Data & characterisation using FTIR partial columns from NDACC

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- Quality Assessment of FTIR data (example Izaña)
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Who are we?

- Ground-based FTIR group in Karlsruhe (Germany)
- Team: T. Blumenstock, F. Hase, M. Schneider, S. Barthlott
  & PhD students: S. Dohe, M. Gisi, R. Kohlhepp
- Retrieval code development: PROFFIT *(Hase et al., JQSRT, 2004)*
- Measurement sites:
  - Kiruna (Sweden) [since 1996]
  - Izaña (Tenerife) [since 1999]
  - Addis Ababa (Ethiopia) [since 2009]
  - Karlsruhe (Germany) [since 2009]
  - Coming soon: Mexico [starting this year]
NDACC InfraRed working group (IRWG)

- Collection of over twenty high resolution FTIR spectrometers
- Regularly recorded atmospheric absorption spectra
- Retrieval of several gaseous atmospheric components (e.g. $O_3$, $HNO_3$, HCl, HF, CO, ...)
- Common retrieval strategy within the IRWG for all sites
- Public data access via database (data format: hdf)
Common NDACC FTIR retrieval approach for $O_3$

- Spectroscopy: HITRAN 2008
- $p$, $T$ profiles: NCEP daily profiles
- Retrieval codes: SFIT2 or PROFFIT
- Microwindows: 1000-1005 cm$^{-1}$ + optional narrow MWs
- Climatology: WACCM (one for all seasons)
- Interfering species: $H_2O$ (+ $CO_2$, $C_2H_4$, O668, O686)
- Common layering
- Results reported in new IRWG-HDF data format, includes exhaustive characterisation (e.g. random + systematic errors, AVKs)

Optimised Retrieval strategy (requires PROFFIT9)

- Optional additional temperature fit
- Interspecies constraint (O666, O668, O686)
**Vertical information - Sensitivity**

- **Averaging kernel (AVK):** answer of the profile to a change in a specific height
- **4-5 DOFs (trace of AVK matrix)**
- **Layers that can be resolved:** e.g. ground-10 km, 10-20 km, 20-28 km, and >28 km
- **High sensitivity up to 50-60 km**
- Temperature error is leading
- Spectroscopic error is main systematic error source (i.e. pressure broadening coeff. and line intensity)
- Not shown: smoothing error (up to 25% in tropopause) → smoothing with AVK when comparing with other instruments

**Assumed uncertainties:**

<table>
<thead>
<tr>
<th></th>
<th>random</th>
<th>systematic</th>
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<tbody>
<tr>
<td>Baseline offset</td>
<td>0.1%</td>
<td>0.1%</td>
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<tr>
<td>Channeling</td>
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<td>0.2%</td>
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<tr>
<td>T profile ground-7 km</td>
<td>0.7 K</td>
<td>0.3 K</td>
</tr>
<tr>
<td>7-30 km</td>
<td>1.4 K</td>
<td>0.6 K</td>
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<tr>
<td>above 50 km</td>
<td>3.5 K</td>
<td>1.5 K</td>
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<tr>
<td>ILS</td>
<td>1%</td>
<td>1%</td>
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<tr>
<td>LOS</td>
<td>0.09%</td>
<td>0.01%</td>
</tr>
<tr>
<td>Solar lines</td>
<td>0.8%</td>
<td>0.2%</td>
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<tr>
<td>Line intensity</td>
<td>--</td>
<td>2%</td>
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<tr>
<td>Press. broadening coeff.</td>
<td>--</td>
<td>5%</td>
</tr>
</tbody>
</table>
Izaña observatory

- Izaña observatory on Canary Island of Tenerife
- Located at 2370 m.a.s.l. (close to Pico del Teide)
- Run by the Spanish Weather Service (AEMET)
- WMO/GAW station
- Regional Brewer Calibration Centre for Europe of WMO/GAW
- Ozone is measured with several observing systems:
  - Brewer, ECC sondes, FTIR, and DOAS are all part of NDACC
  → Especially for ozone perfect conditions for intercomparisons
Intercomparison of FTIR and Brewer total columns

- Comparison period: January 2005 - February 2007
- Coincidence within 30 minutes → 240 measurements
- FTIR data measured with Bruker 125 HR, common retrieval strategy

“Comparison of ground-based Brewer and FTIR total column O3 monitoring techniques”, M. Schneider et al., ACP, 2008.
Intercomparison of FTIR and Brewer total columns

- **Common strategy:** agreement good but large scattering
- **New strategy:** simultaneous fit of temperature with additional small MWs containing CO₂ lines → Much less scattering
- **Systematic difference of 5%:** mainly caused by differences in spectroscopic parameters
- **scatter of about 0.5%** is root sum square of precision of both instruments [Brewer: 0.3%] → FTIR precision better than 0.4% (<1.5 DU!!)
Comparison of FTIR and ECC sondes data

“Quality assessment of O3 profiles measured by a state-of-the-art ground-based FTIR observing system“, M. Schneider et al, ACP, 2008

- Comparison period between January 2005 and December 2006
- 53 coincidences (criterion: same day & sonde reached 30.5 km)
- New retrieval strategy used (incl. simultaneous temperature fit)
- General problem: comparing two datasets with different vertical resolution
  - degrade the high resolved dataset (sondes) to the FTIR dataset by smoothing with FTIR-Kernel
  - only compare rough structures that are resolvable by the FTIR (partial columns)
Comparison of FTIR and smoothed ECC profiles

Fig. 7. Difference between FTIR and smoothed ECC sonde profiles. Shown are mean and standard deviation of the difference for the 53 FTIR/ECC coincidences. The grey shaded area indicates the expected FTIR error (excluding the smoothing error); the light grey shaded area indicates the expected random error of (FTIR-ECC)/ECC.

- Sonde data above 30.5 km extended with FTIR a priori profile
- Due to smoothing with FTIR AVK, no smoothing error in difference
- Up to 27 km slight difference (not significant) (+2% up to -10%): due to error in pressure broadening coefficient
- Above 28 km significant systematic error up to 16%: several sources possible, e.g. underestimation of ECC sondes or systematic FTIR errors (line parameterisation)
- Scatter mean is 5% with maximum around 12 km: reason may be different airmasses
Comparison of partial column amounts

Original partial columns of ECC sondes are used (unsmoothed)

- General good agreement: correlation coefficients is at least 0.96 up to 20 km, above correlation coefficient of 0.92
- Scatter agrees well with FTIR random errors.
- Differences between FTIR and ECC and between Brewer and ECC are similar: possibly due to different airmasses (Brewer and FTIR have same observation geometry)

Fig. 8. Correlation between FTIR and ECC measurements. Black squares: individual measurements; red lines: linear regression line of least squares fits. (a) TR layer, (b) TP layer, (c) MS layer, (d) layer from surface – 30.5 km.
Outlook: time series of Ozone above Kiruna

- More than 15 years of measurement
- Different seasonal cycles resolvable
- No significant trend in layers up to 20 km
- Above 28 km clear positive tendency with a significant increase of 1%

→ Combination with other datasets from the IRWG enables assessment of temporal development of ozone in different layers and its latitudinal dependency (see WMO/UNEP Scientific Assessment 2010 & Vigouroux et al., 2008)
Summary & Key-Questions:

- **Is the data set suitable for assessing long-term changes?**
  - Long-term records available at several sites (e.g. Jungfraujoch, Kitt Peak, and Kiruna).
  - Total columns very reliable; vertical trend determination requires ILS monitoring.

- **How internally consistent is it & evidence for consistency?**
  - Same retrieval strategy for all sites.
  - Complete reprocessing possible for the whole time series.
  - Regular cell measurements to check instrumental line shape.
  - Cross validation with other long-term datasets (e.g. Brewer).

- **How can it be used to evaluate other data sets?**
  - HDF reporting provides all information required for sensible validation.
  - Limited vertical resolution / sensitivity has to be taken into account.
  - Various validations have been performed (satellite, balloon, sondes, Brewer, ...).

- **Can it be used in conjunction with other data sets to provide a long record?**
  - Can be fused with other observations reporting total columns.

- **What has been learnt that is relevant in assessing other data sets?**
  - Solar absorption measurement is self-calibrating, unrevealing drifts in other data sets.
  - Despite lower resolution there is enough information to resolve different trends in vertical layers.
Thank you for your attention!

References:


APPENDIX

Seasonal cycle of Ozone above Kiruna

- Gd-10 km: max. spring, min. fall due to STE
- 10-20 km: Brewer-Dobson circulation dominates (transport of Ozone from Tropics to winter-pole)
- 20-28 km: no significant seasonal cycle
- Above 28 km: max. summer, min. winter, photolytic production