OCO-2 Absorption Cross sections

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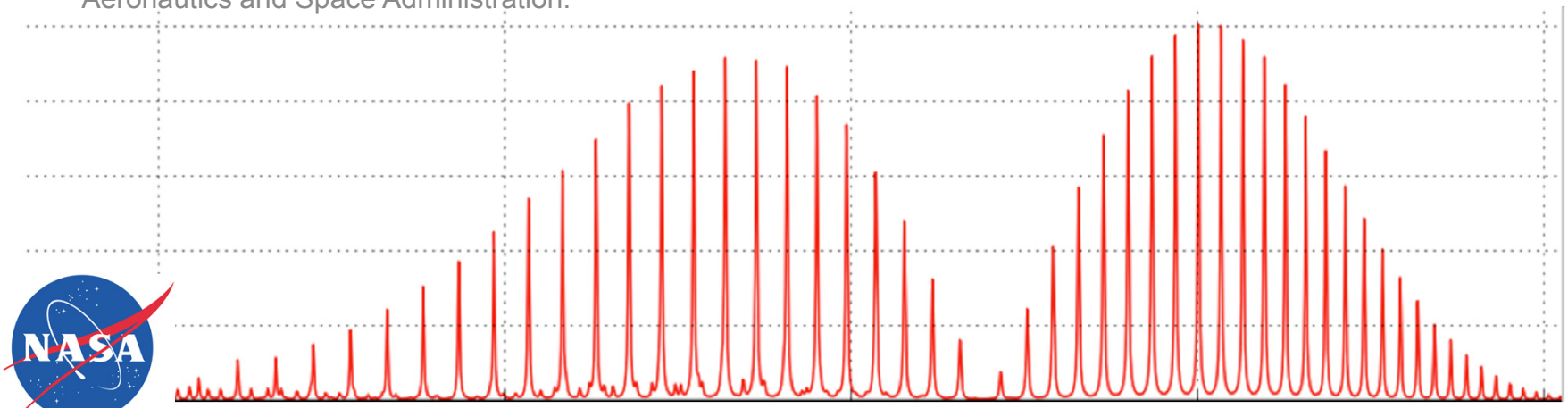
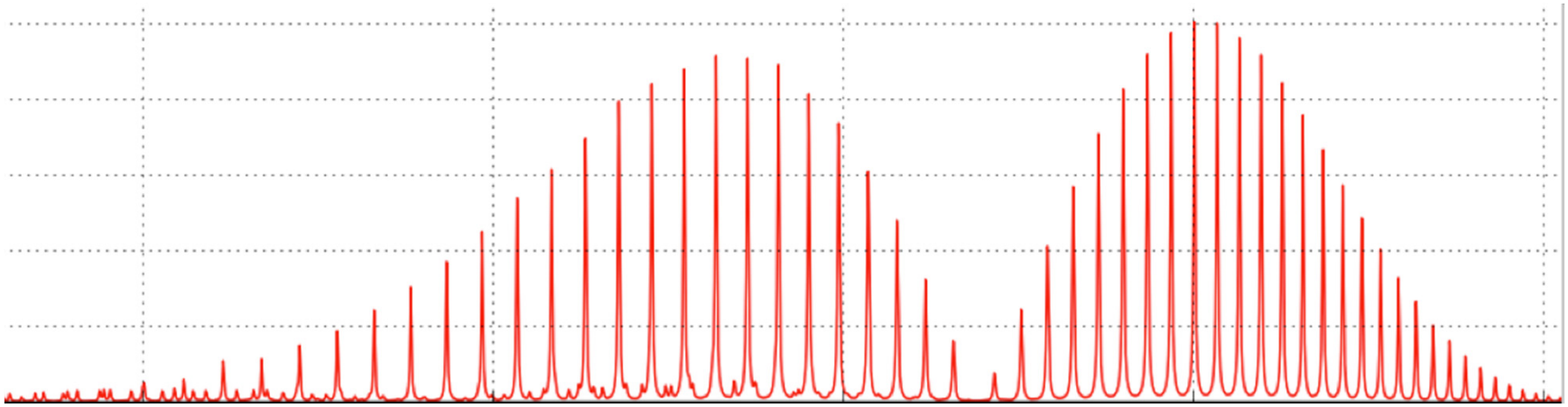


Agenda

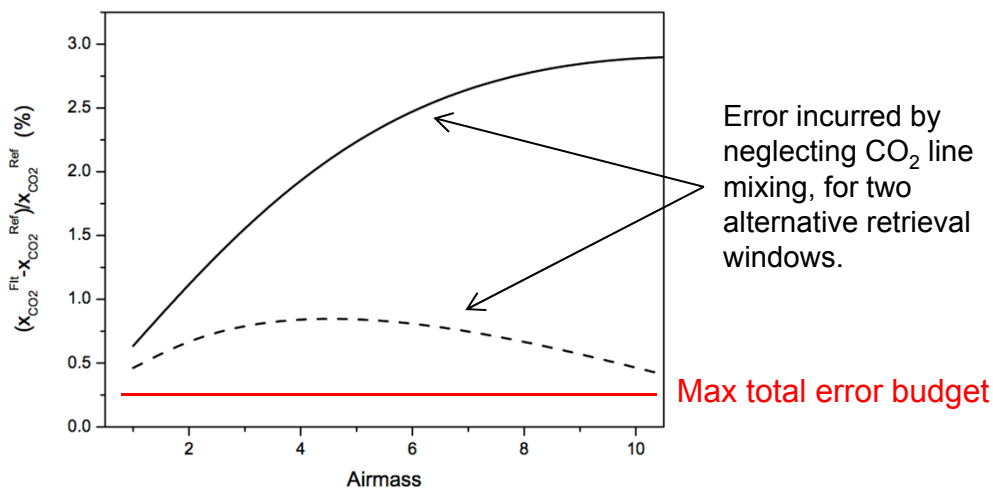
1. Spectroscopy in OCO-2 retrievals
   - Parameter sources and computation
   - Validation and testing

2. Pending challenges

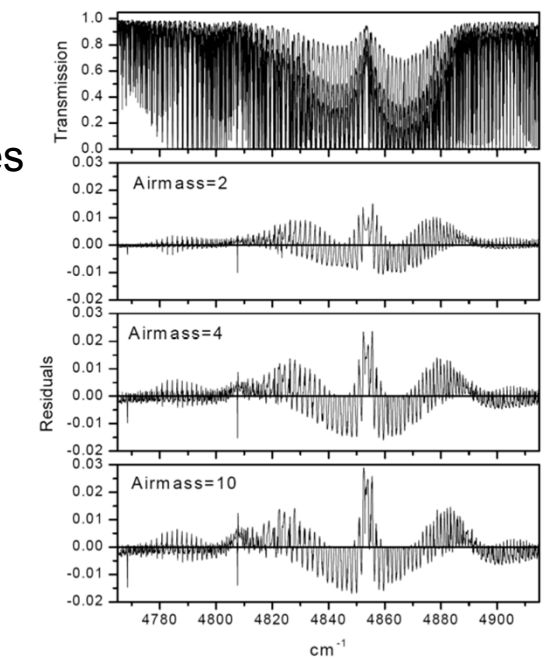


Why spectroscopy matters

- 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



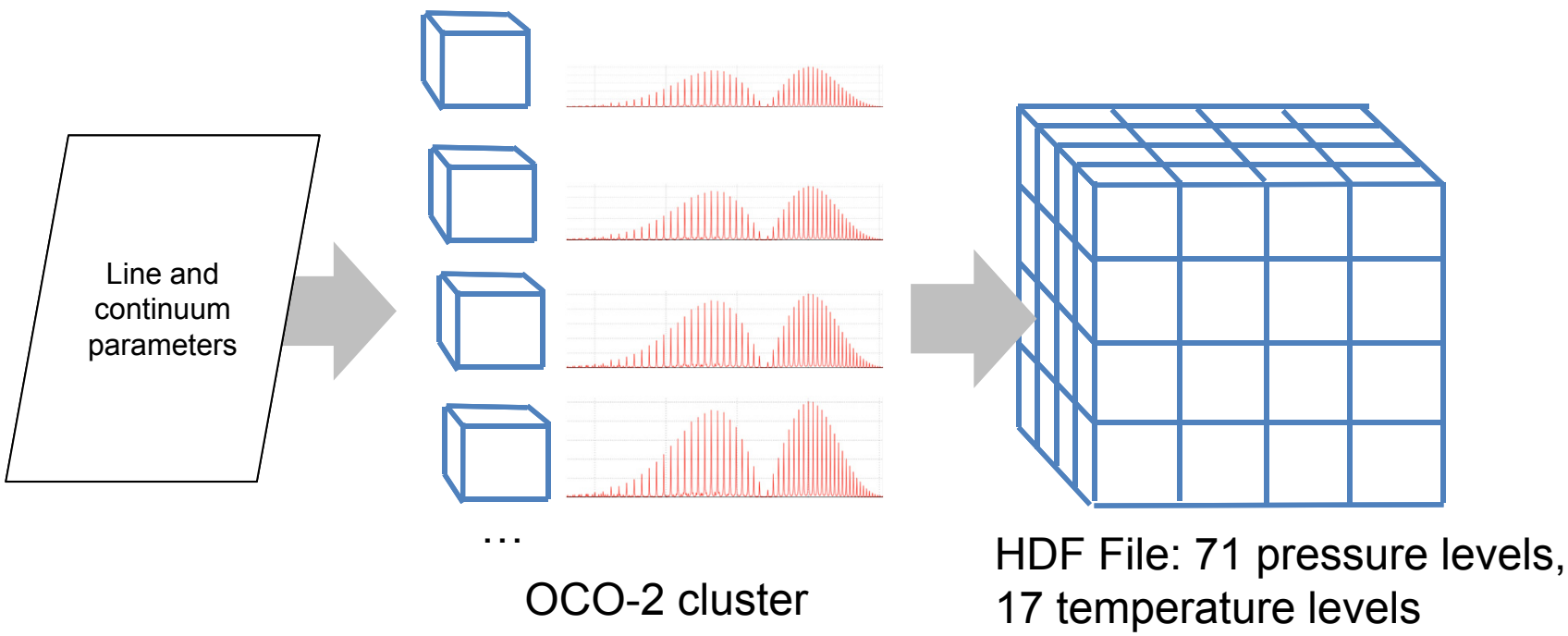
From Hartmann, J.-M., Tran, H., and Toon, G. C.: Influence of line mixing on the retrievals of atmospheric CO2 from spectra in the 1.6 and 2.1 µm regions, Atmos. Chem. Phys., 9, 7303-7312.



Residuals due to neglecting line mixing

Table construction process

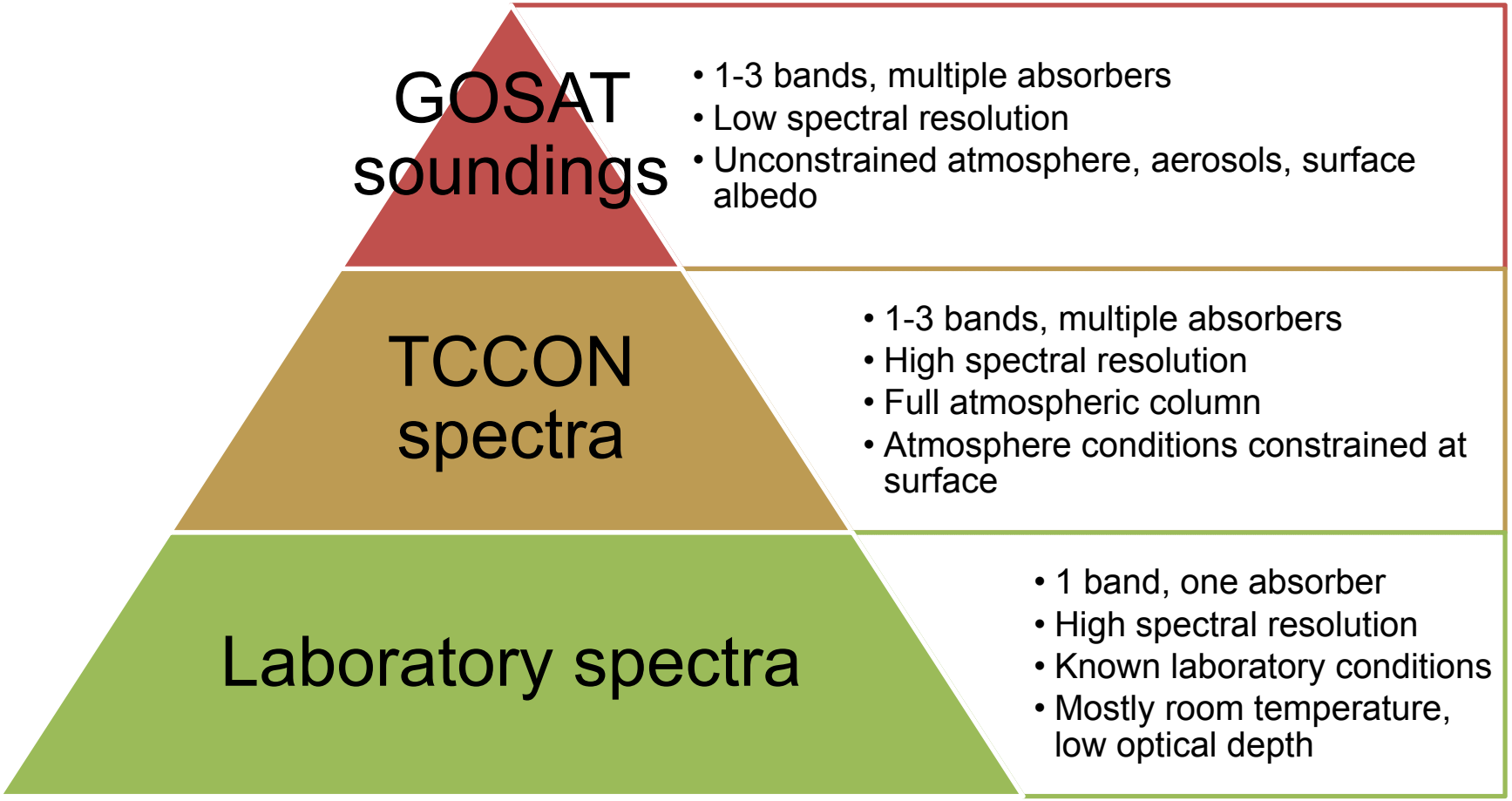
- Problem: Advanced spectroscopic models too slow for online use
- Solution: pre-computed lookup table for linear interpolation
- OCO-2 supercomputer computes cross sections at independent temperature and pressure levels (~1 month of CPU time)



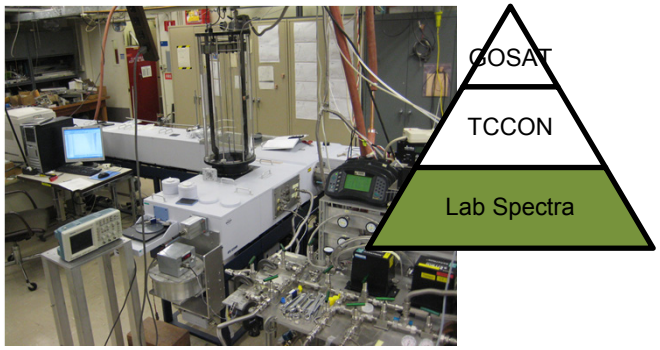
Parameter sources

ABSCO Tables		v3.3	v4.0
4850cm^{-1} CO_2	**Line shape**	Voigt, Toth 2008	**SDV [Benner/Devi]** **Minor isotopes** **via Toth et al.**
	mixing	[Hartmann 2008]	**Multi-spectrum** **[Benner/Devi]**
	continuum		**additional continuum**
6200cm^{-1} CO_2	**Line shape**	SDV [Devi et al. 2007]	
	mixing	[Hartmann 2008]	**Multi-spectrum** **[Devi et al. 2007]**
13200cm^{-1} O_2	**Line shape**	Voigt [Tran 2006]	
	mixing	[Tran 2006]	
	rescaling		**rescaled to match *a priori* surface pressure**

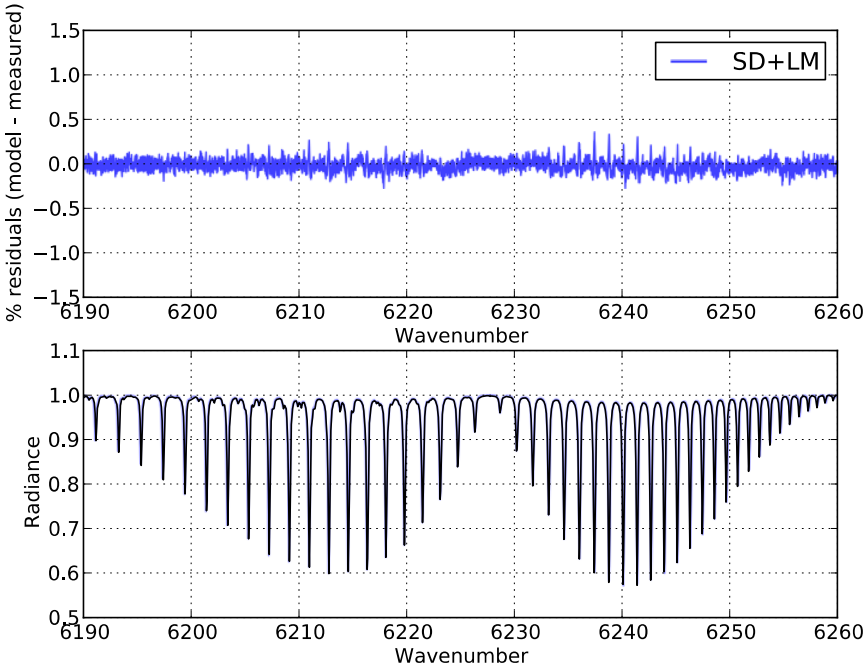
ABSCO Evaluation



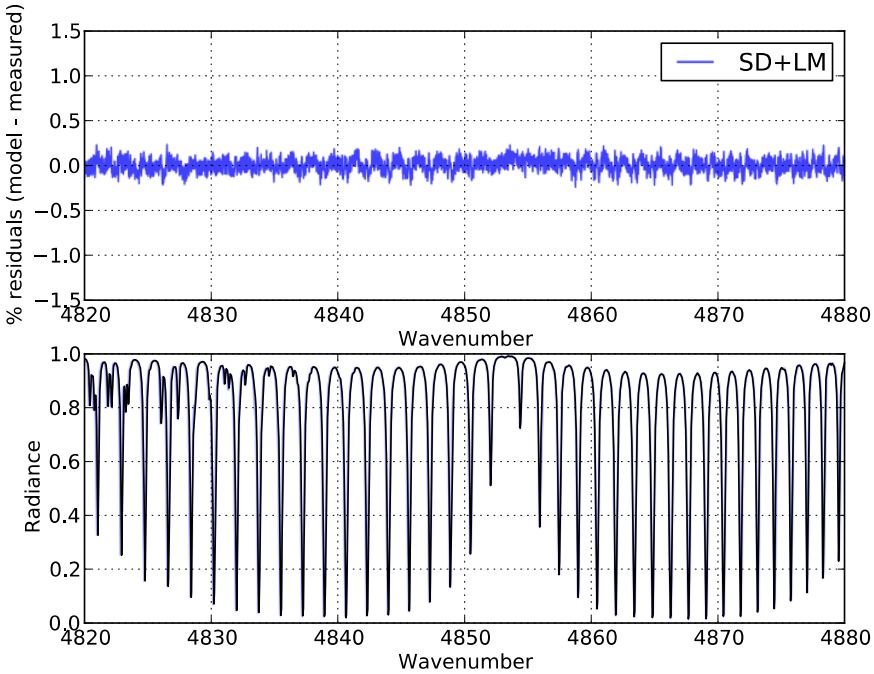
Evaluation with lab spectra



JPL Bruker FTS

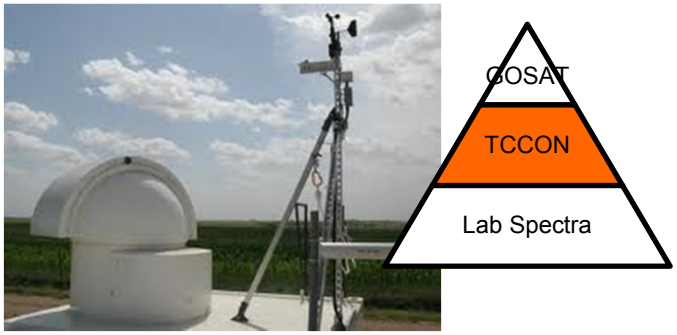


1.6 μm band, path length 32.54m
optical path difference 75cm
Total cell pressure is 742 Torr
Sample is 9.03% air-broadened $^{16}O^{12}C^{16}O$



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

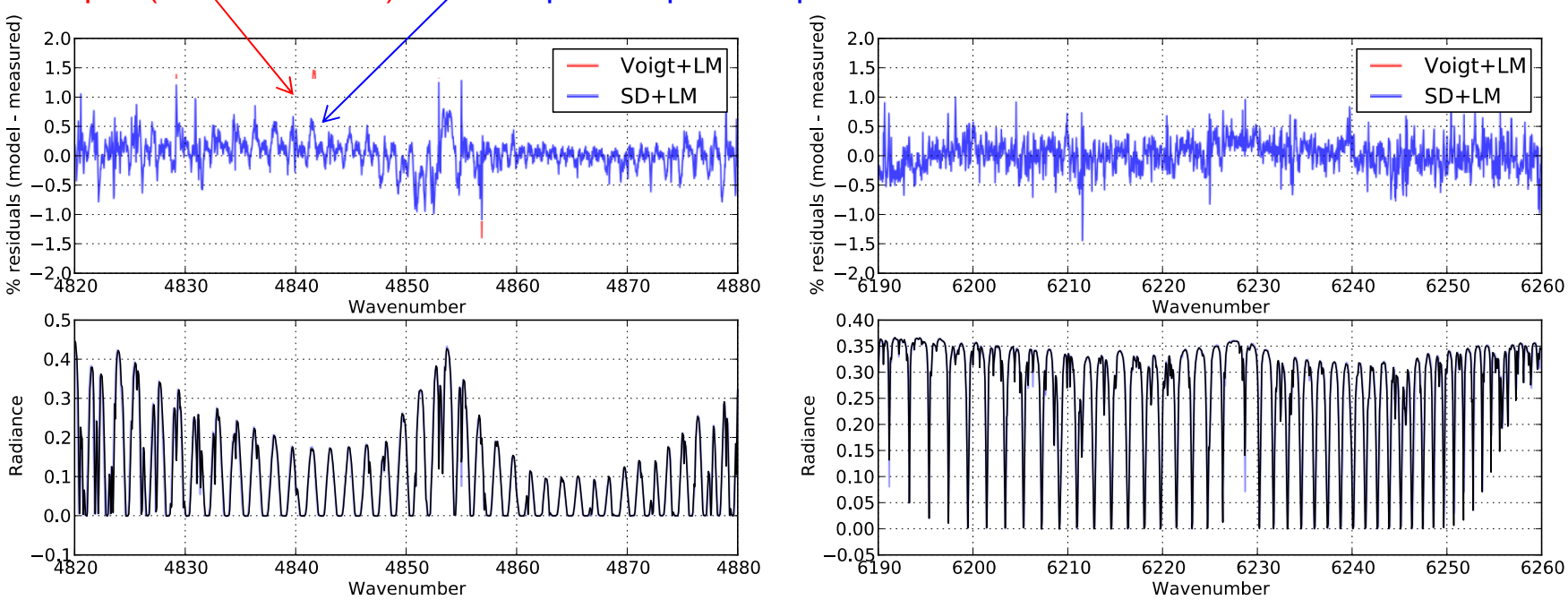
Evaluation with TCCON network data



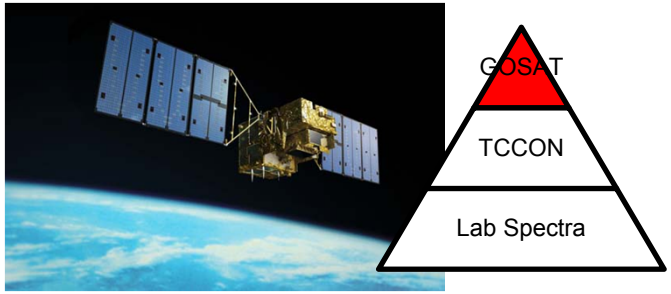
TCCON retrieval for Park Falls 22 Dec. 2004
~12 airmasses

State of the art
First-order line mixing, Voigt shapes (HITRAN 2012?)

ABSCO v4.0
Nearest-neighbor line mixing
Speed dependent profile

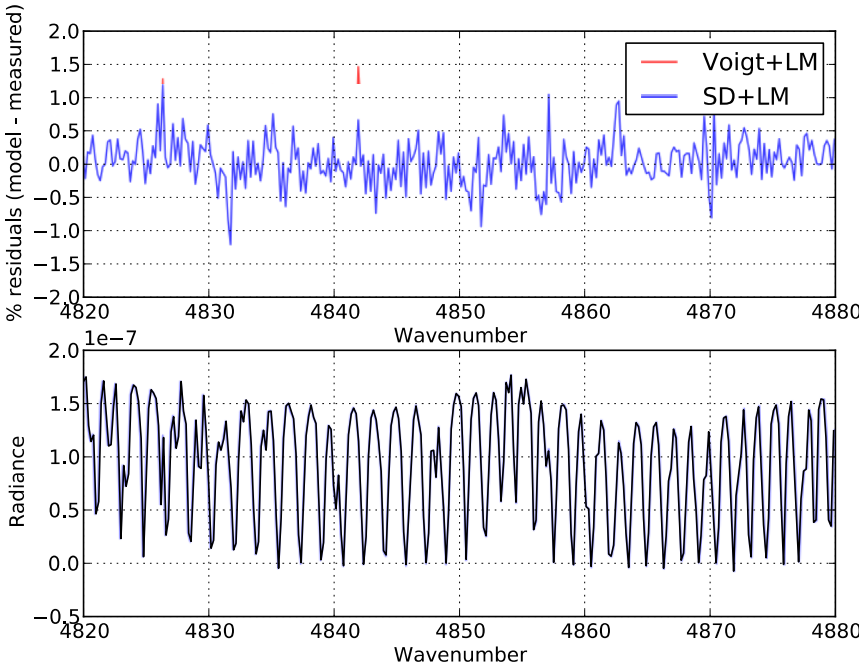


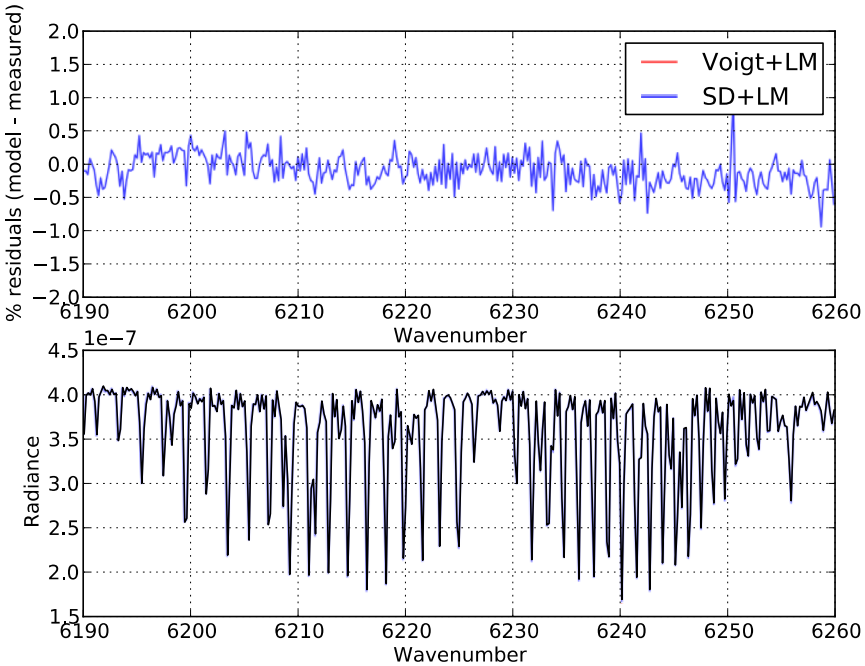
Evaluation with GOSAT data



Mean of soundings over TCCON stations

# Converged		Scatter v. TCCON		Correlation	
V+LM	V4.0	V+LM	V4.0	V+LM	V4.0
279 (65.6%)	300 (70.6%)	1.50 ppm	1.39 ppm	0.767	0.781





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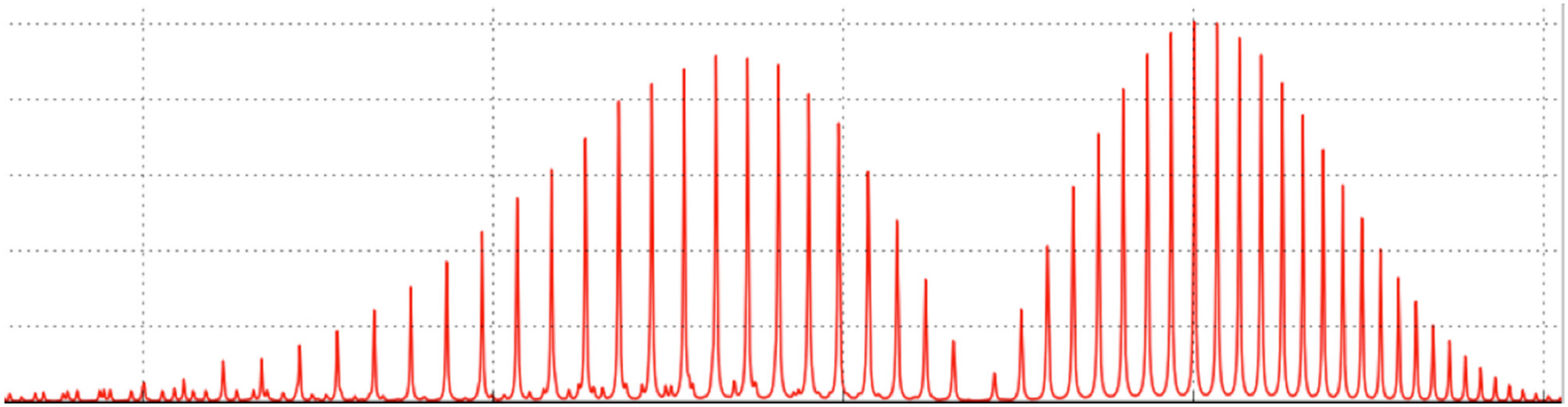
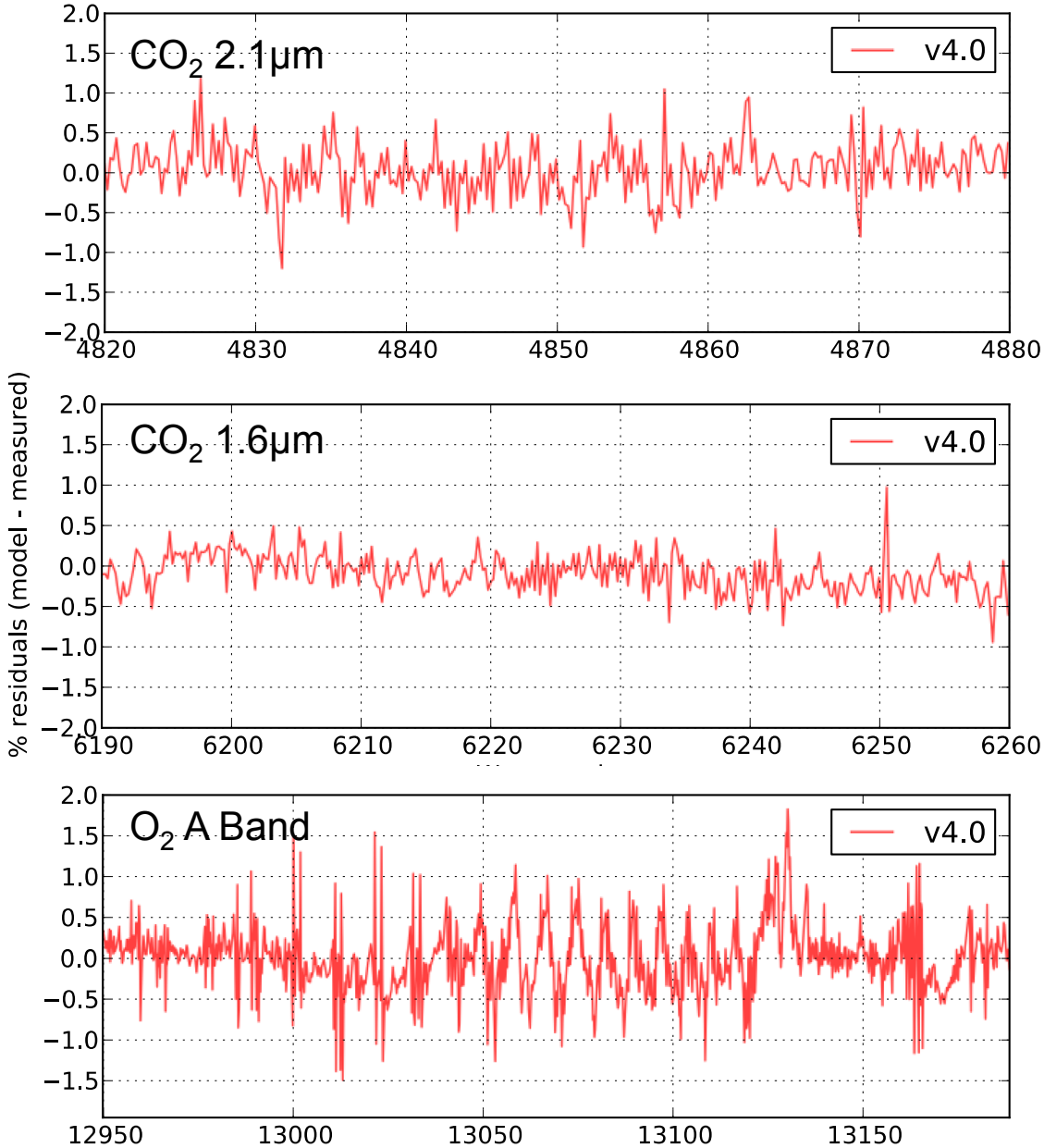


Pending challenges

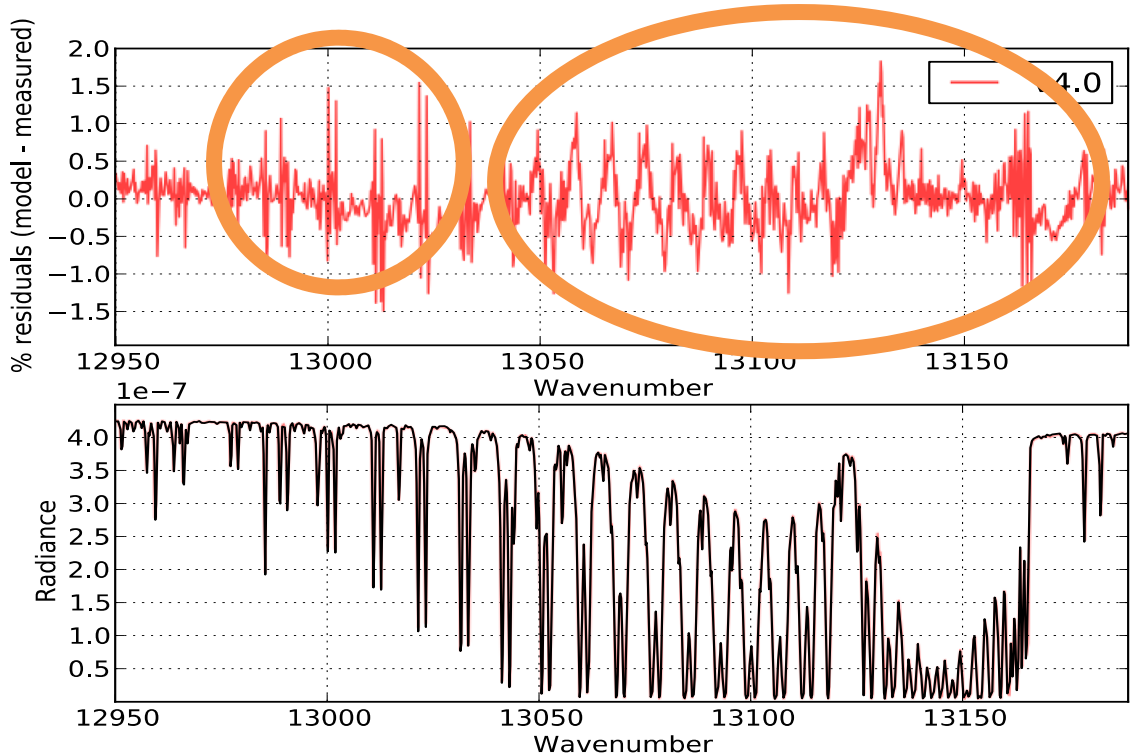
10hPa bias in surface pressure

Airmass bias in single-band CO_2 retrievals (especially in the 2.1μm band)



The A Band surface pressure bias

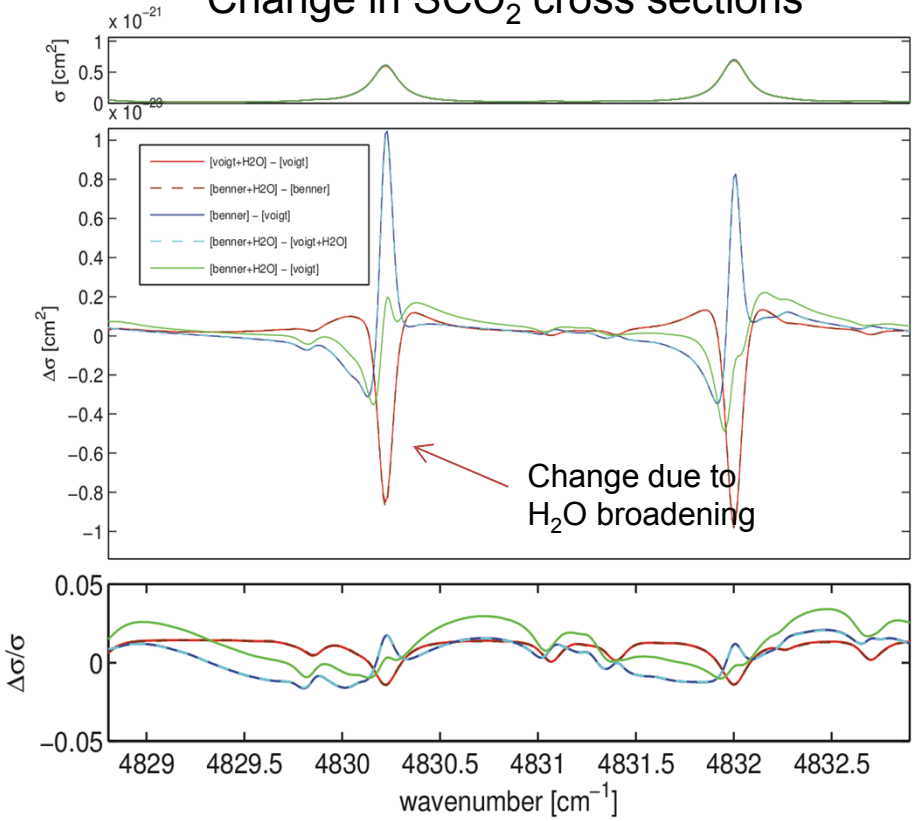
- Errors currently addressed by rescaling cross sections to remove the empirical mean error
- Line mixing and Dicke narrowing may both play a role
- Future models will model these effects directly



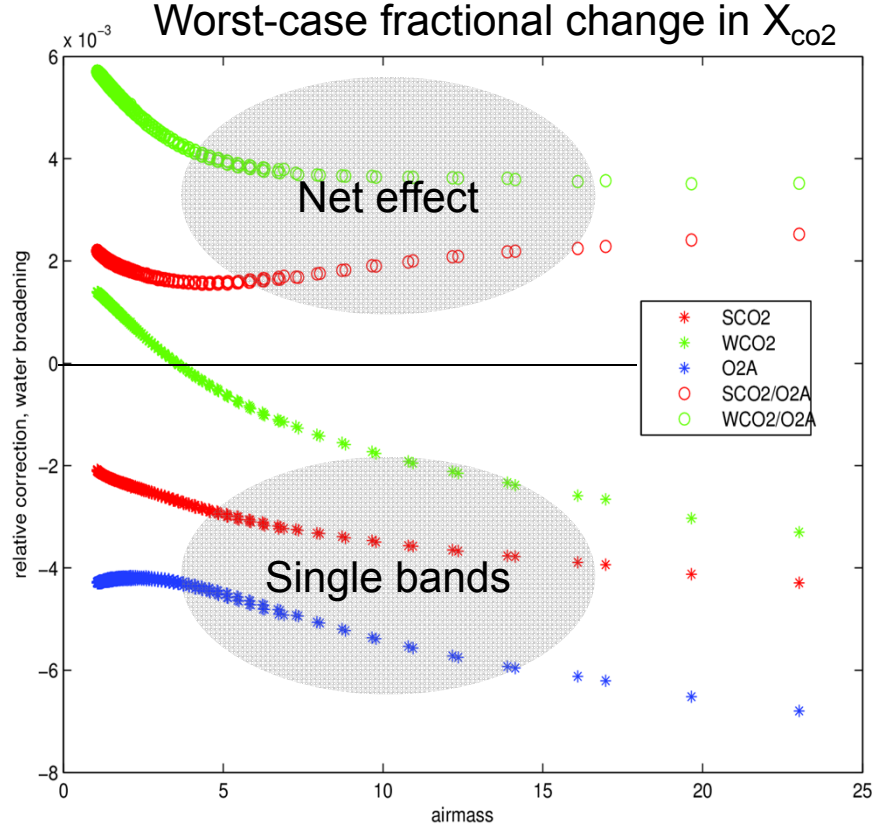
Current challenges: H_2O broadening

Broadening by water (Sung 2009) appears significant

Change in SCO_2 cross sections



Worst-case fractional change in X_{co2}



Courtesy Fabiano Oyafuso, JPL

H_2O broadening of CO_2

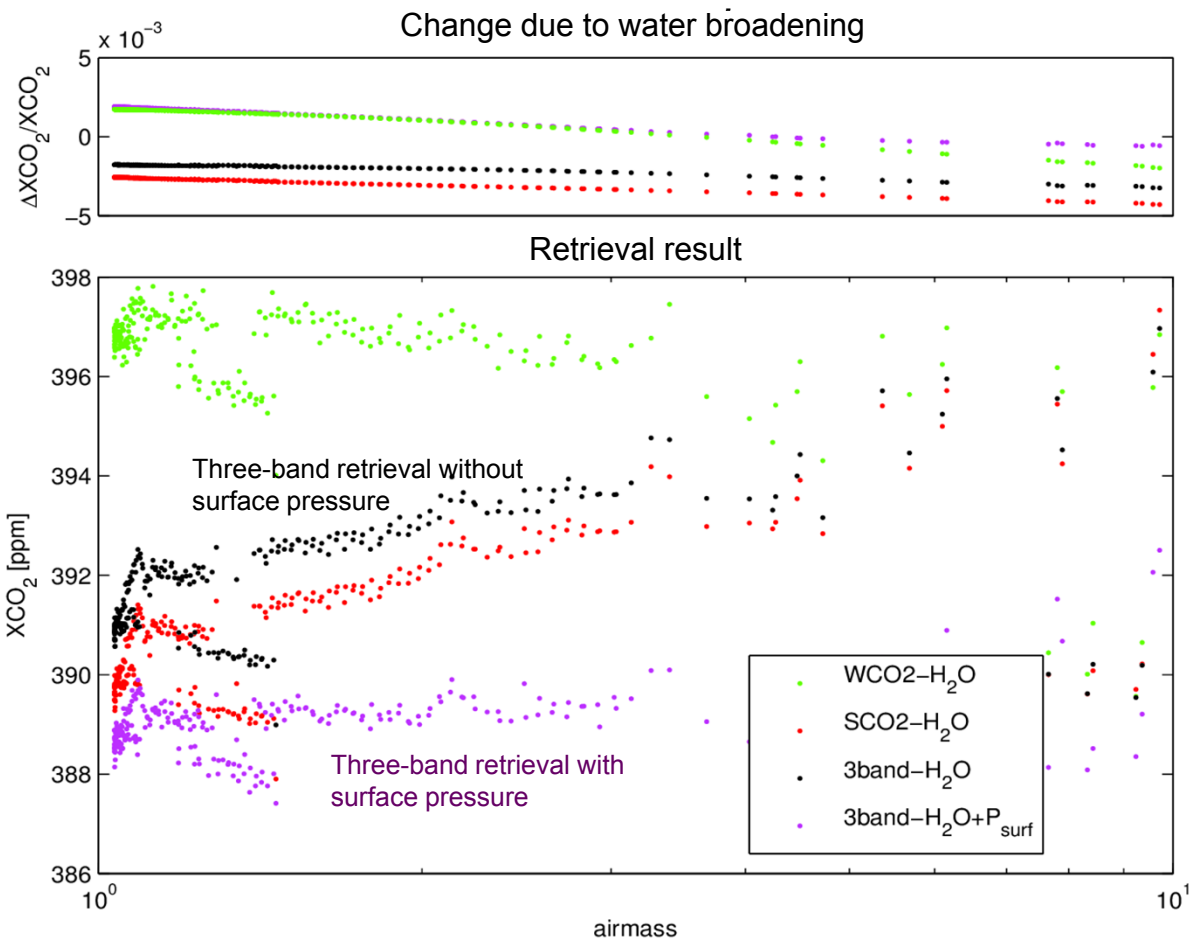
Water broadening now implemented

- O_2 from Fanjoux
- CO_2 from [Sung 2009]

Single band results agree with an implementation in GFIT.

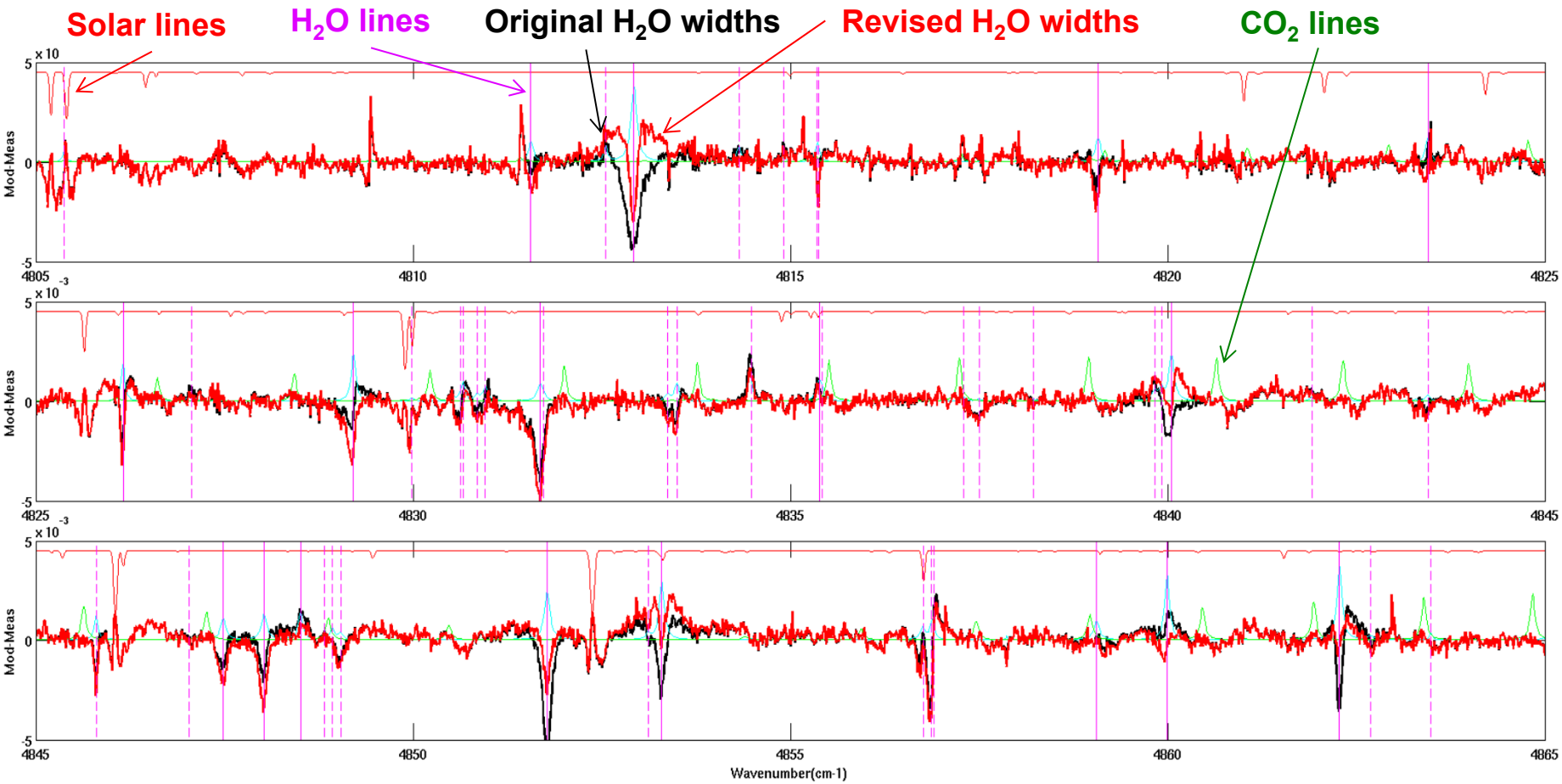
Changes X_{CO2} by up to ~0.4%, though residuals still dominated by other spectroscopic effects.

For L2, start with linear interpolation for the VMR interval from 0 to 5%?



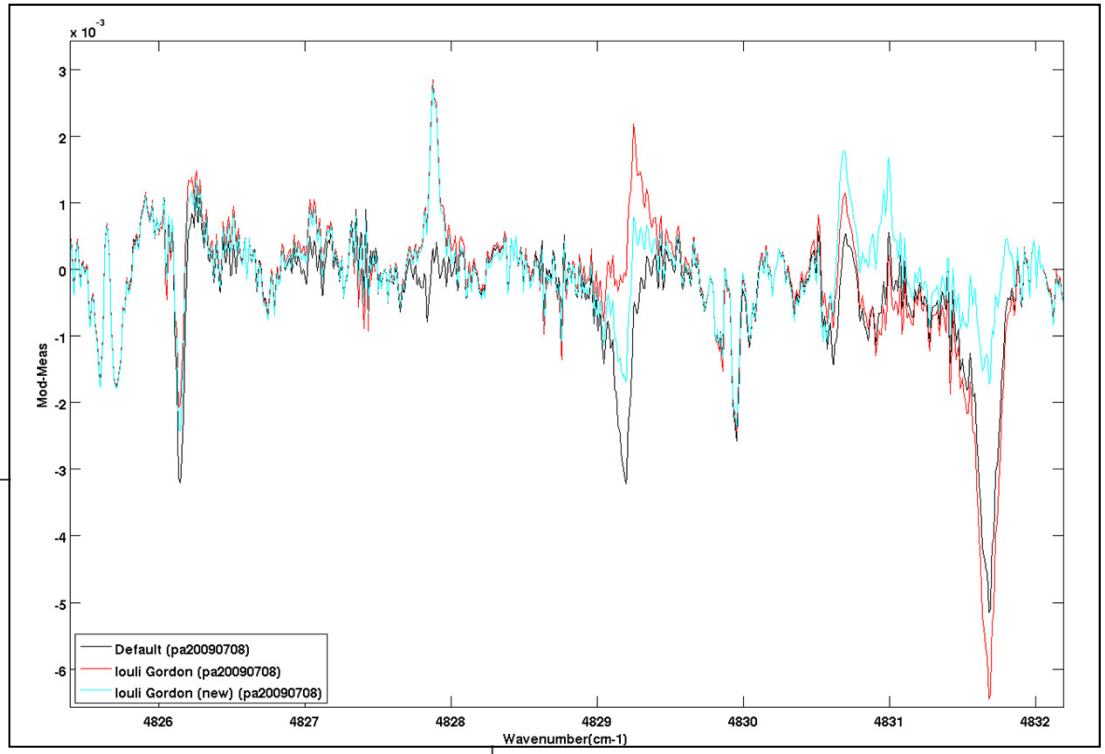
Courtesy Fabiano Oyafuso

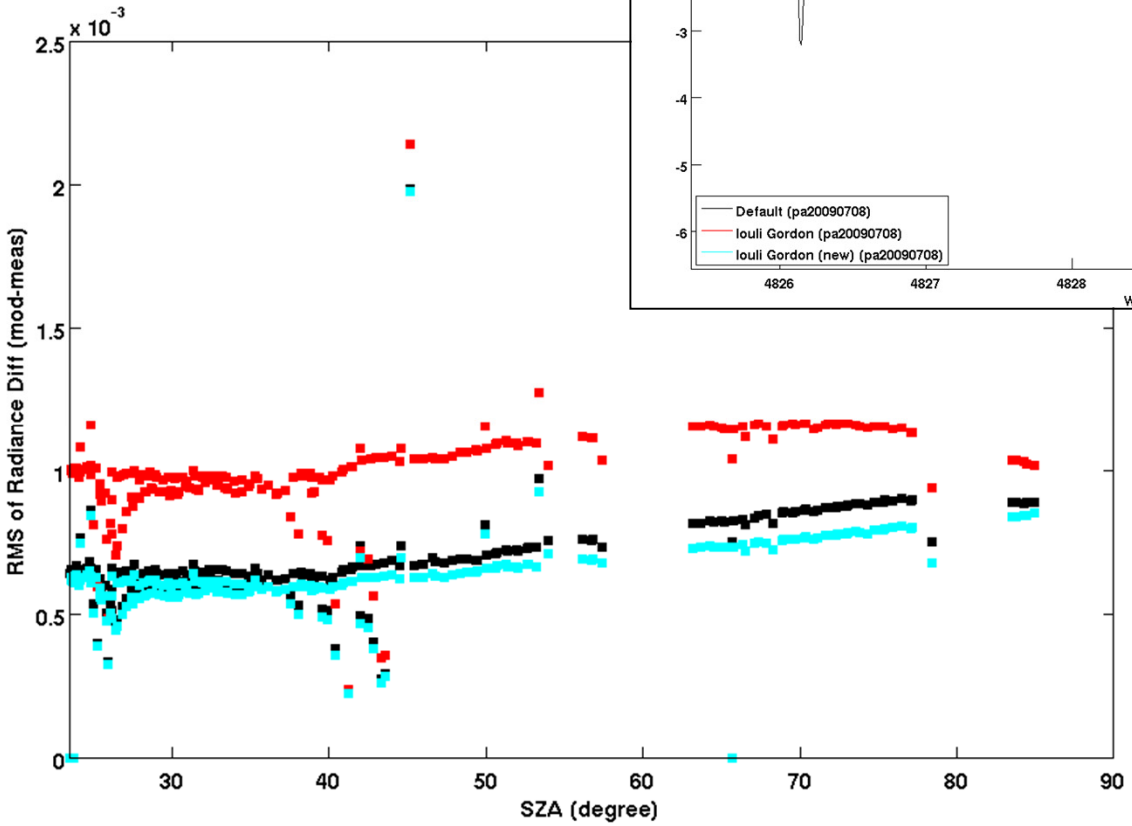
Line-by-line residual inspections



Courtesy Yibo Jiang, Linda R. Brown

Improving H_2O intensities



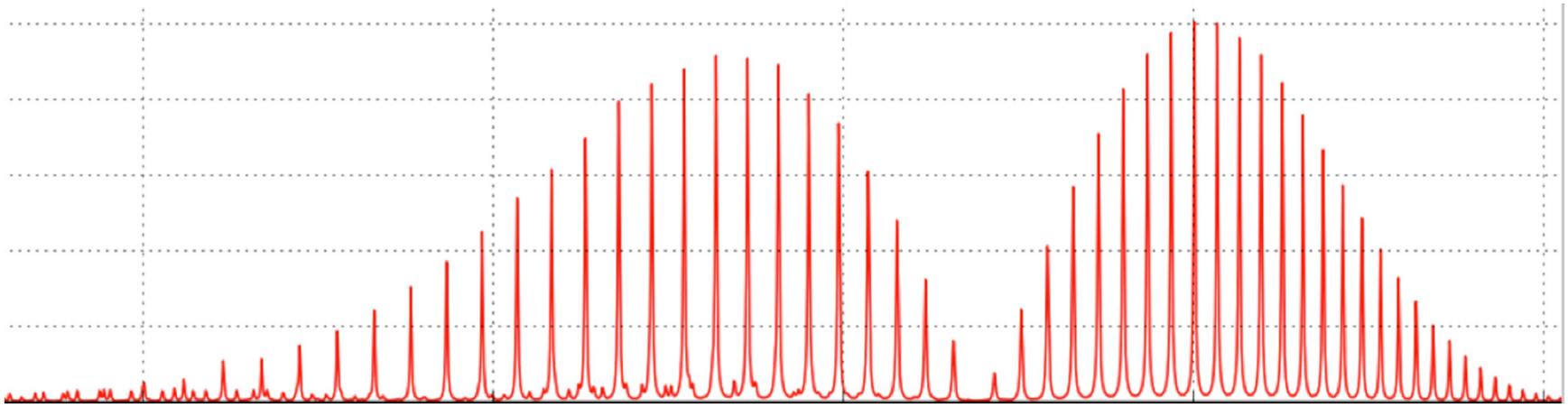


Work in progress, courtesy Lorenzo Lodi and Jonathan Tennyson from UCL, Iouli Gordon from SAO, Yibo Jiang from JPL

Moving to v4.1

ABSCO Tables		V4.0	V4.1
4850cm^{-1} H_2O	**Line parameters**	HITRAN 2008	**Revised widths and intensities**
4850cm^{-1} CO_2	**Line shape**	SDV [Benner/Devi] Minor isotopes via Toth et al.	**Foreign broadening by H_2O**
	mixing	Multi-spectrum [Benner/Devi]	
6200cm^{-1} CO_2	**Line shape**	SDV [Benner/Devi]	**Foreign broadening by H_2O**
	mixing	Multi-spectrum [Devi et al. 2007]	
13200cm^{-1} O_2	**Line shape**	Voigt	**Rautian or Galatry**
	mixing	First-order	**Nearest Neighbor**
	rescaling	rescaled to match *a priori* surface pressure	

Discussion

- Recent improvements are a step in the right direction
- Radiometric accuracies are not yet to the desired 0.1% level, and some systematic errors remain
- New measurements (CRDS) can better constrain line shapes
- Major priorities:
  - The A Band
  - H_2O broadening (for which we'll need accurate H_2O retrievals)

Questions?