H_2O retrievals from Jungfraujoch infrared spectra: some spectroscopic problems.

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GOALS

- evaluate the long-term evolution of H_2O total column above Jungfraujoch, from IR solar absorption spectra recorded in the last 50 years.
- extract vertical information from more recent FTIR spectra.

INSTRUMENTATION

Infrared solar absorption spectra have been recorded since 1950 at the Jungfraujoch observatory (Swiss Alps, 3580 m a.s.l.), with various instruments operated by the University of Liège:

- 1950-1951: 1-m focal length infrared grating spectrometer
- 1958-1989: 7-m focal length IR, visible and UV grating single-pass then double-pass spectrometer
- 1974-1976: prototype near-infrared Fourier transform spectrometer
- from 1984 onwards: home-made FTIR spectrometer
- from 1990 onwards: Bruker IFS-120HR FTIR spectrometer

The FTIR spectrometers are an essential component of the primary Alpine Station of the NDACC (Network for the Detection of Atmospheric Composition Change).

OBSERVATIONAL DATABASE

Grating spectra:

- a few hundreds of paper recordings from 1950 to 1967
- about 8000 spectra from 1968 to 1989 (see example in Figure 1)
  - H_2O lines @ 694.38 nm and in narrow windows encompassing lines of atmospheric interest (about 10 cm^{-1} wide)
  - resolution: about 15 mK

FTIR spectra:

- a few dozen of near IR spectra (1974-1976)
- more than 40 000 high resolution spectra (since 1984)
  - resolution 2.85 mK to 6.10 mK (i.e. OPD 175.4 cm to 81.9 cm)
  - between 2 and 14 micrometers (700 to 5000 cm^{-1})

SEARCH FOR H_2O LINES

Intensive work: find appropriate H_2O lines, in different spectral regions (selection criteria: temperature insensitive, free of interferences…)

Grating spectrometer:
- very few H_2O lines available, due to narrow spectral domains recorded by this instrument.

FTIR spectrometer: too many lines !
- first selection based on the linefinder code from J. Notholt (IUP, Bremen): 10278 lines selected from 700 to 4300 cm^{-1}
- second selection: 63 micro-windows kept (see Table 1)
- combination of micro-windows with strong and weak lines, to improve the DOFS (Degree Of Freedom for Signal, i.e. the number of independent atmospheric layers that can be retrieved from the spectra) (see examples in Figures 2 and 3).

To be carefully addressed: lines in the different spectral ranges need to be intercalibrated with great care !

ANALYSIS

- spectroscopic database : Hitran 2004, including latest updates for H_2O (August 2006, www.hitran.com)

Grating spectra
- SFIT1 [old version] (non linear least squares iterative fit) (see Figure 4)
- ILS = gaussian function (0.025 cm^{-1} HWHM)
- retrieval of H_2O TOTAL COLUMN only

FTIR spectra
- retrieval software SFIT2 v3.91 (optimal estimation method)
- lines profile = Voigt function
- p, T vertical profiles from NCEP
- a priori profile: ACE-FTS extended down to the ground based on US standard atmosphere
- a priori profile covariance: ACE-FTS above troposphere, 200 % in the troposphere
- retrieval of H_2O TOTAL COLUMN and VERTICAL PROFILE INFORMATION (see Figure 5)

Spectral domain (cm^{-1})	Number of selected microwindows
700 – 1300	16
1900 – 2200	8
2500 – 3100	10
3100 – 3500	17
4000 – 4300	12

Table 1

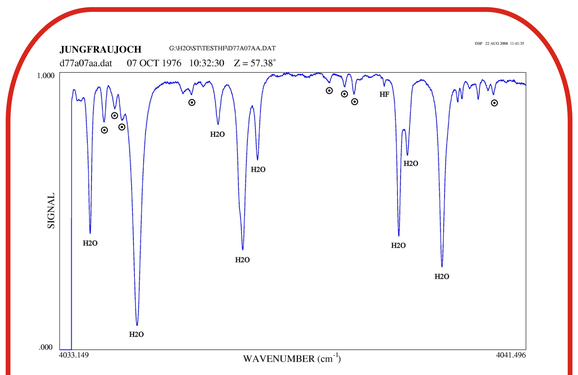

Figure 1. Example of a spectrum recorded in 1977 with the Jungfraujoch grating spectrometer, in the region of the R1 line of HF.

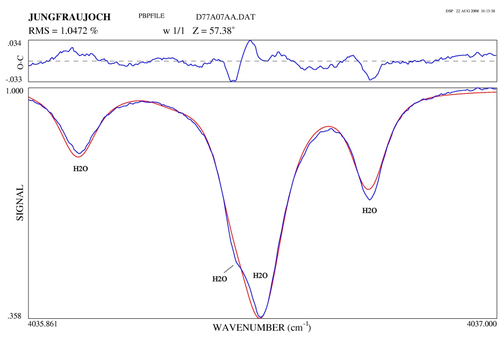

Figure 4. Fit of H_2O lines in the HF window, recorded with the Jungfraujoch grating spectrometer on October 7, 1977. The fit quality improved considerably when position of the first line was changed from 4035.97653 cm^{-1} to 4035.98276 cm^{-1} and position and strength of the last line were changed from 4036.69703 cm^{-1} and 9.521 E-24 cm^{-1} /(molecule×cm^{-2}) to respectively 4036.69078 cm^{-1} and 6.990 E-24 cm^{-1}/(molecule×cm^{-2}) [preliminary results !!].

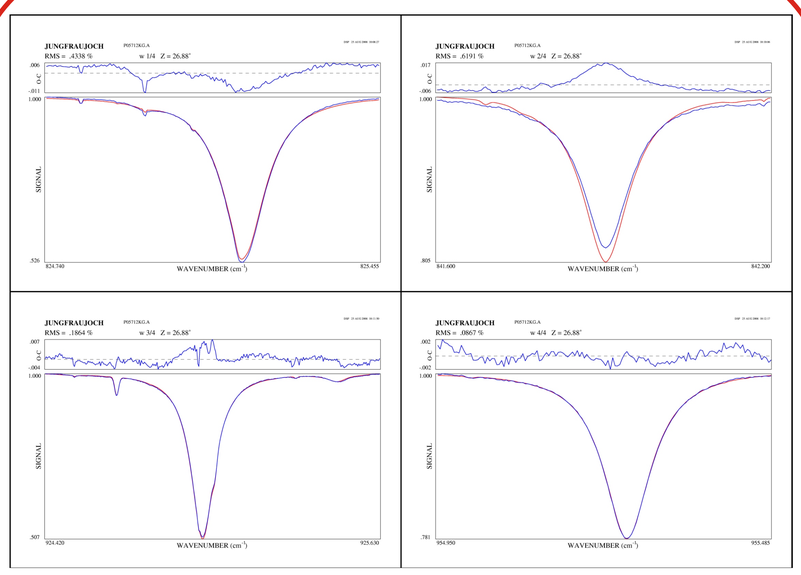

Figure 2. Simultaneous fit of 4 H_2O micro-windows (DOFS = 2.89) from a FTIR absorption spectrum recorded at the Jungfraujoch on July 12, 2005, at a solar zenith angle of 26.88°. Blue curves correspond to observed spectrum, red curves to computed spectrum. The upper frames of each micro-window show the residuals (observed-computed spectrum). Notice the vertical scales of the residuals and of the spectrum, different for each micro-window. Obviously, the spectroscopic parameters of the 841.9028 cm^{-1} line (top right panel) need to be revised !

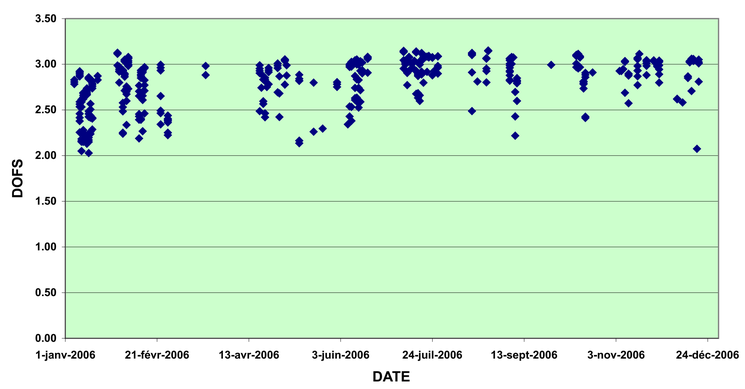

Figure 6. DOFS obtained from the micro-windows combination of Figure 2, for all the spectra recorded in 2006. This micro-windows combination provides a mean DOFS of 2.8. The DOFS is reasonably constant over the seasons, despite very high difference in atmospheric H_2O contents between winter and summer.

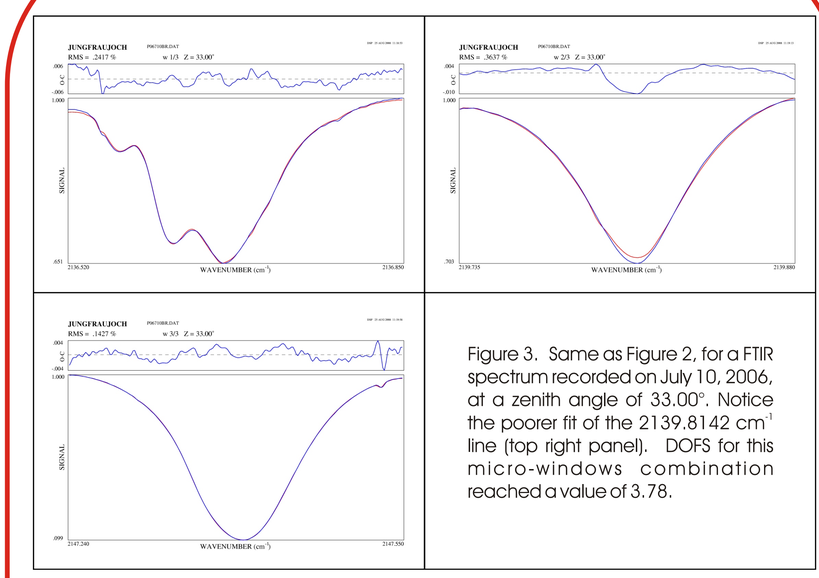

Figure 3. Same as Figure 2, for a FTIR spectrum recorded on July 10, 2006, at a zenith angle of 33.00°. Notice the poorer fit of the 2139.8142 cm^{-1} line (top right panel). DOFS for this micro-windows combination reached a value of 3.78.

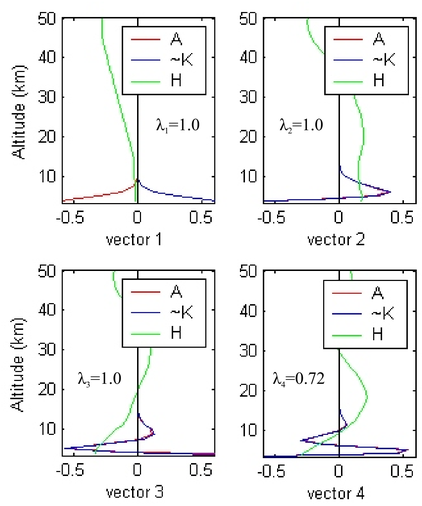

Figure 5. Typical eigenvectors (red and blue curves) for the micro-windows combination of Figure 3, providing a DOFS of 3.78. Corresponding eigenvalues equal 1.0, 1.0, 1.0 and 0.72 respectively, meaning than even for the fourth layer, 72 % of the information come from the retrieval.
At least 3 independant layers can be deduced: from 3.58 to 4.3 km, from 4.3 to 6.5 km and from 6.5 to 11 km. In the best cases, a fourth layer, from 11 to 18 km, can be retrieved.

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