Spectroscopic challenges for the OCO-2 mission

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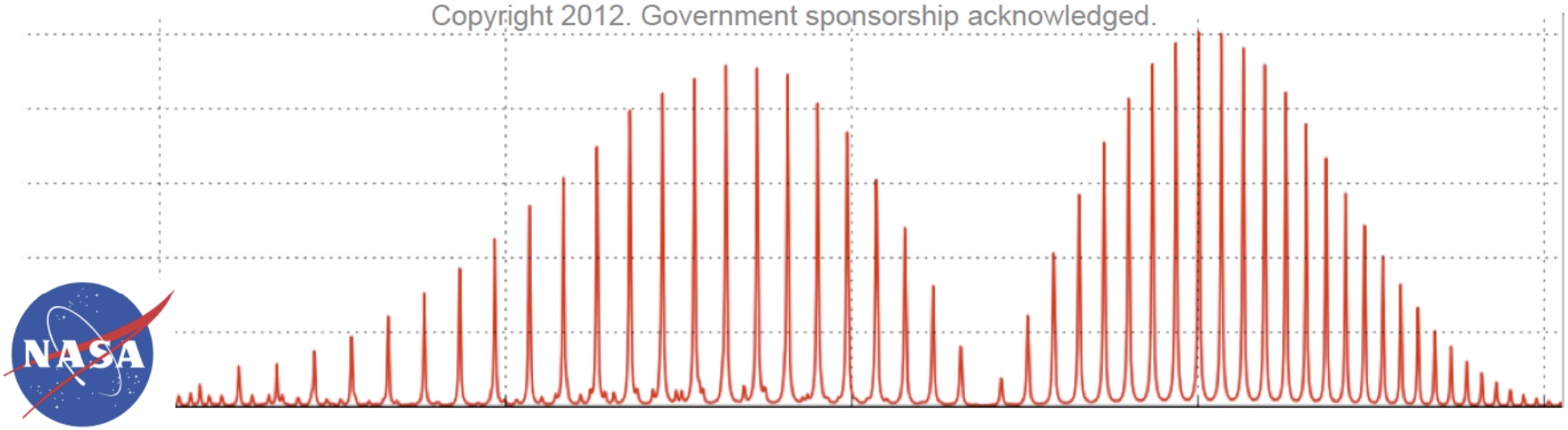
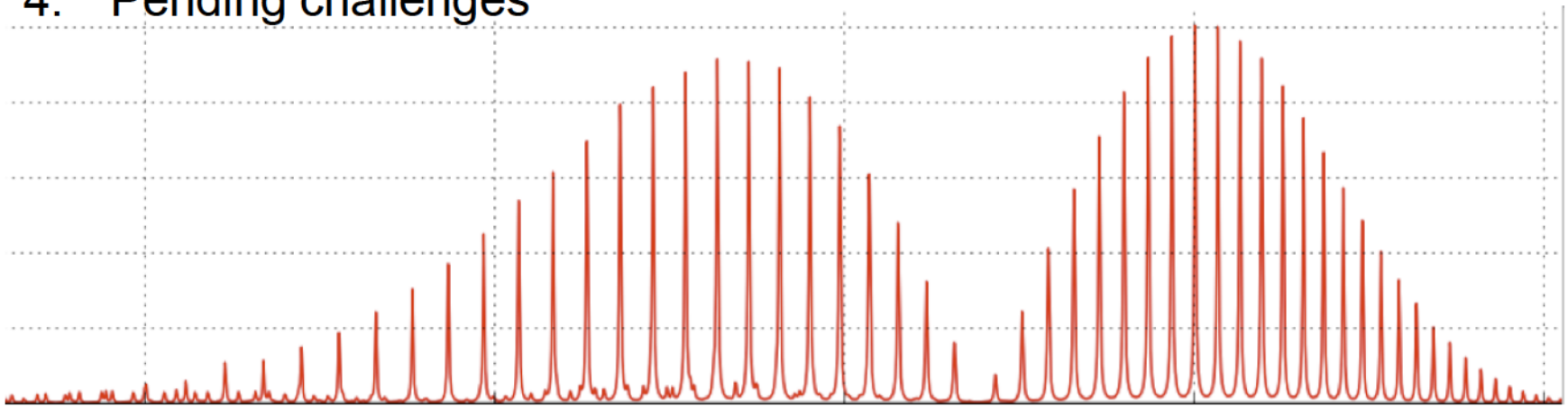


Overview

1. Motivation
2. Spectroscopic input to the forward model
   - 1.61 and 2.06 micron CO_2 bands
   - 0.76 micron O_2 A band
3. Validation and testing method
   - Lab Spectra
   - Upward-looking FTS spectrometers
   - GOSAT orbital measurements
4. Pending challenges



The OCO-2 Mission

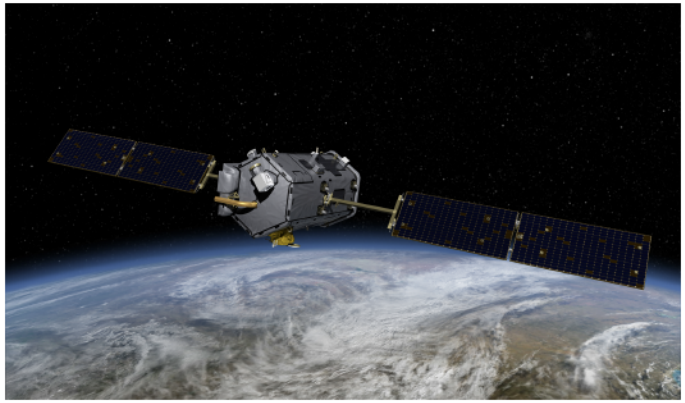
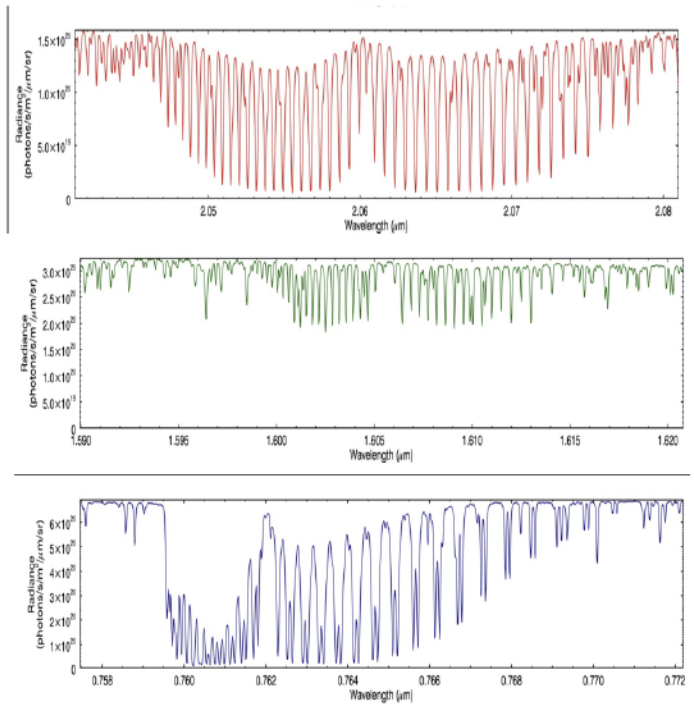


Image: NASA / Orbital

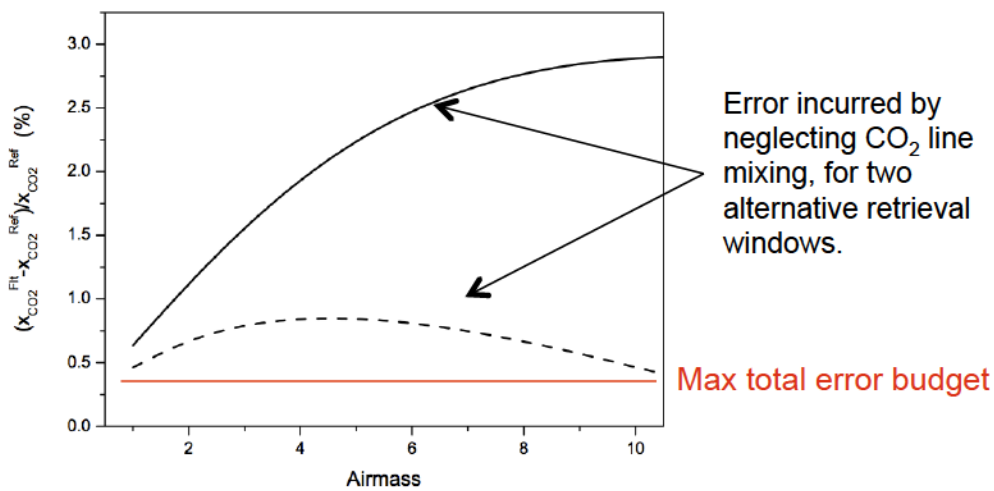
- Launch expected in late 2014
- Sounding spectrometer monitors three spectral regions
  - CO_2 in the 4850 cm^{-1} (2.06 micron) band
  - CO_2 in the 6220 cm^{-1} (1.6 micron) band
  - O_2 in the 13100 cm^{-1} (0.76 micron) band
- Will estimate dry air mole fraction (X_{CO2})
  - Provides unprecedented coverage to estimate regional-scale CO_2 sources and sinks (Crisp et al., 2012)
- High precision requirements
  - Goal ~ 0.3% (1 ppm out of 400)

This talk: Our process for evaluating spectroscopic models for the three OCO-2 bands

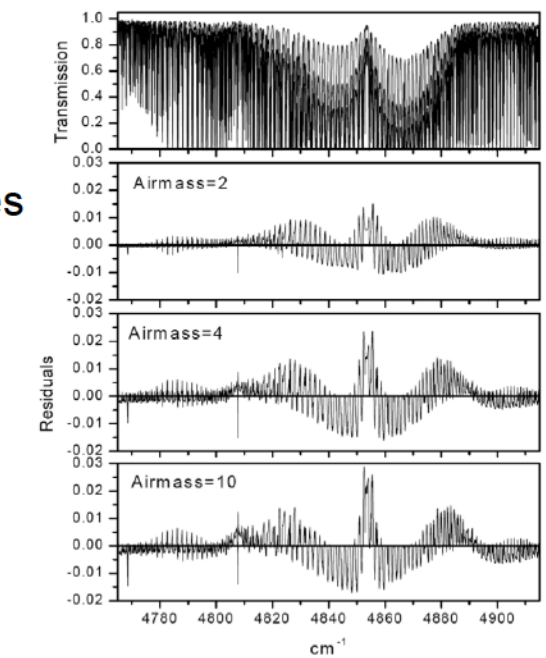


Why accurate spectroscopy matters

- 0.3% OCO-2 accuracy requirement requires 0.1% reference spectroscopic accuracy (Miller et al., 2005)
  - 0.3 % CO_2 variation rarely produces radiance variations > 0.1 % at OCO-2 resolution
- This challenges measurement accuracy AND our understanding of the physics
- Many subtle physical effects come into play at this level (Miller et al., 2007)
  - Line Mixing (O_2, CO_2)
  - Speed Dependence (CO_2)
  - Dicke Narrowing (O_2)
- Getting it wrong can introduce airmass/regional biases



From Hartmann, J.-M., Tran, H., and Toon, G. C.: Influence of line mixing on the retrievals of atmospheric CO2 from spectra in the 1.6 and 2.1 µm regions, Atmos. Chem. Phys., 9, 7303-7312.



Residuals due to neglecting line mixing

CO_2

Speed dependent profiles adjust pressure broadening to account for molecules having various speeds at collision

Absorption cross section

Integration over angular velocities

Doppler half width

$$\kappa(\nu) = \sum_{i=0}^{16} \frac{v_i e^{-v_i^2}}{\pi^{3/2}\alpha_D} \tan^{-1}\left\{\frac{\nu - \nu_0 + v_i \alpha_D}{\alpha_L\left[1 + S\left(v_i^2 - 1.5\right)\right] + H}\right\}$$

$$v_i = -4 + i/2$$

Lorenz half width

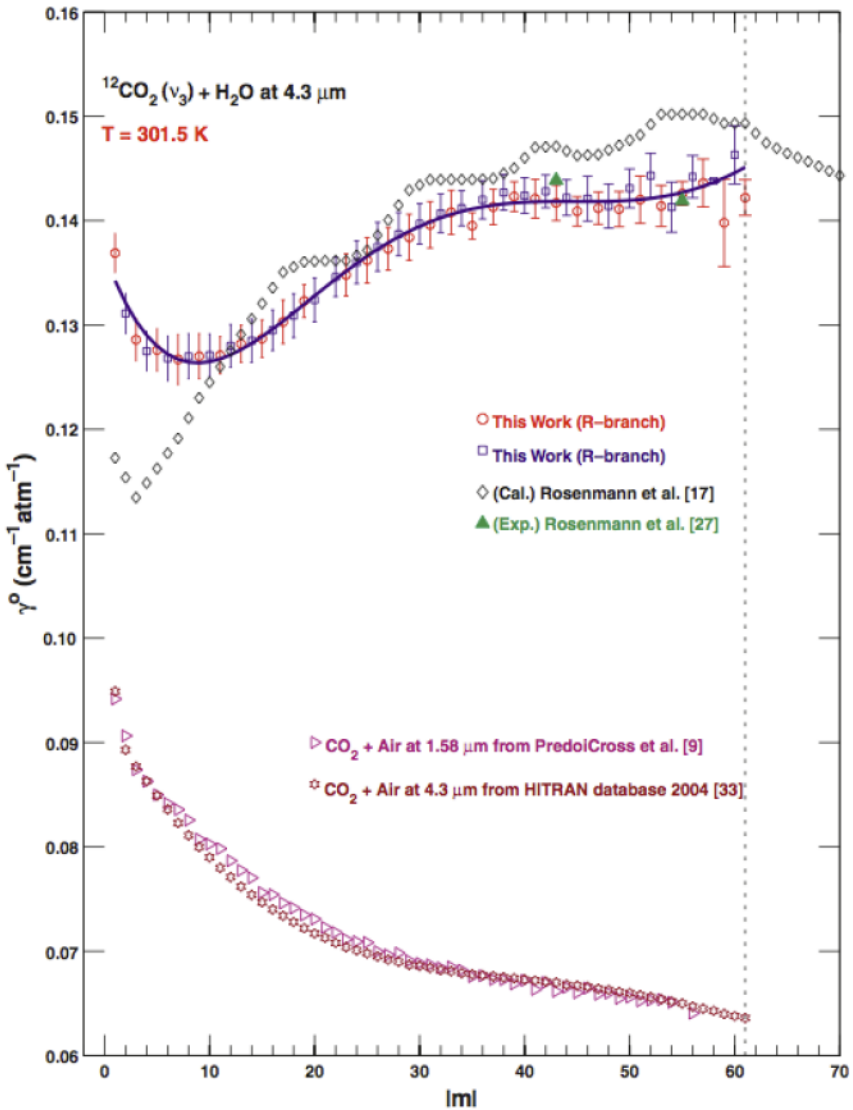
We set Dicke narrowing to zero

Spectral Region		Benchmark	Ongoing
4850cm^{-1} CO_2	**Line shape**	Voigt profile [Toth 2008]	**Speed Dependent Voigt profile [Benner/Devi] Minor isotopes via [Toth 2008]**
	Line mixing	ECS model [Lamouroux 2010]	**Nearest-neighbor line mixing (tridiagonal) from multi-spectrum least squares fit [Benner/Devi]**
6220cm^{-1} CO_2	**Line shape**	Voigt profile [Toth 2008]	**Speed Dependent Voigt profile [Devi et al. 2007] Minor isotopes via [Toth 2008]**
	Line mixing	ECS model [Lamouroux 2010]	**Nearest-neighbor line mixing (tridiagonal) from multi-spectrum least squares fit [Devi et al. 2007]**

Future: Updated multi-spectrum fits using new CRDS measurements

6220 cm^{-1} band: Long et al. (NIST) 4850 cm^{-1} band: Bui et al. (Caltech)

H_2O broadening of CO_2



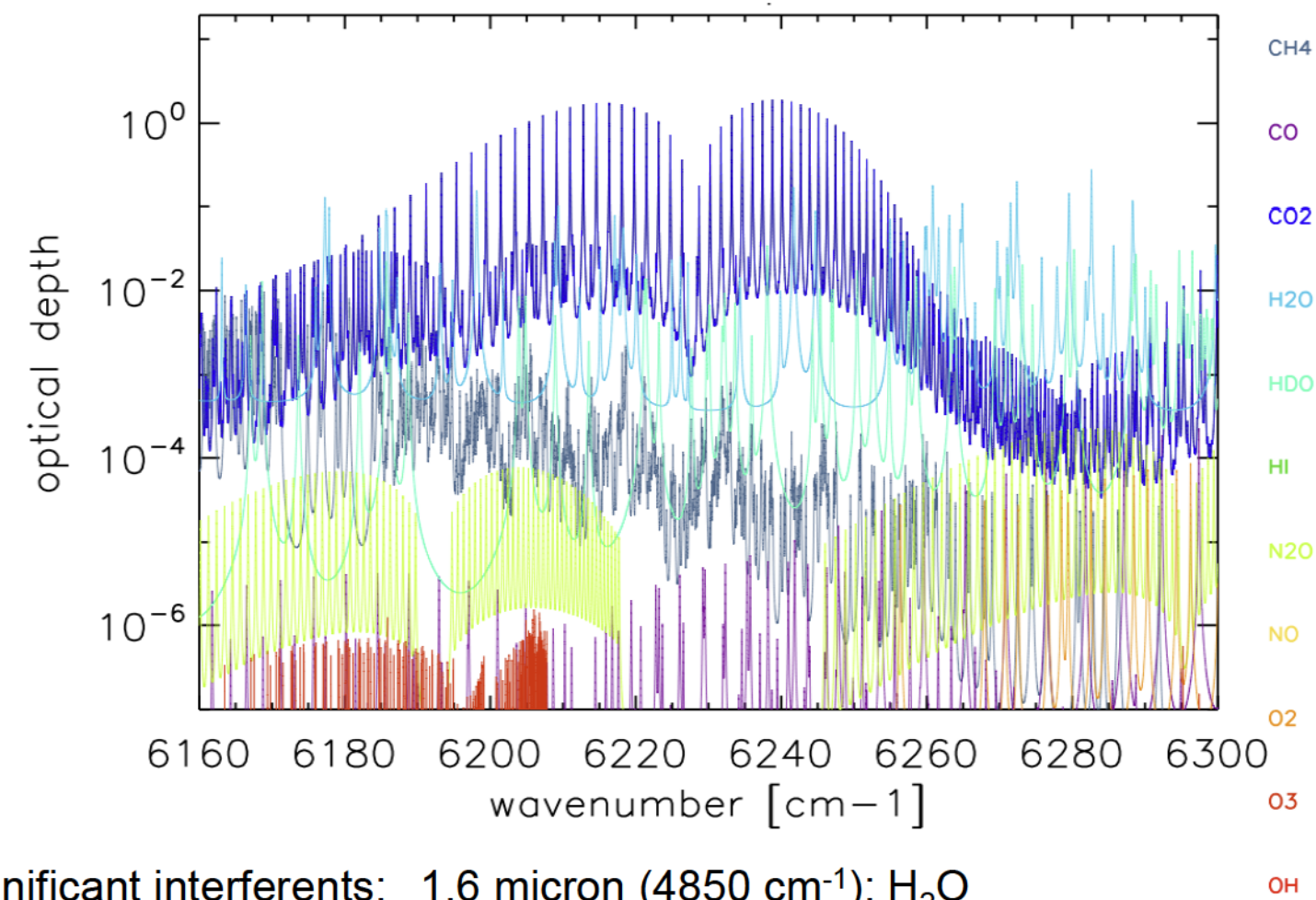
H_2O broadening of CO_2 included in the OCO-2 model

Left: Fig 6 from Sung et al. [2009]

Sung et al: Measurements at 4.3 μm

Assume widths are not vibrationally dependent.

Interferents



Significant interferents: 1.6 micron (4850 cm^{-1}): H_2O
2.06 micron (6220 cm^{-1}): H_2O, CH_4
0.76 micron (13100 cm^{-1}): H_2O

O_2 A band (0.76 micron)

Spectral region		Benchmark	Ongoing
13100 cm^{-1}	Line shape	Voigt	Voigt for main isotopologue. Galatry for minor isotopologues. Positions, intensities from Long [2010; 2011]
	Line mixing	Tran & Hartmann [2008]	Tran & Hartmann [2008]
	CIA	Tran & Hartmann [2008]	Tran & Hartmann [2008]
	H_2O broadening of O_2	None	Vess [2012]

Future

- Multi-spectral fitting, including new measurements
  - Cavity ringdown spectroscopy (CRDS): NIST, Caltech
  - Photo-acoustic spectroscopy (PAS): Caltech
  - Fourier Transform Spectrometer (FTS): JPL
- **Line shape is an active area of research!**

Evaluation Methodology

Image: JAXA

GOSAT soundings

- 1-3 bands, multiple absorbers
- Low spectral resolution
- Unconstrained atmosphere, aerosols, surface albedo

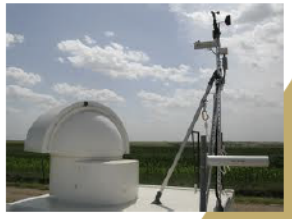


Image: Caltech

TCCON spectra

- 1-3 bands, multiple absorbers
- High spectral resolution
- Full atmospheric column
- Atmosphere conditions constrained at surface

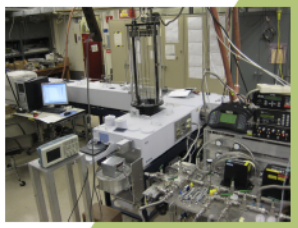
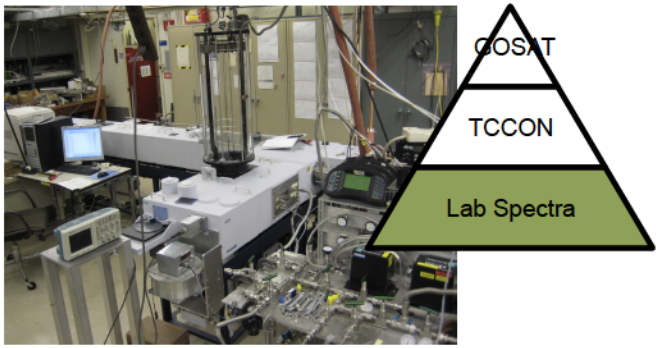


Image: JPL

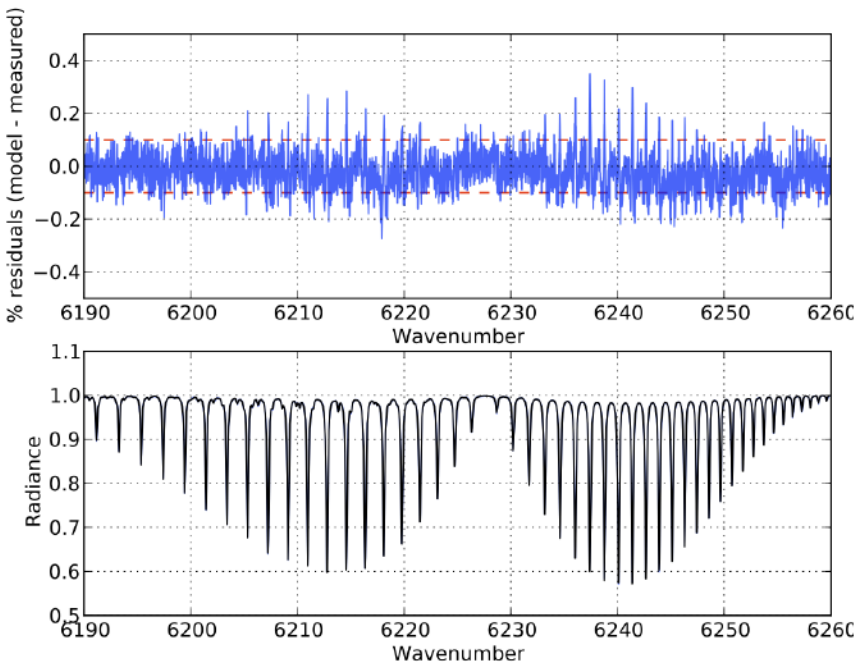
Laboratory spectra

- 1 band, one absorber
- High spectral resolution
- Known laboratory conditions
- Mostly room temperature, low optical depth

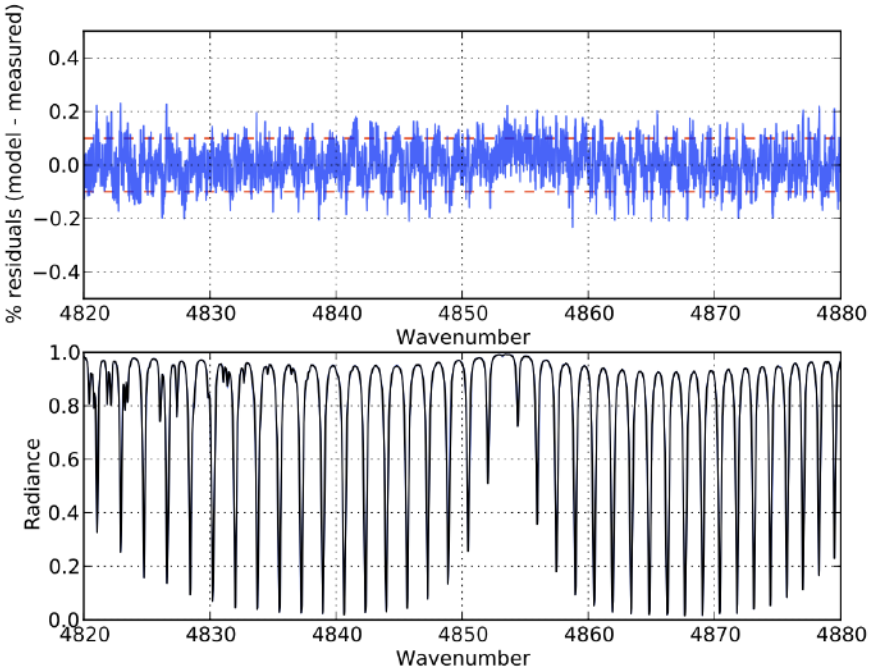
Evaluation with lab spectra



JPL FTS

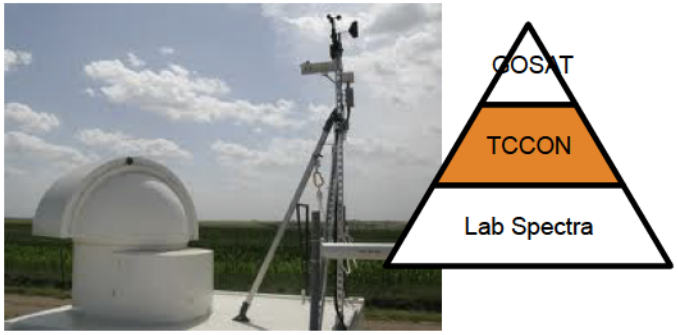


1.6 µm band, path length 32.54m
optical path difference 75cm
Total cell pressure is 742 Torr
Sample is 9.03% air-broadened $^{16}O^{12}C^{16}O$



2 µm band, path length 29.3m
Optical path difference 112.5 cm
Total pressure 599.8 Torr
Sample: 4.95% air-broadened $^{16}O^{12}C^{16}O$

Evaluation with TCCON network data

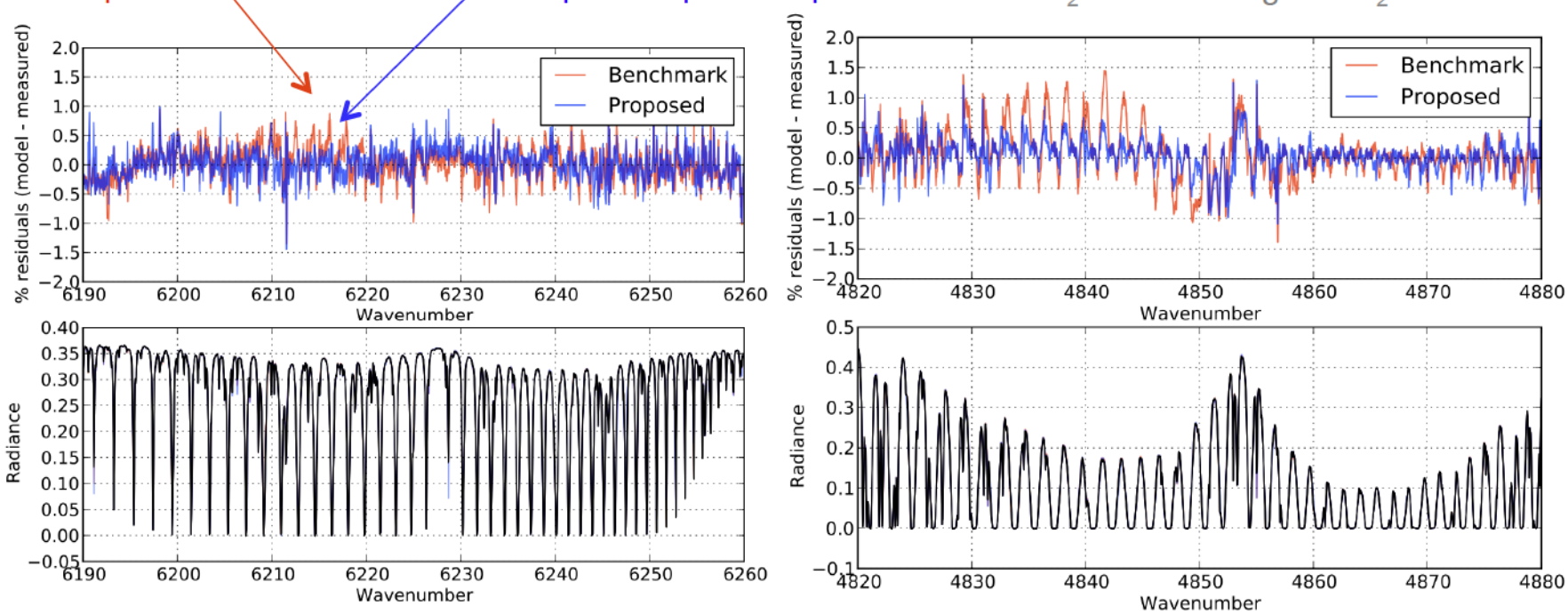


TCCON retrieval for Park Falls 22 Dec. 2004
~12 airmasses

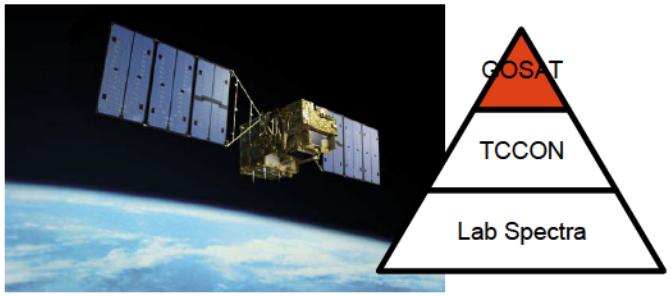
State of the art
First-order line mixing, Voigt shapes

"Ongoing" model
Nearest-neighbor line mixing
Speed dependent profile

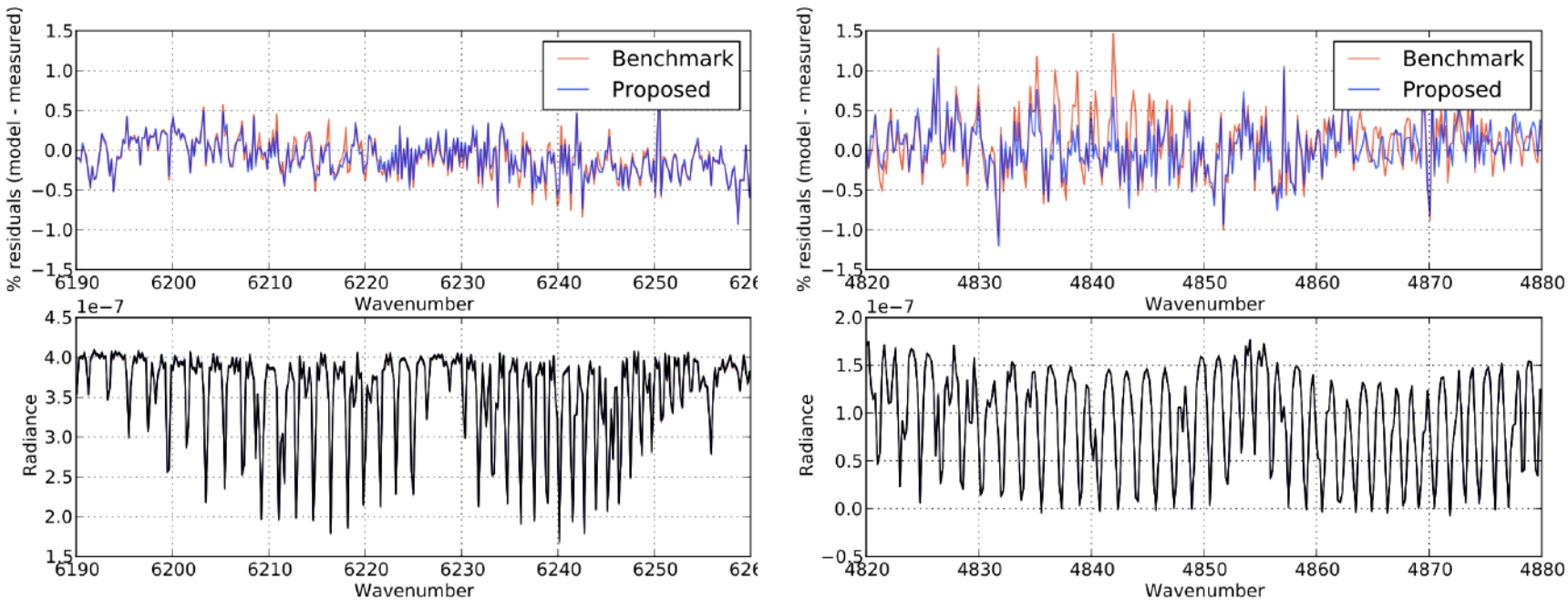
Thompson et al., *JQRST* [2012]
Results shown here do not include H_2O broadening of CO_2.



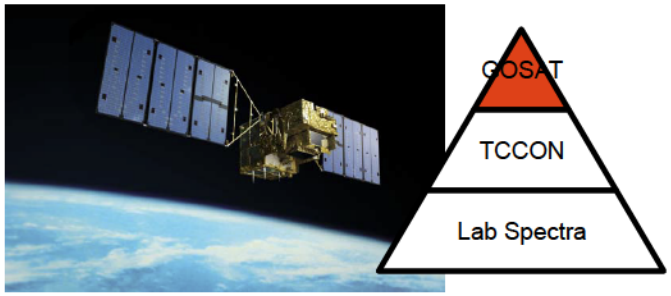
Evaluation with GOSAT data



- Mean of soundings over TCCON stations
- Three-band retrieval using surface pressure to estimate Column-averaged dry mole fraction $\mathbf{X_{co2}}$

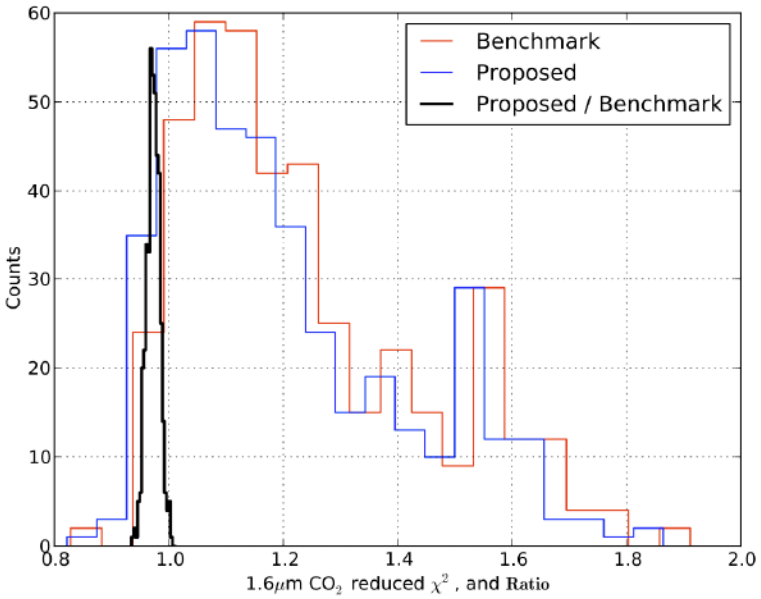


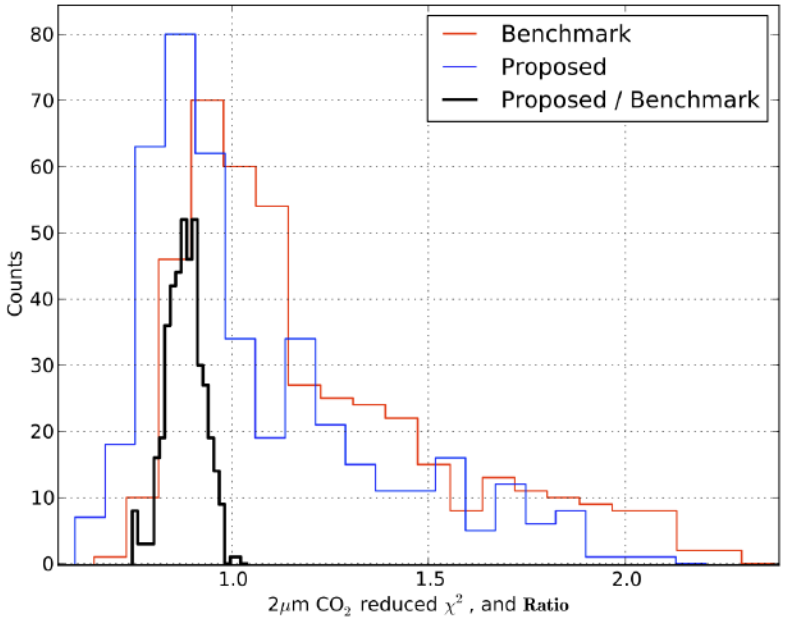
Evaluation with GOSAT data



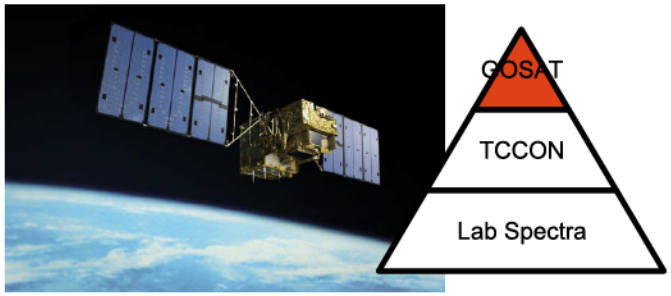
Mean of soundings over TCCON stations, after zeroing out the mean bias

# Converged		Scatter v. TCCON		Correlation	
Benchmark	"Ongoing"	Benchmark	"Ongoing"	Benchmark	"Ongoing"
279 (65.6%)	300 (70.6%)	1.50 ppm	1.39 ppm	0.767	0.781

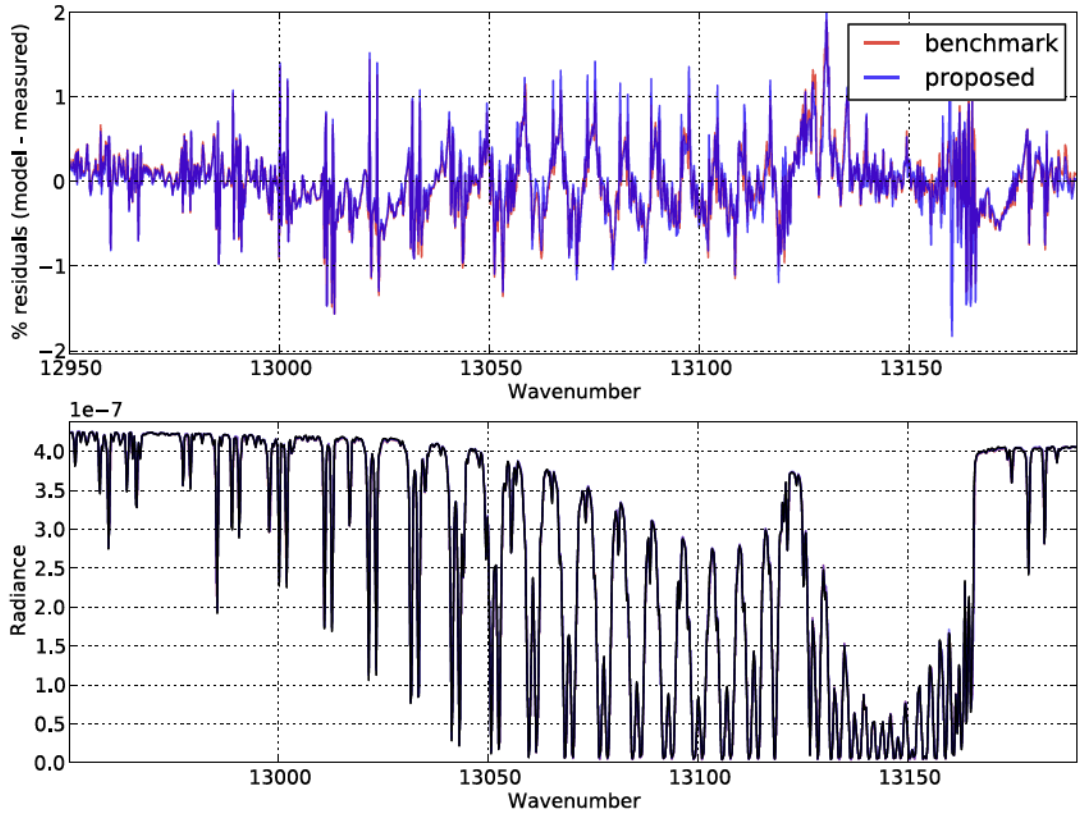




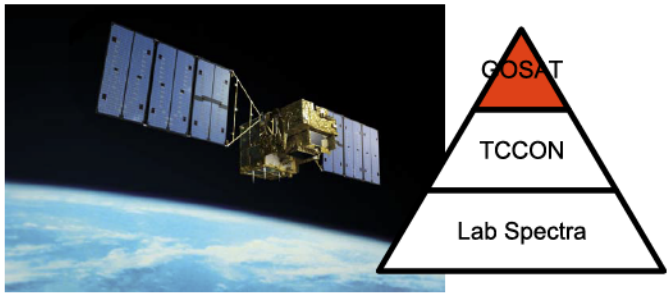
Evaluation with GOSAT data



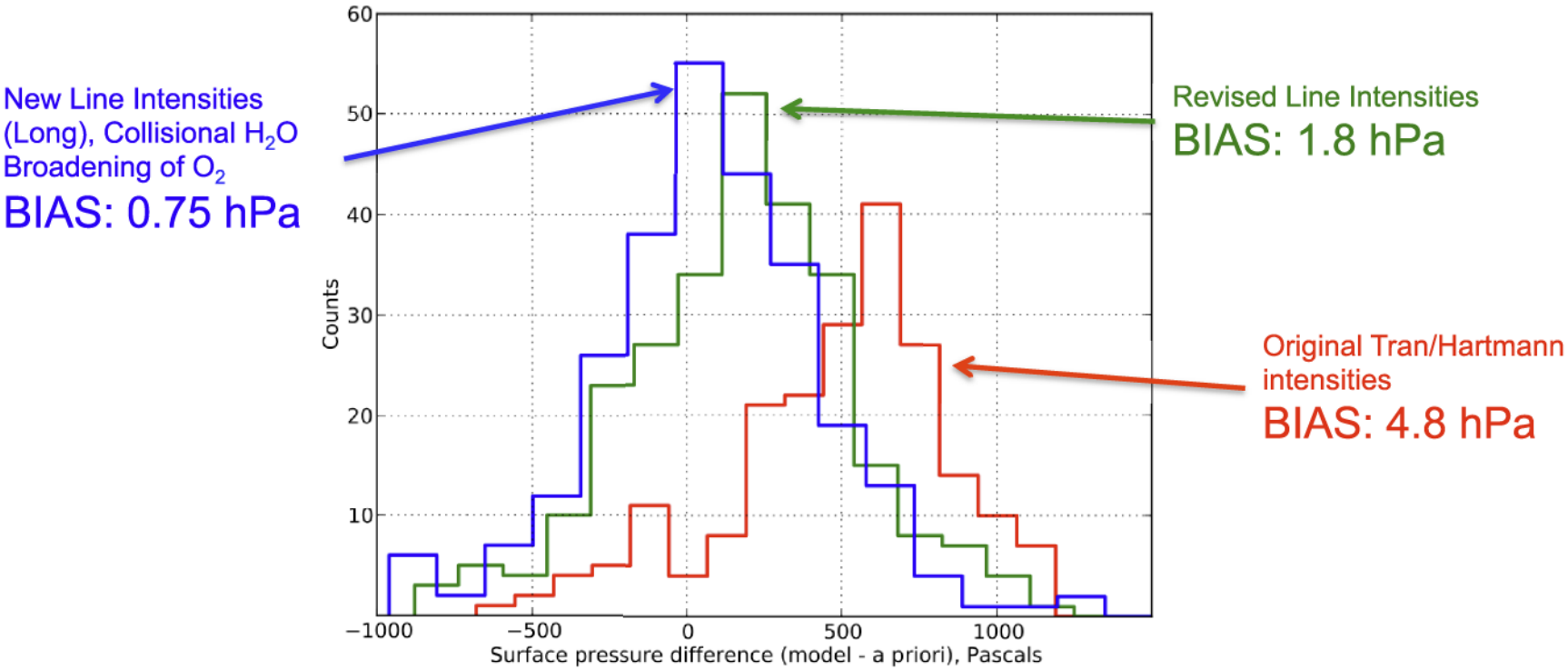
Estimation of Xco_2 requires surface pressure information.
O_2 A band is used for surface pressure information (amongst other things).



Evaluation with GOSAT data



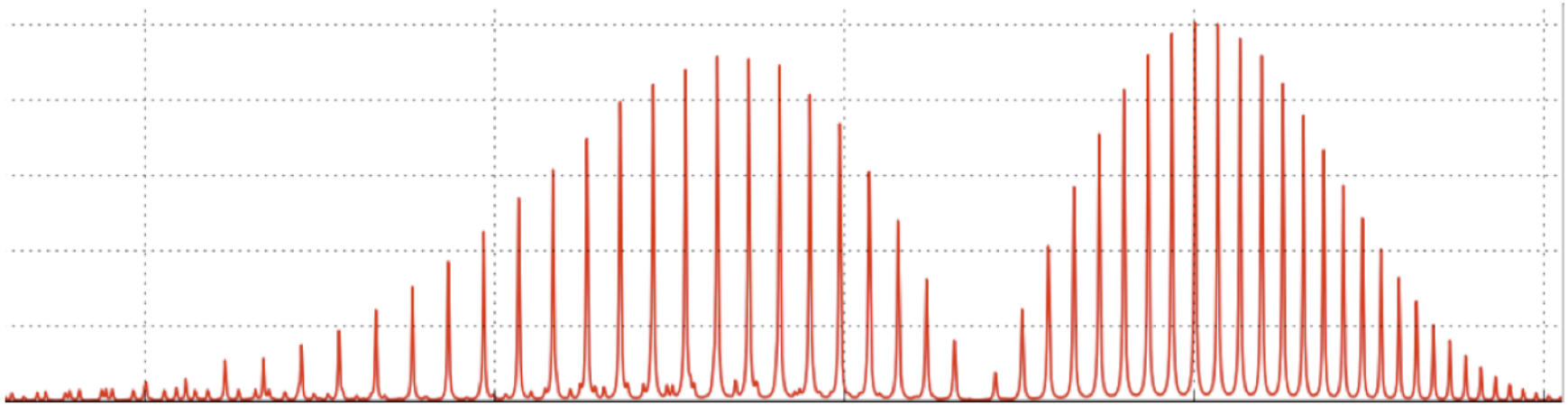
Surface pressure bias with respect to ECMWF values:



Note that in moving from red to blue about 28% more soundings pass filter

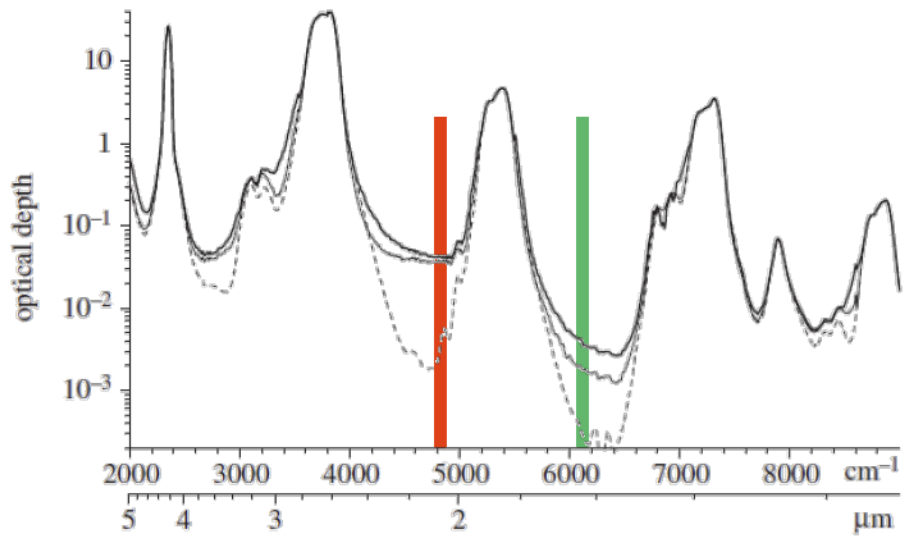
Comments

- The new models seem a step in the right direction
  - Qualitatively similar improvements for three instruments and retrieval codes
- Accuracies are not yet to the desired 0.1% level
  - Some systematic errors remain
- New measurements (CRDS, PAS) may help constrain line shapes
- **Key components of the approach:**
  - **Consistent use of line parameters with line shape used in their determination**
  - **Use of multiple spectra in the fitting of line shape and line parameters**



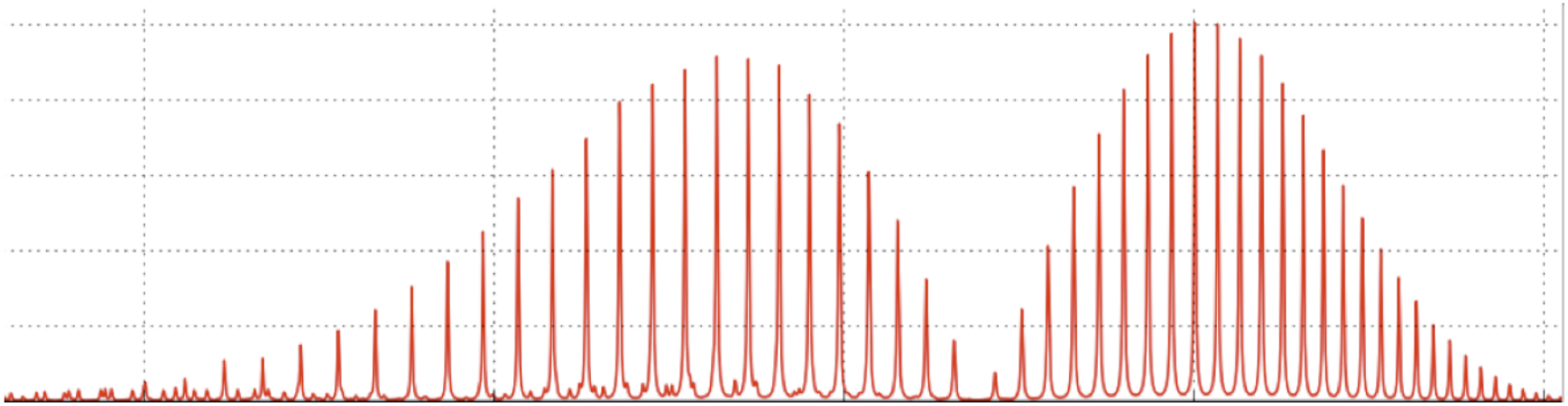
Some pending challenges

- Significant uncertainties in continuum effects,
  - Especially the H_2O contribution
  - May contribute to difficulties in fitting atmospheric spectra in the 1.6 micron band?
- Intense focus on improving Oxygen A band spectroscopy
  - Incorporating new measurements in a multi-spectrum fit
  - Simultaneous retrieval of Galatry line profile with nearest-neighbor line mixing
  - Validation of models for Collision-Induced Absorption



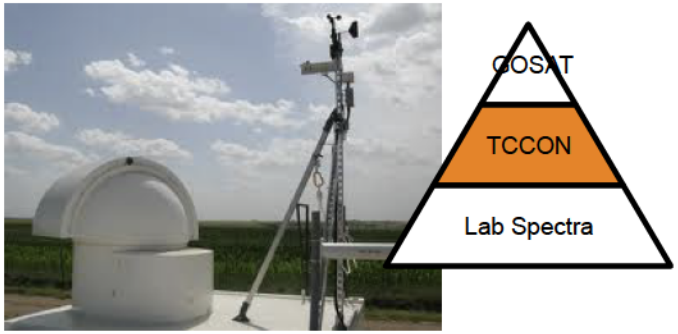
Uncertainties in the H_2O continuum is large in CO_2 bands (Ptashnik et al. 2011;2012)

Questions?



Backup slides

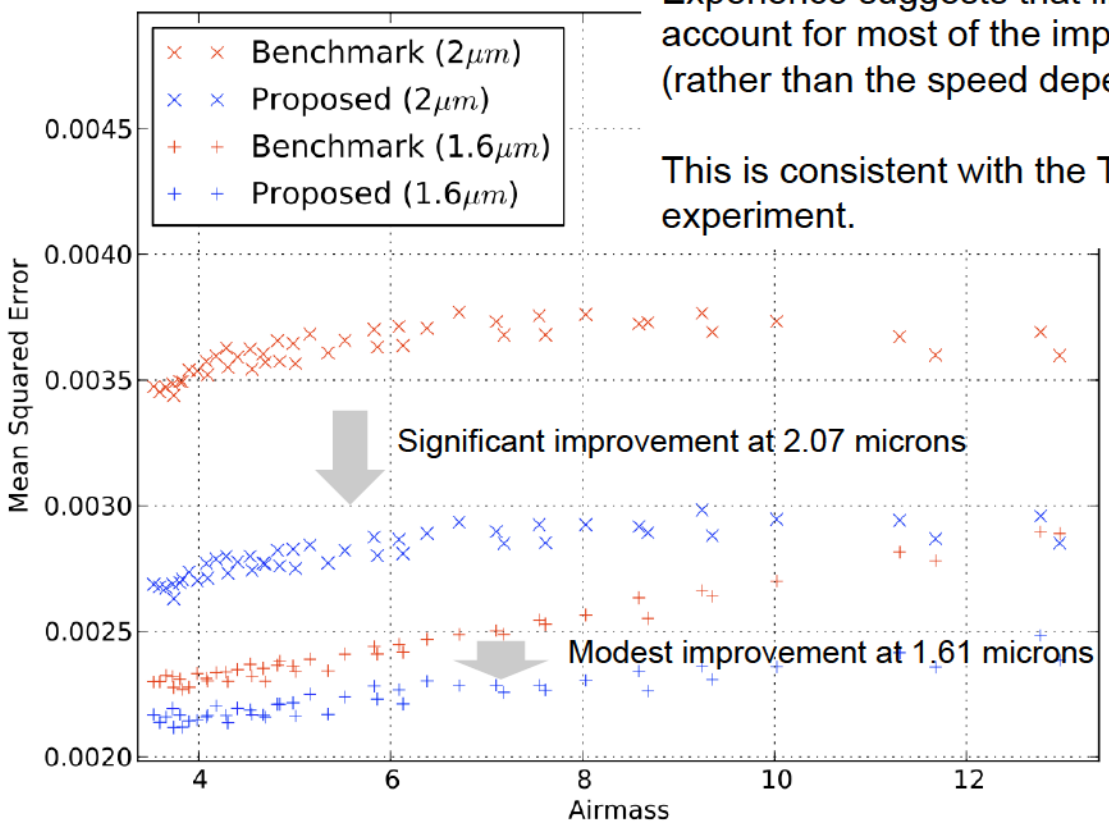
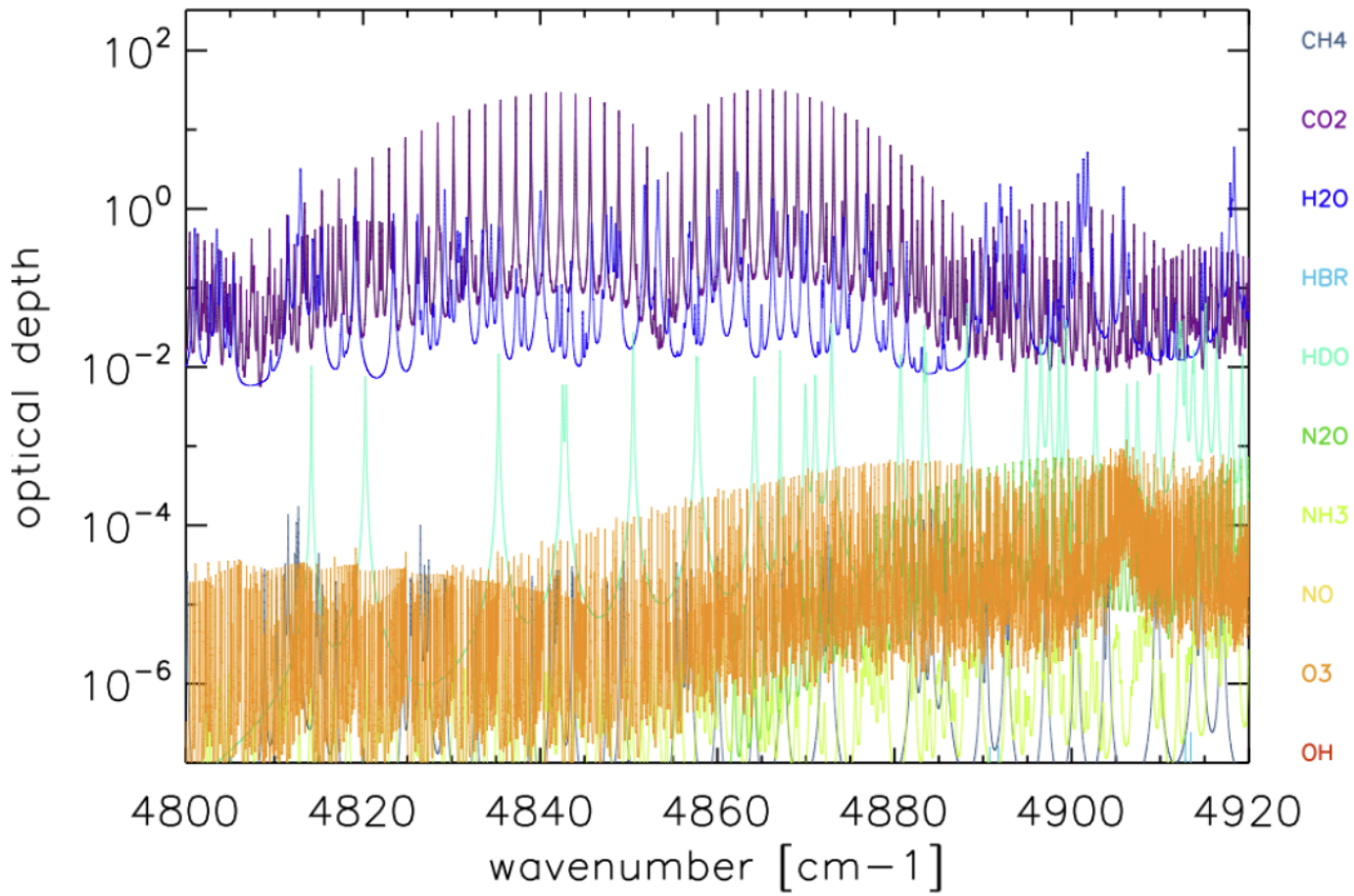
Evaluation with TCCON network data



TCCON retrievals for Park Falls 22 Dec. 2004

Experience suggests that line mixing may account for most of the improvement (rather than the speed dependent profile).

This is consistent with the TCCON experiment.



Interferents