ACOS/OCO-2 Progress on Gas Absorption Cross Sections

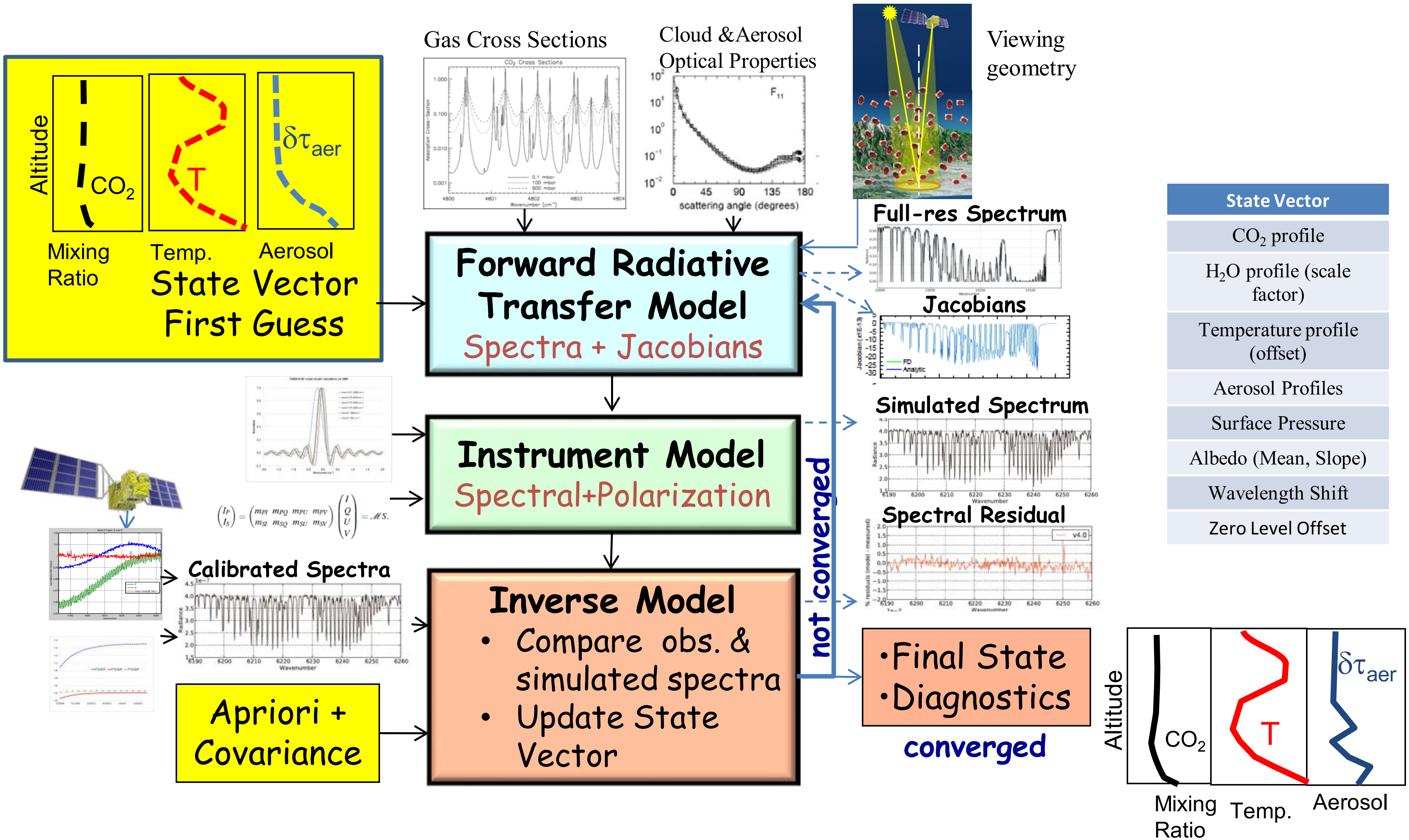
The OCO-2 Gas Absorption Coefficient (ABSCO) Group

29 November, 2012

The ABSCO Group

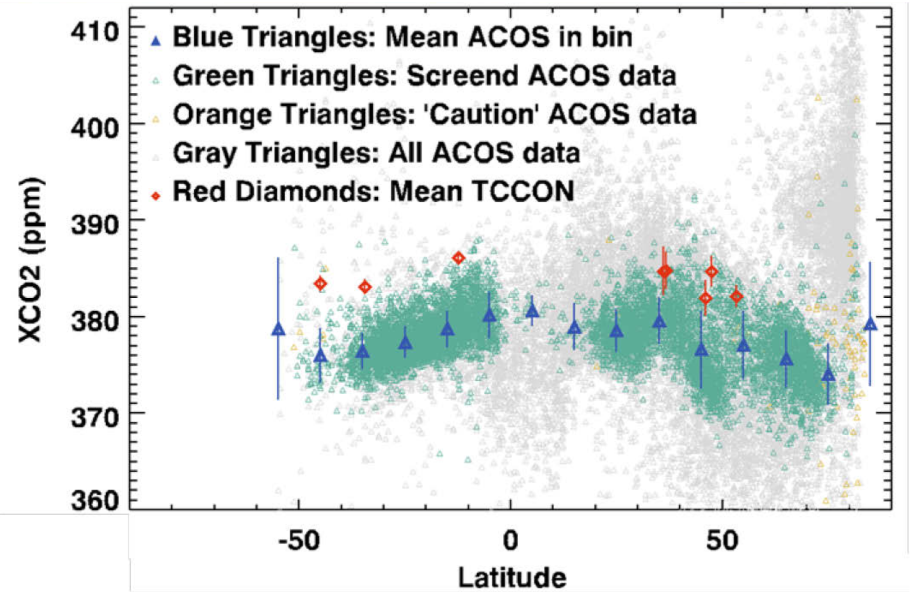
- David Thompson (JPL/Caltech)
- Chris Benner (William and Mary)
- Linda Brown (JPL/Caltech)
- David Crisp (JPL/Caltech)
- Malathy Devi (William and Mary)
- Brian Druin (JPL/Caltech)
- Iouli Gordon (Harvard)
- John Hodges (NIST)
- Yibo Jiang (JPL/Caltech)
- David Long (NIST)
- Eli Mlawer (AER)
- Charles Miller (JPL/Caltech)
- Fabiano Oyafuso, (JPL/Caltech)
- Vivienne Payne (JPL/Caltech)
- Keeyoon Sung (JPL/Caltech)

The ACOS “Full Physics” X_{CO2} Retrieval Algorithm

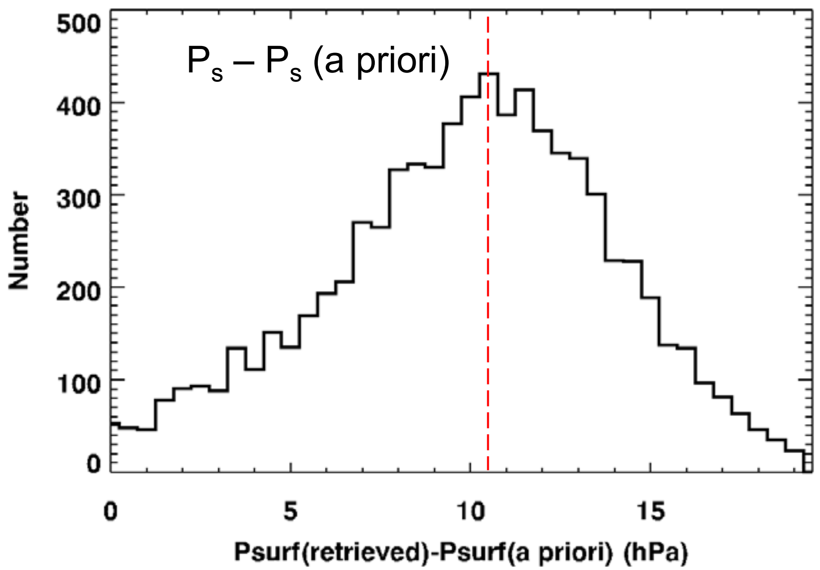


State Vector
CO_2 profile
H_2O profile (scale factor)
Temperature profile (offset)
Aerosol Profiles
Surface Pressure
Albedo (Mean, Slope)
Wavelength Shift
Zero Level Offset

Biases in Early ACOS X_{CO2} Products



ACOS GOSAT X_{CO2} estimates (green and grey triangles) and their zonal averages (blue triangles with 1σ errors) are compared to TCCON X_{CO2} estimates (red diamonds).

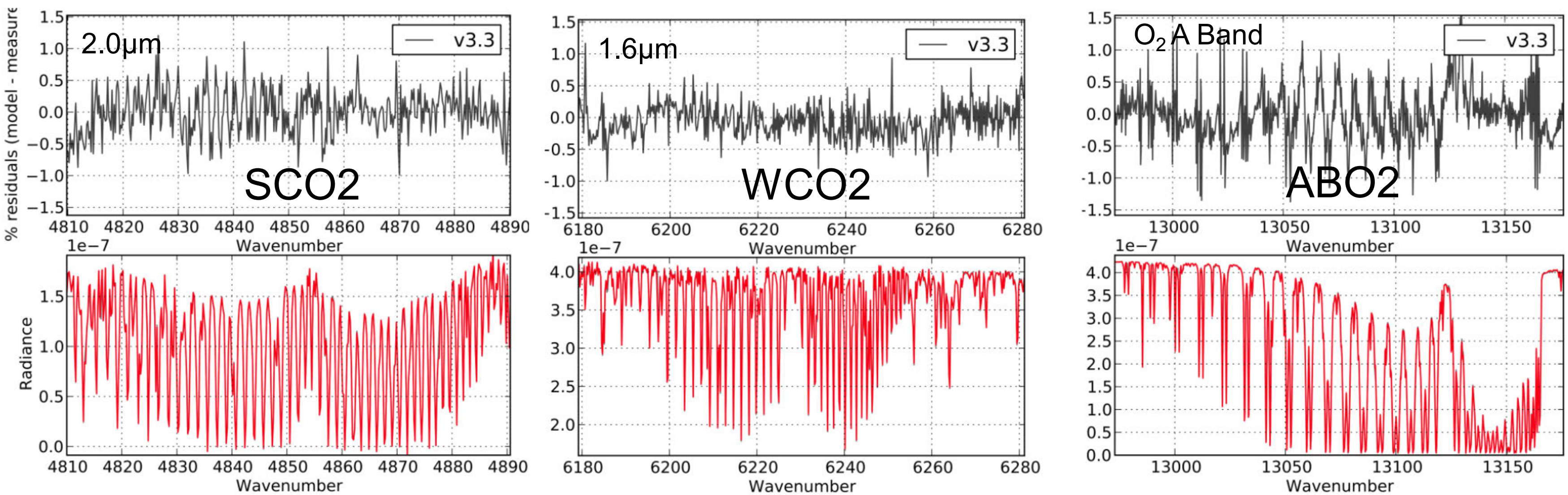


Global histogram of differences between retrieved surface pressures and a priori (ECMWF) surface pressures show a ~10 hPa bias.

- Initial comparisons of ACOS GOSAT and TCCON retrievals showed a consistent global bias of ~2% (7 ppm) in X_{CO2} when compared with TCCON and aircraft measurements.
- About 2/3 of this bias is associated with a ~10 hPa (1%) high surface pressure bias, that was traced to limitations in the Oxygen A-band spectroscopy.
- Much of the remaining bias is associated with uncertainties in CO_2 spectroscopy

Evidence of Shortcomings in Gas Absorption Coefficients

- Persistent spectrally-dependent residuals in ensembles of GOSAT and TCCON retrievals provide additional evidence of shortcomings gas absorption cross sections
  - Residuals correlated with spectral features limit the retrieval algorithm's ability to exploit the full information content of the spectra, and converge to a unique, best estimate of X_{CO2}



Persistent spectral residuals are seen in all 3 bands used to retrieve X_{CO2} from GOSAT spectra. Those in the SCO2 and ABO2 are most strongly correlated with the band structure. These issues do not impair TCCON X_{CO2} retrievals, because TCCON uses the WCO2 and O2 $^1\Delta_g$ band instead of the A-band in these retrievals.

Improved Gas Absorption Cross Sections

The ACOS ABSCO team embarked on a three-element approach to improve our understanding the CO_2 and O_2 absorption bands needed to retrieve X_{CO2}, including:

- New laboratory measurements (Long path FTS, Cavity Ring-down, Photoacoustic)
- Ground-based direct solar observations from TCCON
- GOSAT measurements

GOSAT soundings

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

TCCON spectra

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

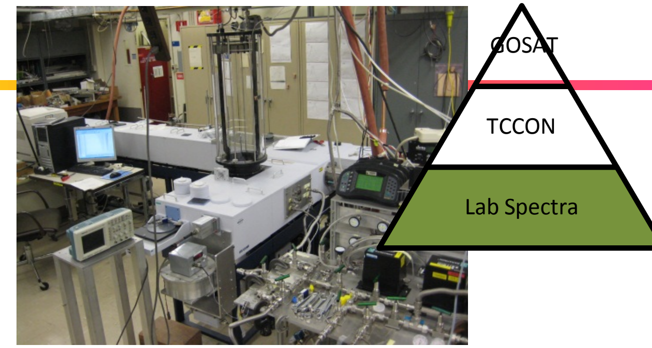
Laboratory spectra

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

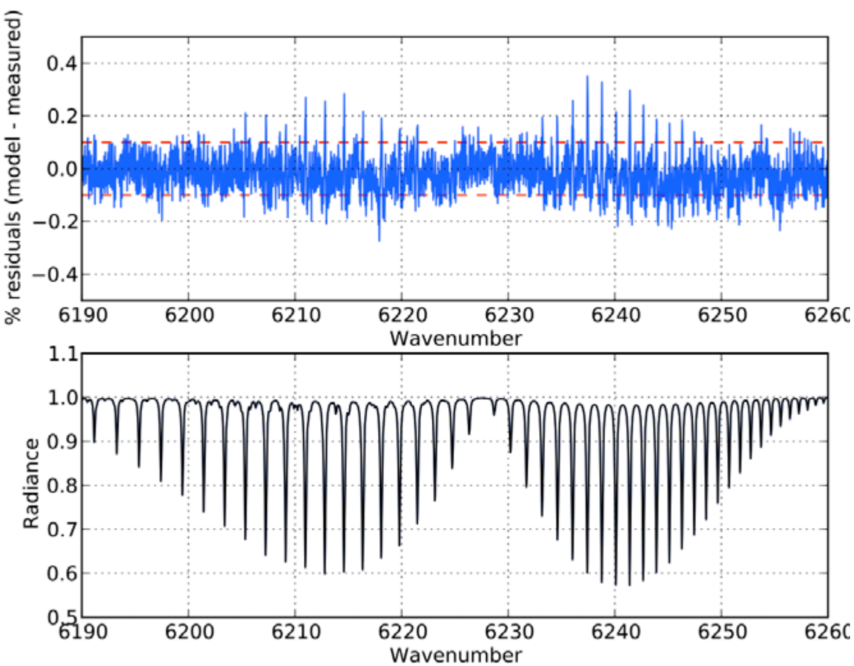
Advances in Laboratory Measurements

- The initial focus was on the CO_2 bands at 1.61 and 2.06 microns
  - Exploiting available measurement capabilities and recent advances in instrumentation and measurement techniques
    - Improved characterization of trace gas composition, temperature, and optical path length in convention, long-path absorption cells
    - New methods, including Frequency Stabilized Cavity Ring-Down (FS-CRDS) and Photoacoustic methods, that provide high signal-to-noise ratios over a wide dynamic range, facilitating measurements of weak absorption
    - Advanced, multi-spectral fitting techniques, that derive spectral line parameters (positions, strengths, widths, pressure shifts) from ensembles of spectra collected for a range of optical paths, pressures, temperatures, and absorbing gas concentrations
    - Self-consistent treatment of line mixing and line shapes that include speed-dependence and collisional narrowing as well as pressure and Doppler broadening effects
  - This investigation has yielded dramatic improvements in our ability to fit laboratory measurements of CO_2

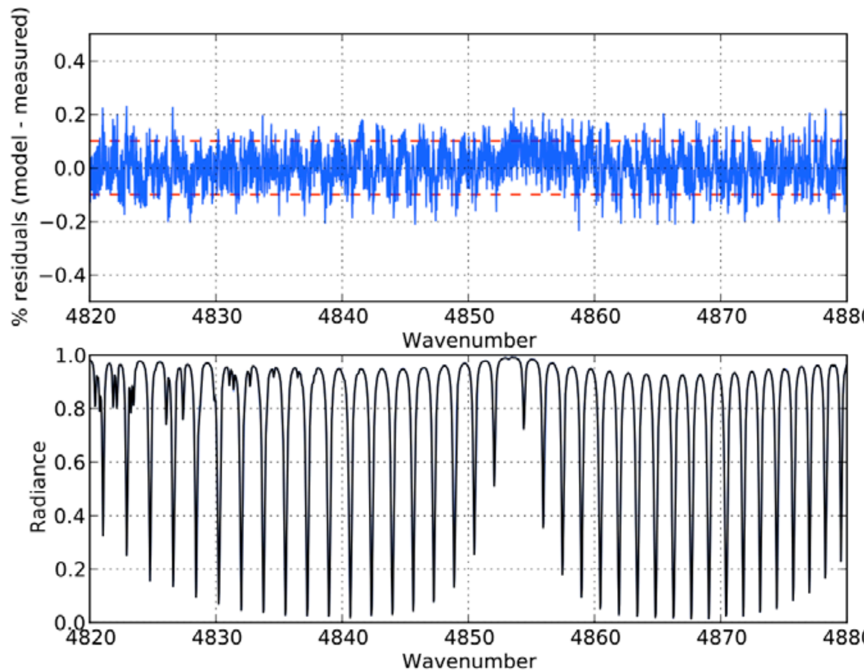
Evaluation with lab spectra



JPL FTS

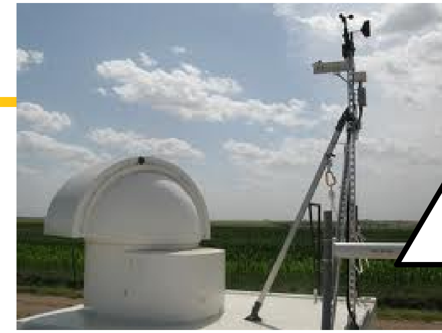


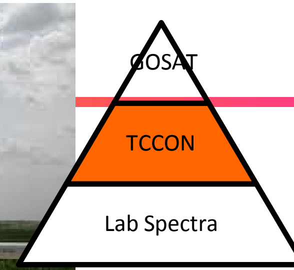
1.6 μm band, path length 32.54m
optical path difference 75cm
Total cell pressure is 742 Torr
Sample is 9.03% air-broadened $^{16}O^{12}C^{16}O$



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



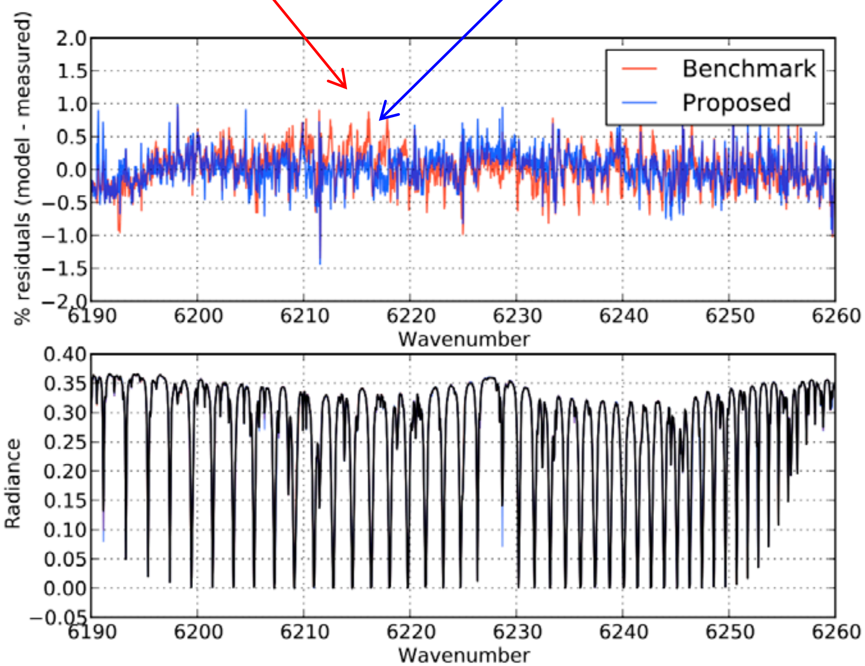


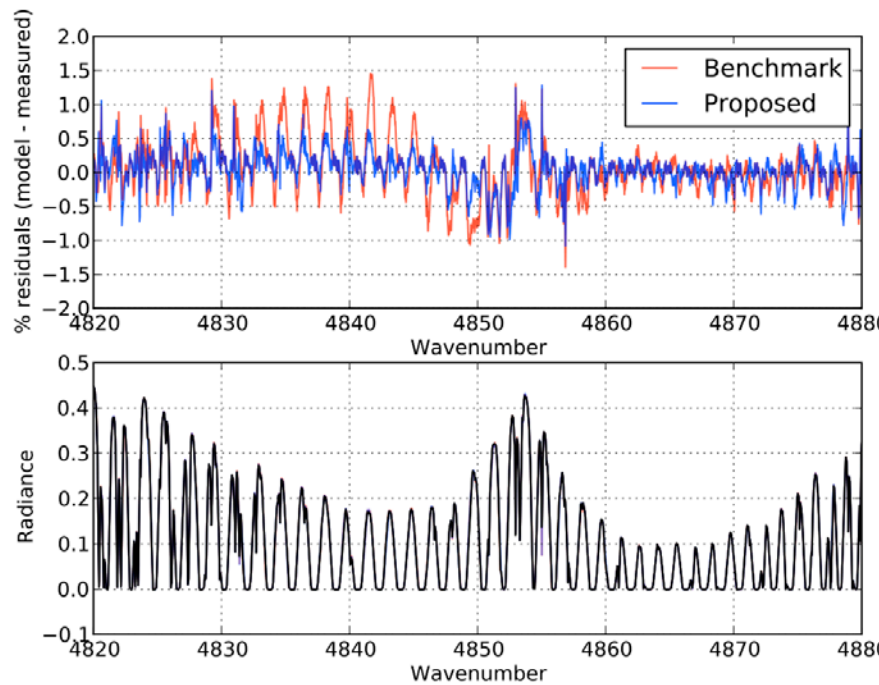
TCCON retrieval for Park Falls 22 Dec. 2004
~12 airmasses

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

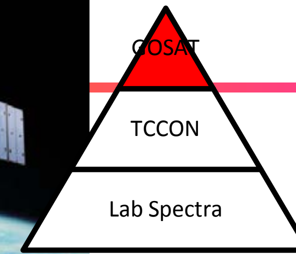
“Ongoing” model
Nearest-neighbor line mixing
Speed dependent profile

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

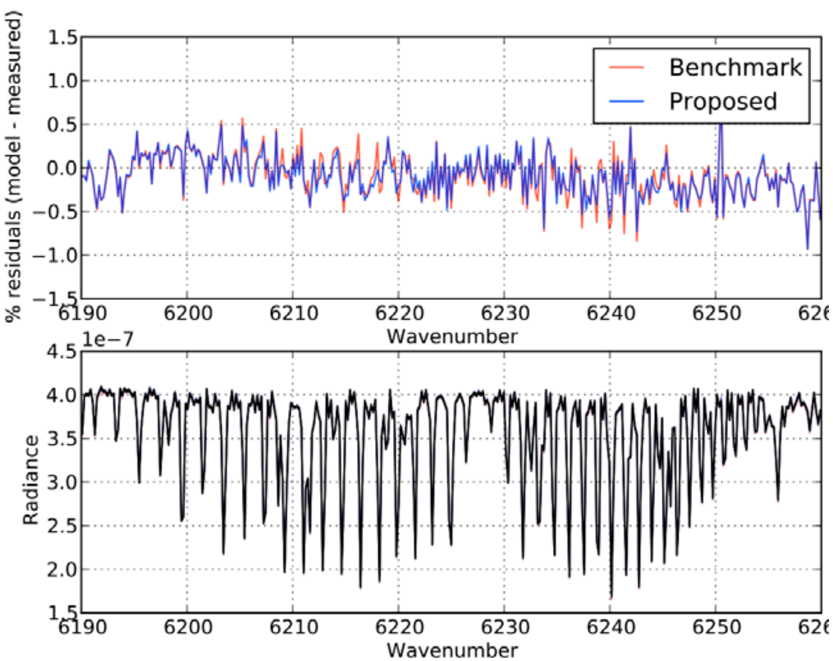


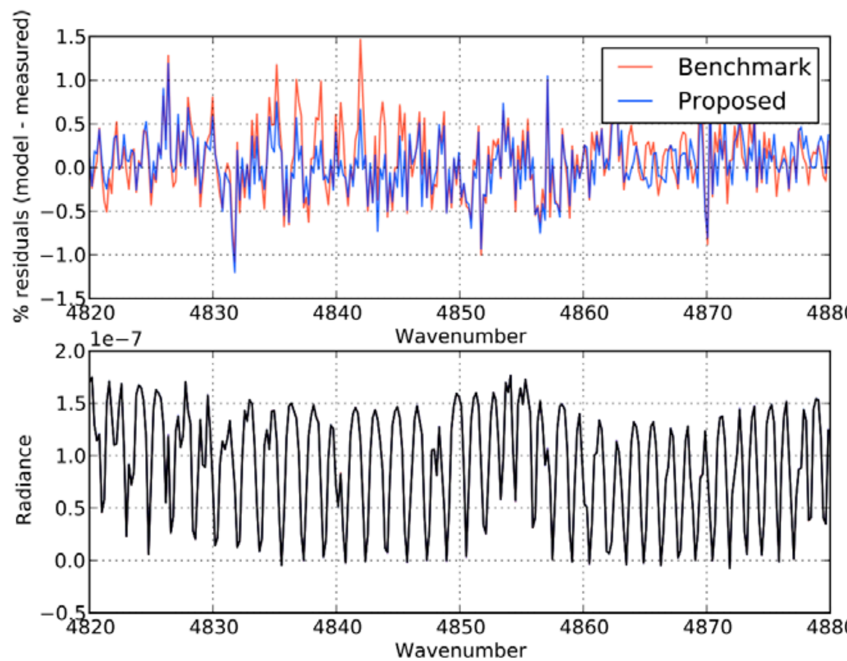


Evaluation with GOSAT data



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



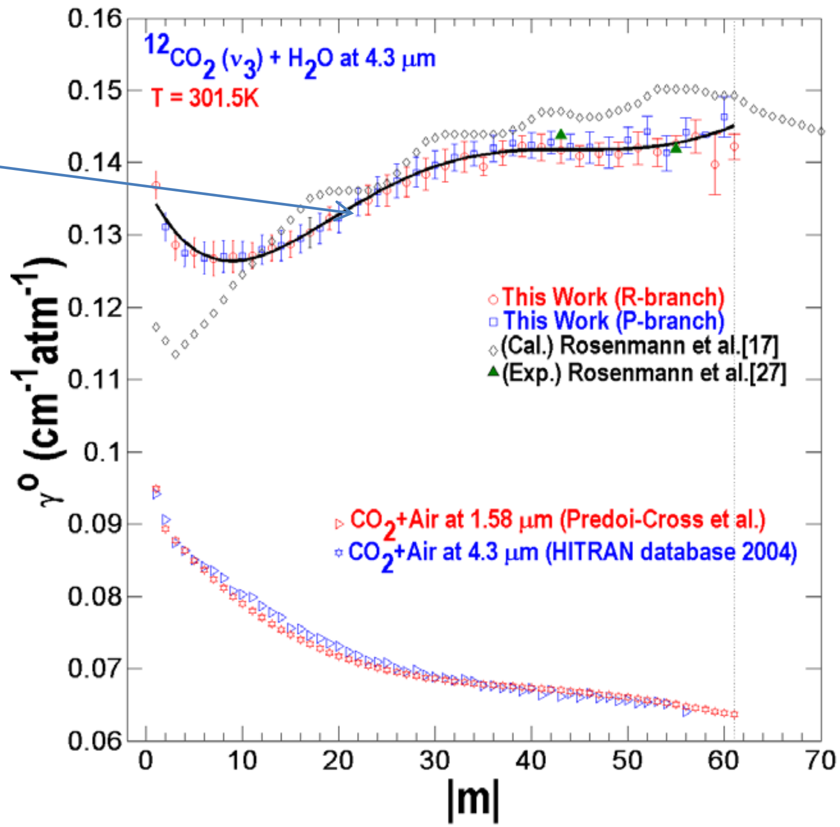


CO_2 lines broadening by H_2O

- Two recent publications suggest that water vapor broadens CO2 lines much more effectively than air (~1.8x).
- Consistent results now available from 2 different experiments

	Sung et al. (4.3 μm) half widths (cm^{-1})	Wallace et al. (1.6 μm) halfwidth (cm^{-1})
R14	0.1287 (±1.4 %)	0.136 (±19.8 %)
R16	0.1303 (±1.6 %)	0.134 (±17.9 %)
R18	0.1323 (±1.2 %)	0.133 (±20.3 %)

- Unlike air broadening and self broadening, which decrease with increasing rotational quantum number |m|, water broadening of CO_2 increases with increasing |m|.
- New measurements are being conducted to confirm these results and assess their impact on XCO2 retrievals from TCCON and GOSAT.



Water broadened half-widths of CO_2 (top) is compared to air broadened half widths (bottom) as function of rotational transition, |m|.

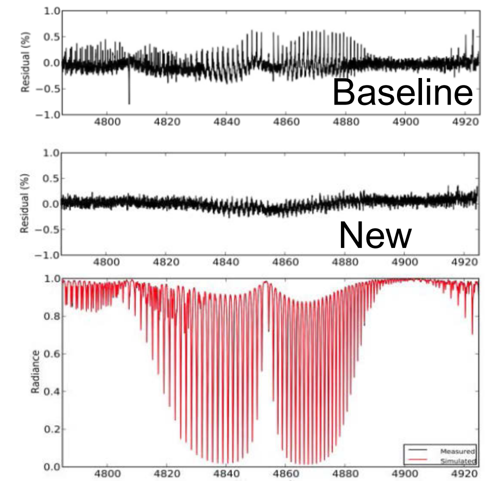
* K. Sung, L. Brown, RA Toth, T. J. Crawford, *Can J. Phys*, **87**, 469-484 (2009)

Measurements of CO_2 Spectra

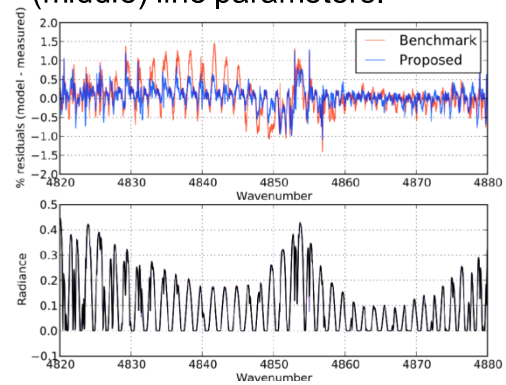
- The new, self-consistent line parameters yielded substantial improvements in fits to laboratory measurements of CO_2
  - Typical peak-to-peak residuals were reduced from 0.5% to 0.1%

- The use of these new line parameters in X_{CO2} retrievals from TCCON and GOSAT spectra also yielded reductions in both bias and spectrally-dependent residuals, but these reductions were more modest than those seen in the lab.

- These differences in performance may be associated with the physical conditions (e.g. vertical variations in p, T, or gas amount) or absorbers (e.g. water vapor line and continuum absorption) that were not included in the lab measurements.



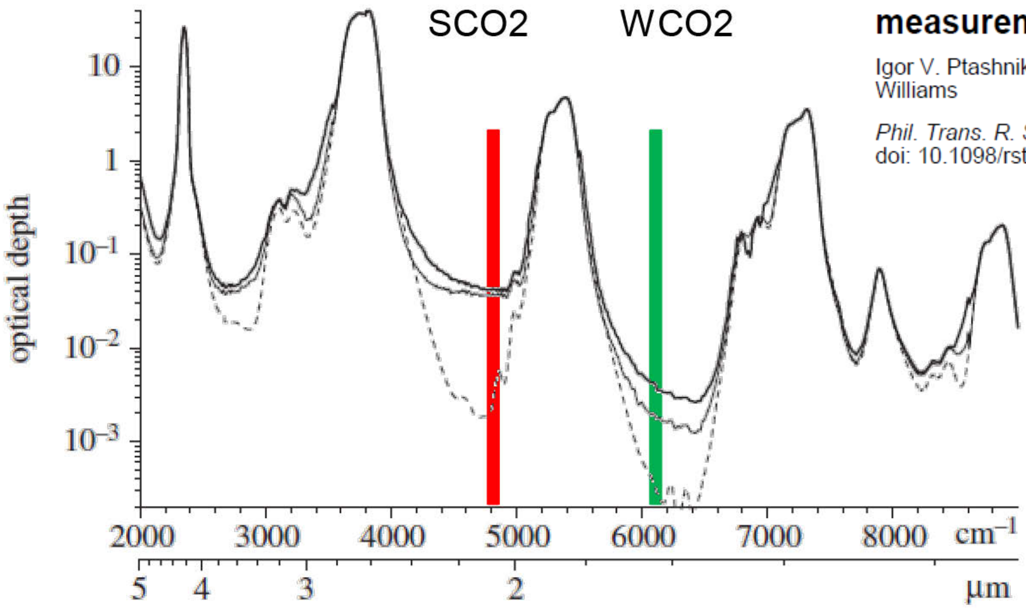
Lab measurements of the SCO2 band (bottom) shown with residuals for baseline (top) and revised (middle) line parameters.



TCCON measurements of the SCO2 band (bottom) shown with residuals for baseline (red) and revised (blue) line parameters.

Other Spectroscopy Issues

- Recent laboratory measurements indicate that the self- and air-broadened water continua absorption in the SCO2 (and WCO2) band may be much stronger than previously assumed.
- This continuum absorption could contribute to both the spectrally-dependent residuals, and observed biases between X_{CO2} retrievals using the SCO2 and WCO2 bands



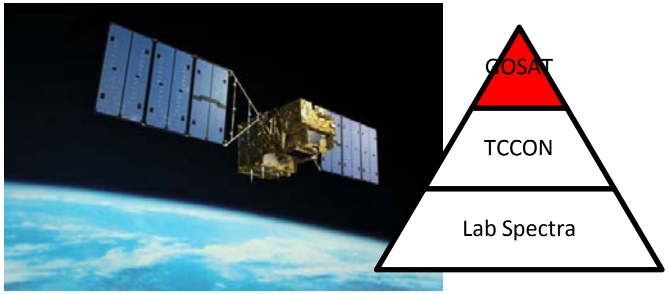
Water vapour foreign-continuum absorption in near-infrared windows from laboratory measurements

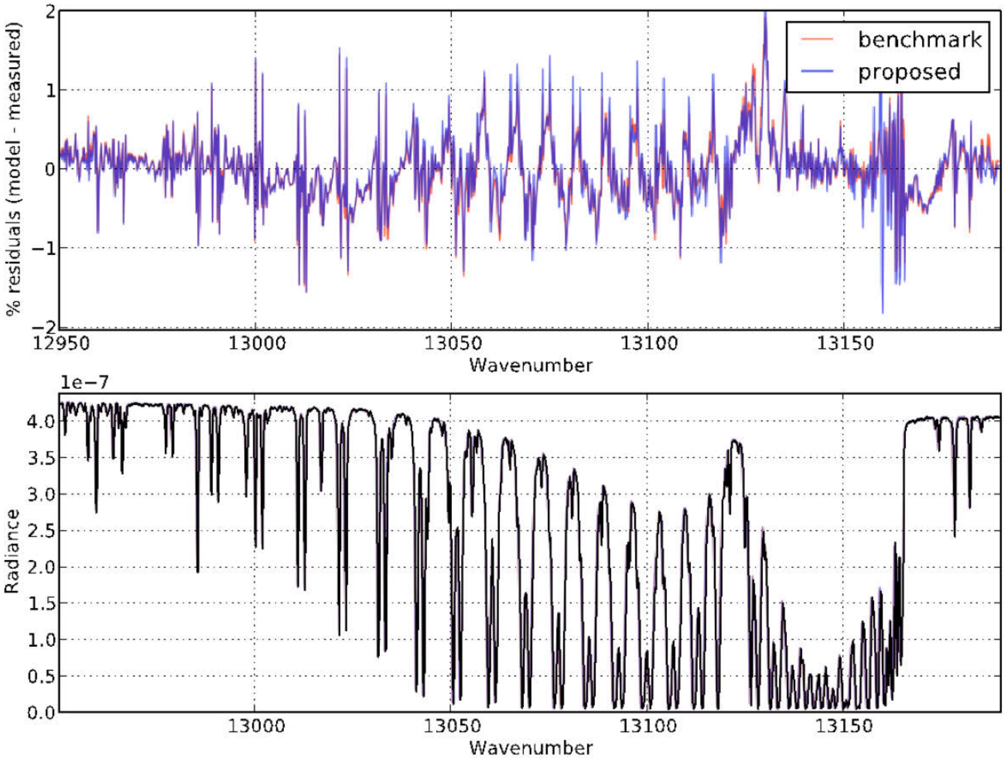
Igor V. Ptashnik, Robert A. McPheat, Keith P. Shine, Kevin M. Smith and R. Gary Williams

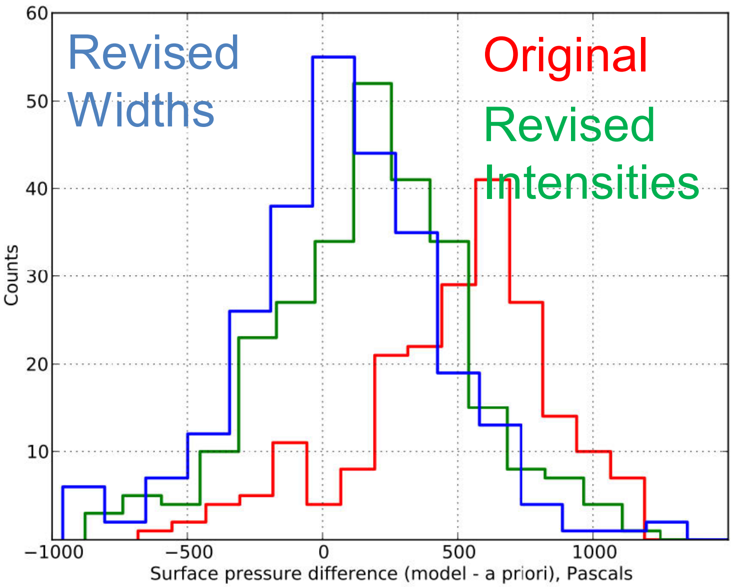
Phil. Trans. R. Soc. A 2012 **370**, 2557-2577
doi: 10.1098/rsta.2011.0218

Evaluation of O_2 with GOSAT data

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

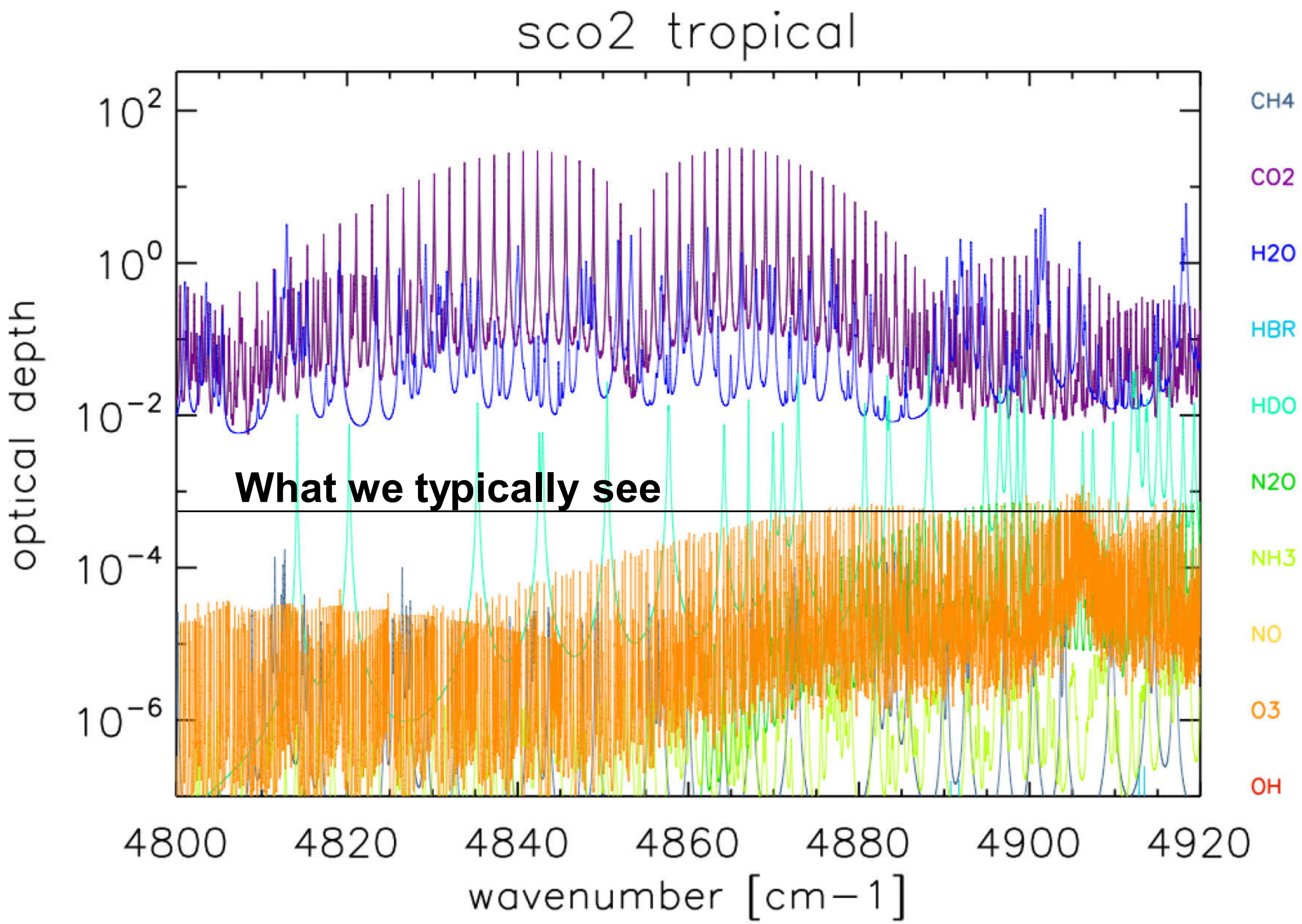






Surface pressure biases due to uncertainties in line strengths and widths.

3. Sensitivity to trace gases

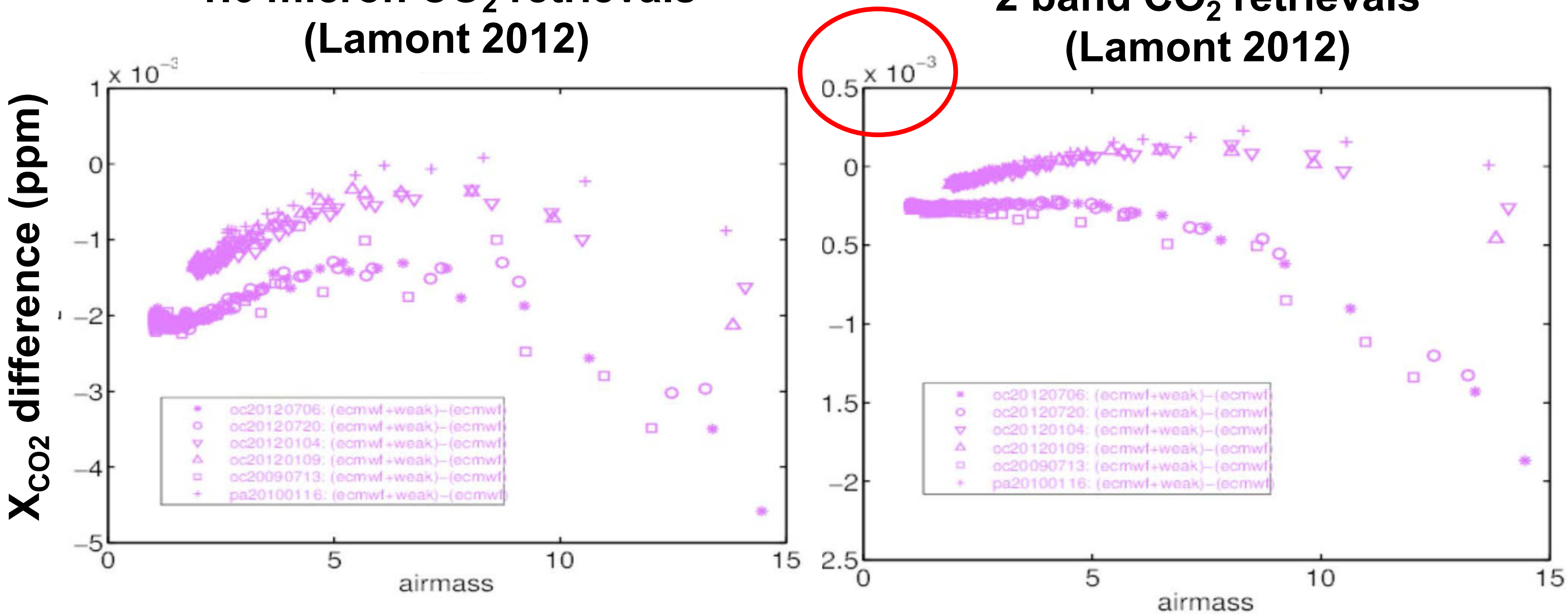


2. Sensitivity to weak CO_2 lines

Neglecting lines below HITRAN 2004 intensity cutoff of 10^{-26} has negligible impact

1.6 micron CO_2 retrievals (Lamont 2012)

2 band CO_2 retrievals (Lamont 2012)



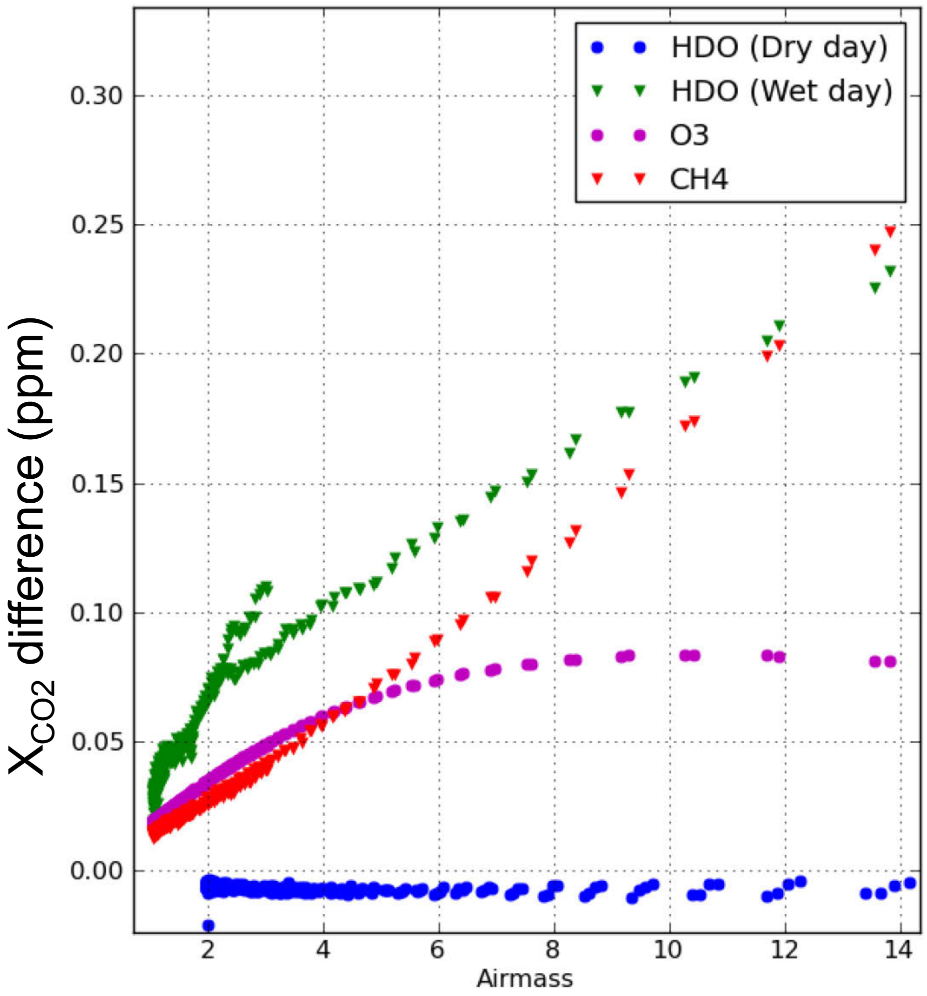
3. Sensitivity to trace gases

Preliminary evaluations on Lamont TCCON spectra, holding surface pressure fixed

Each gas contributes a *very* subtle benefit to spectrum fit residuals

Worth testing on GOSAT spectra?

Change in X_{CO2} from introducing trace gases

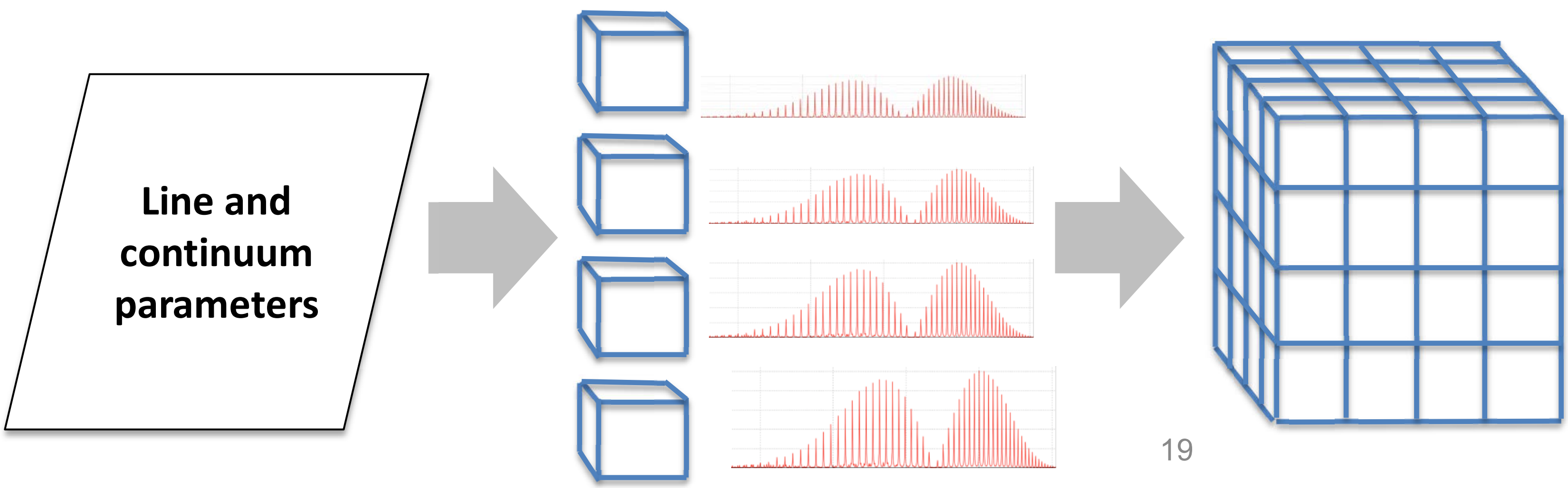


Summary of ACOS Gas Absorption Line Lists

	0.76µm O_2	1.61µm CO_2	2.06µm CO_2	H_2O
Spectral range	12745-13245 cm^{-1}	4700-6500cm^{-1}	4700-6500cm^{-1}	**12745-13245 cm^{-1}** 4700-6500cm^{-1}
Spectral resolution	0.01cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}	0.01 cm^{-1} or 0.002cm^{-1}
Position	**Long (2010), Long (2011)**	Devi (2007)[1]	Benner/Devi (2011)[1]	**Gordon (2012), Rothman (2010)**
Intensities	"	"	"	"
Air-widths	Tran (2008)	Predoi-Cross (2009)[1]	"	"
Air-shifts	Brown (2009) Robichaud (2008a) Predoi-Cross (2008)	Devi (2007b)[1]	"	"
Temp. dep.	Brown (2000)[1,2]	Predoi-Cross (2009)[1]	"	"
Line shapes	Voigt / **Galatry**	Speed-dependent Voigt	Speed-dependent Voigt	Voigt
Isotopologue abundance	Rothman (2009)[1]	Rothman (2009)	**Rothman (2009)**	Rothman (2009)
H_2O broadening	**Vess (2012)**	**Sung (2009)**	**Sung (2009)**	-
Air-Line mixing	Tran (2008)	Devi (2007)	Benner/Devi (2011)	-
" Temp. dep.	Tran (2008)	-	-	-
Speed dep.	-	Devi (2007)[1]	Benner/Devi (2011)[1]	-
Continuum	CIA via Tran (2008)	-	*	**Mlawer (2012)**

Absorption coefficient (ABSCO) Tables

- **Pre-computed ABSCO look-up tables**
  - **Problem:** Advanced spectroscopic models too slow for online use
  - **Solution:** pre-computed lookup table for linear interpolation
  - 71 Pressure levels, 17 Temperature
  - Recently expanded from 3-dimensions (wavenumber, pressure, temperature) to add a 4th dimension, to accommodate water variable amounts of water vapor broadening



Preliminary Conclusions

- 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**