HFC-23 long-term trend derived from FTIR solar spectra at the Jungfraujoch NDACC station: Comparing independent datasets and retrieval algorithms.

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26.06.2026

Overview

- Research context
- HFC-23 retrieval window
- SI-haloVOCs project
- Independent datasets
  - ACE-FTS satellite data
  - AGAGE *in situ data*
  - TOMCAT-SLIMCAT model simulation
- Long-term intercomparison
- Conclusions and outlook

Research context

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- **HFCs as alternatives to CFCs and HCFCs**: **HFC-23 (CHF_3)** emerged as a **chlorine-free** alternative with **no ozone depletion potential** but a **potent GHG** (GWP_{100} of **14,700**, total atmospheric lifetime of **228 years** [5]).

- **Regulation**: HFC-23 regulated under the **Kigali Amendment (MP)** and **Kyoto Protocol (1997)**.

- **HFC-23 main sources and applications**:

  By-product of HCFC-22 production (2% to 4% rate).

  Low temperature specialist refrigerant.

  Firefighting agent.

- **Impact**: **CFC levels declining**, **HCFC concentrations stabilizing**, but **HFC-23 rising** → high-precision monitoring is critical for Kigali Amendment assessment.

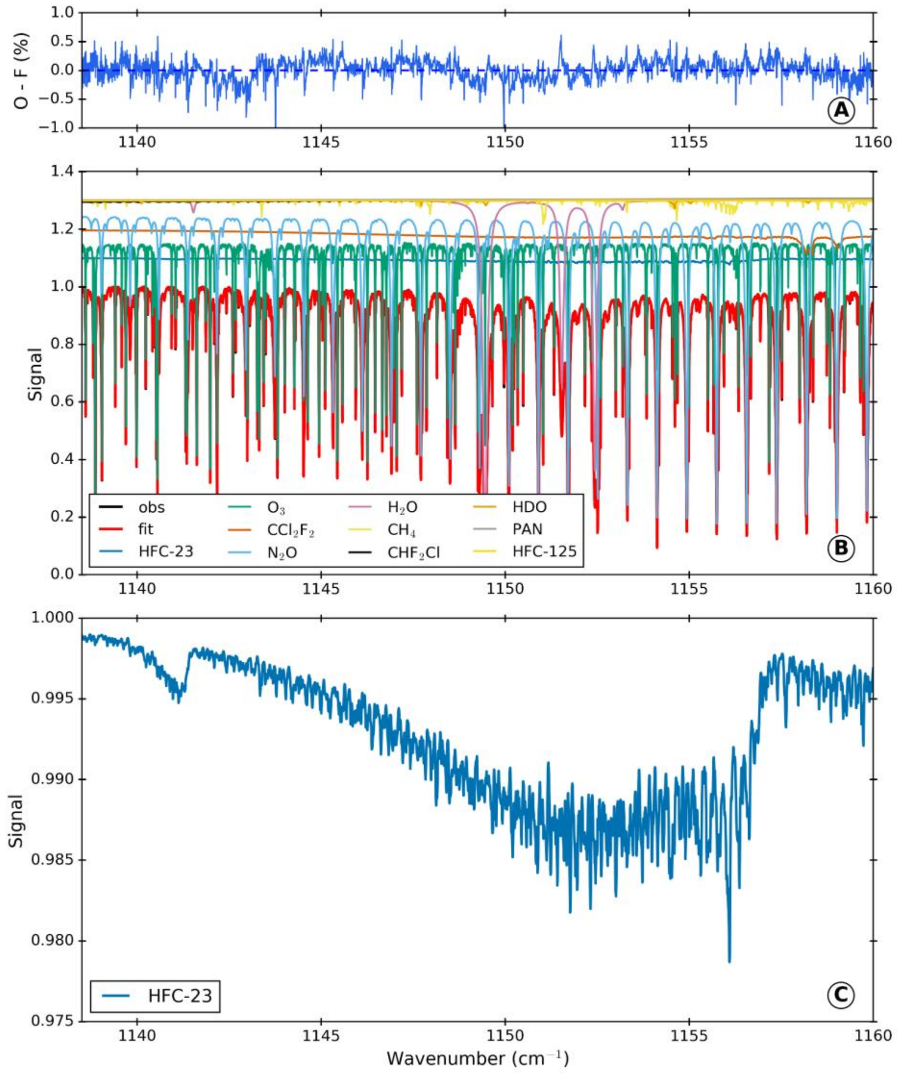
HFC-23 retrieval window

HFC-23 retrieval window

- HFC-23 total columns derived from clear-sky FTIR measurements at **Jungfraujoch station** (46.55°N, 7.98°E, 3580 m a.s.l.).

- Spectroscopic monitoring by the **University of Liège**, with high-resolution FTIR observations since **1984** [1].

- HFC-23 retrieval strategy: **4272** spectra.



Simulation of the 1138.5-1160.0 cm^{-1} spectral window from a spectrum recorded on March 3, 2025 with the Bruker IFS-125HR FTIR instrument at Jungfraujoch station. The root-mean-square of the residuals (RMS) is 0.18% (panel A). The main interfering species (H_2O, O_3, CCl_2F_2, N_2O, CH_4, $CHClF_2$, HDO, PAN, and HFC-125) are shifted vertically for clarity (panel B). Note the difference in vertical scale in panel C, where the HFC-23 absorption is greatly amplified.

SI-haloVOCs project

SI-haloVOCs project

Standardizing long-term remote sensing and *in-situ* measurements of atmospheric halogenated VOCs based on SI-traceability

- **Context:** Need to assess the regulation of halogenated **VOCs** at global and European levels ➔ Use of ***in-situ*** and **remote-sensing** measurements.

- **However:** measurements of halogenated VOCs require sophisticated equipment which is sparse.

- **Combining** long-term ***in-situ*** and **remote-sensing** measurements would increase global coverage. **However,** to ensure comparability between the ≠ measurement techniques in time and location, **traceability to the SI** must be ensured.

- **Aim:** Conduct the first direct intercomparison between **SI-traceable *in-situ*** measurements and **FTIR** time series.

SI-haloVOCs project

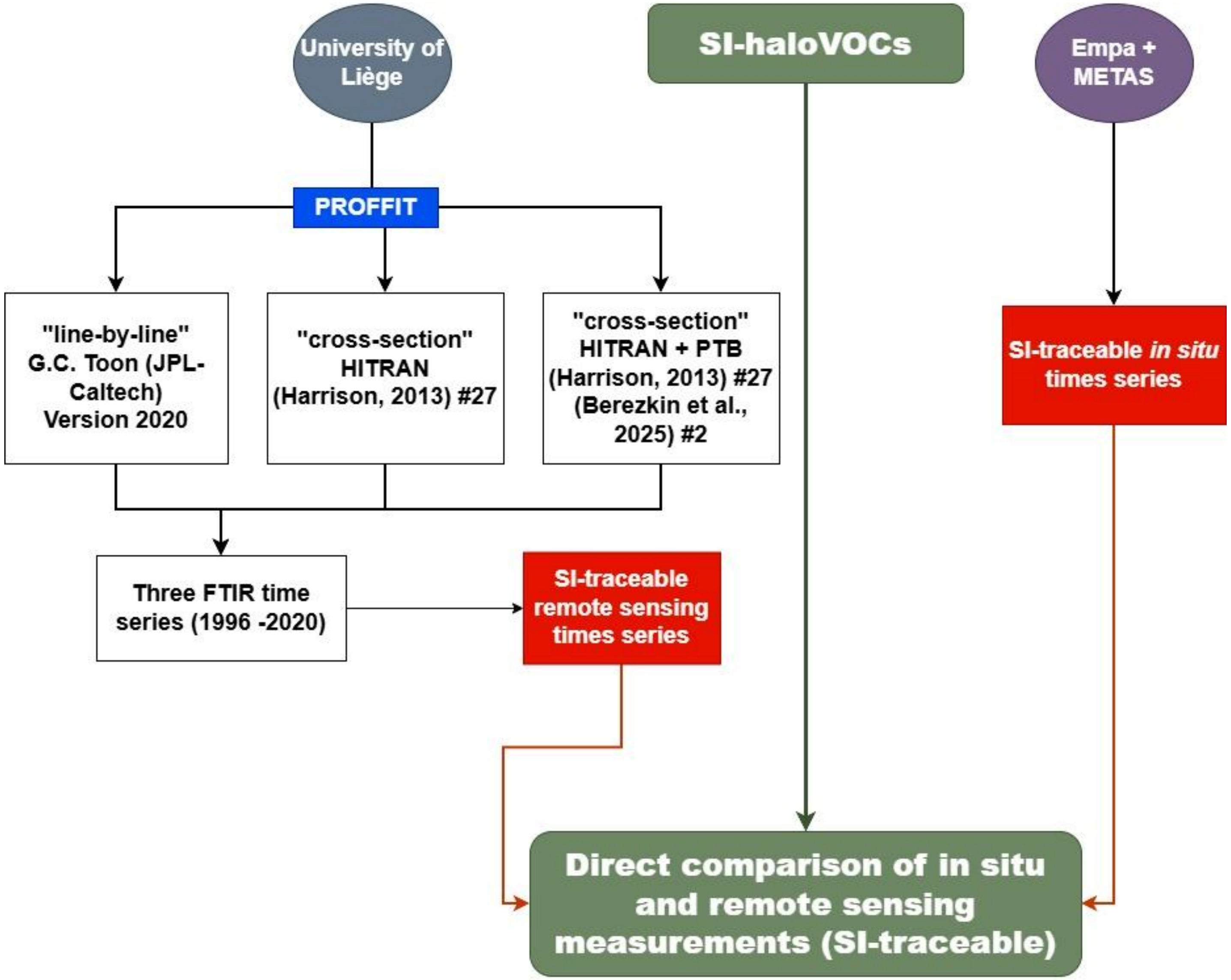
Standardizing long-term remote sensing and *in-situ* measurements of atmospheric halogenated VOCs based on SI-traceability

- Collaboration between **METAS, Empa** (Switzerland) and the **University of Liège** (Belgium) with the **Physikalisch-Technische Bundesanstalt** (PTB) providing SI-traceable spectroscopic reference data.

- **University of Liège's objectives:**
  - Implementation of SI-traceable information for remote-sensing measurements (**PROFFIT**).
  - Generate SI-traceable time series of remote sensing measurements (**PROFFIT**).
  - Comparison of long-term, SI-traceable *in-situ* (Empa) and remote-sensing measurements.

SI-haloVOCs project

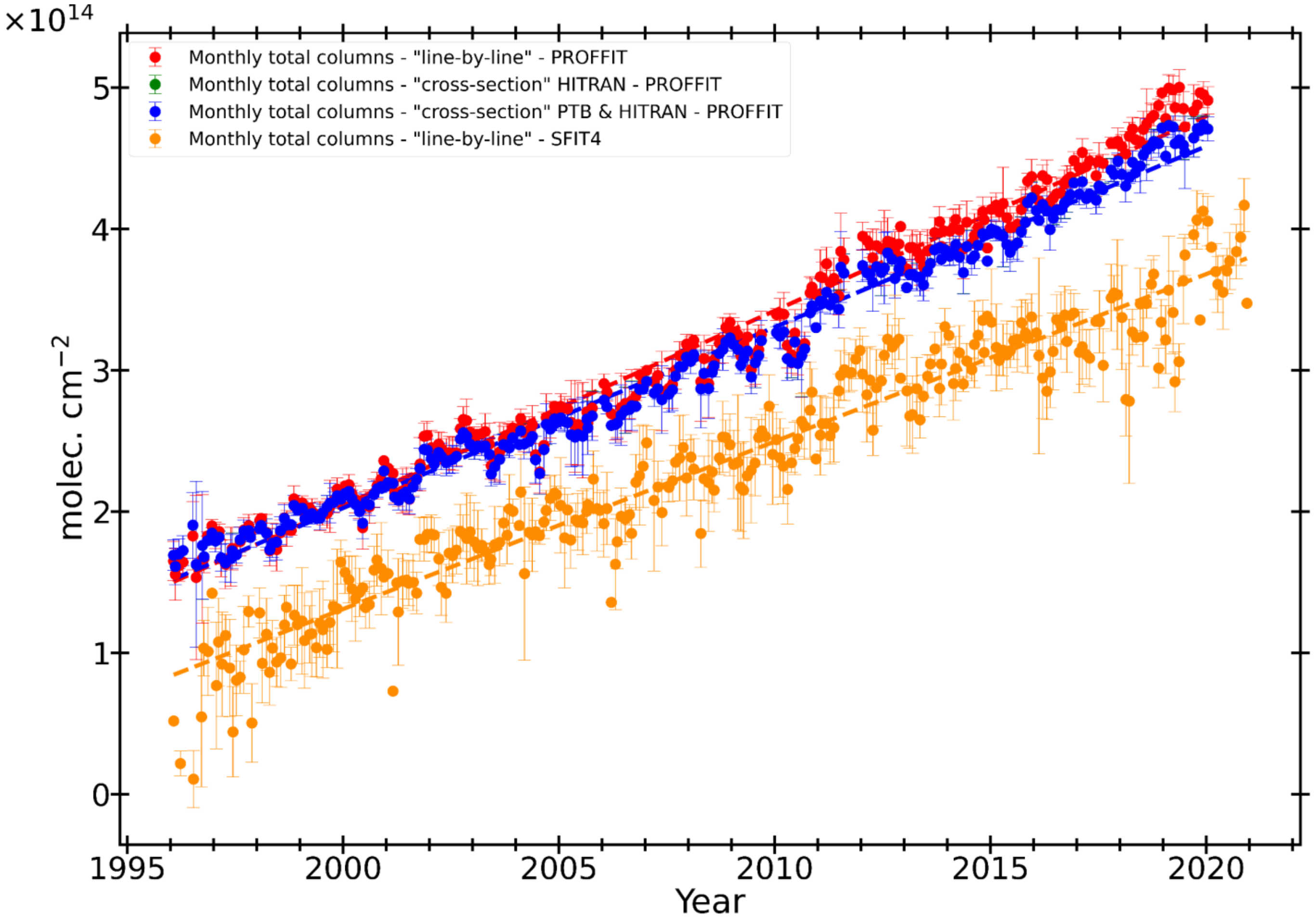
Roadmap



SI-haloVOCs project

PROFFIT and SFIT4 intercomparison

Dataset	Absolute trend (10^{13} molec. cm^{-2})	Relative Trend (%.yr^{-1})
PROFFIT « line-by-line »	1.38 ± 0.02	4.38 ± 0.07
PROFFIT « cross-section » HITRAN	1.28 ± 0.02	4.20 ± 0.07
PROFFIT « cross-section » HITRAN + PTB	1.28 ± 0.02	4.20 ± 0.07
SFIT4 « line-by-line »	1.19 ± 0.04	5.08 ± 0.17



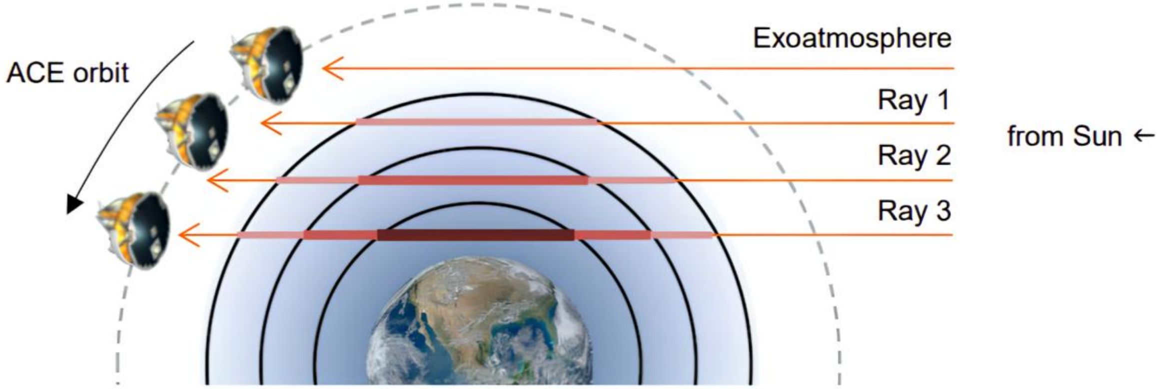
Monthly means atmospheric HFC-23 total columns (expressed in number of HFC-23 molecules cm^{-2}) from 1996 to 2020. Red, green, blue, and orange dots represent PROFFIT "line-by-line", PROFFIT "cross-section" HITRAN, PROFFIT "cross-section" PTB & HITRAN, and SFIT4 "line-by-line" approaches, respectively. The monthly mean HFC-23 values retrieved via the PROFFIT "cross-section" HITRAN and "cross-section" PTB & HITRAN methods show no statistically significant difference. Vertical error bars indicate ± 1σ variability around the monthly mean, while dashed lines display the linear trends for each dataset.
Note: the PTB abbreviation refers to the implementation of SI-traceable cross-sections (SI-haloVOCs project)

Independent datasets

Datasets: ACE-FTS satellite data

Key features

- **ACE-FTS** aboard the **Canadian SCISAT satellite**, operational since **2004** [2].
- The FTIR spectrometer uses **solar occultation** to measure atmospheric profiles [2].
- Covers **750–4400 cm^{-1}** spectral range at **0.02 cm^{-1} resolution**, retrieving profiles from the upper atmosphere down to **5 km** (clear-sky conditions).
- **Level 2 v5.3** (research product) [6], analyzed for **6.5–12.5 km altitude** in the **40–55°N** mid-latitude band.



Limb sounding from orbit around the Earth (Lahance et al., 2013).

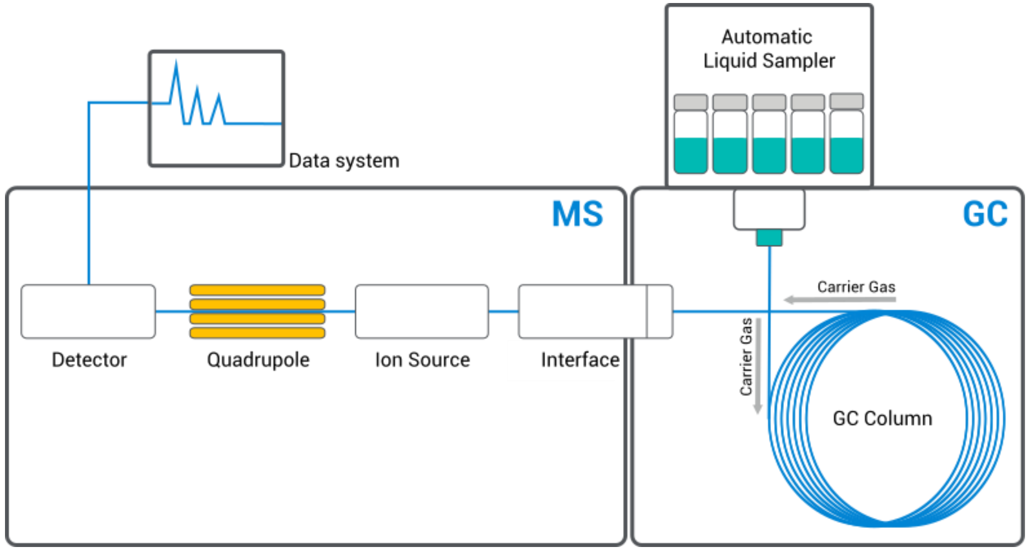
Datasets: AGAGE *in-situ* data

Key features

- *In-situ* HFC-23 measurements at **Jungfraujoch** using a **GC-MS system** [7].

- **Medusa system** preconcentrates **2 L air samples** at **-160°C**, desorbs at **100°C**, and injects into GC-MS for analysis.

- Reported on the **SIO-07 scale** with **0.6% precision** and **3% accuracy**.

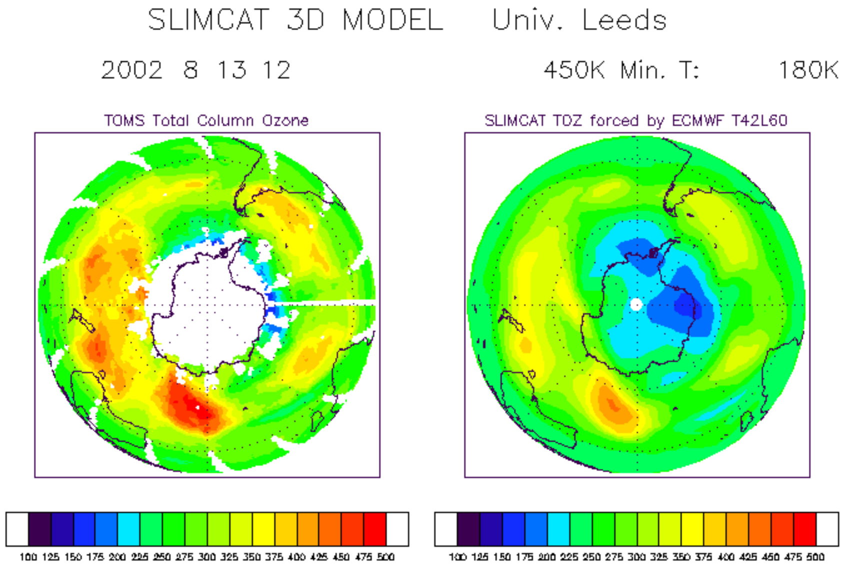


https://www.agilent.com/en/product/gas-chromatography-mass-spectrometry-gc-ms/gcms-fundamentals

Datasets: TOMCAT-SLIMCAT model simulation

Key features

- **Chemical transport model (CTM)** developed by Pr. Martyn Chipperfield, University of Leeds [3].
- **2.8° × 2.8° horizontal grid**, **32 vertical levels** up to **60 km**.
- Driven by **ECMWF ERA5 meteorology** [4], with stratospheric chemistry and **WMO/NOAA surface fluxes** for HFCs [9].
- **Daily sampling** at Jungfraujoch coordinates for direct comparison with FTIR observations.



TOMCAT – SLIMCAT Antarctic Ozone simulation for 2002
(https://tomcat.leeds.ac.uk/tomcat/animations/anim_antarc_o3_2002_toz/)

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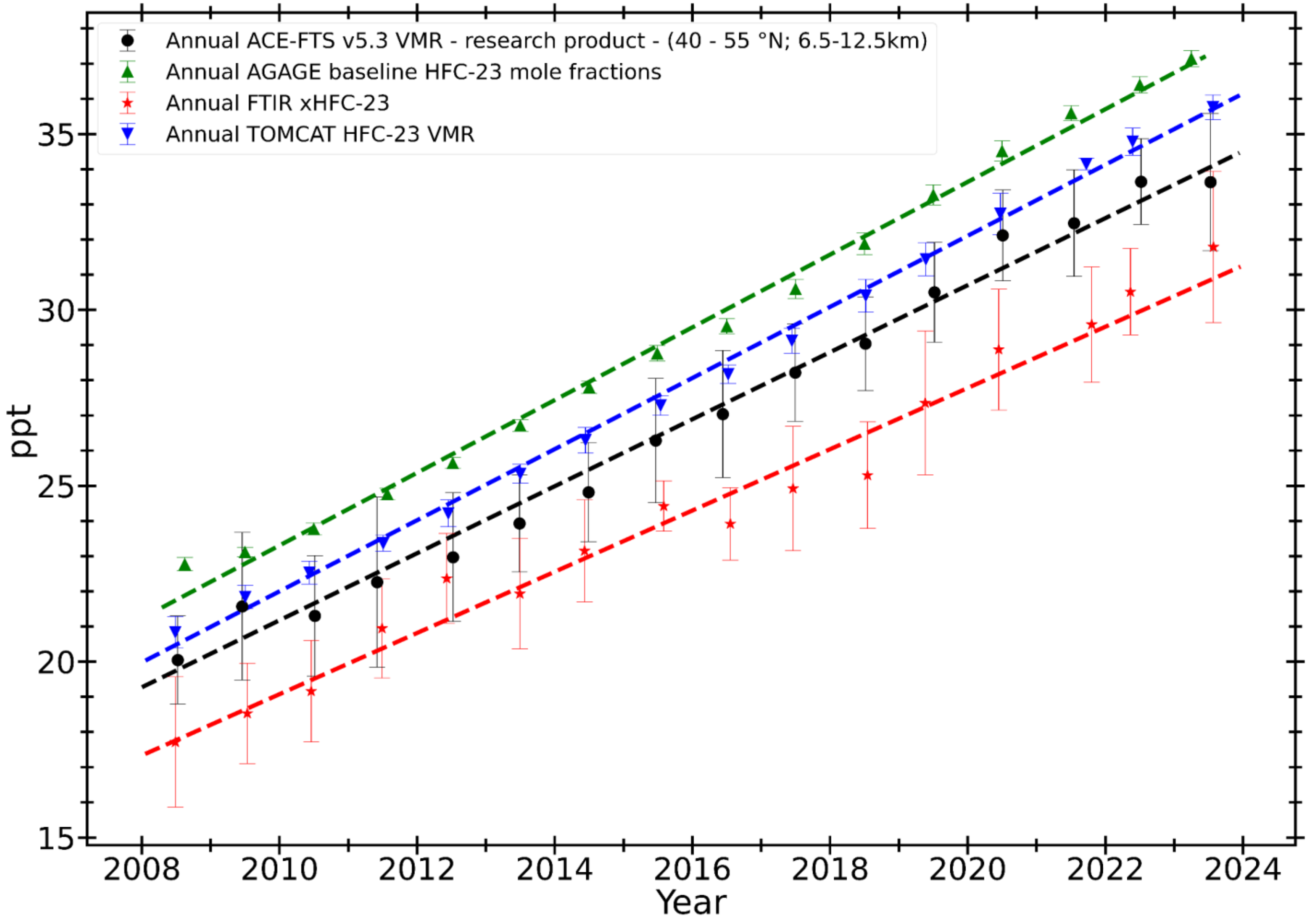
Long-term intercomparison

Long-term intercomparison

Remote sensing, *in-situ* and model datasets

Dataset	Absolute trend (ppt. yr^{-1})	Relative Trend (%.yr^{-1})
ACE-FTS	0.98 ± 0.06	3.66 ± 0.23
AGAGE	1.04 ± 0.04	3.52 ± 0.15
FTIR	0.86 ± 0.08	3.52 ± 0.35
TOMCAT	0.99 ± 0.03	3.53 ± 0.10



Annual mean atmospheric HFC-23 mole fractions from 2008 to 2024. Black dots represent ACE-FTS v5.3 (research version) data. Green upward-pointing triangles correspond to AGAGE in-situ measurements at Jungfraujoch. Red stars indicate xHFC-23 from Jungfraujoch FTIR measurements and blue inverted triangles depict xHFC-23 derived from the TOMCAT-SLIMCAT model simulations. One standard deviation around the monthly mean is shown by the vertical error bars. The dashed lines show the linear trends from each dataset.
Note: The linear trend analysis was performed using the algorithm developed by [8]

Conclusions and outlook

Conclusions and outlook

- A strategy for retrieving HFC-23 has been updated and implemented for FTIR observations at the Jungfraujoch station.

- The cross-validation of independent data revealed similarities (both absolute and relative trends), confirming the validity of our strategy.

- HFC-23 time series was determined using two retrieval algorithms for the Jungfraujoch, implementing three distinct spectroscopic approaches.

- Further work is needed to investigate the systematic difference between PROFFIT and SFIT4 algorithms.

Appendix: references

- [1]: **Zander et al. (2008)** *Our changing atmosphere: Evidence based on long-term infrared solar observations at the Jungfraujoch since 1950* **Journal:** *Science of The Total Environment* **DOI:** 10.1016/j.scitotenv.2007.10.018

- [2]: **Bernath et al. (2005)** *Atmospheric Chemistry Experiment (ACE): Mission overview* **Journal:** *Geophysical Research Letters* **DOI:** 10.1029/2005gl022386

- [3]: **Chipperfield (2006)** *New version of the TOMCAT/SLIMCAT off-line chemical transport model: Intercomparison of stratospheric tracer experiments* **Journal:** *Quarterly Journal of the Royal Meteorological Society* **DOI:** 10.1256/qj.05.51

- [4]: **Hersbach et al. (2020)** *The ERA5 global reanalysis* **Journal:** *Quarterly Journal of the Royal Meteorological Society* **DOI:** 10.1002/qj.3803

- [5]: **WMO (2018)** *GAW Report No. 58: WMO Global Atmosphere Watch (GAW) Implementation Plan: 2016–2023* **Type:** Rapport

- [6]: **Boone et al. (2023)** *Version 5 retrievals for ACE-FTS and ACE-imagers* **Journal:** *Journal of Quantitative Spectroscopy and Radiative Transfer* **DOI:** 10.1016/j.jqsrt.2023.108749

- [7]: **Keller et al. (2011)** *Evidence for under-reported western European emissions of the potent greenhouse gas HFC-23* **Journal:** *Geophysical Research Letters* **DOI:** 10.1029/2011gl047976

- [8]: **Friedrich et al. (2020)** *A statistical analysis of time trends in atmospheric ethane* **Journal:** *Climatic Change* **DOI:** 10.1007/s10584-020-02806-2

- [9]: **Prinn et al. (2018)** *History of chemically and radiatively important atmospheric gases from the Advanced Global Atmospheric Gases Experiment (AGAGE)* **Journal:** *Earth System Science Data* **DOI:** 10.5194/essd-10-985-2018
  - Available at https://gml.noaa.gov/aggi/aggi.html