EM27 Retrieval Pipeline: Automated EM27/SUN Data Processing

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Software

- Review
- Repository
- Archive

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Summary

The EM27/SUN (Gisi et al., 2011; Hase et al., 2016) is an FTIR spectrometer used to perform solar absorption measurements to derive column-averaged atmospheric concentrations of greenhouse gases (GHGs). In support of ESA, the COllaborative Carbon Column Observing Network (COCCON) (Alberti et al., 2021; Frey et al., 2019; Herkommer et al., 2024) has been established to offer a framework for the operation and data analysis of the EM27/SUN, ensuring the generation of fiducial GHG observations. The process of estimating the column-averaged concentration of GHGs from the interferograms recorded by the EM27/SUN is called retrieval. The retrieval algorithm established in the COCCON community is PROFFAST (Hase et al., 1999; Hase, 2023; Sha et al., 2020). PROFFASTpylot (Feld et al., 2024) is an interface around PROFFAST that significantly reduces the complexity of running PROFFAST retrievals.

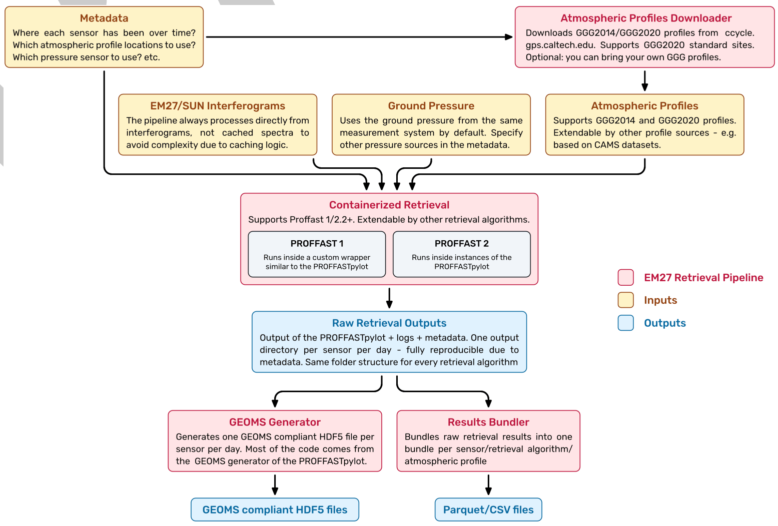

Figure 1: Modules of the EM27 Retrieval Pipeline.

The Munich Urban Carbon Column network (MUCCnet) consists of 5 EM27/SUN spectrometers deployed in and around Munich, Germany (Aigner et al., 2023; Dietrich et al., 2021; Heinle & Chen, 2018). Due to its autonomous operation since 2019, our research group generates a significant amount of EM27/SUN data. Processing this data in an automated and scalable way required us to extend the functionality of the PROFFASTpylot. Under the hood, we use the PROFFASTpylot to ensure consistency with the COCCON community.

State of the Field

The EM27 Retrieval Pipeline is complementary to the PROFFASTpylot (Feld et al., 2024). In general, the more EM27/SUN measurement data one has to retrieve, the more benefits come from the higher degree of automation the pipeline offers. While not implementing 100% of the flexibility the PROFFASTpylot provides, this pipeline is flexible enough to be used by any EM27/SUN setup, adhering to COCCON processing standards. Since the EM27 Retrieval Pipeline is an automation layer on top of the underlying retrieval algorithm, it is algorithm-agnostic and could be extended to support GFIT (Connor et al., 2016; Zeng et al., 2021) or other algorithms.

GGG2014/GGG2020 (J. L. Laughner et al., 2024; Wunch et al., 2015) is the data processing suite of the Total Carbon Column Observing Network (TCCON) (Toon et al., 2009). It is built around the GFIT retrieval algorithm and offers a similar degree of automation as the PROFFASTpylot. Since the TCCON instruments are significantly larger and more complex to deploy than the EM27/SUN, the GGG processing suite does not explicitly account for frequent instrument redeployments.

Statement of Need

Human-induced climate change is one of the most pressing issues of our time, as it puts the stability of our Earth system at risk. Our civilization is built on that stability. Anthropogenic GHG emissions, as well as natural sources and sinks of GHGs, have to be quantified to create targeted reduction policies, measure policy effectiveness, and identify new emission sources (Calvin et al., 2023).

The EM27/SUN is widely used to achieve these GHG flux estimations (Butz et al., 2017; Chen et al., 2016; Dietrich et al., 2021; Doc et al., 2025; Forstmaier et al., 2023; Hase et al., 2015; Jones et al., 2021; F. Klappenbach et al., 2015; Luther et al., 2019, 2022; Stauber et al., 2025; Tu et al., 2022; Vogel et al., 2019). Unlike the HR125 used by TCCON (Toon et al., 2009), the EM27/SUN can be transported and deployed at different and remote locations without much effort. Since 2016, the instruments of our permanent urban sensor network MUCCnet have been deployed at 3 locations in San Francisco (Friedrich Klappenbach et al., 2021), 4 in Hamburg (Forstmaier et al., 2023), 4 in Vienna (Luther et al., 2023), 12 in Poland (Luther et al., 2019, 2022), and 11 locations in Munich (Chen et al., 2018; Dietrich et al., 2021).

Figure 2 shows the XCO2 timeseries of the MUCCnet instruments since September 2019. Running the retrievals for various instrument deployments and keeping track of all deployments over time requires an organizational system that this pipeline provides. To enable a large number of long-term observations with EM27/SUN spectrometers, such as the upcoming sensor networks of COCCON-Spain (García et al., 2024) and GEMINI-UK (Humpage et al., 2024), an improvement in automation is crucial. The EM27 Retrieval Pipeline addresses this.

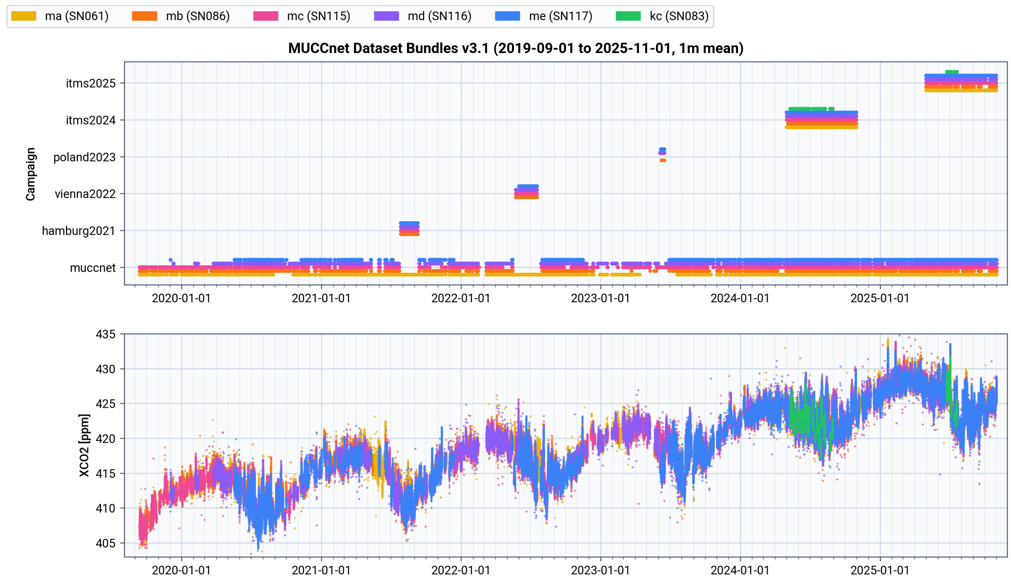

Figure 2: XCO2 of the MUCCnet instruments from 2019-09-01 to 2025-11-01

Software Design

We made the following architectural decisions to achieve this higher degree of automation and ease of use:

- **Configuration:** JSON configuration files are used to specify input/output paths, retrieval algorithm, start/end dates, and so on. These files are validated against JSON schemas (Pydantic, 2025; Wright et al., 2022) representing a strict set of rules for their structure and content. A misconfiguration will be detected at program start, instead of failing only once the code tries to use an invalid configuration parameter. The JSON schema is rendered as an API reference in the documentation, enabling us to adequately document a large number of configuration parameters.
- **Metadata Management:** Metadata (where/when/how each sensor was set up) is provided as JSON files as well. These files can be stored locally or pulled from a GitHub repository, enabling centralized, version-controlled tracking of sensor deployments. Metadata systems used in different EM27/SUN teams can be easily translated into this pipeline's schema, which largely agrees with the schema proposed in Zeeman et al. (2024).
- **Parallelization and Containerization:** While the PROFFASTpylot parallelizes the individual steps of PROFFAST, the pipeline parallelizes the whole retrieval process by running one isolated retrieval job per instrument per day. Every result folder maintains the structure of an individual PROFFASTpylot run, but also contains all configuration files required to reproduce it.
- **Algorithm Support:** While each tagged release of the PROFFASTpylot supports a specific range of PROFFAST versions, the EM27 Retrieval Pipeline keeps support for all implemented retrieval algorithms and versions.
- **Caching/Implicit Scheduling:** Users do not have to define an explicit queue of jobs, but instead define a date range and a list of sensors. The downloading/retrieval/bundling will decide which jobs to run, i.e., only run the jobs where no output exists yet.
- **Testing:** The codebase is statically typed and checked with strict MyPy (Python, 2025) and Pyright (Microsoft, 2025), and includes unit- and end-to-end tests (using PyTest (Krekel et al., 2024)) covering all major functions and retrieval scenarios.

Furthermore, the pipeline adds features required to produce long-term EM27/SUN datasets:

- **A fully automated interface to obtain Ginput data:** It automates requests for atmospheric profiles in the GGG2014 or GGG2020 format from a Ginput server (J. Laughner et al., 2021; J. L. Laughner et al., 2023; TCCON, 2025).
- **Bundling of retrieval results:** The raw retrieval outputs can be distributed over thousands of folders. The bundling routine merges these outputs into one file per sensor/retrieval algorithm/atmospheric profile, suitable for distribution.

Figure 1 shows the current building blocks of the EM27 Retrieval Pipeline. For the full feature set of the pipeline, please refer to its GitHub repository at github.com/tum-esm/em27-retrieval-pipeline and documentation. For example, starting with version 1.8, the pipeline extracts important parameters from the given OPUS files using the OPUS-file reader of the `tum-esm-utils` library (Makowski et al., 2025).

Research Impact Statement

The pipeline was first established in 2021 (Rißmann et al., 2022) and has been used for our entire EM27/SUN dataset since 2022 (Chen et al., 2024; Chen, Stauber, et al., 2025; Friedrich Klappenbach et al., 2024; Löw, Feld, et al., 2025; Luther et al., 2023; Stauber et al., 2025; Tang et al., 2024). Multiple journal publications using MUCCnet for inverse modeling are currently in preparation. The data generated by MUCCnet and the EM27 Retrieval Pipeline has been published to the ICOS Carbon Portal (Makowski et al., 2023, 2024) and the EVDC Portal (Chen, Makowski, et al., 2025a, 2025b; Löw, Makowski, et al., 2025) and is a cruicial data input for the GHG modeling approaches developed with the grants listed below.

AI Usage Disclosure

GitHub Copilot was used for single line code-completions, but not to write any complete functions or modules. All code was reviewed and tested by human developers.

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