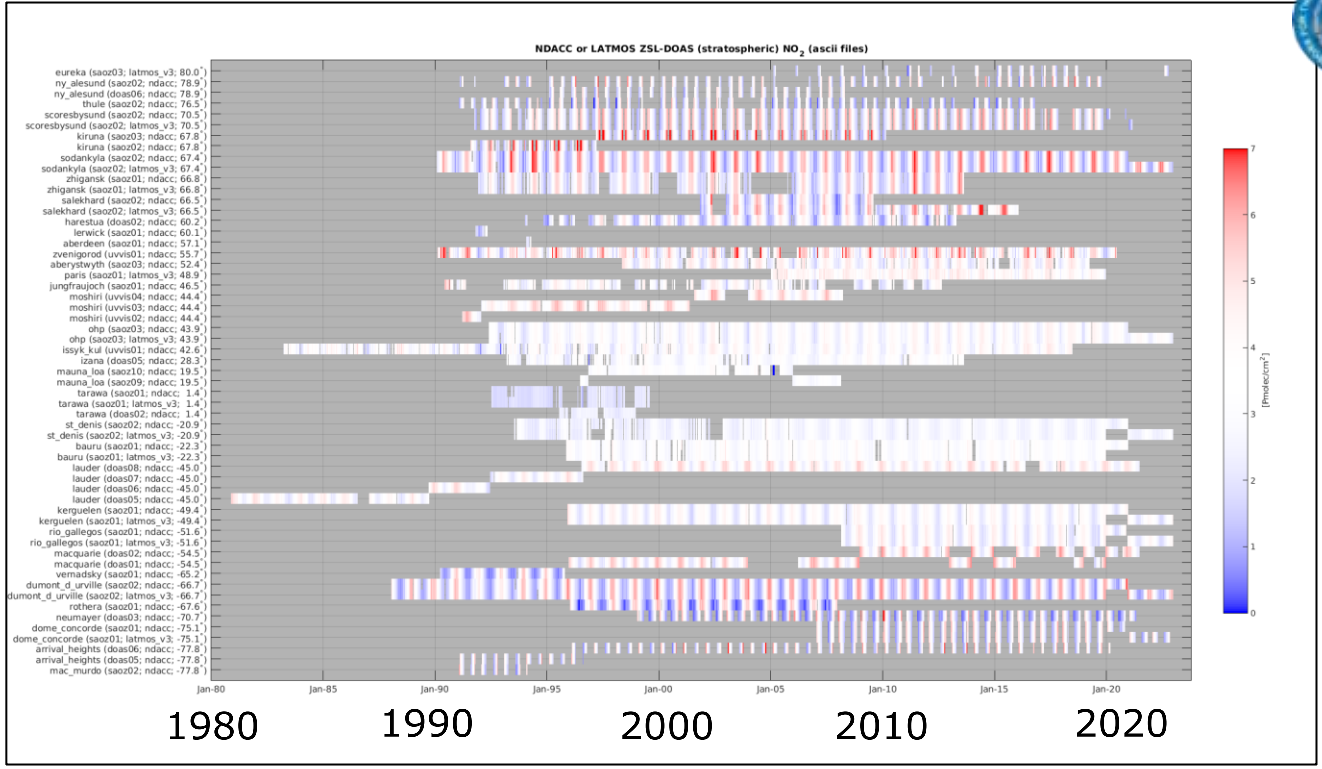
GOME2A HCHO vs MAX-DOAS

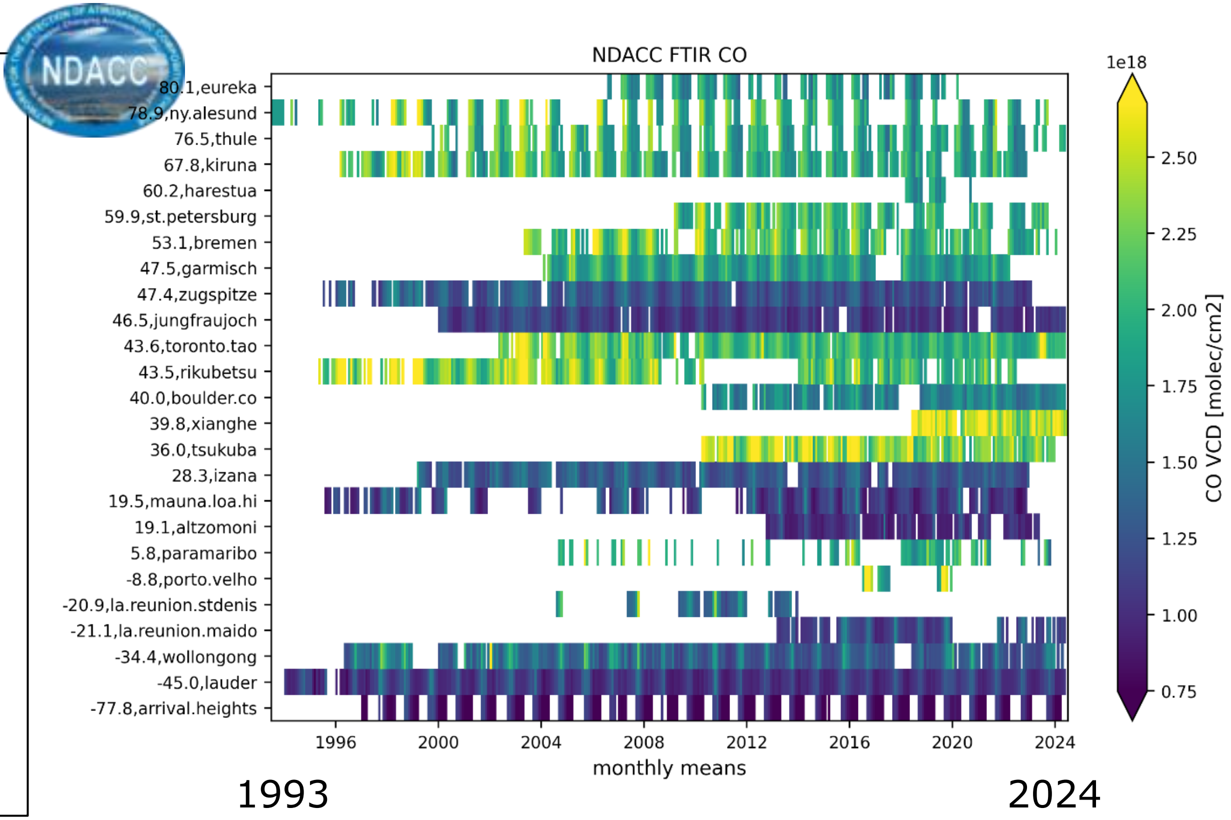


Long FRM Records: Strong Asset!

Stating the obvious:

Assessments of satellite-based Climate Data Records stability require long-term, continuous, sustained acquisition of FRM records like, e.g., NDACC FTIR and ZSL-DOAS / SAOZ





Progress in FRM Harmonization & Completeness

FRM4DOAS

https://frm4doas.aeronomie.be/

CINDI-3

Third Cabauw INtercomparison of DOAS-type Instruments

NDACC

Atmos. Meas. Tech., 11, 5049–5073, 2018
https://doi.org/10.5194/amt-11-5049-2018

Atmospheric Measurement Techniques

NDACC harmonized formaldehyde time series from 21 FTIR stations covering a wide range of column abundances

Corinne Vigouroux[1], Carlos Augusto Bauer Aquino[2], Maite Bauwens[1], Cornelis Becker[3], Thomas Blumenstock[4], … Michel Grutter[6], César Guarin[6], James Hannigan[7], Frank Hase[4]

PGN

PANDONIA GLOBAL NETWORK

Reference Measurements of Atmospheric Composition

https://www.pandonia-global-network.org

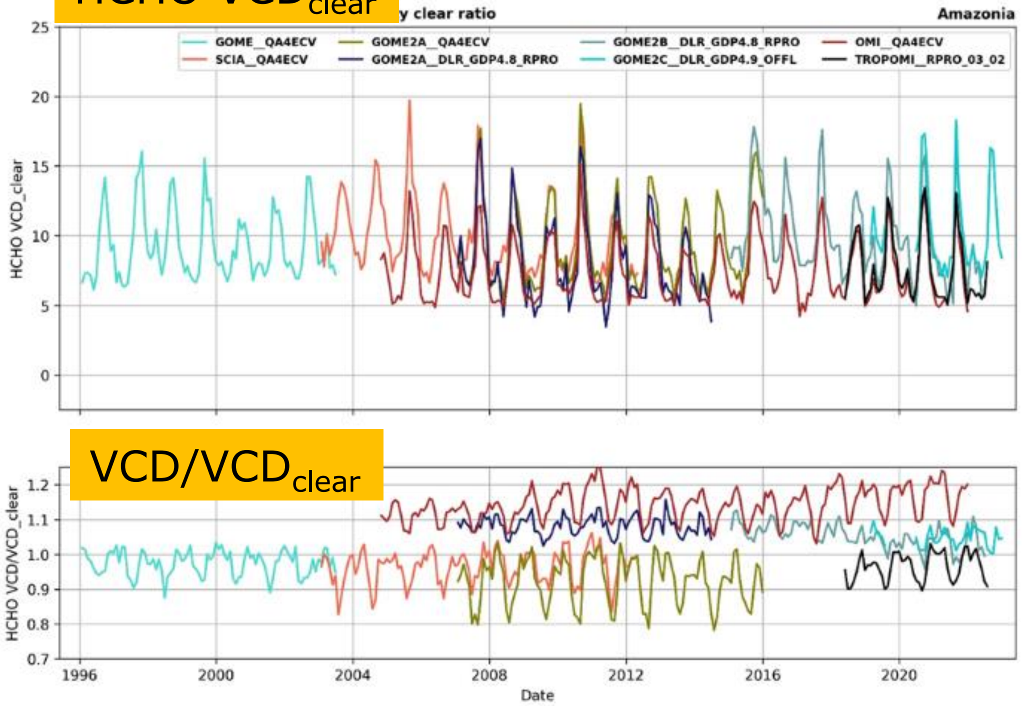
- FRM4DOAS: MAX-DOAS NO_2 & HCHO: central processing service to produce homogenized data
  - See also recent CINDI-3 campaign, targeting harmonization among teams
  - Pilot project for CEOS-FRM Maturity Assessment Framework
- Recent addition of harmonized FTIR HCHO to the NDACC Data Host Facility
- PGN Pandora: centrally processed data with detailed uncertainty budget

- We encourage further harmonization efforts (e.g., through ESA FRM4xxx projects)
  - To include more stations and more measurement series
  - To rescue and preserve data on the long term – and prevent loss of historical datasets!
  - To expand to other measurement targets, such as MAX-DOAS SO_2 and FTIR NH_3

End-to-end Validation: Cloud Correction

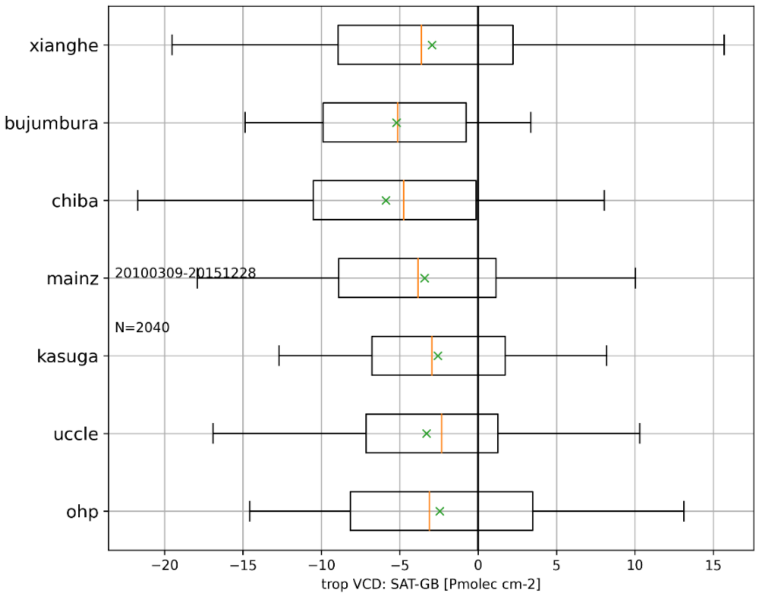
GOME-2 QA4ECV HCHO vs MAX-DOAS

HCHO VCD_{clear}

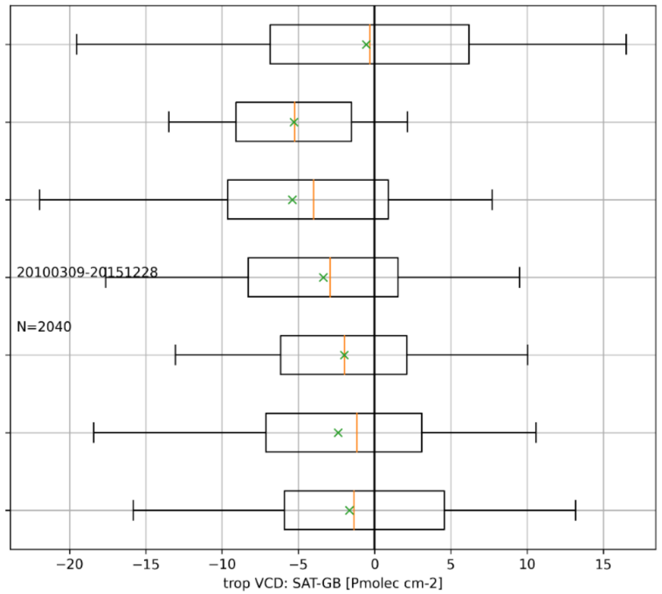


VCD/VCD_{clear}

Cloud corrected



clear-sky



Size and sign depend on algorithm and sensor.
Better multi-sensor continuity with clear-sky assumption

Feedback from round-robin validation

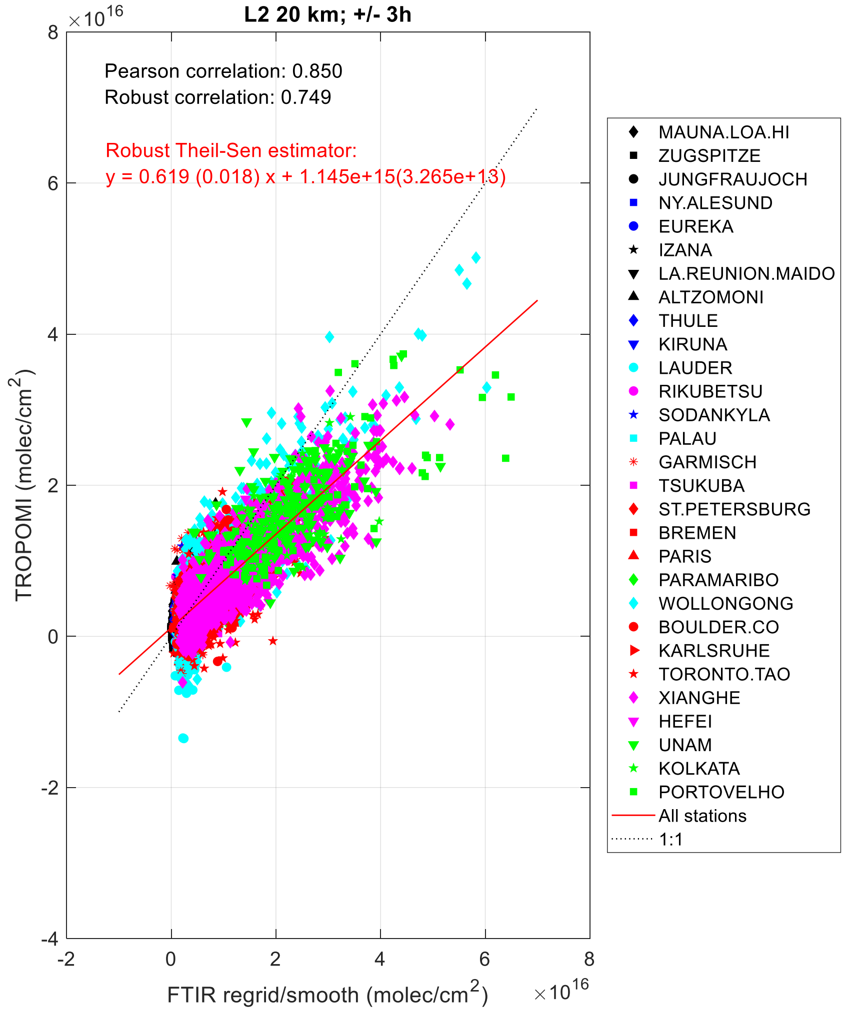
clear-sky adopted for HCHO CDR

GOME-2 QA4ECV HCHO:
cloud corrected vs clear-sky
→ clear-sky: better bias & correlation

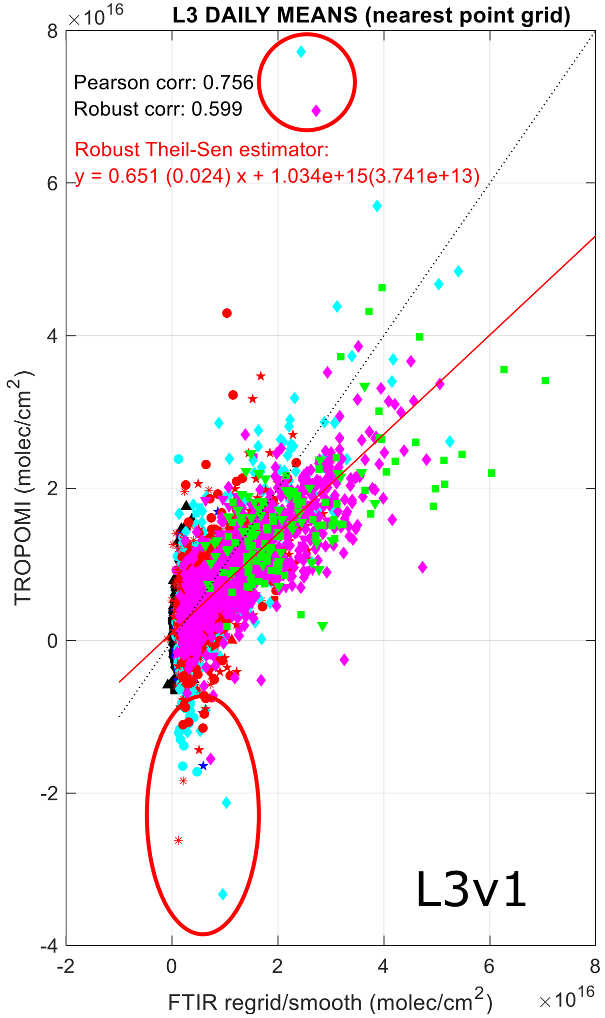
GOME-2 AC SAF HCHO:
cloud corrected vs clear-sky
→ No difference

End-to-end Validation: L2 & L3

- **TROPOMI: L2**



- **TROPOMI: L3 DAILY**



Feedback from round-robin validation

Outliers in L3 due to poorly sampled grid cells

L3-specific quality filter included in L3v2

Also L2-to-L3 representativeness fields included

Validation of Prognostic Uncertainties

$$\sigma^2(\text{SAT-FRM}) = \sigma^2(\text{eSAT}) + \sigma^2(\text{eFRM}) + \underline{\sigma^2(\text{mismatch errors})}$$

?

1/ SAT and FRM uncertainties need to be harmonized and sufficiently complete (random + systematic)

2/ Full uncertainty validation needs quantification of mismatch errors (co-location + smoothing). OSSSMOSE tool demonstrated for ozone => **Adaptation to precursors is needed.**

— Chapter 10 — 2012

Comparing and Merging Water Vapour Observations: A Multi-dimensional Perspective on Smoothing and Sampling Issues

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§ Now at Advanced Mechanical and Optical Systems, Liège, Belgium

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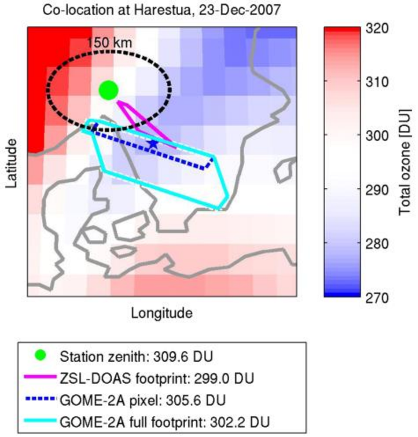

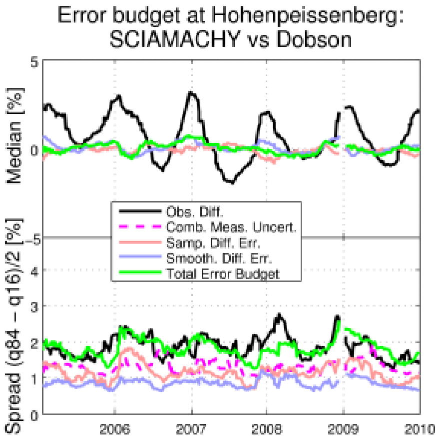

Atmos. Meas. Tech., 8, 5039–5062, 2015
www.atmos-meas-tech.net/8/5039/2015/
doi:10.5194/amt-8-5039-2015

Atmospheric Measurement Techniques

Metrology of ground-based satellite validation: co-location mismatch and smoothing issues of total ozone comparisons

T. Verhoelst[1], J. Granville[1], F. Hendrick[1], U. Köhler[2], C. Lerot[1], J.-P. Pommereau[3], A. Redondas[4], M. Van Roozendael[1], and J.-C. Lambert[1]

Conclusions

- Round-robin and end-to-end validation of not only the final product but also intermediate processing steps give helpful insight into the quality of both L2 *and* L3 Climate Data Records.
- Cloud correction is highly dependent on sounder and algorithm; in some cases clear-sky assumption can be the better choice.
- Close iteration between data providers and validators lead to better final CDRs.

Challenges in assessing the quality of ECV Climate Data Records

Recommendations for ATMOS 2024

- Validation of satellite-based CDRs of atmospheric ECVs requires rescue, harmonization and preservation of historical Fiducial Reference Measurements. The FRM4DOAS project is an example of appropriate framework.
- Long-lasting atmospheric monitoring programmes (e.g., SAOZ network for NO_2) are a unique source of FRM for the accurate validation of satellite-based CDRs, and a reference for new FRM networks currently in development. Their termination will endanger our ability to validate long-term and multi-satellite CDRs.
- Recent progress in FRM harmonization, uncertainty assessment, metadata completeness… needs continuation, and expansion to new species (incl. SO_2 and NH_3). The CEOS-FRM Maturity Assessment Framework may serve as an inter- and intra-network harmonization tool.