

Outline

1. PROFFAST and PROFFASTpylot
current developments
2. ITMS Project
Support from the German COCCON
community

PROFFAST and PROFFASTpylot

upcoming updates



Lena Feld, COCCON Telecon
03.05.2025

```
lenaf@imk-asf-bodllf: ~/Projects/proffastpylot/exam...
(prf_venv) lenaf@imk-asf-bodllf:~/Projects/proffastpylot/example$ python r
un_tsukuba.py
Example data are already available on disk
2025-03-04 10:04:50,859, INFO: +++ Welcome to PROFFASTpylot +++
Cite this software as

Feld et al., (2024). PROFFASTpylot: Running PROFFAST with Python. Journal
of Open Source Software, 9(96), 6481, https://doi.org/10.21105/joss.06481

2025-03-04 10:04:50,890, INFO: Run information:
Retrieval for Instrument SN063 at Tsukuba with time offset 9.0.
The following dates will be processed:
2024-06-19, 2024-07-22.

2025-03-04 10:04:52,125, INFO: Running preprocess with 2 task(s) ...
2025-03-04 10:05:02,978, INFO: Finished preprocessing.

2025-03-04 10:05:02,987, INFO: Running pcxs with 2 task(s) ...
2025-03-04 10:12:13,377, INFO: Finished pcxs.

2025-03-04 10:12:13,383, INFO: Running invers with 2 task(s) ...
2025-03-04 10:12:18,543, INFO: Finished invers.

2025-03-04 10:12:19,387, INFO: The combined results of PROFFAST were writt
en to /home/lenaf/Projects/proffastpylot/example/results/Tsukuba_SN063_240
619-240722/comb_invparms_Tsukuba_SN063_240619-240722.csv.
2025-03-04 10:12:19,388, INFO: Removing temporary files ...
2025-03-04 10:12:19,597, INFO: Done.

(prf_venv) lenaf@imk-asf-bodllf:~/Projects/proffastpylot/example$
```

Changes currently under development

- Output
 - **HDF files** following the GEOMS conventions (EVDC requirement)
 - NetCDF file following the cf convention (similar to TCCON output)
 - Extended variables in comb_invparms csv file
- Recording near dateline
 - Extended use cases and new example
- Moving observer
- Diagnosis for sun centering
 - Investigation of the residuals to detect Doppler shift

Recording Near the Dateline

- Recording in UTC leads to unintuitive folder structure
 - Recommended: Recording in Local Time Zone (without using daylight saving time)
- Three options available in PROFFASTpylot
 - Using UTC for the Interferograms and the folder structure
 - Using a specific time zone (Local Time) for interferograms and folder structure
 - New: Using UTC for the interferograms and Local Time for the folder structure

Moving Observer

- New version of preprocess can use different coordinates for each spectrum
- PROFASTpylot adaption in development
 - Input mechanism
 - Similar to the pressure input

Thank you

for the helpful comments, questions and ideas.

Citing PROFFASTpylot

- When using PROFFASTpylot, cite the software as

Feld et al., (2024). PROFFASTpylot: Running PROFFAST with Python. Journal of Open Source Software, 9(96), 6481, <https://doi.org/10.21105/joss.06481> .

COCCON in support of ITMS

Lena Feld, Darko Dubravica, Carlos Alberti, Jochen Gross, Frank Hase (KIT)

Moritz Makowski, Andreas Luther, Friedrich Klappenbach, Josef Stauber, Junwei Li, Jia Chen (TUM)

Lukas Grosch, Winfried Markert, Christof Petri, Thorsten Warneke (UB)

Benedikt Löw, Ralph Kleinschek, Rebekka Held, Nicolas Neumann and André Butz (UH)



Integrated Greenhouse Gas Monitoring System (ITMS)

- Creation of **observation based greenhouse-gas emission estimates** for Germany



ITMS General Assembly 2023, Picture by DWD

Integrated Greenhouse Gas Monitoring System (ITMS)

National Inventories



Atmospheric Observations



Models



spatially, temporally resolved,
observation based **emission estimates**
for different sectors

Atmospheric GHG observation systems

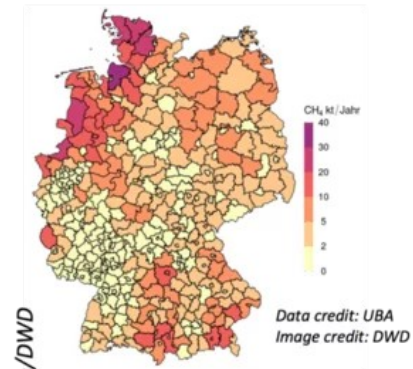
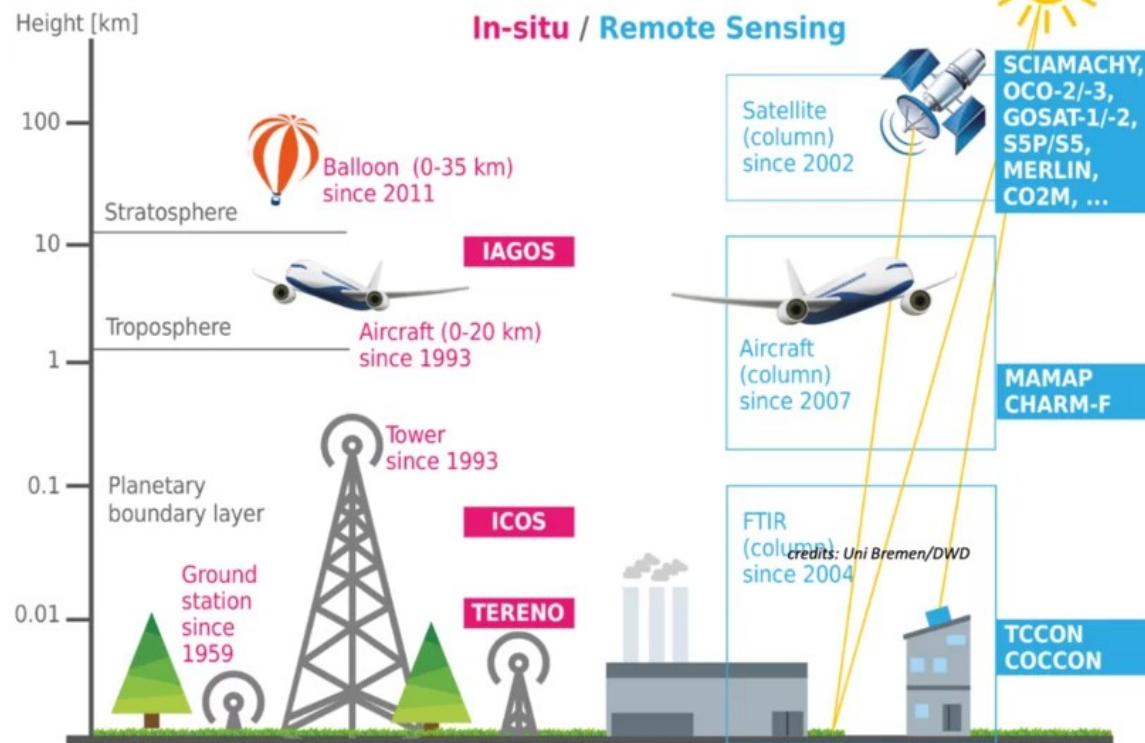


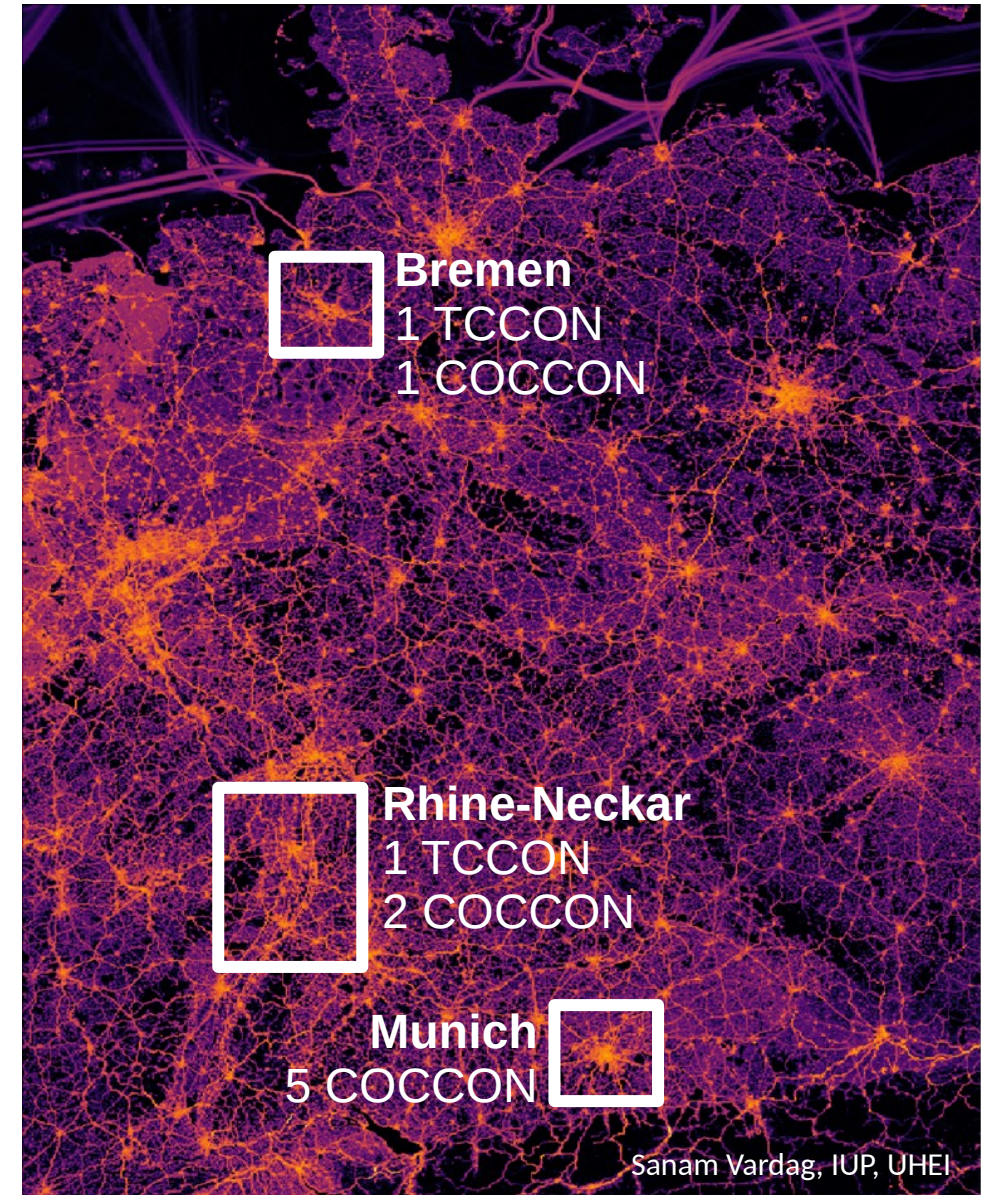
Image credits: Uni Bremen/DWD

ITMS-B-FTIR

- Collaboration between



- Data provision for ITMS
 - Inter-Calibration
 - Precision and uncertainties
 - Interpretation of the recorded dataset



Inter-calibration between the stations

- One EM27/SUN dedicated for traveling between the stations
- Traveling pressure sensor



Inter-calibration between the stations

- Determine calibration factors (f) with 10 minute binning
 - Calibration factor and standard deviation of every bin (f_i and σ_i)
 - Weighted average for overall calibration factor
- Calibration uncertainty determined from consistency of the f_i

per bin:

$$f_i = f_{\text{ref}}^{\text{SN}}|_i = \frac{X_{\text{ref}}}{X_{\text{SN}}}$$

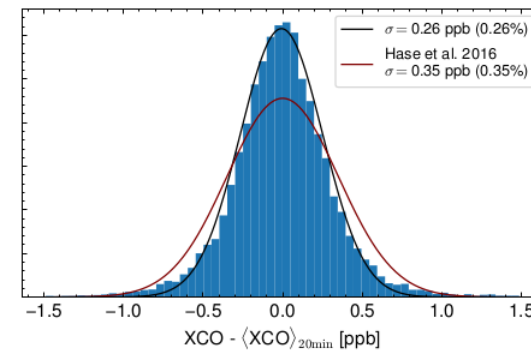
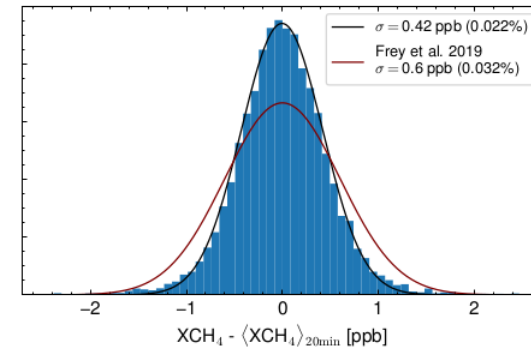
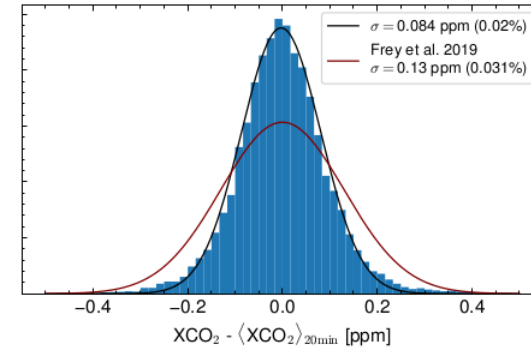
$$\sigma_{f_i} = \Delta f_{\text{ref}}^{\text{SN}}|_i = f_{\text{ref}}^{\text{SN}}|_i \cdot \sqrt{\left(\frac{\Delta X_{\text{SN}}}{X_{\text{SN}}}\right)^2 + \left(\frac{\Delta X_{\text{ref}}}{X_{\text{ref}}}\right)^2}$$

overall:

$$f = f_{\text{ref}}^{\text{SN}} = \frac{\sum_i \frac{f_i}{\sigma_{f_i}^2}}{\sum_i \frac{1}{\sigma_{f_i}^2}}$$

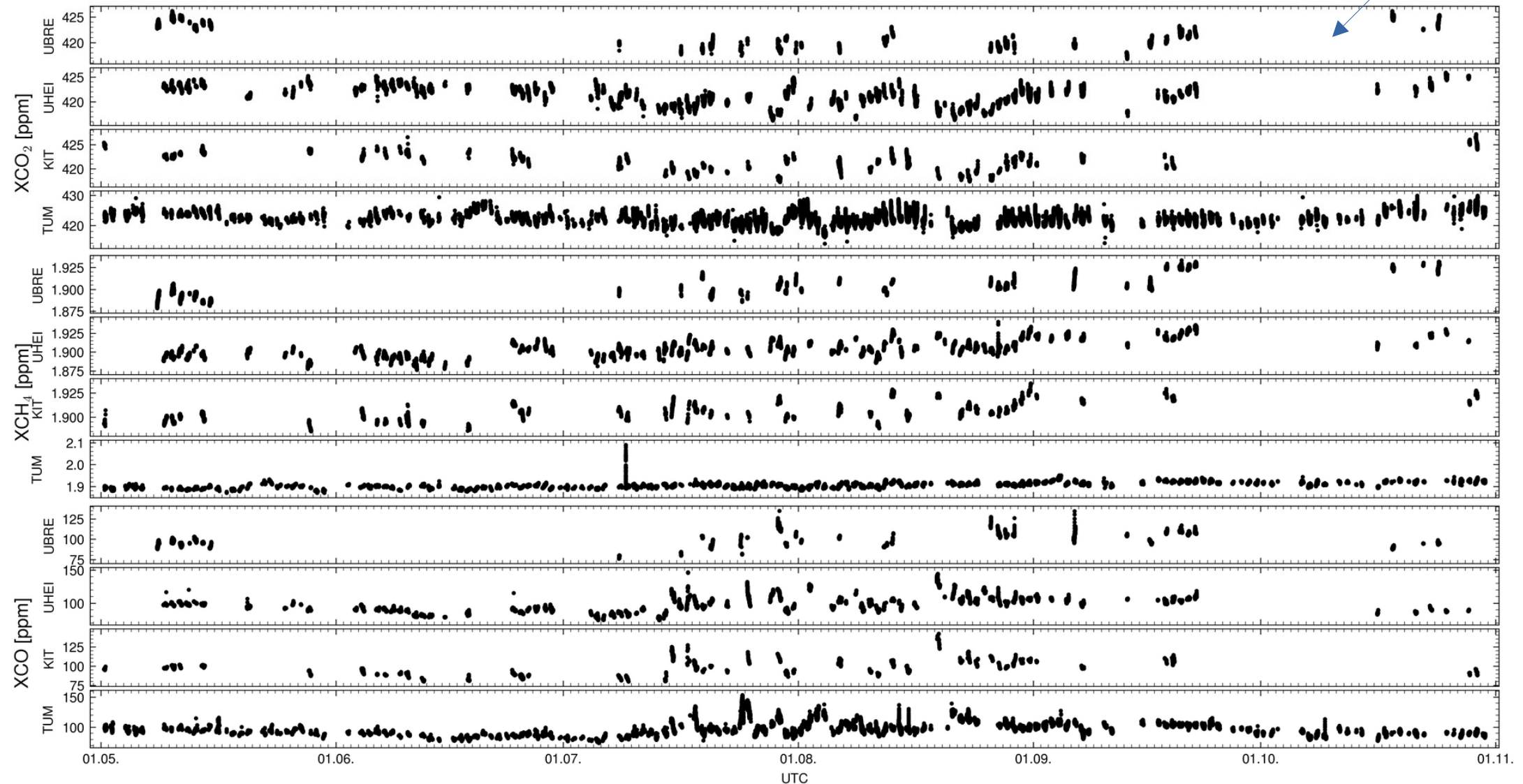
Precision of the Spectrometers

- Distribution of difference to rolling average (20 min)
 - Gaussian Fit
- Communication to the ITMS Modeling Group
 - Instrument-specific precision estimates
 - Calibration uncertainty



Published Dataset (May - Oct 2024)

Löw et al.: ITMS-B-FTIR Dataset (Version 1): COCCON observations in support of ITMS. COCCON [Dataset], EVDC - ESA Atmospheric Validation Data Centre, <https://doi.org/10.48477/COCCON.ITMS-B-FTIR.R01,2025>.



Outlook:

Investigating Observed Gradients

- Different Scales
 - Urban ~10 km (Munich),
 - Regional ~100 km (Karlsruhe ↔ Heidelberg) and
 - German-wide ~1000 km (Munich ↔ Bremen)
- Comparison to
 - Satellites
 - Models