Water vapor line parameters: Some feedback from atmospheric users

S. Fally

http://www.ulb.ac.be/cpm

A. C. Vandaele

http://aeronomie.be

S. Trabelsi, E. Mahieu, P. Demoulin

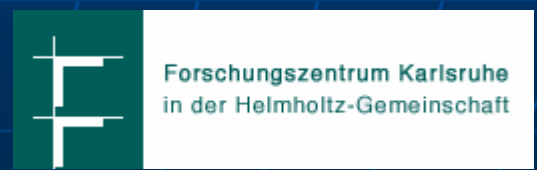
http://girpas.astro.ulg.ac.be

C. Frankenberg

http://www.sron.nl

H. Vogelmann, T. Trickl

http://imk-ifu.fzk.de



Outline

- gb-FTIR @ Junfraujoch, Swiss Alps
  → Discrepancies between ≠ H_2O μwindows
- Near-IR DIAL @ Zugspitze, Germany
  → HITRAN compared to Ponsardin & Browell
- Near-IR SCIAMACHY / ENVISAT
  → Effect of H_2O parameters on CH_4 retrievals
- IR SOIR / Venus Express
  → Spectroscopic needs for CO_2 broadened H_2O


gb-FTIR @ Jungfraujoch, Swiss Alps (46.5°N, 8°E, 3580 m a.s.l.)

gb-FTIR @ Jungfraujoch …

- Numerous wv lines in the 700-4300 cm^{-1} range
- Best retrieval strategy to retrieve H_2O vertical information?

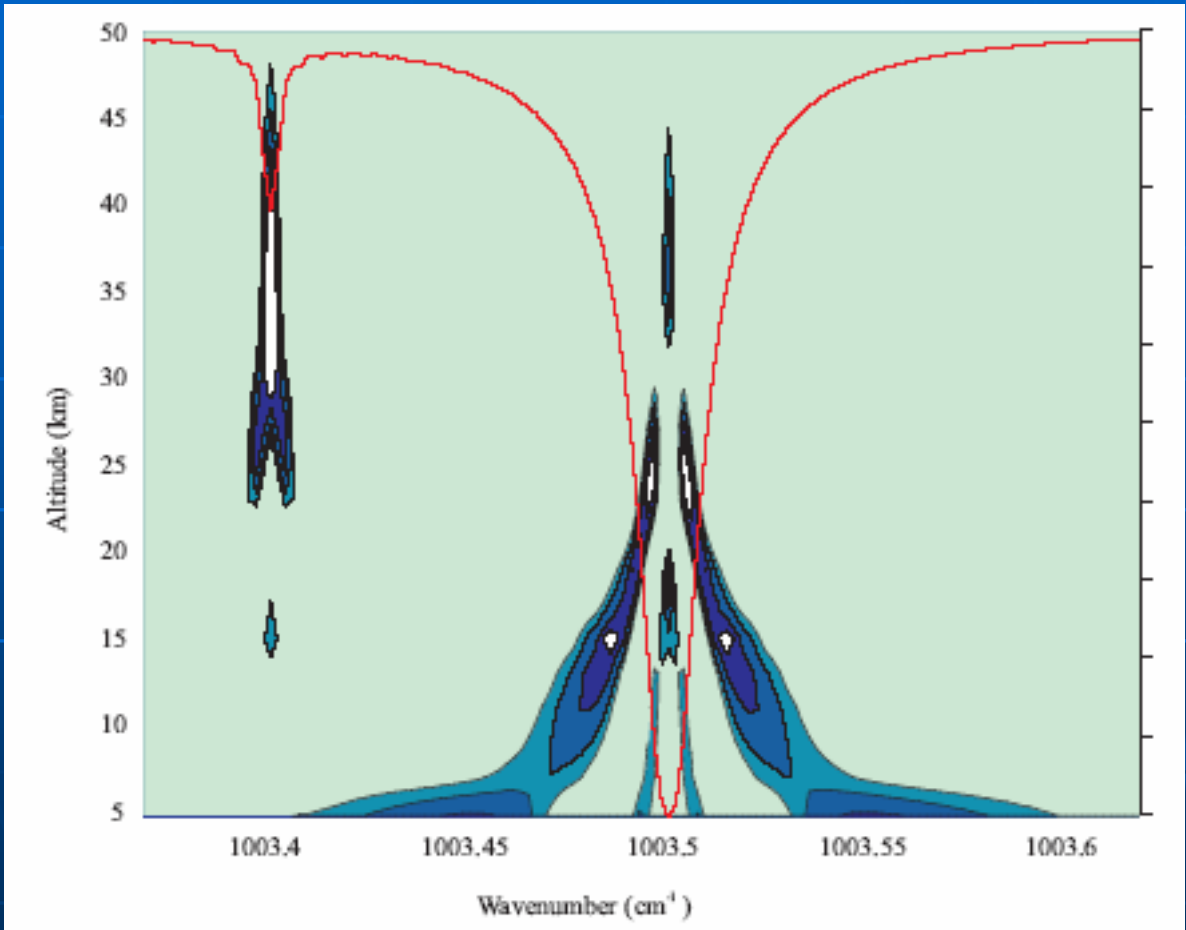
→ Find suitable lines in ≠ spectral domains (T° insensitive, free of interferences, ...)

→ Lot of μwindows investigated

Spectral domain (cm^{-1})	Nb H_2O lines	Selected μw (mainly $H_2{}^{16}O$)
700 - 1300	2130	16
1900 - 2200	1236	8
2500 - 3100	2348	10
3100 - 3500	2727	17
4000 - 4300	1837	12

gb-FTIR @ Jungfraujoch …

- ↗ vertical sensitivity ?



Matrix of the contribution functions for O_3 profile inversion (from B. Barret, PhD thesis, 2003)

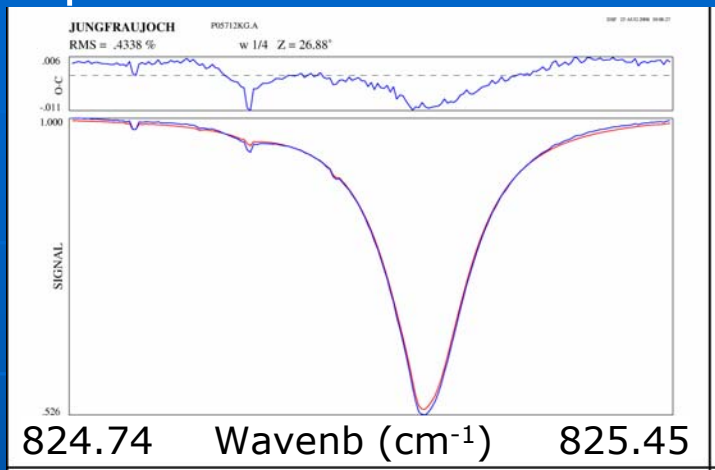
✓ Info close to the ground in the wings of strong line

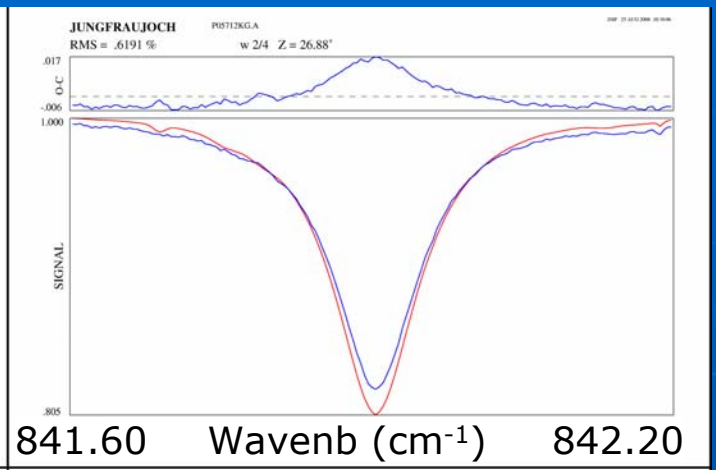
✓ Info at high altitude at the center of weak & strong lines (but strong is saturated)

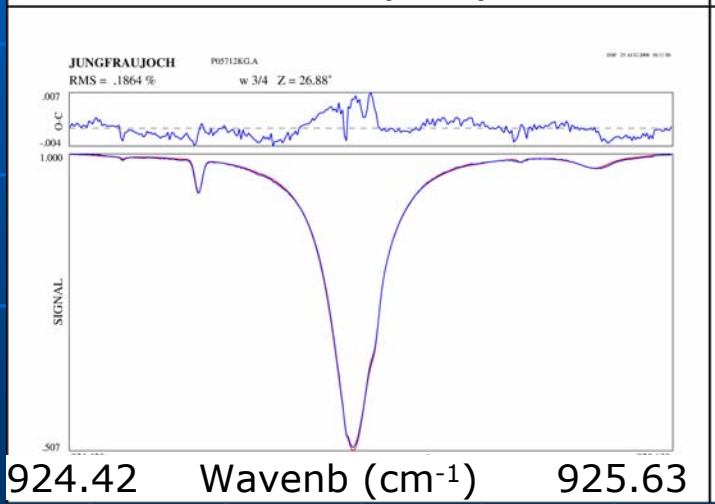
→ Combination of μwindows including strong & weak lines

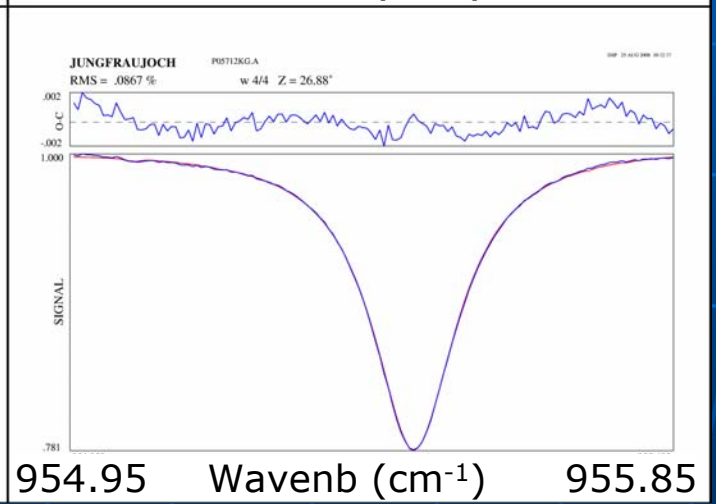
gb-FTIR @ Jungfraujoch …

- Multi-μwindows fits:









→ Poor quality (poorer than with single μwindow)

→ HITRAN line parameters must be modified

→ Tuned line parameters have been adopted

→ Detailed results: See poster 2-3 by P. Demoulin *et al.*

→ Inconsistencies between different regions

Outline

- gb-FTIR @ Jungfraujoch, Swiss Alps

  → Discrepancies between ≠ H_2O μwindows

- Near-IR DIAL @ Zugspitze, Germany

  → HITRAN compared to Ponsardin & Browell

- Near-IR SCIAMACHY / ENVISAT

  → Effect of H_2O parameters on CH_4 retrievals

- IR SOIR / Venus Express

  → Spectroscopic needs for CO_2 broadened H_2O

Near-IR DIAL @ Zugspitze, Germany (47.42 °N, 10.98 °E)

Near-IR DIAL @ Zugspitze …

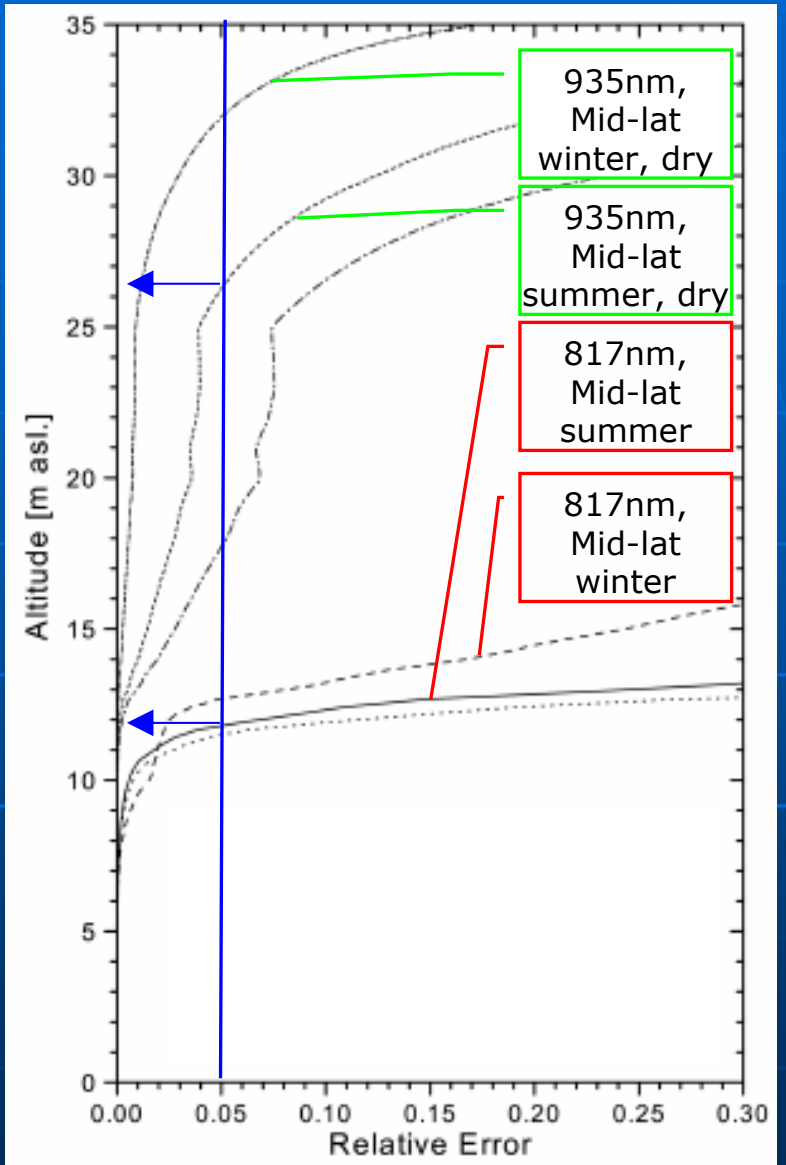
- Optimum line choice ?

✓ Simulations of the LIDAR performance in 3 spectral regions: 725, 817, 935 nm (13800, 12200, 10700 cm^{-1}) using mid-lat summer & winter H_2O profiles (LOWTRAN5 model)

✓ Error analysis:
Minimize error at high altitude

Abs. cross-section
= strong enough to get significant light loss
= weak enough to avoid too much attenuation at low alt.
Error next to the tropopause < 5%

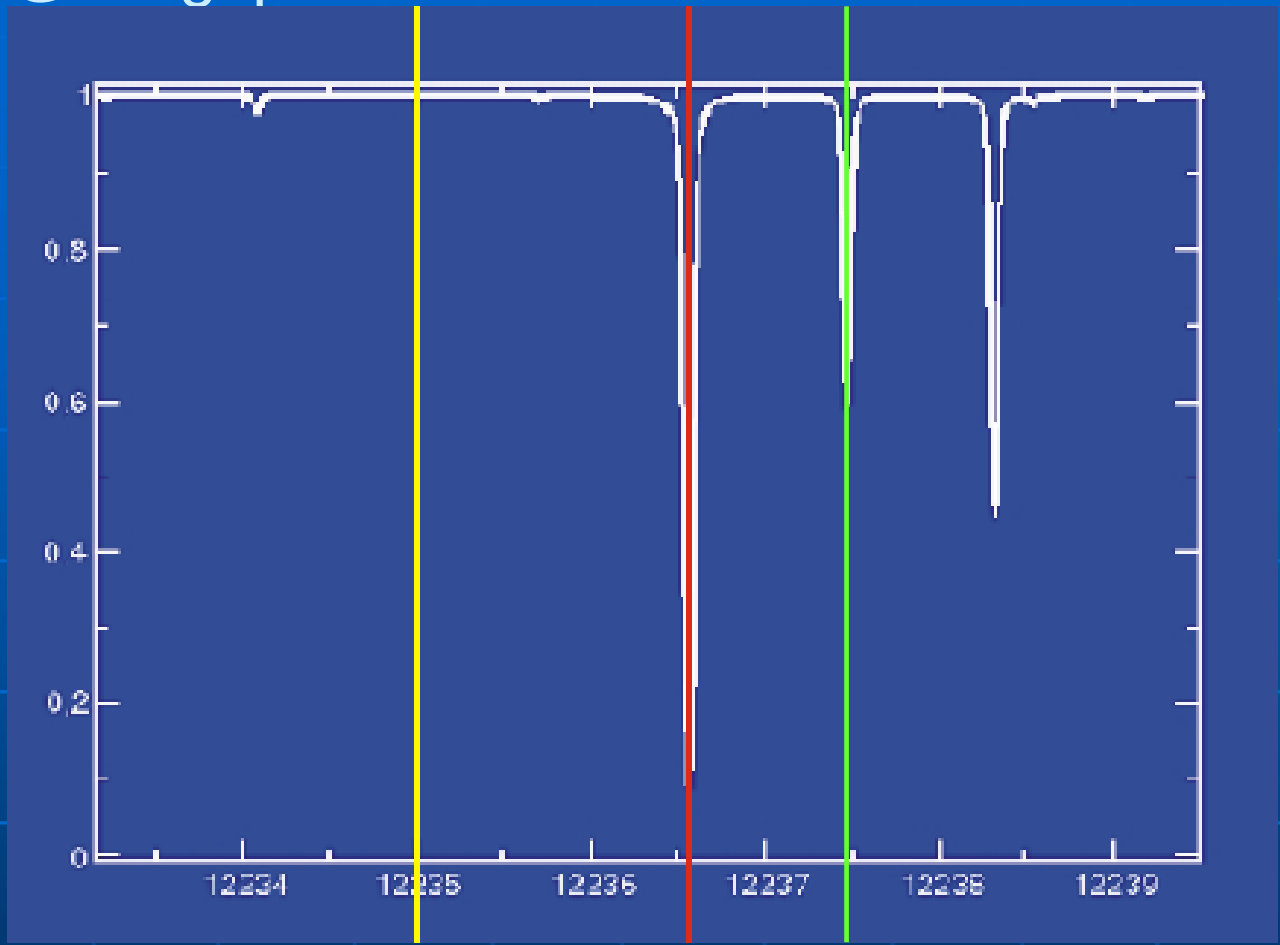
→ Both criteria# met by the 817 nm range



Altitudinal profile of the relative meas. error (noise neglected) (from Vogelmann & Trickl, Appl. Optics47, 2116-2132, 2008)

Near-IR DIAL @ Zugspitze …

→ Chosen lines



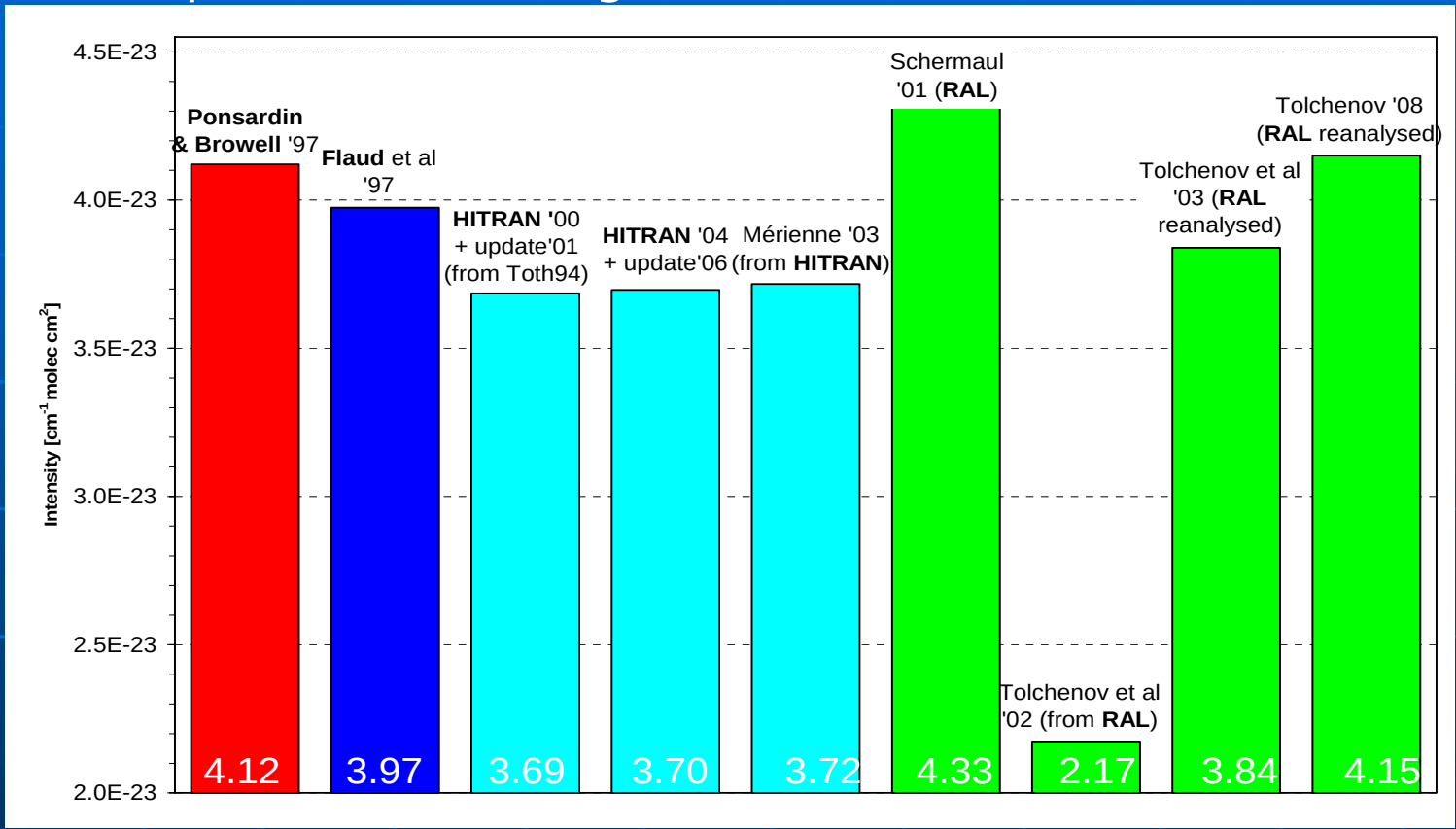
λ_{on} = 817.223nm = 12236.6 cm^{-1} winter (dry)
λ_{on} = 817.162nm = 12237.5 cm^{-1} summer
λ_{on} = 816.757nm = 12243.5 cm^{-1} summer (not shown)
λ_{off} = 817.351nm = 12235.0 cm^{-1}
(from http://gap-vm-pub1.gap.fzk.de/305.php)

- Exp. details in Vogelmann & Trickl, Appl. Opt., 47, 2116-2132, 2008

Near-IR DIAL @ Zugspitze …

- Dataset choice for line parameters ?

✓ Comparison of strengths for 1 line @ 12236.56 cm^{-1}



HITRAN= Toth'94

Tolchenov'08 ≈ Ponsardin & Browell'97

ICLAS (Mazzotti'06): only weak lines (≤ 5e-26)

TDLS (Ibrahim'08): Not reported

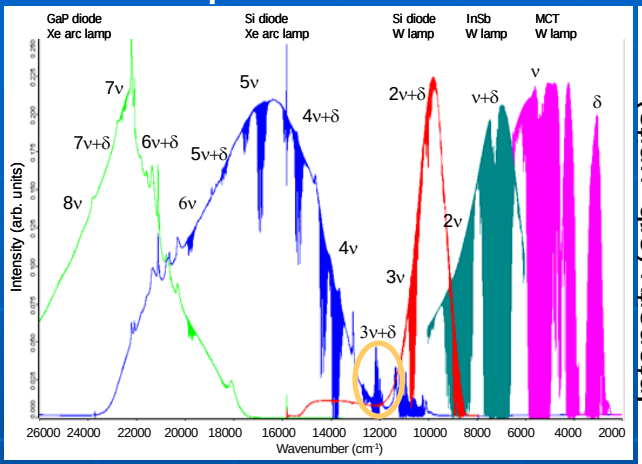
✓ Toth & Mérienne / Ponsardin: Avg 7 lines around 12200cm^{-1} = 0.897 & 0.899 (±0.015 & 0.011)
→ ~ 10% systematic diff. (although high internal precision)
→ linked to meas. technique & lineshape ?

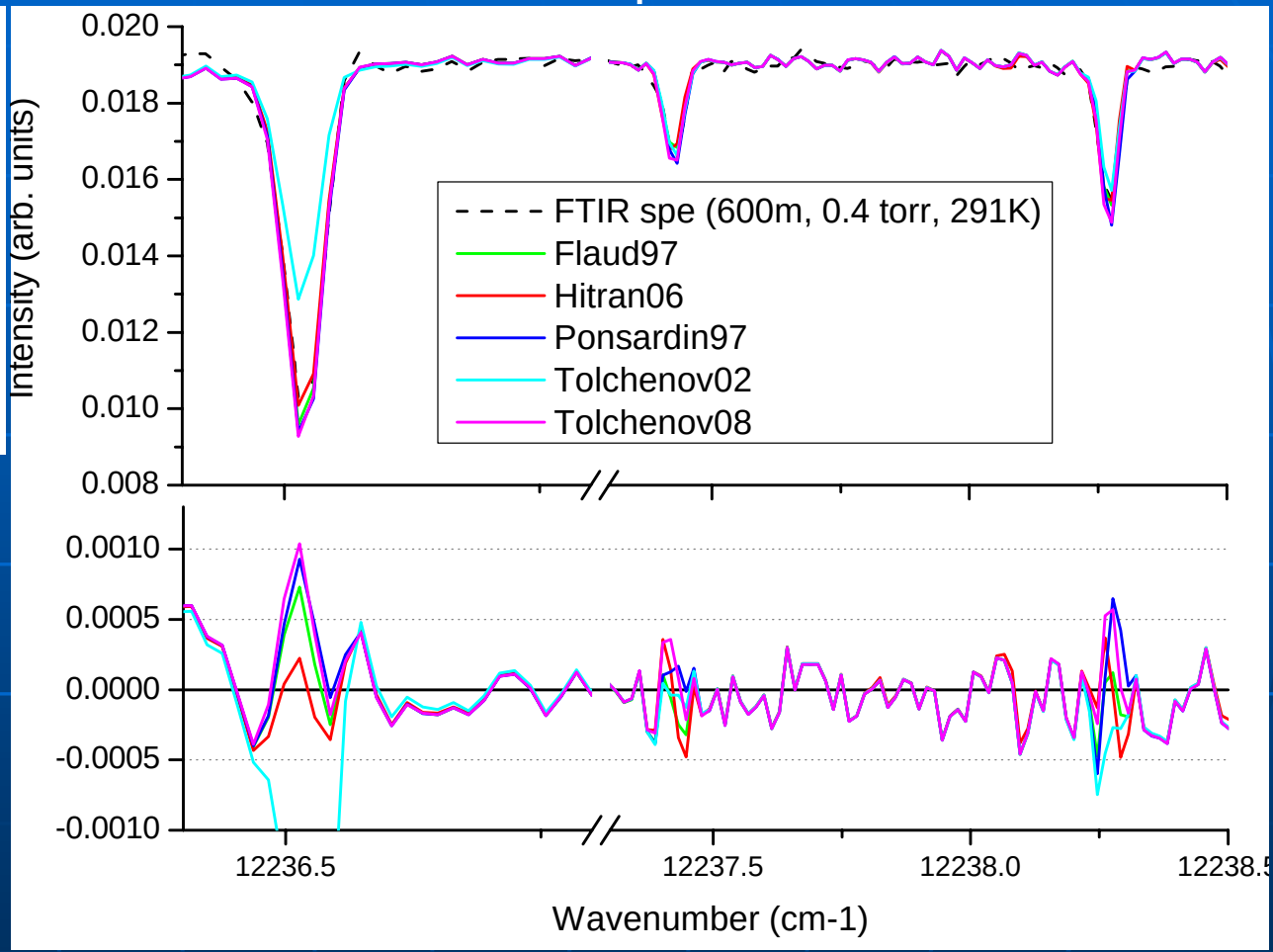
→ Inconsistencies between different databases

Near-IR DIAL @ Zugspitze …

- Dataset choice for line parameters?

✓ Comparison between lab. FTS & simulated spectra





→ Stronger line @ 12236.5 simulates worse than the 2 weaker ones

→ HITRAN = best results

→ Others (exc. Tolch02)= similar results (with peak err~10%)

→ Inconsistencies both within each database (strong><weak) between different databases

Outline

- gb-FTIR @ Jungfraujoch, Swiss Alps

  → Discrepancies between ≠ H_2O μwindows

- Near-IR DIAL @ Zugspitze, Germany

  → HITRAN compared to Ponsardin & Browell

- Near-IR SCIAMACHY / ENVISAT

  → Effect of H_2O parameters on CH_4 retrievals

- IR SOIR / Venus Express

  → Spectroscopic needs for CO_2 broadened H_2O

SCIAMACHY / ENVISAT

SCIAMACHY / ENVISAT…

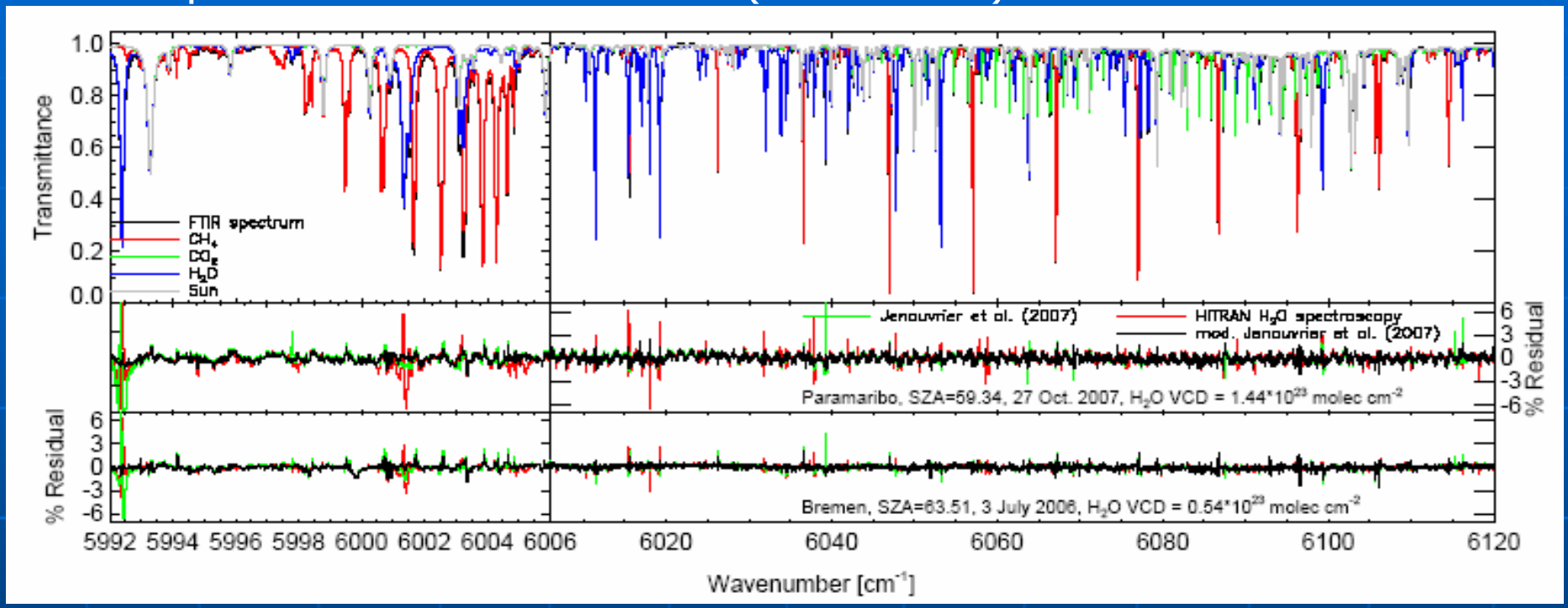
- SCIAMACHY / ENVISAT :
  - ✓ 8 channel grating spectrometer
  - ✓ UV → VIS → IR (240-2380 nm)
  - ✓ http://envisat.esa.int/instruments/sciamachy/

- CH_4 retrievals :
  - ✓ Nadir spectra
  - ✓ 1630-1670 nm (5990-6130 cm^{-1}) → Interfering spe= CO_2 & H_2O
  - ✓ See Frankenberg *et al.*,ACP, 2005; JGR, 2006; ACPD, 2008

- Context :
  - ✓ Unresolved seasonal bias in the SH
    → Impact of wv spectroscopy on CH_4 retrievals ?
  - ✓ See Frankenberg *et al.*, GRL35, L15811, 2008 (Aug. 12)

SCIAMACHY / ENVISAT…

- Comparison of HITRAN & BR (Bxl-Reims) databases



Retrievals from 2 g-b high resolution FTIR solar absorption spectra (Paramaribo, Suriname & Bremen, Germany) (from Frankenberg *et al.*, GRL35, 2008)

→ Systematic residuals with HITRAN mostly vanish with modified BR
= up to 6% @ Paramaribo; < @ Bremen due to < wv

→ Very strong residuals for few strong lines with BR, esp. 5975-5998 cm^{-1} (γ_{air}<< or unprovided) + same for 4200-4350cm^{-1}

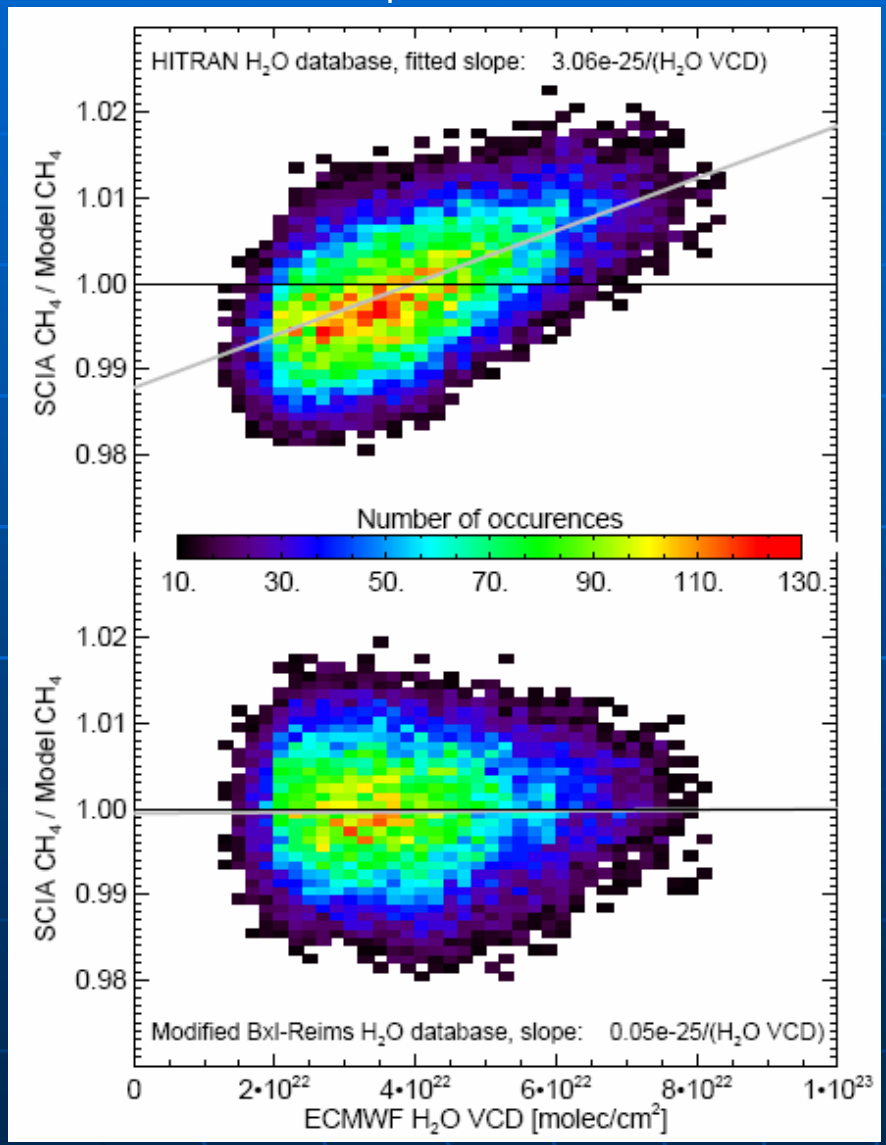
→ Proposed modifications to BR list

→ Overall, substantial reduction of systematic errors with BR as compared to HITRAN

SCIAMACHY / ENVISAT…

- Impact of wv spectroscopy on SCIAMACHY CH_4 retrievals

✓ Retrieved CH_4 vs total wv column over Sahara:



Exclude latitudinal bias
Exclude true correlation CH_4 emissions/specific humidity

→ + correlation if HITRAN

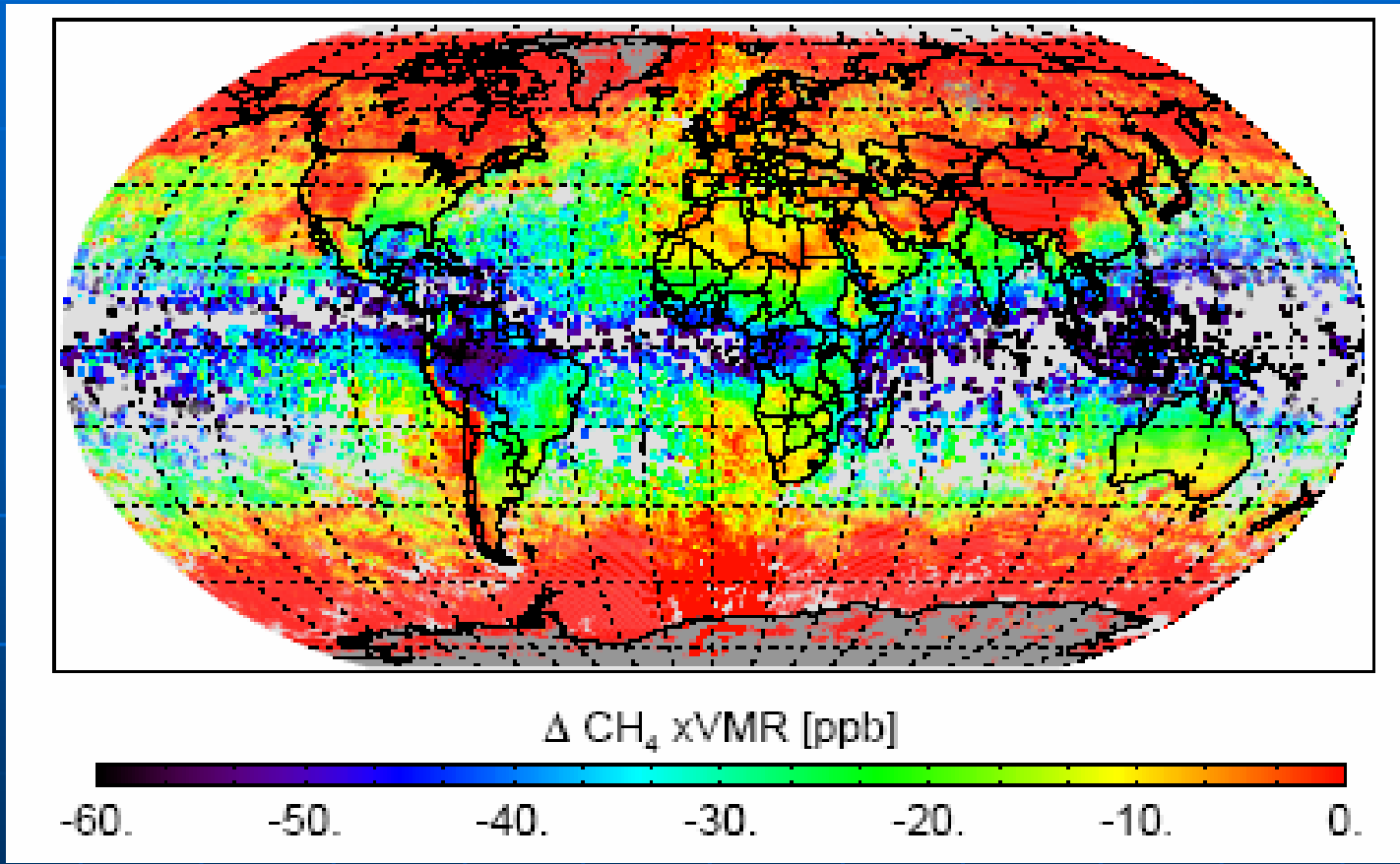
→ No correlation if modified BR list

→ Retrieval bias caused by erroneous wv HITRAN database

SCIAMACHY / ENVISAT…

- Impact of wv spectroscopy on SCIAMACHY CH_4 retrievals

✓ BR – HITRAN for column yearly averaged mixing ratio:



(from Frankenberg *et al.*, GRL35, 2008)

→ up to -60ppb in the tropics
= 3% overestimation with HITRAN over tropics

→ Significant -& surprisingly big !- impact of wv on CH_4 retrievals in the 5990-6150 cm^{-1} range

Outline

- gb-FTIR @ Jungfraujoch, Swiss Alps

  → Discrepancies between ≠ H_2O μwindows

- Near-IR DIAL @ Zugspitze, Germany

  → HITRAN compared to Ponsardin & Browell

- Near-IR SCIAMACHY / ENVISAT

  → Effect of H_2O parameters on CH_4 retrievals

- IR SOIR / Venus Express

  → Spectroscopic needs for H_2O

SOIR / Venus Express

SOIR / Venus Express …

- **SPICAV** = **Sp**ectroscopy for **I**nvestigation of **C**haracteristics of the **A**tmosphere of **V**enus
  = 3 UV-IR spectrometers ground → H corona (> 40000km alt)
  = SPICAV-UV (SUV), SPICAV-IR (SIR), SOIR (Solar Occultat° at InfraRed)

- Key questions:
  ✓ Why such a ≠ evolution compared to Earth ?
  ✓ High D/H (150 x terresrial) → dramatic H_2O escape
  → Which scenario? Dry from the beginning OR H_2O lost?

  → New measurements are necessary
  → SOIR: simult. meas. H_2O & HDO → H_2O, HDO, H/D vertical profiles retrievals

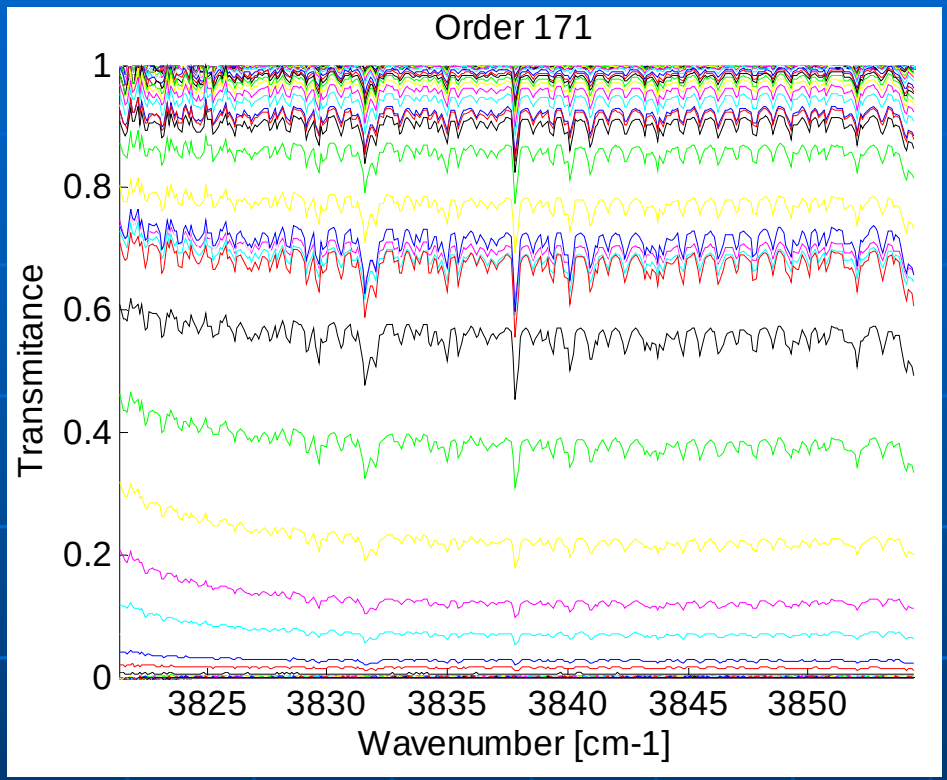
- Best candidates:

✓ H_2O	3830 cm^{-1}	ν1 & ν3 fund. bands	70-110 km
✓ HDO	2715 cm^{-1}	ν1 fund. band	70- 95 km

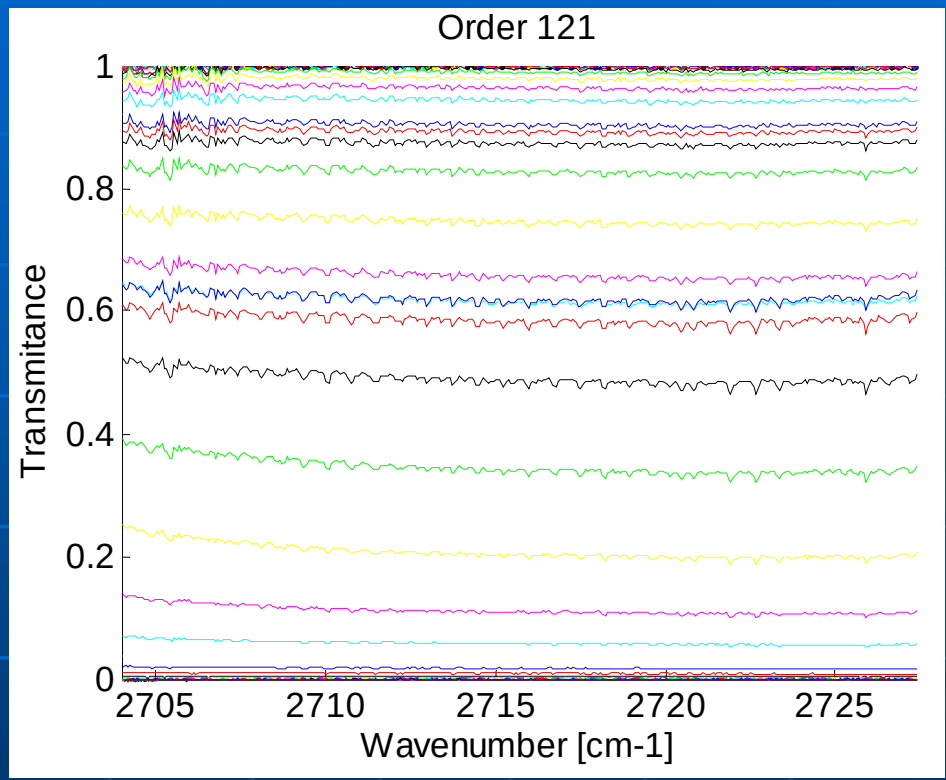
- More info:
  ✓ Friday talk by A. C. Vandaele
  ✓ H_2O, HDO, CO_2: Fedorova *et al.*, JGR, in press, 2008
  ✓ CO, CO_2, HCl, HF: Vandaele *et al.*, JGR, in press, 2008
  ✓ Venus Express: http://sci.esa.int & http://www.venus.wisc.edu

SOIR / Venus Express …

H_2O

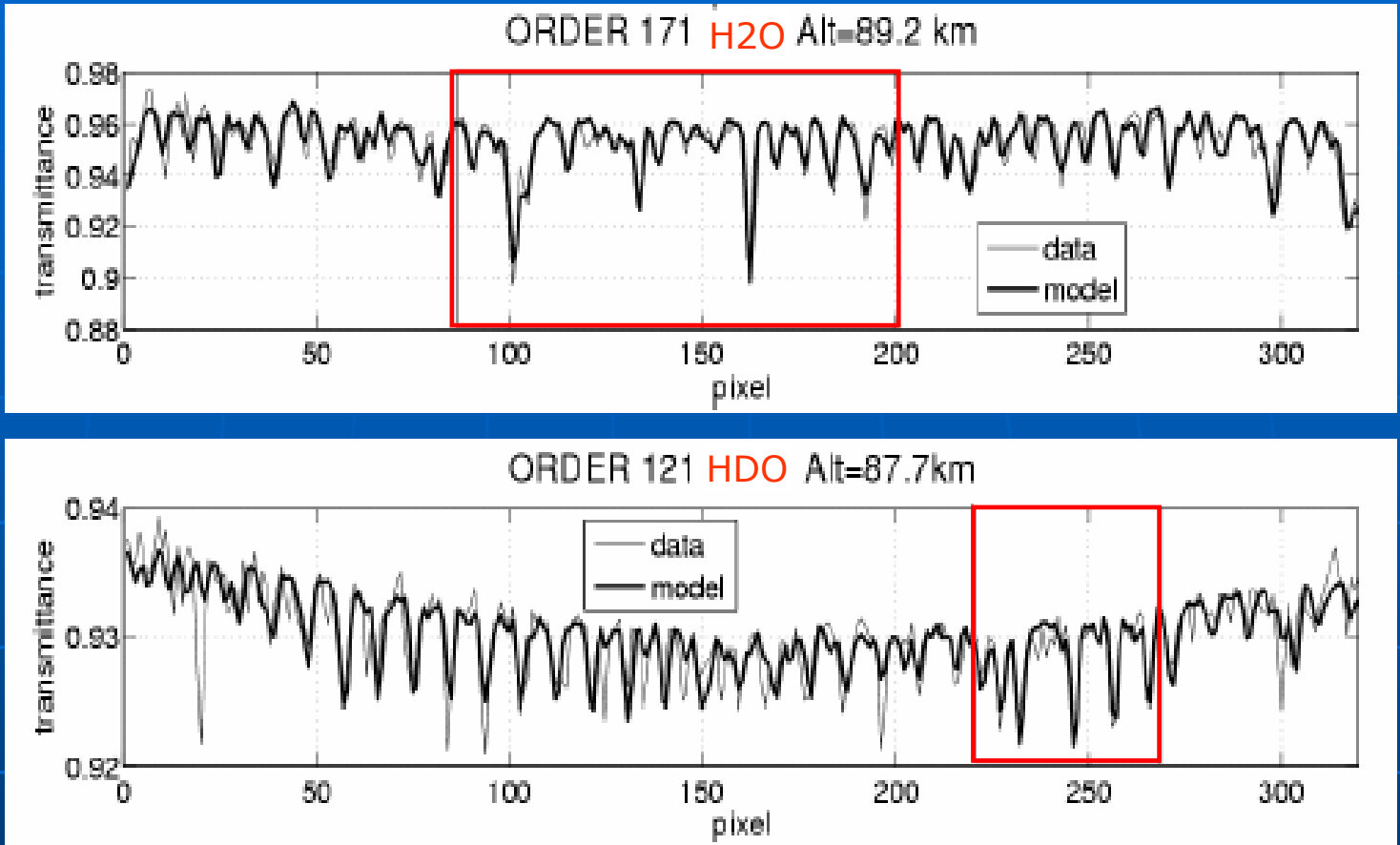


HDO



Evolution of 1 occultation at sunset Aug. 20th 2007:
Transmittance spectra in specific ranges of H_2O (left) & HDO (right) absorptions (from Vandaele *et al.*, 2008)

SOIR / Venus Express …



Examples of best fit on July 27th 2007 (from Fedorova *et al.*, 2008)
□ = chosen region because lines=higher intensity, lower sensitivity to T°, poor CO_2 contamination

→ Broader lines in the model: # uncertainties in the T° profile
instrument function width & resolut°
lineshape

SOIR / Venus Express …

- Literature data for γ_{CO2} ?

✓ Howard *et al.*, J.Opt.Soc.Am, '56 → $\gamma_{CO2}/\gamma_{air}$= 1.3

✓ Gamache *et al.*, JMS, '95 1.0-2.5μm → $\gamma_{CO2}/\gamma_{air}$= 1.3 → 2.0

✓ Brown *et al.*, JMS, '07 5.0-7.7μm → $\gamma_{CO2}/\gamma_{air}$= 1.67(.95 →3.07)

→ NO experimental / calculated values in our region

→ Chosen value: γ_{air}(HITRAN) x 1.7

→ BUT accurate γ_{CO2} needed to reduce uncertainties

→ γ_{CO2} for wv 2.3-4.2 μm (2250-4360 cm^{-1}) required

''Spectroscopic'' conclusions

- H_2O spectroscopic problems Improvements Needs

✓ Discrepancies between μwindows in HITRAN for 700-4300 cm^{-1}
(FTS spectra @ Jungfraujoch)
→ Tuned HITRAN line parameters proposed
→ More consistent parameters

✓ Discrepancies between literature data @ ~12300 cm^{-1}
(DIAL measurements @ Zugspitze)
→ More consistent parameters

✓ Inaccuracies in wv parameters for 5990-6130 cm^{-1}
(CH_4 retrievals with SCIAMACHY)
→ BR list better than HITRAN + update for spurious lines proposed

✓ No γ_{CO2} in 2250-4360 cm^{-1}
(SOIR/SPICAV/VENUS Express)
→ γ_{CO2}

General conclusions

→ Importance of :

- inter-comparisons, cross-validations
- feedback from users
- close collaborations between experimentalists & atmospherists
- new dedicated measurements

→ Importance of high quality
water spectroscopy & lab-work,
both for wv retrieval itself & for other species

Acknowledgments

- Colleagues
  - ✓ A. C. Vandaele & SPICAV/SOIR team,
  - ✓ S. Trabelsi, E. Mahieu, P. Demoulin,
  - ✓ C. Frankenberg,
  - ✓ H. Vogelmann, T. Trickl

- Funding
  - ✓ Belgian Federal Science Policy Office (SSD program/AGACC project, ESA-PRODEX program/C90268, C90113, C17645 contracts)
  - ✓ European Space Agency ESA (ESA-PRODEX program)
  - ✓ National Fund for Scientific Research, Belgium (FRFC program)
  - ✓ Communauté Française de Belgique (Actions de Recherche Concertées)
  - ✓ GAW-CH Programme, MeteoSwiss, Zurich

- Thank YOU for …  your attention !