Overview of the geophysical data derived from long-term FTIR monitoring at the Jungfraujoch NDACC site (46.5°N)

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INSTRUMENTATION, SITE, OBSERVATIONAL DATABASE AND TOOLS

-- Very high resolution (up to 0.003 cm^{-1}) infrared solar spectra are recorded year-round, at the high-altitude International Scientific Station of the Jungfraujoch (Swiss Alps, 46.5°N, 8.0°E, 3580m a.s.l.). Clear-sky conditions are mandatory.

-- Fourier Transform InfraRed (FTIR) monitoring activities are conducted at that site within the framework of the Network for the Detection of Atmospheric Composition Change (NDACC, see http://www.ndacc.org).

-- Our FTIR instruments are equipped with cooled HgCdTe and InSb detectors, allowing covering the 650 to 4500 cm^{-1} region of the electromagnetic spectrum. A set of optical filters (color-coded in Figure 1) are used to maximize the signal-to-noise ratios.

-- The retrievals are essentially performed with the SFIT-2 algorithm (v3.91) which is based on the semi-empirical implementation of the Optimal Estimation Method of Rodgers [JGR, 95, 1990], allowing in most cases to retrieve information on the vertical volume mixing ratio (vmr) profile of the target species.

-- Multidecadal FTIR time series are available from the Jungfraujoch (longest FTIR data sets worldwide), with earlier measurements in 1984.

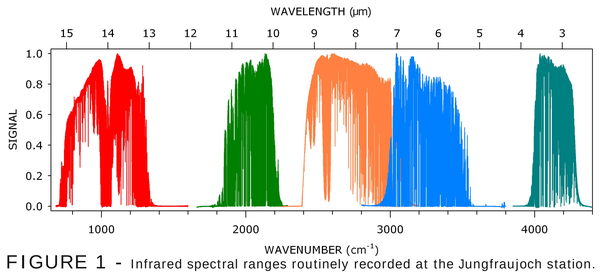


FIGURE 1 - Infrared spectral ranges routinely recorded at the Jungfraujoch station.

FIGURE 2 - NDACC FTIR site locations.

TARGET SPECIES OF THE GROUND-BASED FTIR TECHNIQUE

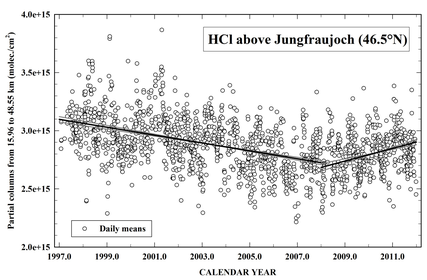


FIGURE 3 - Recent and unexpected upward trend for hydrogen chloride above the Jungfraujoch station. The 2008-2012 increase is significantly positive at the 2-sigma uncertainty level. This feature is confirmed by ACE-FTS IR solar occultation measurements at northern mid-latitudes. For more details, see Mahieu, 2012 (http://hdl.handle.net/2268/132600).

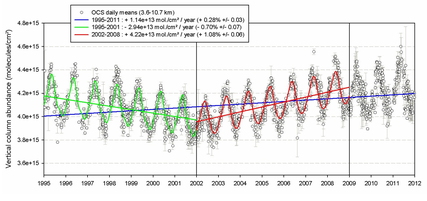


FIGURE 4 - Timely trends for carbonyl sulfide (OCS) in the troposphere, as deduced from long-term monitoring activities at the Jungfraujoch station. Coal combustion and aluminum production, notably in China, are candidate explanations for the OCS increase as of 2002. For more details, see Lejeune, 2012 (http://hdl.handle.net/2268/123804).

Numerous atmospheric species have exploitable spectral signatures in the infrared region routinely recorded by the NDACC-affiliated ground-based FTIR instruments (see map). First priority species include O_3, HNO_3, HCl, HF, CO, N_2O, CH_4, HCN, C_2H_6 and $ClONO_2$. Total and partial column timeseries of all these species are available in hdf and/or NASA-Ames format from the NDACC database (http://www.ndacc.org].

Altogether, about 30 molecules are now routinely retrieved from the Jungfraujoch spectra:

-- major greenhouse gases: H_2O, CO_2, CH_4 and N_2O
-- ozone
-- halogenated compounds: CCl_3F (CFC-11), CCl_2F_2 (CFC-12), $CHClF_2$ (HCFC-22), CH_3CClF_2 (HCFC-142b), CCl_4, CF_4, SF_6, HCl, $ClONO_2$, HF and COF_2
-- nitrogen compounds: N_2, N_2O, NO, NO_2, HNO_3, $ClONO_2$
-- organic compounds: CO, C_2H_2, C_2H_6, CH_3OH, HCN, formaldehyde, formic acid, OCS
-- many isotopologues of H_2O, CH_4, CO, O_3...

Sample results from the Jungfraujoch geophysical database are shown in **FIGURE 3** and **FIGURE 4**.

EXAMPLES OF RECENT ADDITIONS: METHANOL AND HCFC-142b

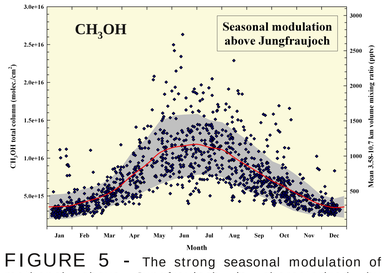


FIGURE 5 - The strong seasonal modulation of methanol above Jungfraujoch is characterized by minimum values (and variability) in December to February and maximum columns in June-July. The ratio between the lowest and highest individual columns exceeds 14. More details in Bader et al., 2013 (http://hdl.handle.net/2268/145478).

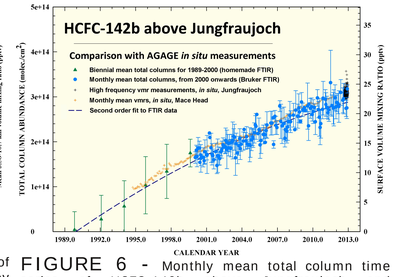


FIGURE 6 - Monthly mean total column time series of HCFC-142b above Jungfraujoch and comparison with AGAGE GC-MS in situ measurements at Mace Head (53°N). Overall, the long-term evolutions of the two sets are in good agreement. The 5% average difference between the 2 sets is within the systematic uncertainty characterizing the FTIR data. See Mahieu et al., 2013 (http://hdl.handle.net/2268/144709).

RETRIEVAL STRATEGIES UNDER DEVELOPMENT: NH_3, PAN, CH_3Cl...

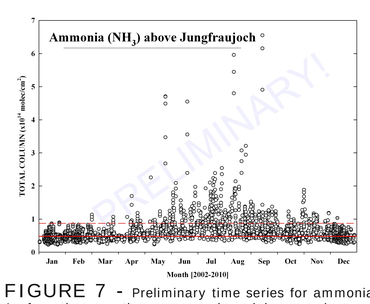


FIGURE 7 - Preliminary time series for ammonia. As for other reactive compounds, minimum values are observed during December-February while the spring and summertime seasons show enhanced columns.

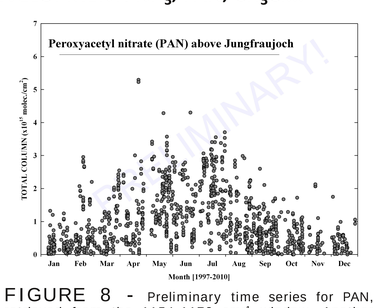


FIGURE 8 - Preliminary time series for PAN, retrieved from the 1154-1173 cm^{-1} window. Another spectral interval spanning a more intense PAN feature -but including a strong water vapor line- has yet to be tested.

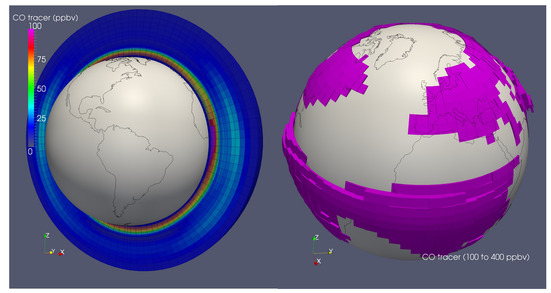
Poster presented at the 6th International GEOS-Chem Meeting, Harvard University, May 6-9, 2013

PYGCHEM:
Development of a new Python interface to GEOS-Chem

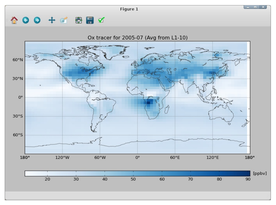
Aim of this project
– provide an alternative to the IDL interface (GAMAP), based on an open-source framework ;
– more than a collection of routines, the proposed interface intends to bundle an object-oriented library with several widgets and a customized shell for common or specific tasks related to GEOS-Chem simulations.

Why a Python interface?
– general and powerful open-source programming language, easy to learn. Object -oriented programming support ;
– a large, still growing, user and developer community ; many extensions including mature scientific libraries ;
– easy connection between Python and other languages as Fortran ;
– a "Pythonic" interface should allow the GEOS-Chem users to focus on the scientific aspects of their model use without spending too much time on technical details.

Examples of features that are planned for the upcoming first release
– reading/writing files used or generated by GEOS-Chem (e.g., binary punch files, netCDF data files, globchem.dat, tracerinfo.dat, diaginfo.dat...) info/from specific Python data structures or Numpy arrays ;
– interactive 1D or 2D plotting of diagnostics (using matplotlib and basemap) ;
– interactive 3D visualization of diagnostics (using Paraview or Mayavi) after export to the VTK format ;
– interactive exploration of the global chemistry mechanism defined for GEOS-Chem simulations, using an independent data structure (with import/export routines) and visualization tools (e.g., creation of a chemical reaction network using NetworkX).



3D Visualizations with Paraview



2D map created with matplotlib/basemap

The global chemistry mechanism visualized as an interactive CRN

The project is currently under development. We need your feedback and/or suggestions!
– Do you have any interest in using a GEOS-Chem Python interface for your research activities ?
– As a GEOS-Chem user – and Python user –, which features do you expect from such an interface ?
– Are you a Python developer ? Do you want to join us in the effort of developing this interface ?

The Github page of the project :
https://github.com/benbovy/PyGChem

Parts of the code are taken from the "gchem" python package that has been developed by Gerrit Kuhlmann (https://github.com/gkuhl/gchem/)

ACKNOWLEDGMENTS

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