Satellite and Ground-based evaluation of 1.61 and 2.07 micron CO_2 absorption models for the OCO-2 mission

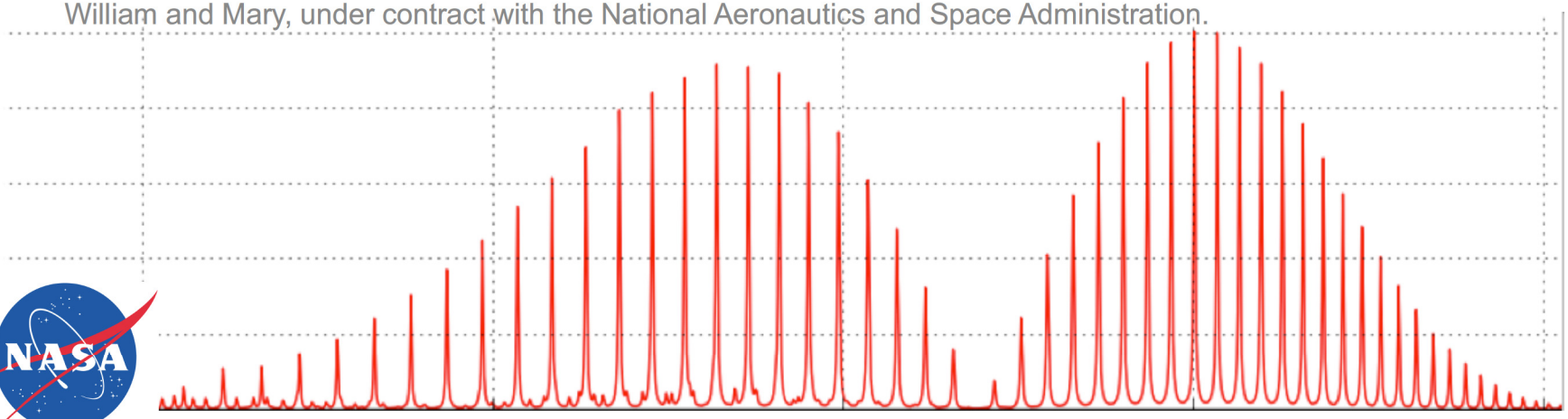
Vijay Natraj, Jet Propulsion Laboratory, California Institute of Technology

David R. Thompson[1] Linda Brown[1] Chris Benner[2] Dave Crisp[1] Malathy Devi[2]
Yibo Jiang[1] Charles E. Miller[1] Fabiano Oyafuso[1] Vivienne Payne[1] Keeyoon Sung[1]

…. and others

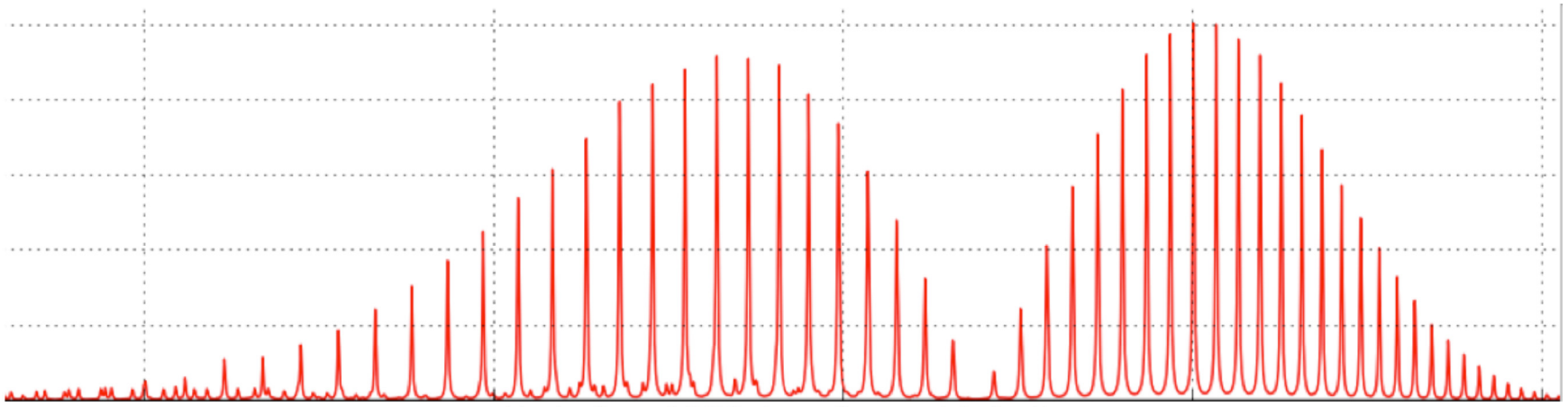
[1]Jet Propulsion Laboratory, California Institute of Technology, [2]College of William and Mary

Copyright 2012 California Institute of Technology. Government sponsorship acknowledged. A portion of this research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, and the College of William and Mary, under contract with the National Aeronautics and Space Administration.



Agenda

1. Motivation
2. New CO_2 models for the 1.61 and 2.07 micron bands
3. Validation and testing method
   - Lab Spectra
   - Upward-looking FTS spectrometers
   - GOSAT orbital measurements
4. Pending challenges



The OCO-2 Mission

- Launch expected in late 2014
- Sounding spectrometer monitors three spectral regions
  - CO_2 in the 4850 cm^{-1} (strong band)
  - CO_2 in the 6220 cm^{-1} (weak band)
  - O_2 in the 13100 cm^{-1} (A 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, illustrated for the two CO_2 bands

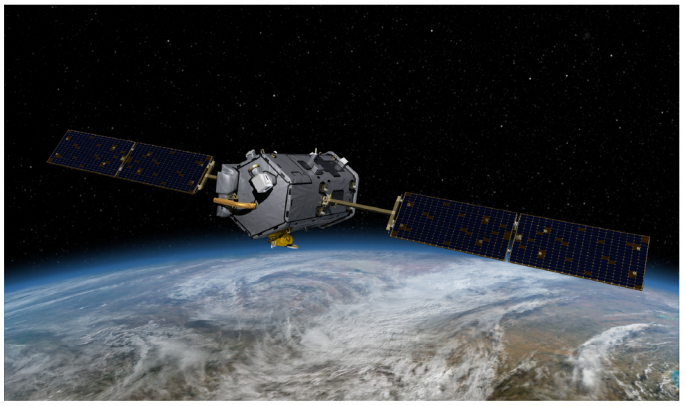
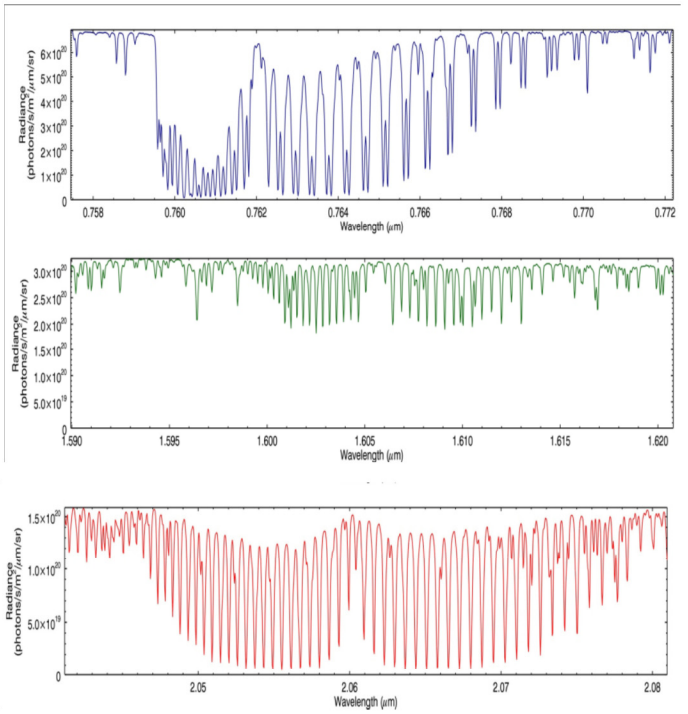


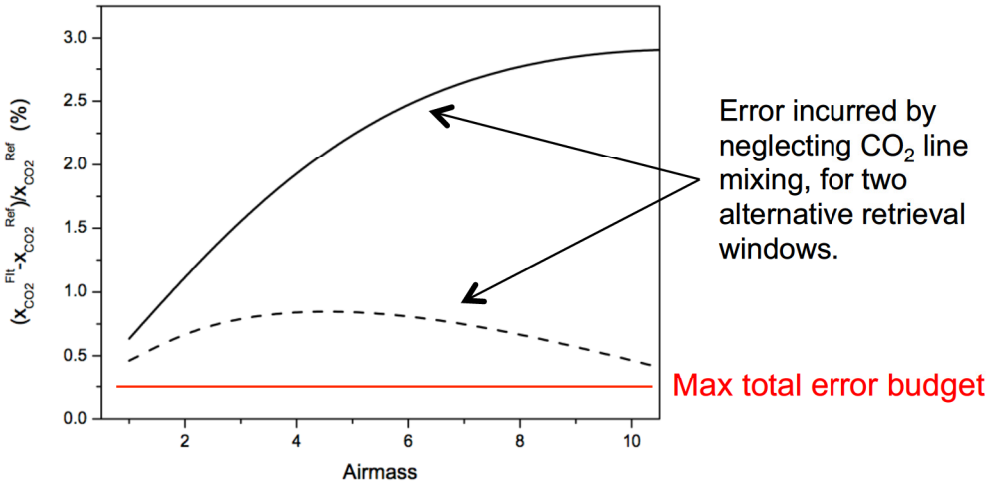
Image: NASA / Orbital

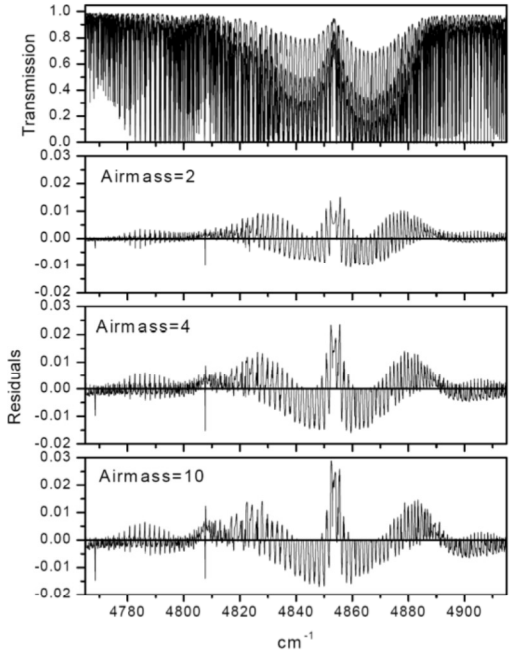
Three OCO-2 bands



Why spectroscopy matters

- 0.25% OCO-2 Accuracy requirement requires 0.1% reference spectroscopic accuracy (Miller et al., 2005)
- 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





Residuals due to neglecting line mixing

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.

New Models

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

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

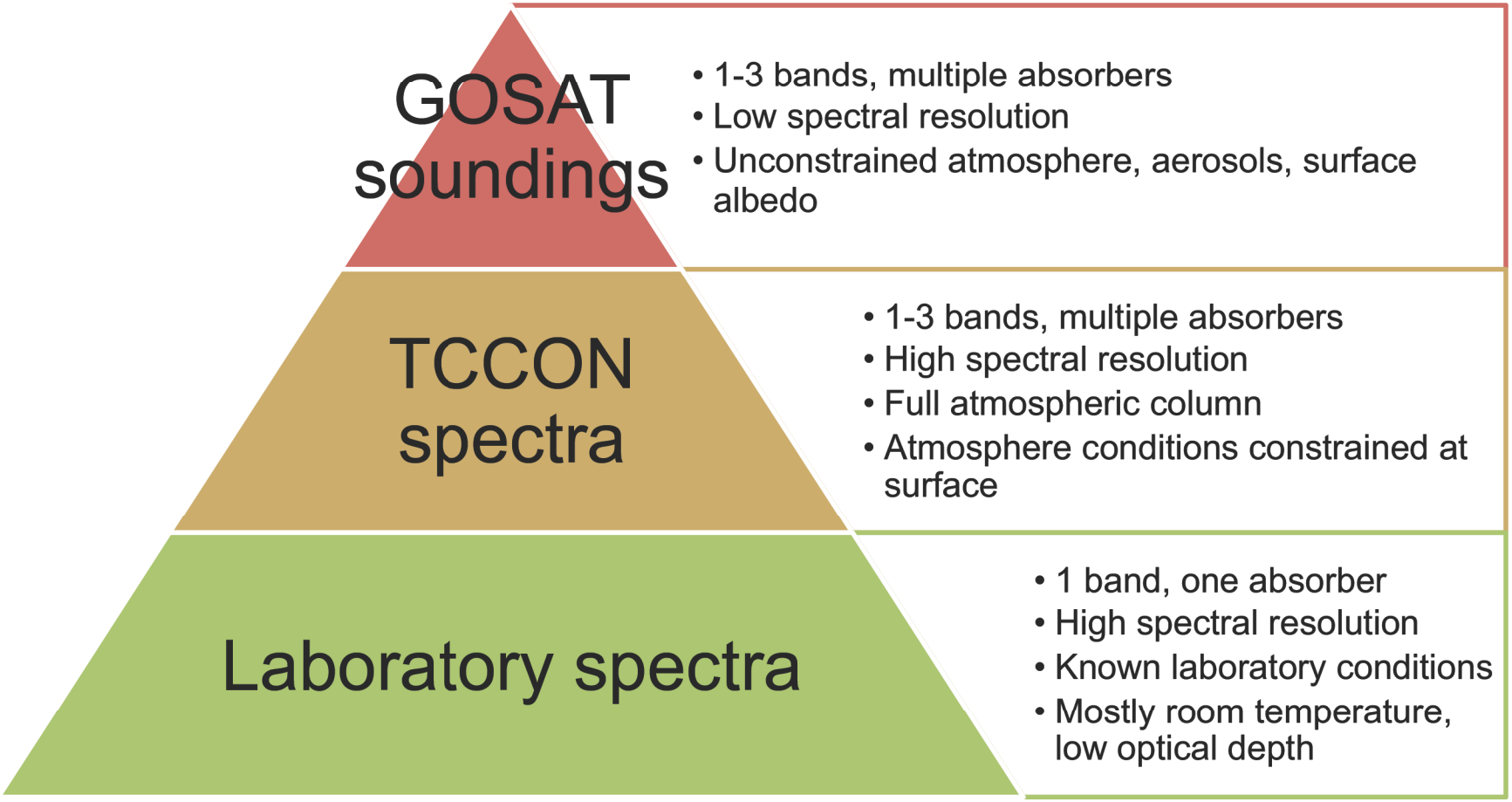
$$v_i = -4 + i/2$$

Lorenz half width

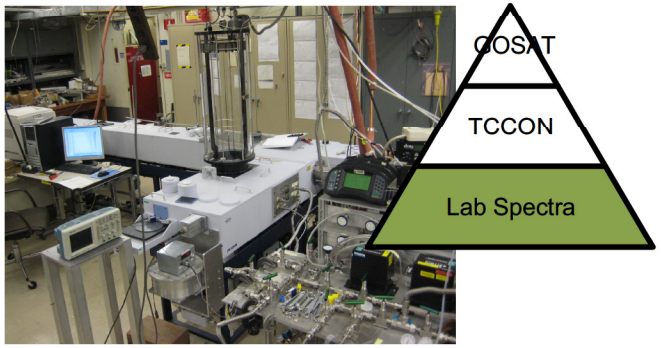
We set Dicke narrowing to zero

Spectral Region		Benchmark	Proposed
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]**
6200cm^{-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]**

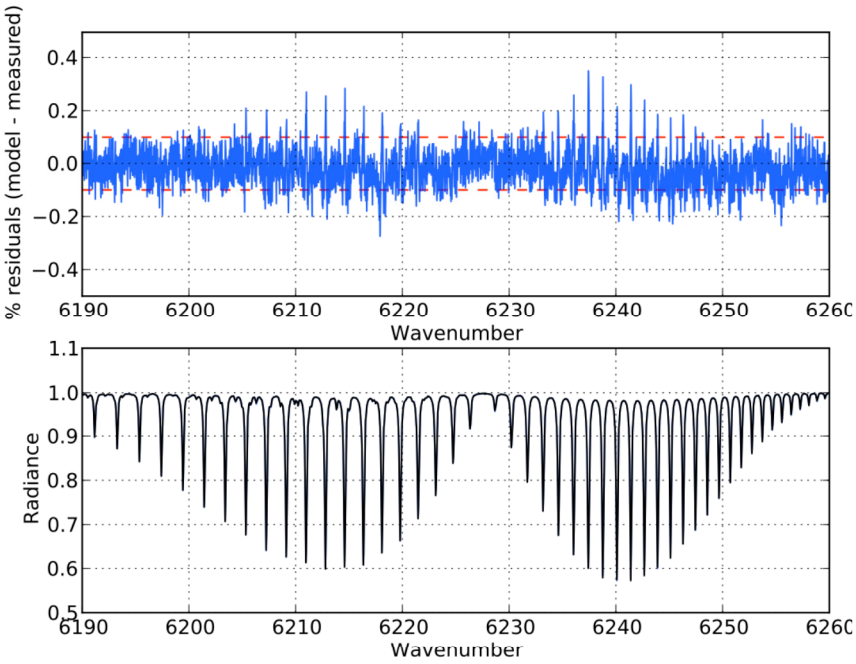
Evaluation Methodology



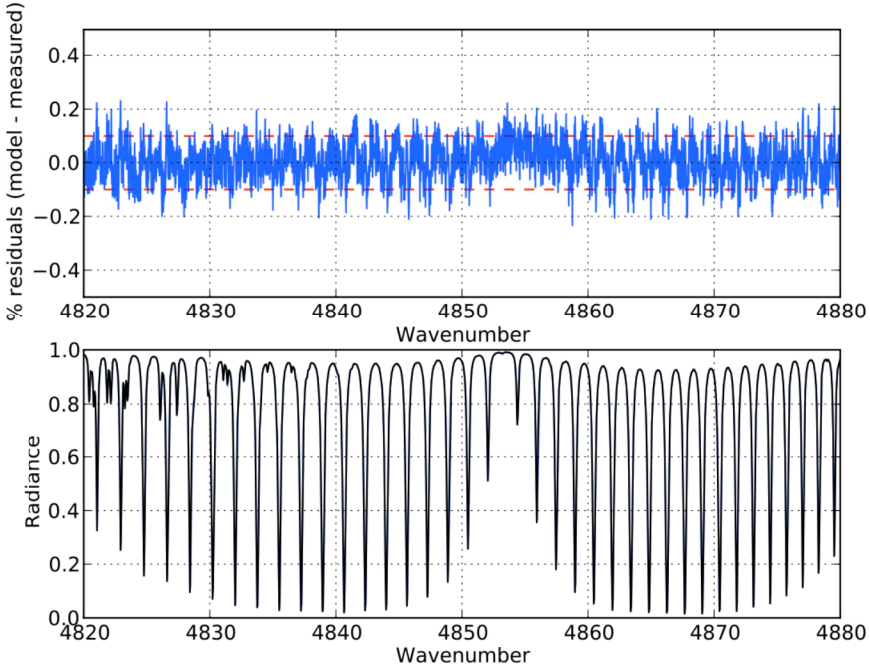
Evaluation with lab spectra



JPL FTS

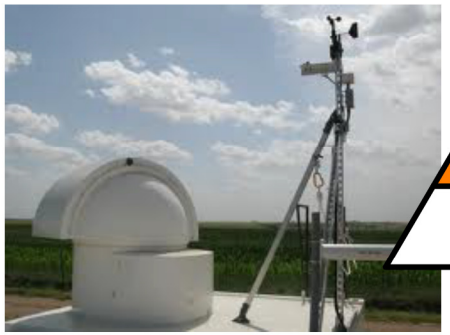


1.6 μm band, path length 32.54m
optical path difference 75cm
Total cell pressure is 742 Torr
Sample is 9.03% air-broadened $^{16}O^{12}C^{16}O$



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

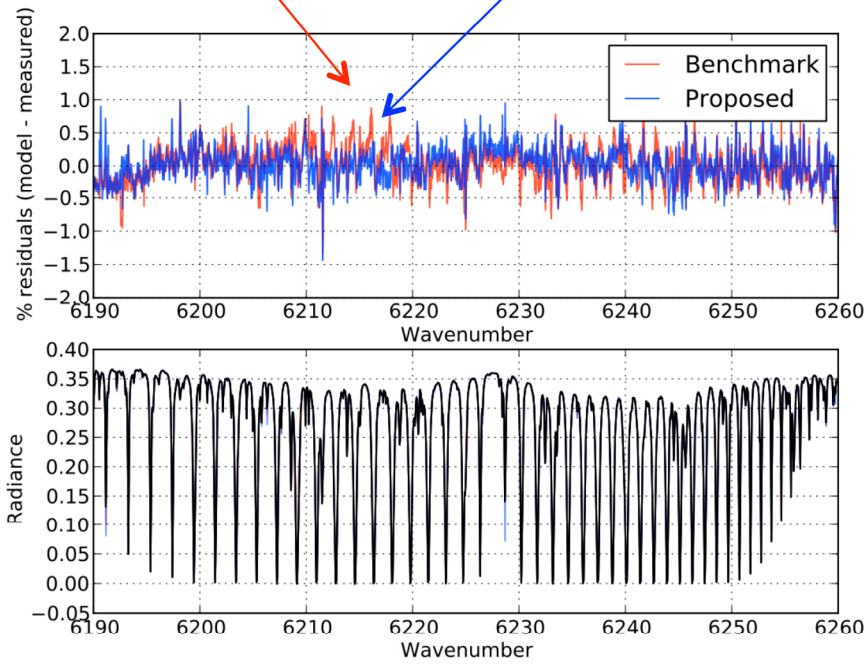


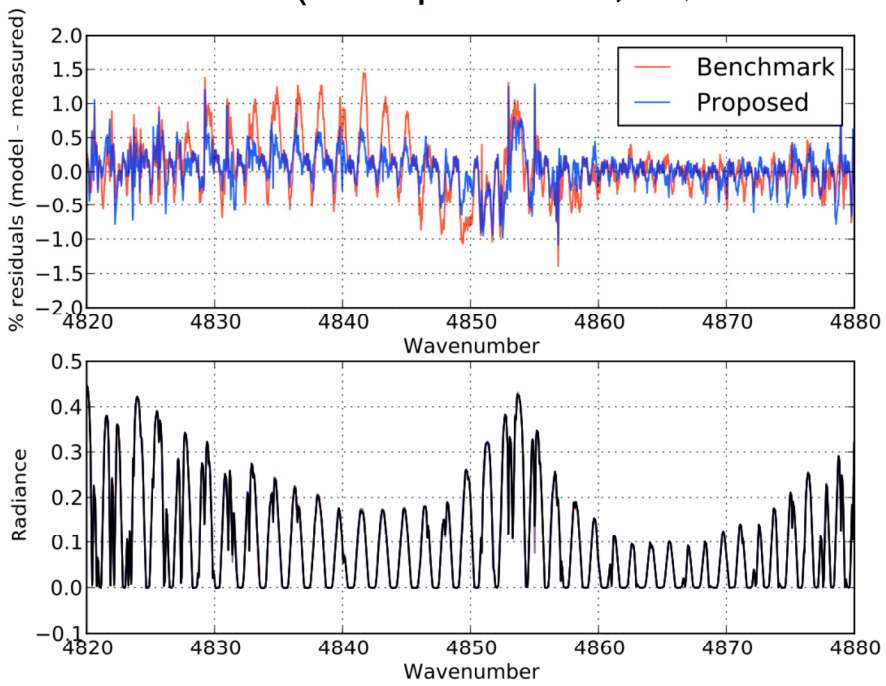
TCCON retrieval for Park Falls 22 Dec. 2004
~12 airmasses

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

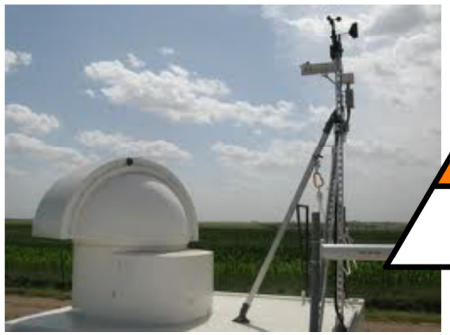
Proposed model
Nearest-neighbor line mixing
Speed dependent profile

(Thompson et al., *JQRST* 2012)

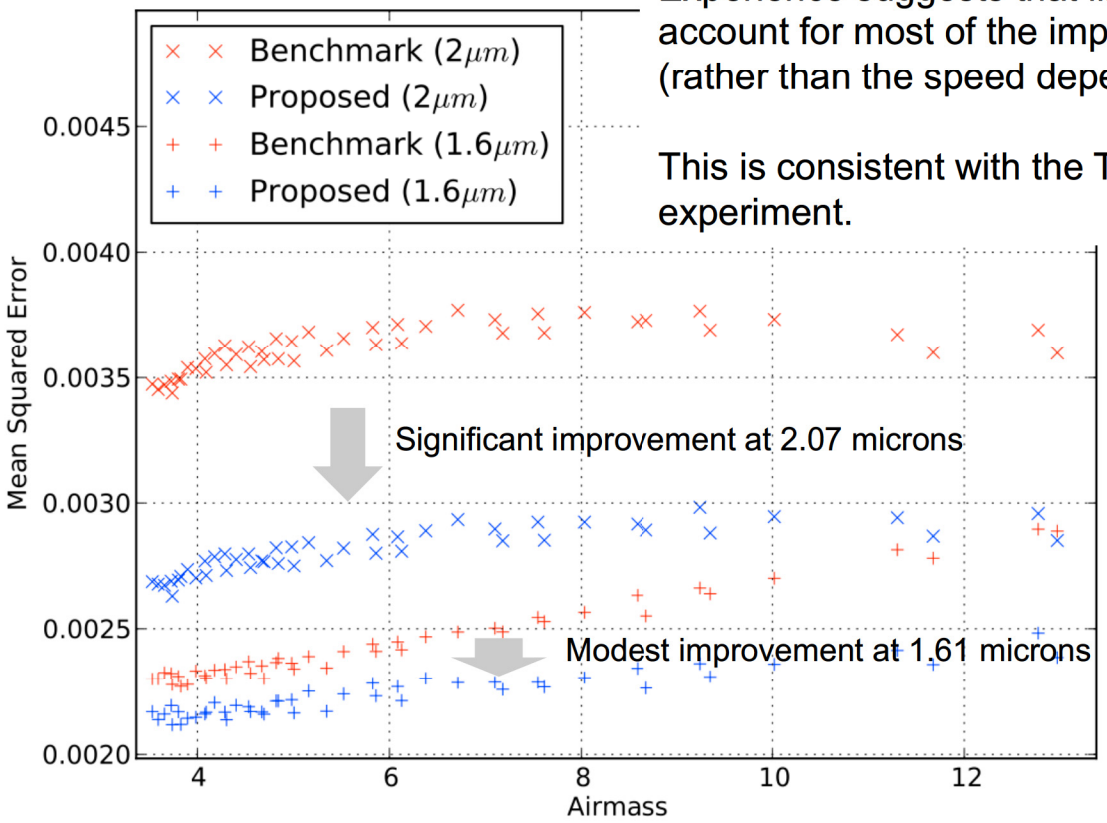




Evaluation with TCCON network data



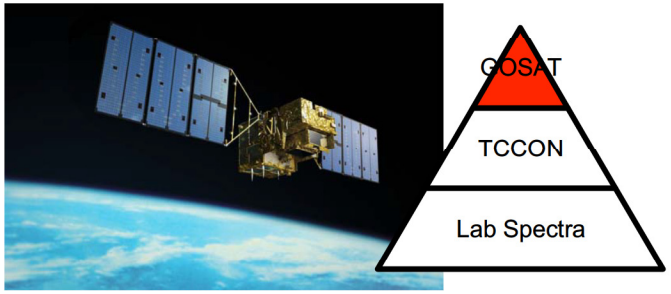
TCCON retrievals for Park Falls 22 Dec. 2004



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

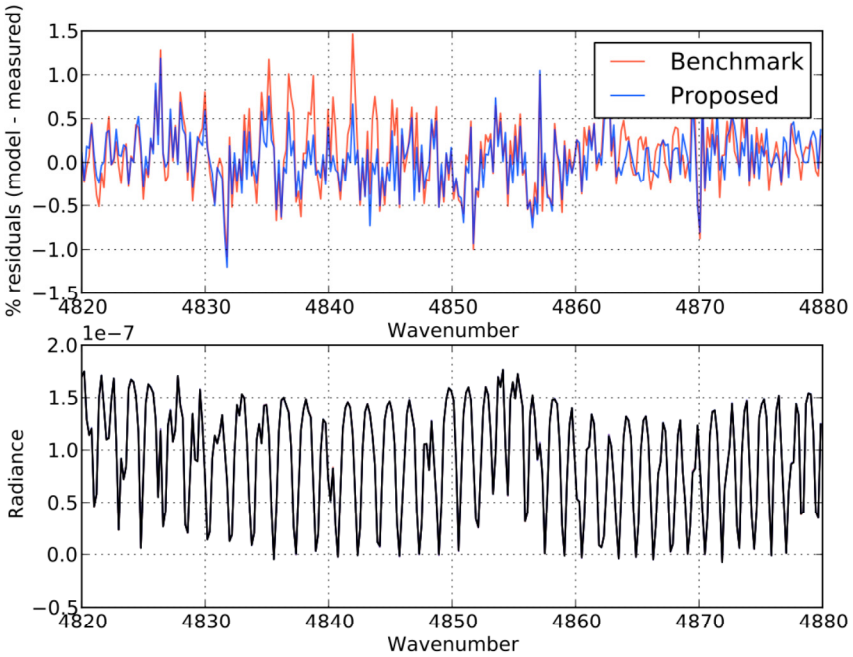
This is consistent with the TCCON experiment.

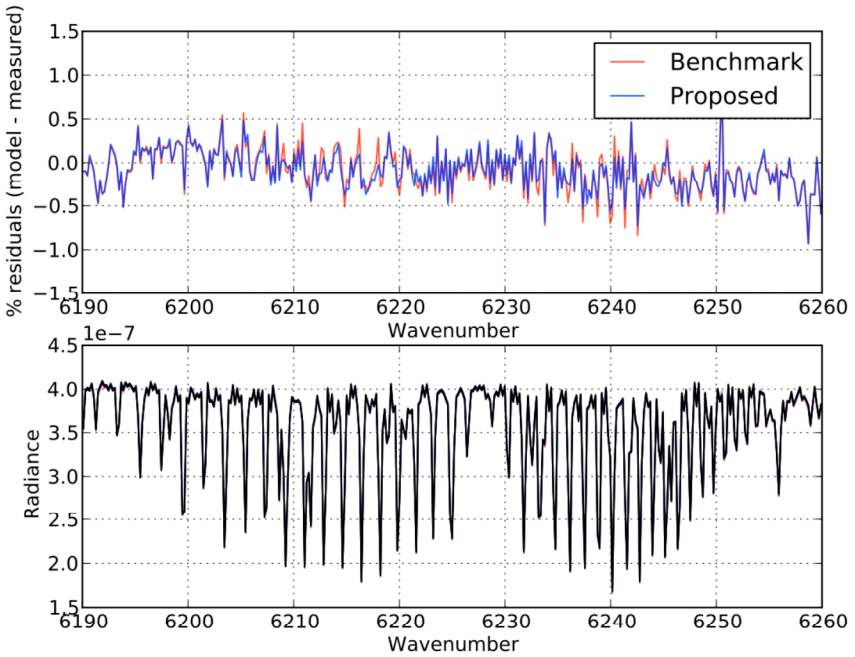
Evaluation with GOSAT data



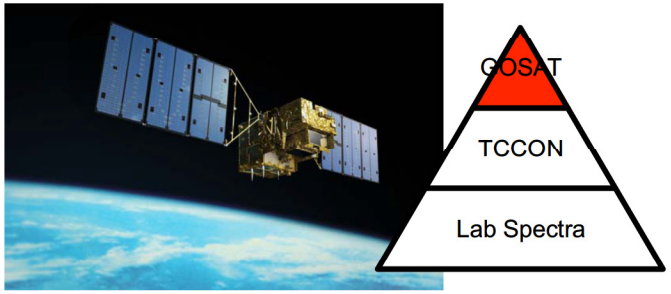
- Mean of soundings over TCCON stations
- Three-band retrieval using surface pressure to estimate Column-averaged dry mole fraction $\mathbf{X_{co2}}$
- O_2 A Band parameters from (Tran et al., 2008)

(Thompson et al., *JQRST* 2012)



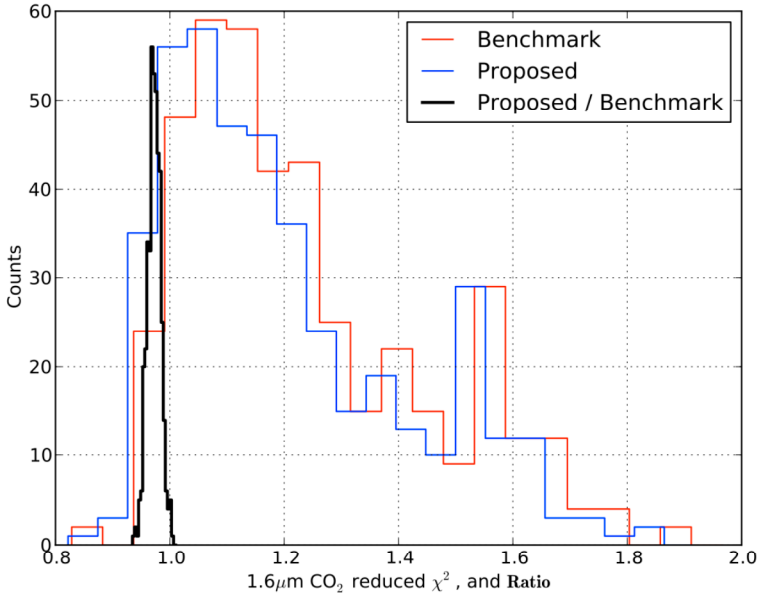


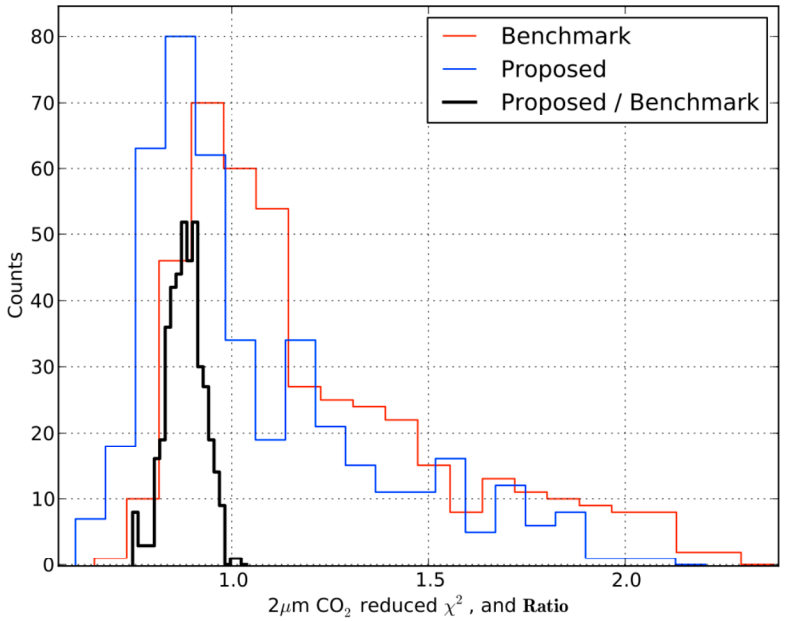
Evaluation with GOSAT data



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

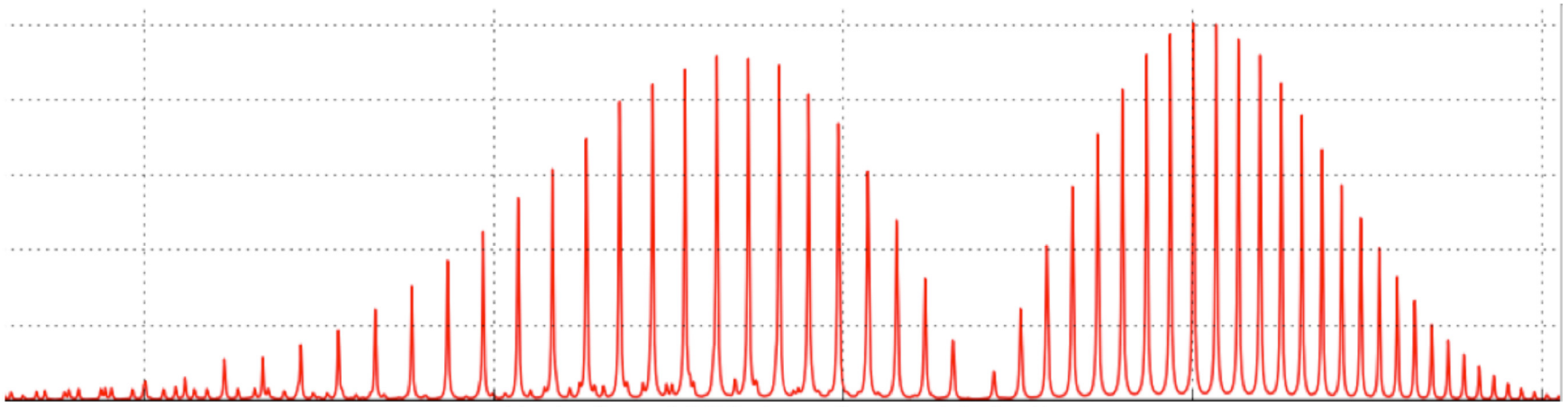
# Converged		Scatter v. TCCON		Correlation	
Benchmark	**Proposed**	**Benchmark**	**Proposed**	**Benchmark**	**Proposed**
279 (65.6%)	300 (70.6%)	1.50 ppm	1.39 ppm	0.767	0.781





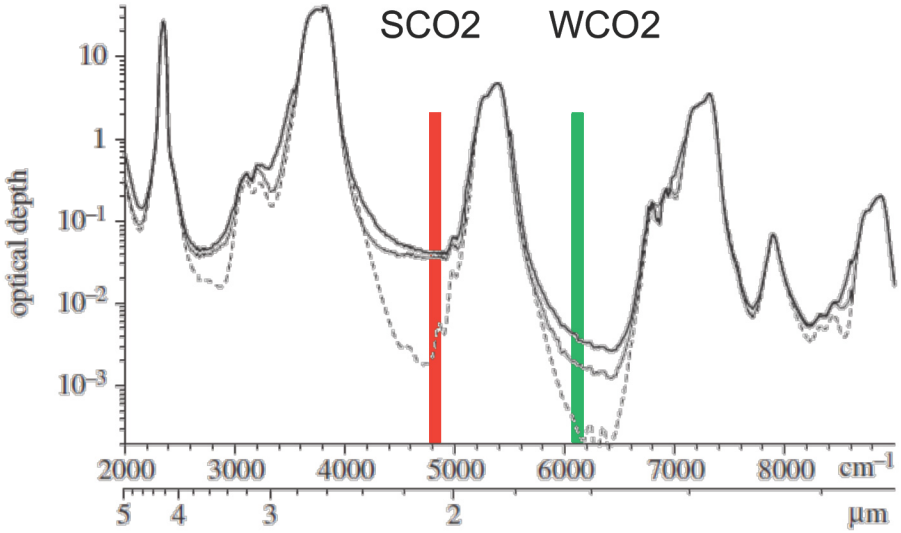
Comments

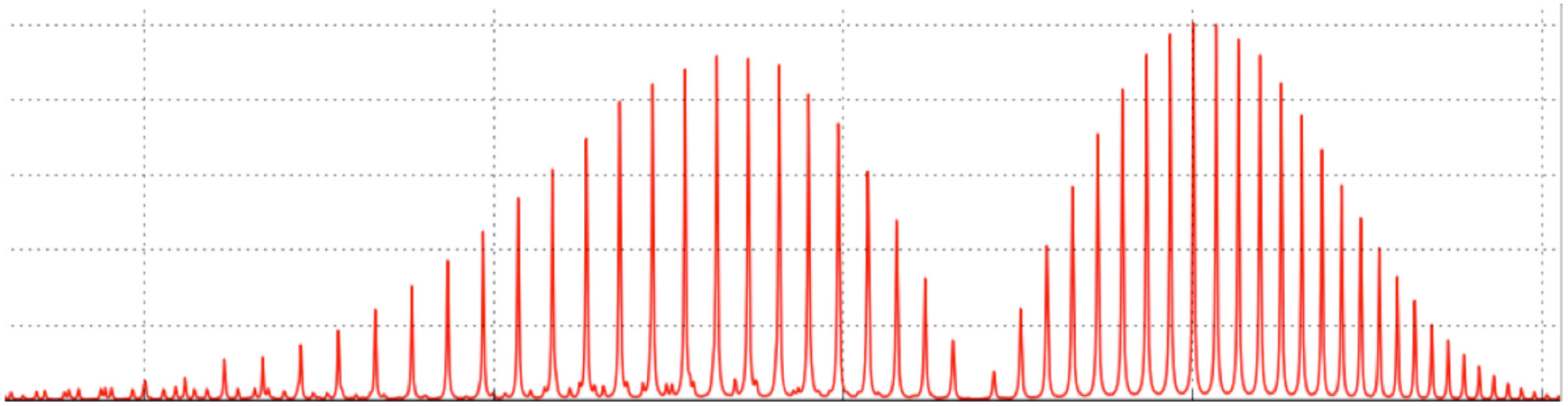
- The new models seem a step in the right direction
  - Qualitatively similar improvements to three instruments and retrieval codes
- Radiometric accuracies are not yet to the desired 0.1% level
  - Some systematic errors remain
- New Cavity Ringdown Spectroscopy (CRDS) may help constrain line shapes



Some pending challenges

- Later upgrades have introduced H_2O foreign broadening of CO_2 (Sung et al. 2009), and O_2 (Vess et al. 2012).
- Significant uncertainties in continuum effects, especially the H_2O contribution
- Intense focus on improving Oxygen A band spectroscopy
  - Incorporating CRDS 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?