Updates to Spectroscopy for OCO-2

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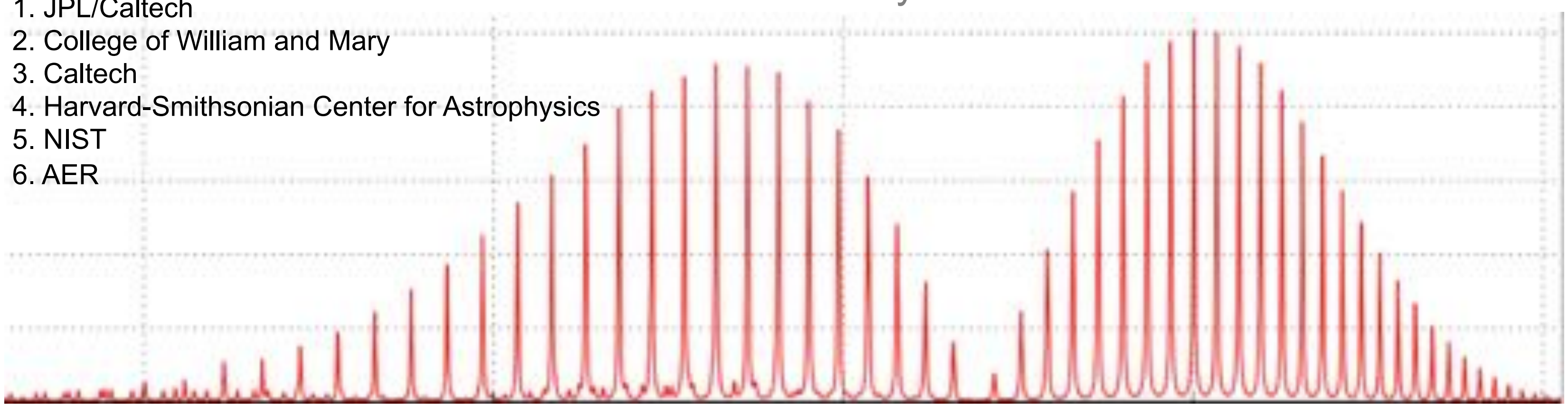
With thanks to many others!

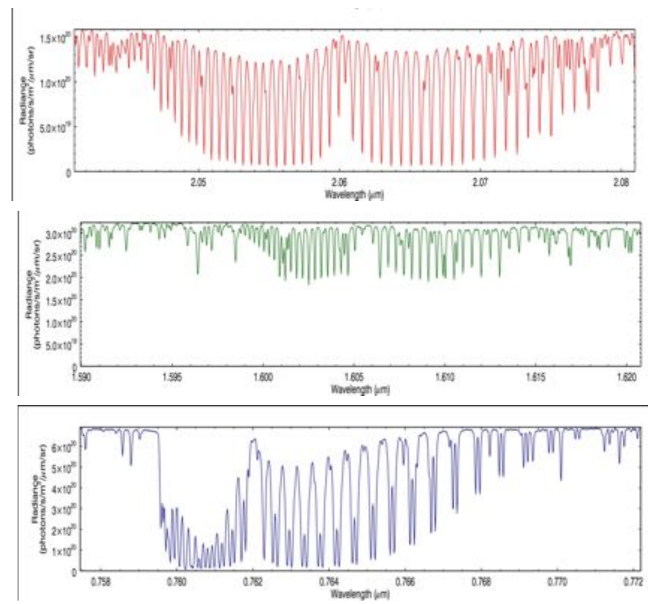
1. JPL/Caltech
2. College of William and Mary
3. Caltech
4. Harvard-Smithsonian Center for Astrophysics
5. NIST
6. AER



The Orbiting Carbon Observatory (OCO-2) Mission

- Grating spectrometer, 3 spectral regions
  - **CO_2 in the 4850 cm^{-1} (2.06 μm) band**
  - **CO_2 in the 6220 cm^{-1} (1.6 μm) band**
  - **O_2 in the 13100 cm^{-1} (0.76 μm) 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 accuracy requirements for X_{CO2}
  - Goal ~ 0.25% (1 ppm out of 400)
- **Goal for accuracy of modeled radiance: 0.1 %**

Image: NASA / Orbital



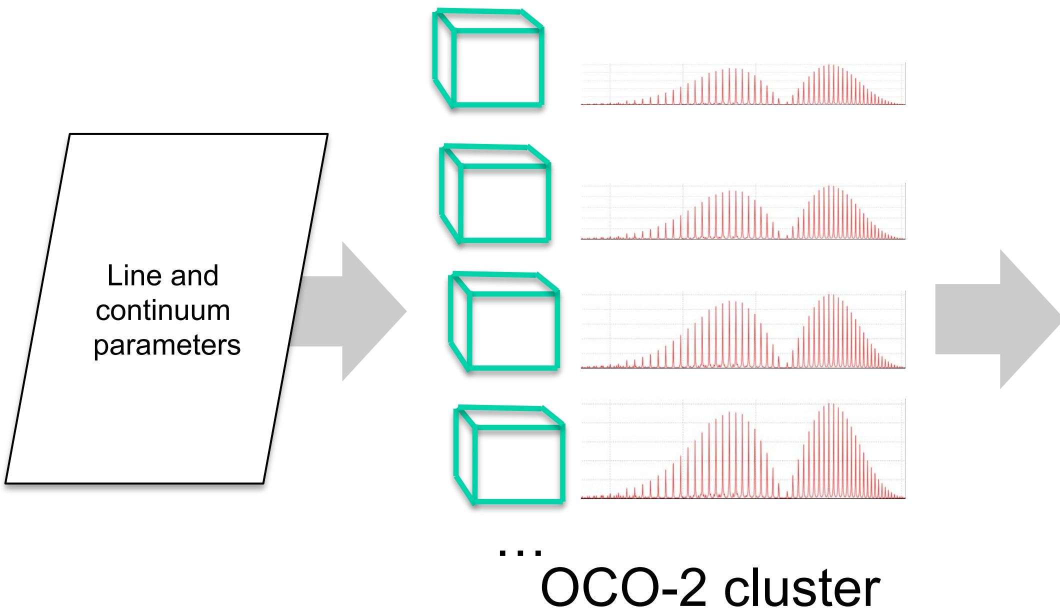
Beyond the Voigt line shape

- 0.1 % on forward-modeled radiances
  - **Stringent requirements on spectroscopic input!**

- "Traditional" line shape model: **Voigt**
  - **Voigt line shape not sufficient for OCO-2 accuracy goals**
- Efforts are underway
  - for OCO-2 and within the community
    - e.g. evolution of the HITRAN database
  - To incorporate **non-Voigt lineshape formulations**
  - To derive **improved experimental line parameters**
- **OCO-2 approach:**
  - **Multispectrum fitting** of laboratory spectra
  - Derive line **parameters that are consistent with the assumed lineshape**

Absorption coefficient (ABSCO) tables

- Problem: Advanced spectroscopic models too slow for online use
- Solution: pre-computed lookup table for linear interpolation
- Compute cross sections at independent temperatures, pressures, H_2O amounts
- **Current ABSCO version used in OCO-2 algorithm v7: ABSCO v4.2**



HDF File with **4 dimensions**:
- Molecule (CO_2, O_2, H_2O, CH_4)
- Pressure
- Temperature
- H_2O amount

Evaluation Methodology

Image: JAXA

Satellite 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

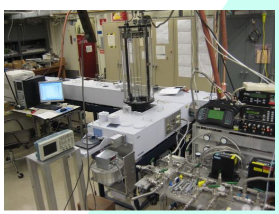


Image: JPL

Laboratory spectra

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

O_2 A band

ABSCO Tables		v4.2 (L2 v7)	v5.0
13200cm^{-1} O_2	Line shape	Voigt for main iso. Galatry for minor iso. Positions, intensities from Long [2010; 2011]	Speed-dependent Voigt from self-consistent set of multi-spectrum fits, utilizing FTS and CRDS measurements **(Drouin et al. 2016, JQSRT)**
	Line mixing	Tran & Hartmann [2008]	
	Collision Induced Absorption (CIA)	Tran & Hartmann [2008]	From ground-based atmospheric measurements at Lamont (E. Mlawer, AER) and CRDS
	H_2O-O_2 broadening	Drouin et al. [2014]	Drouin et al. [2014]

ABSCO v5.0: Self-consistent set of parameters!

Multispectrum fitting approach pioneered by Chris Benner and Malathy Devi

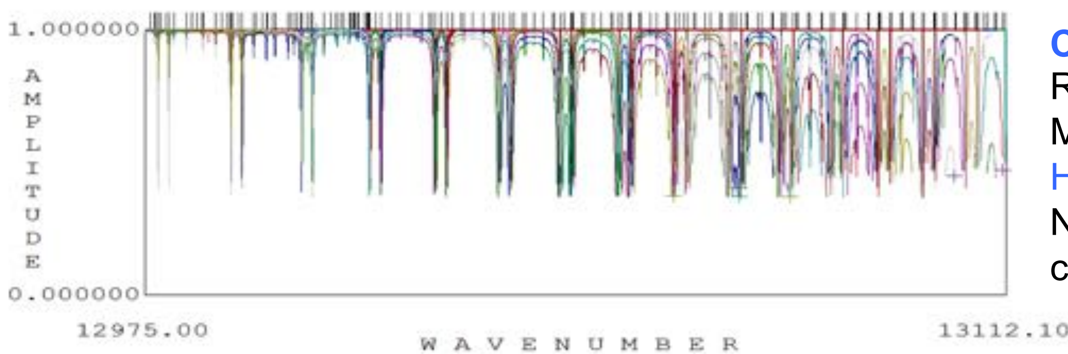
Speed Dependent Voigt (SDV): Accounts for the fact that collisions between molecules take place with velocities spanning some distribution

Line mixing: Accounts for collisional coupling (mixing) between spectral lines. Interactions described by a relaxation matrix.

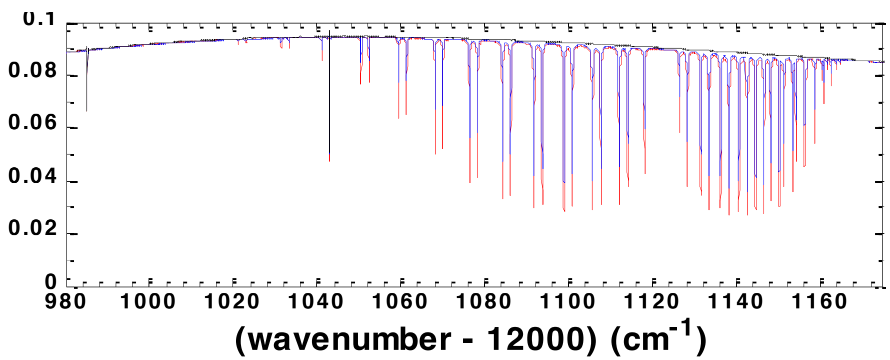
Collision Induced Absorption: Accounts for inelastic collisions between molecules

O_2 multispectrum fitting analysis (Drouin et al. [2016])

- Self-consistent set of O_2 parameters from CRDS and FTS lab spectra
- Reduction in residual rms for laboratory fits



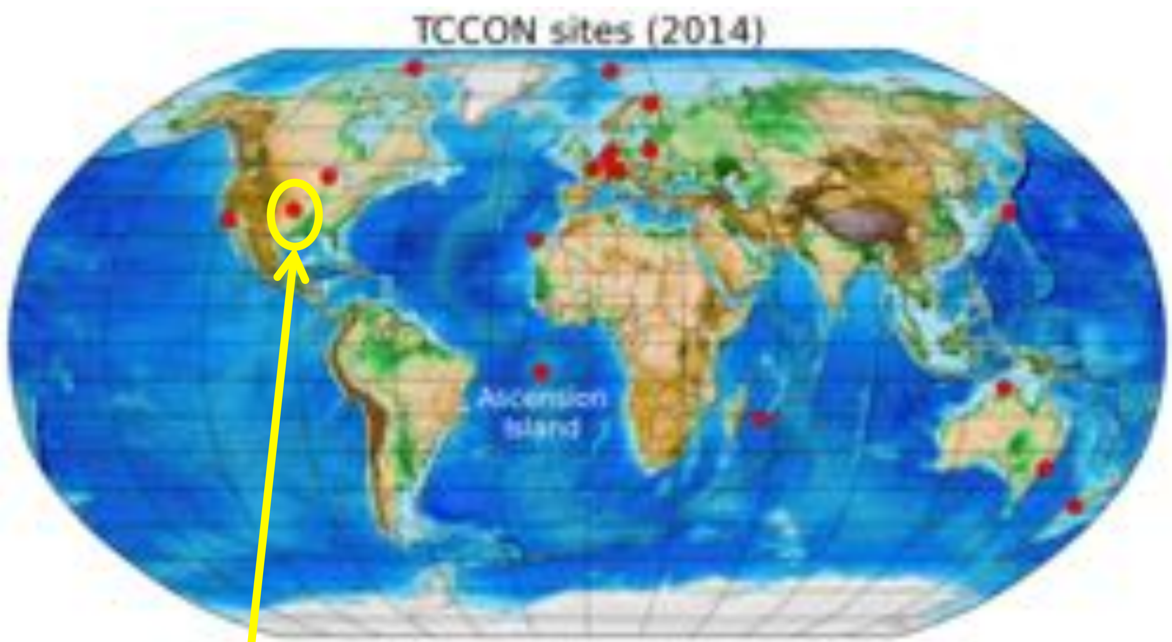
Cavity Ringdown spectra (NIST):
Room temp. only.
Multiple spectral segments.
High precision.
New info on lineshape, mixing, collision-induced absorption (CIA)

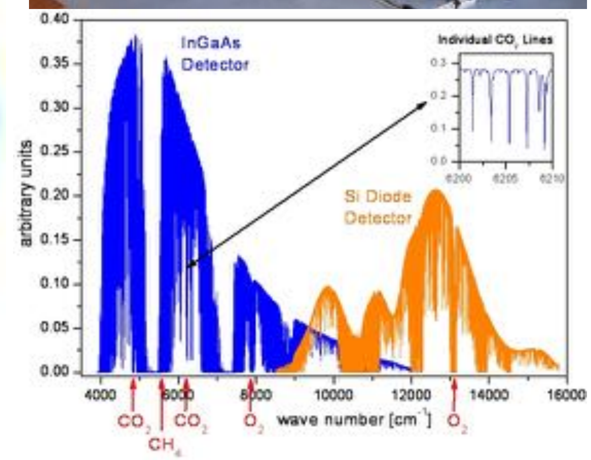


Fourier Transform Spectrometer (JPL):
All features in one spectrum: consistency
New info on lineshape, mixing and T-dependence

ABSCO evaluation using TCCON spectra

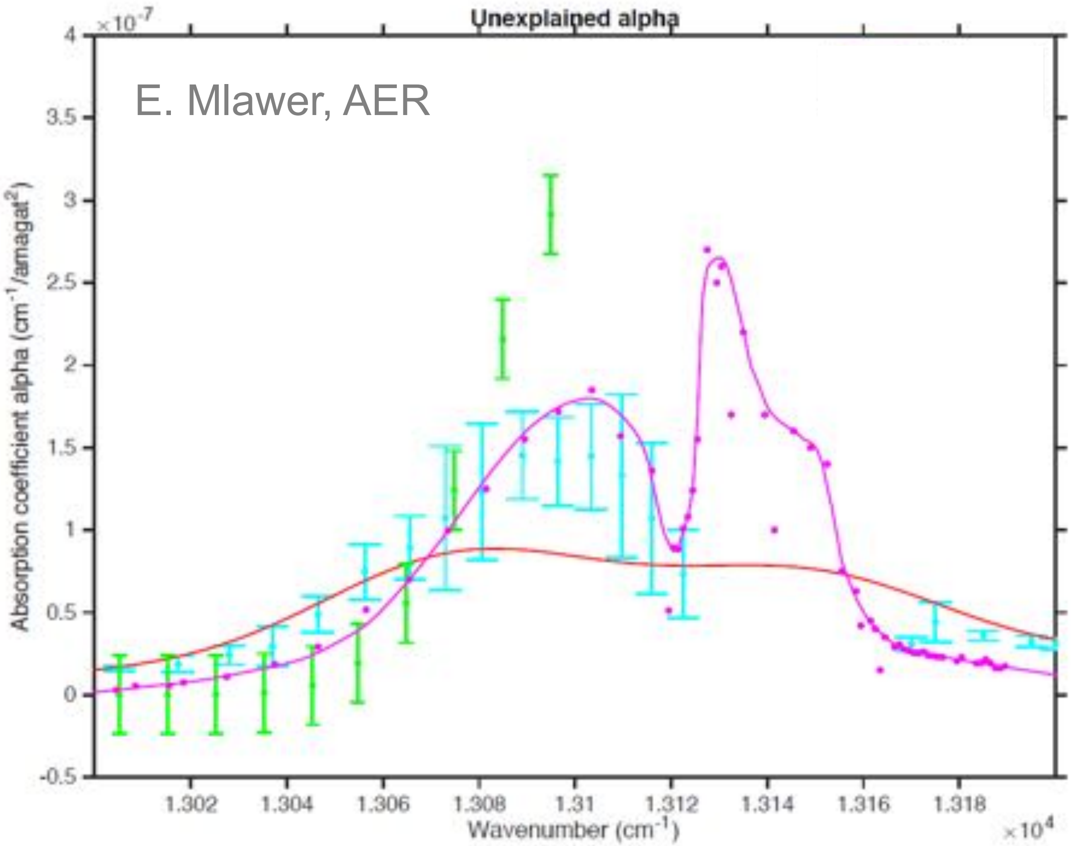
- Atmospheric spectra highly sensitive to far-wing effects
  - Offer additional constraints on line mixing and CIA





Lamont, Oklahoma: Additional instrumentation and "value added products" associated with the DoE ARM Southern Great Plains facility

O_2 CIA: Fits from Lamont measurements



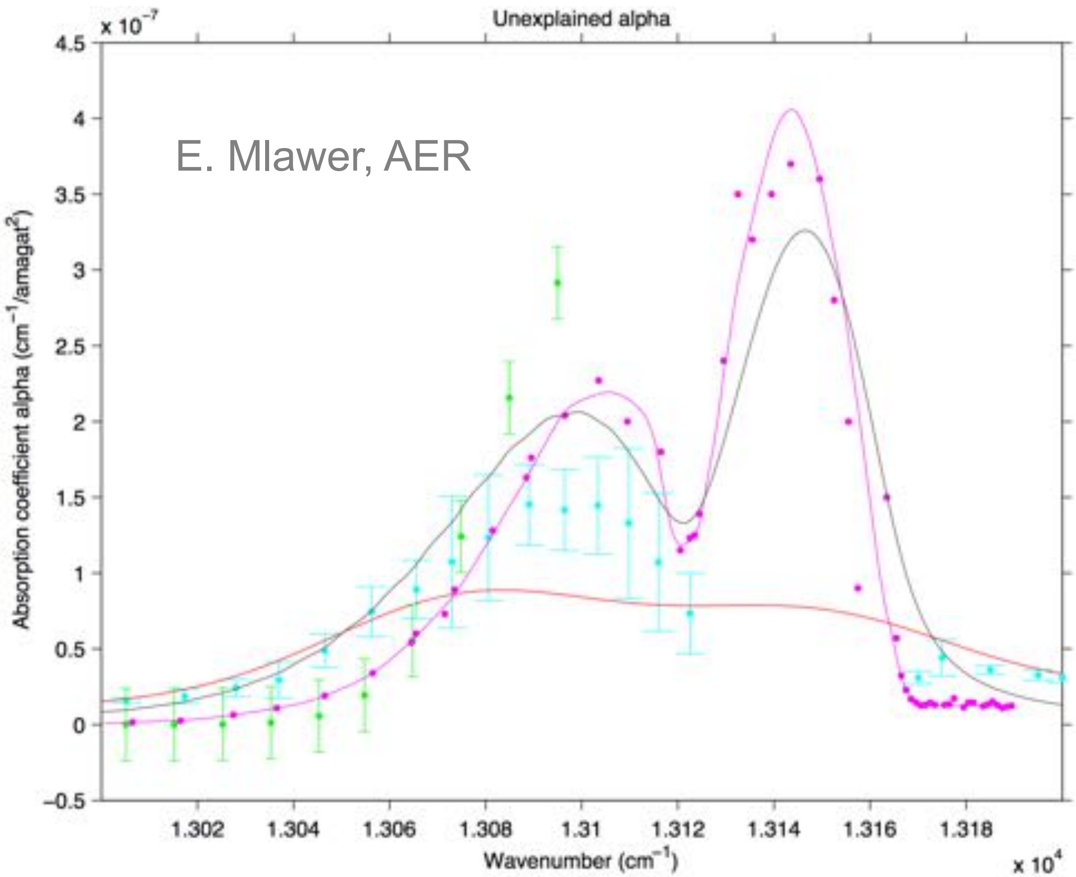
Empirical CIA, based on ABSCO v4.2 lines

Long et al. [2012]

Spiering et al. [2011]

Tran and Hartmann [2008] (from HITRAN 2012)

O_2 CIA: Fits from Lamont measurements



Empirical CIA, based on ABSCO **v5.0** lines

Long et al. [2012]

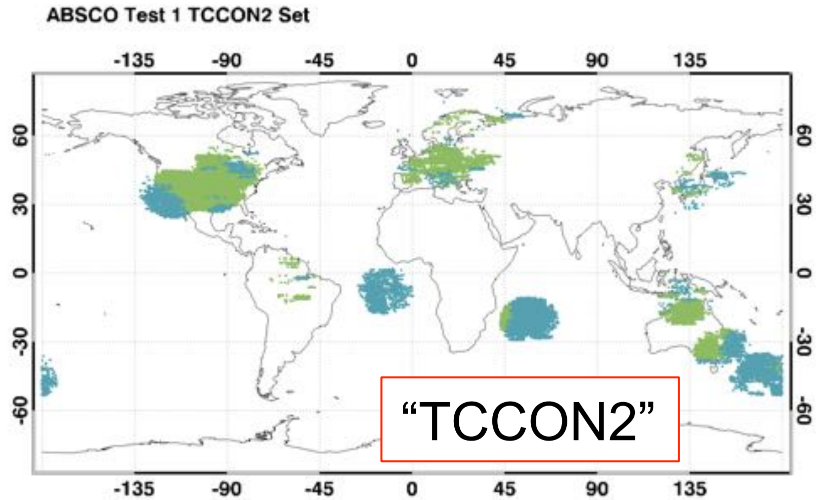
Spiering et al. [2011]

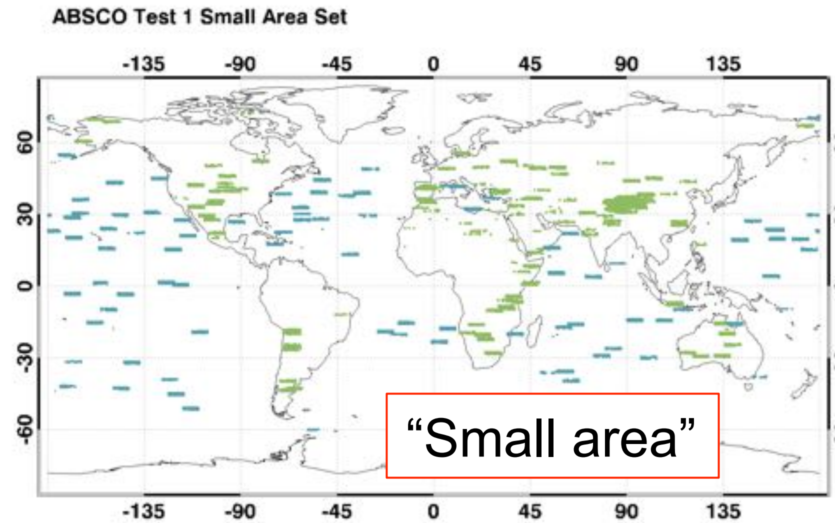
Tran and Hartmann [2008] (from HITRAN 2012)

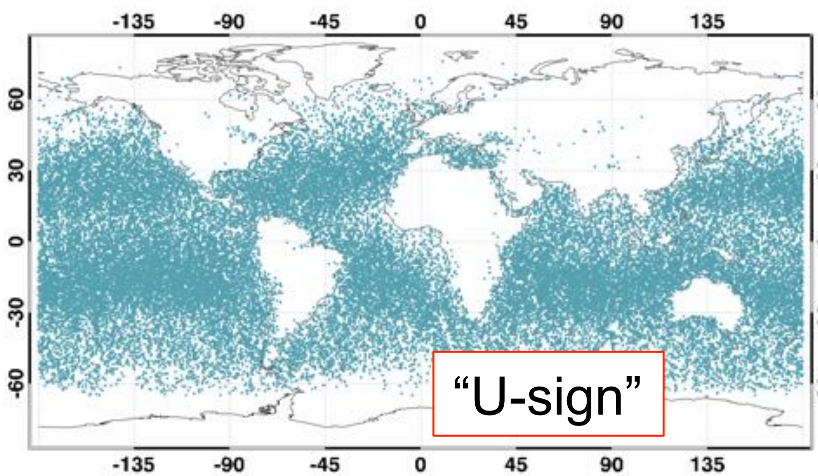
Sum of Lorentzian shapes

ABSCO v5.0 line contributions = more physical CIA estimate

Datasets for testing ABSCO updates in the OCO-2 Level 2 algorithm



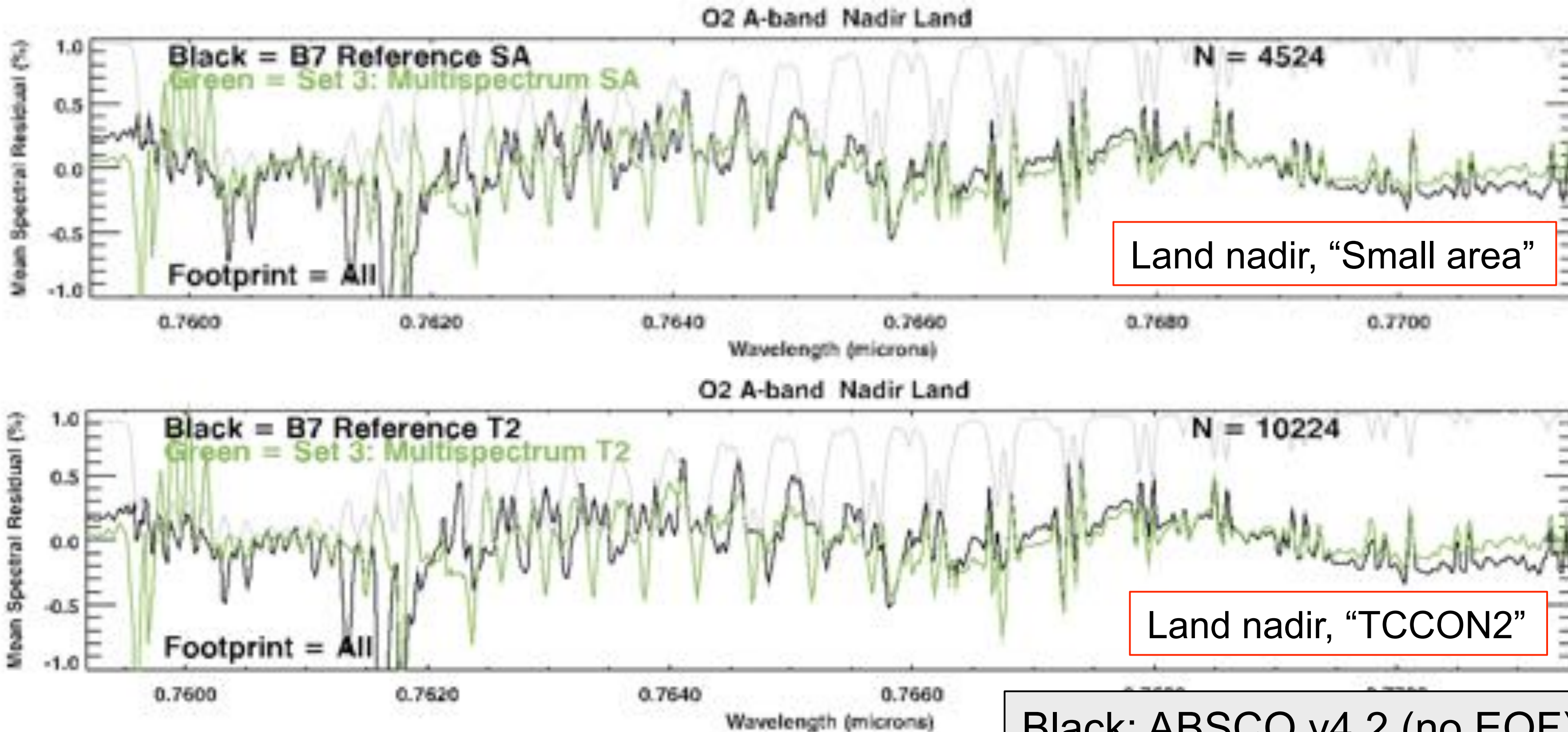




- **<u>Quick Test Sets</u>**
  (Developed by L. Mandrake, JPL)
- **~50,000 cases each**
- **Mixture of observation modes**
- (land nadir, land glint, ocean glint)

- All tests shown here were done with <u>no EOFs</u>

Spectral Residuals:
Examples from 2 different quick test sets



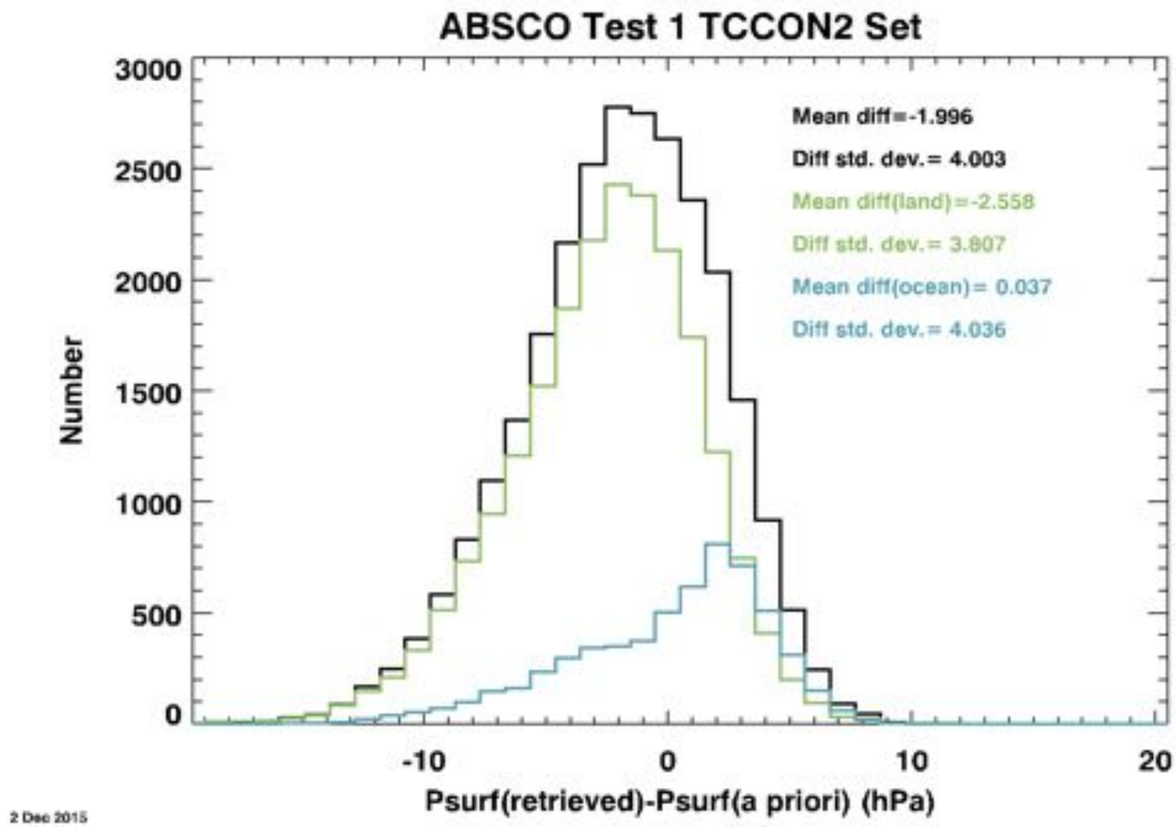
Black: ABSCO v4.2 (no EOF)
Green: ABSCO v5.0

Solar line

- Despite the spikes in the R branch, chi^2 values are lower for ABSCO v5.0

Impact of O_2 A-band ABSCO update on surface pressure retrieval

A priori surface pressure values are from ECMWF.
We expect ECMWF values to be a good estimate of reality, on average.



B7 No-EOF baseline (ABSCO v4.2)

Impact of O_2 A-band ABSCO update on surface pressure retrieval

A priori surface pressure values are from ECMWF.
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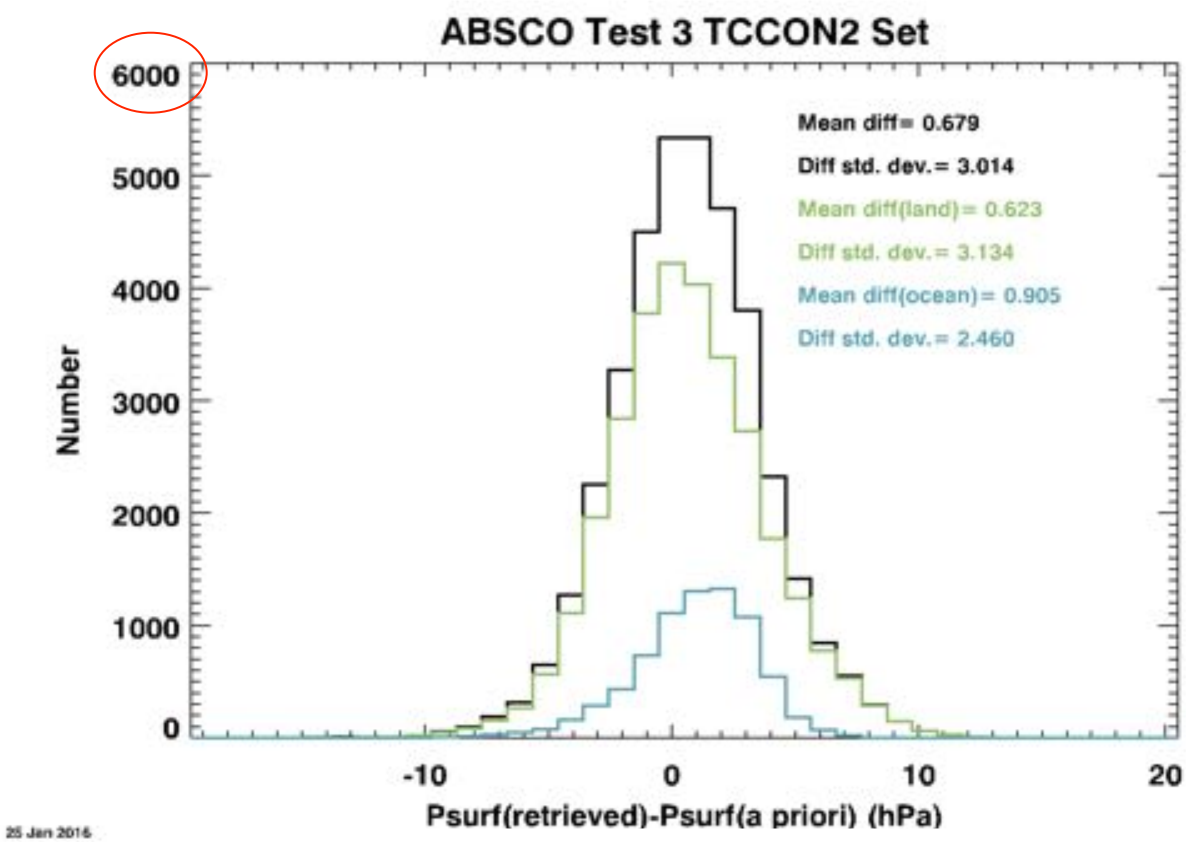


ABSCO v5.0

ABSCO v5.0

- Land and ocean closer
- Peak closer to zero
- Std. dev. reduced
- Distributions more symmetric

ABSCO updates also have a strong impact on the retrieval of aerosol parameters!

CO_2 bands

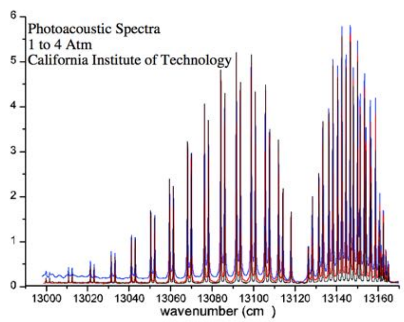
ABSCO Tables		V4.2	V5.0
4850 cm^{-1} CO_2	Line shape	Speed Dependent Voigt from room temp. meas. [Benner et al., 2011] Minor isotopes: Toth 2008	Speed Dependent Voigt, fit to range of temperatures **[Benner et al., 2016]**
	Line mixing	Nearest-neighbor from multi-spectrum fit [Benner et al., 2011]	Nearest-neighbor from multi-spectrum fit [Benner et al., 2015]
	H_2O-CO_2 broadening	Sung et al. [2009]	Sung et al. [2009]
	"CO_2 CIA"	Ad hoc	Ad hoc
6220 cm^{-1} CO_2	Line shape	Speed Dependent Voigt [Devi et al., 2007]. Minor iso: Toth	Speed Dependent Voigt fit to range of temperatures **[Devi et al., 2016]**
	Line mixing	Nearest-neighbor from multi-spectrum fit [Devi et al., 2007]	Nearest-neighbor from multi-spectrum fit **[Devi et al., 2016]**
	H_2O-CO_2 broadening	Sung et al. [2009]	Sung et al. [2009]
H_2O and CH_4 in CO_2 bands	H_2O continuum	Supplied by E. Mlawer	Supplied by E. Mlawer
	H_2O lines	Custom lists from I. Gordon	Custom lists from I. Gordon
	CH_4 lines	Not included	Not included

Summary and future work

- **Publications describing ABSCO v5.0 updates:**
  - **0.76 μm O_2**: Drouin et al. (2016), JQSRT
  - **1.6 μm CO_2**: Devi et al. (2016), JQSRT
  - **2.06 μm CO_2**: Benner et al. (2016), J. Mol. Spec.
- ABSCO v5.0 tables available on request.

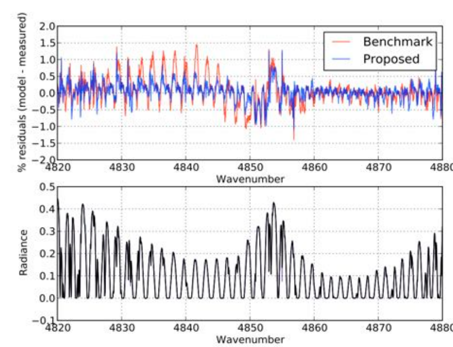
- **Beyond ABSCO v5.0:**

0.76 μm O_2



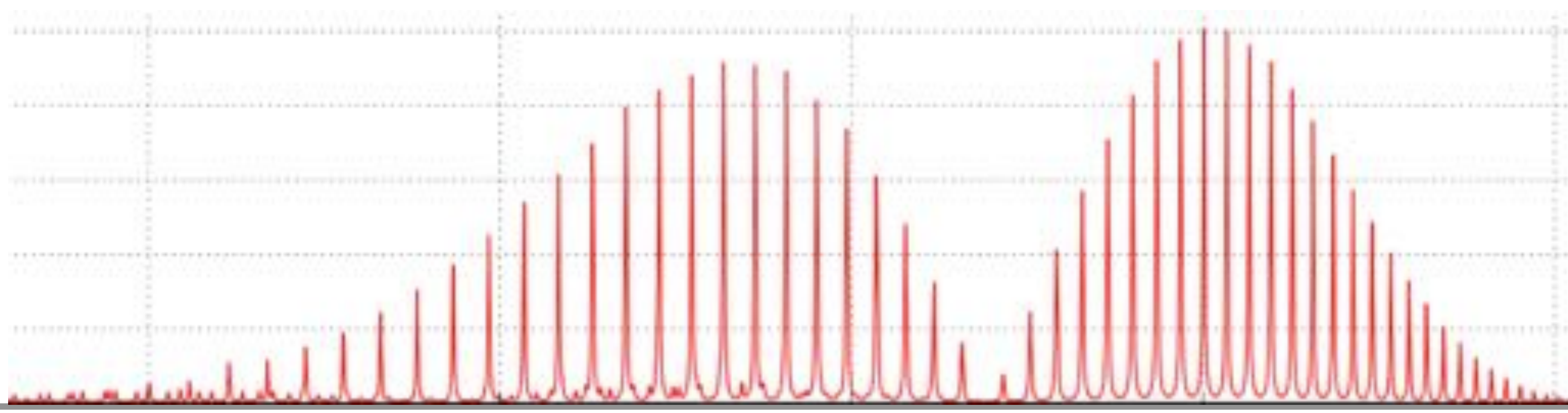
Analysis of new lab measurements
Cavity Ringdown Spectroscopy (NIST)
Photoacoustic Spectroscopy (Caltech)
Range of temperatures
New information on line mixing and CIA

2.06 μm CO_2

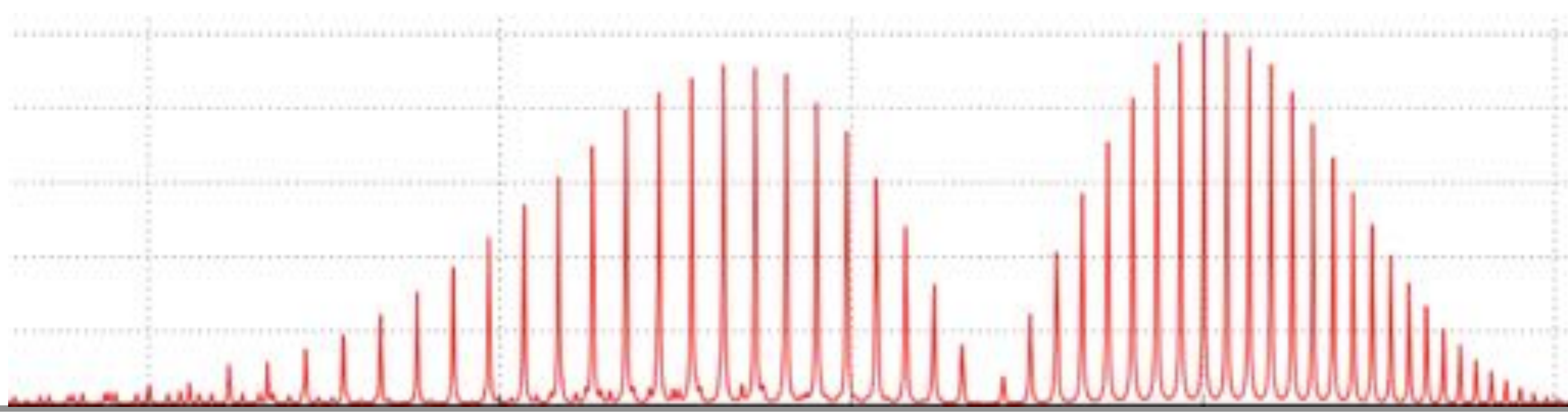


Beyond nearest-neighbor line mixing:
Re-evaluate 2.06 μm line mixing in the context of available measurements & theory

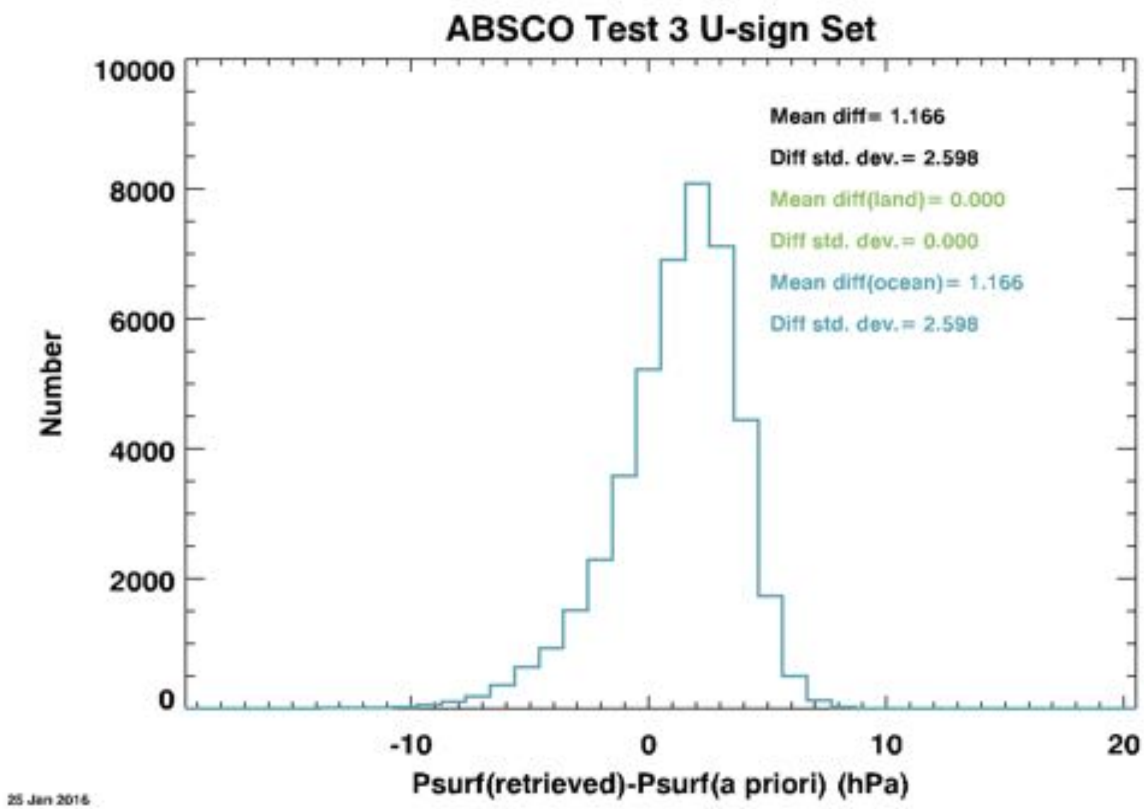
Questions?



Back-up slides



Impact of O_2 A-band ABSCO update on surface pressure retrieval



ABSCO v5.0

ABSCO v5.0

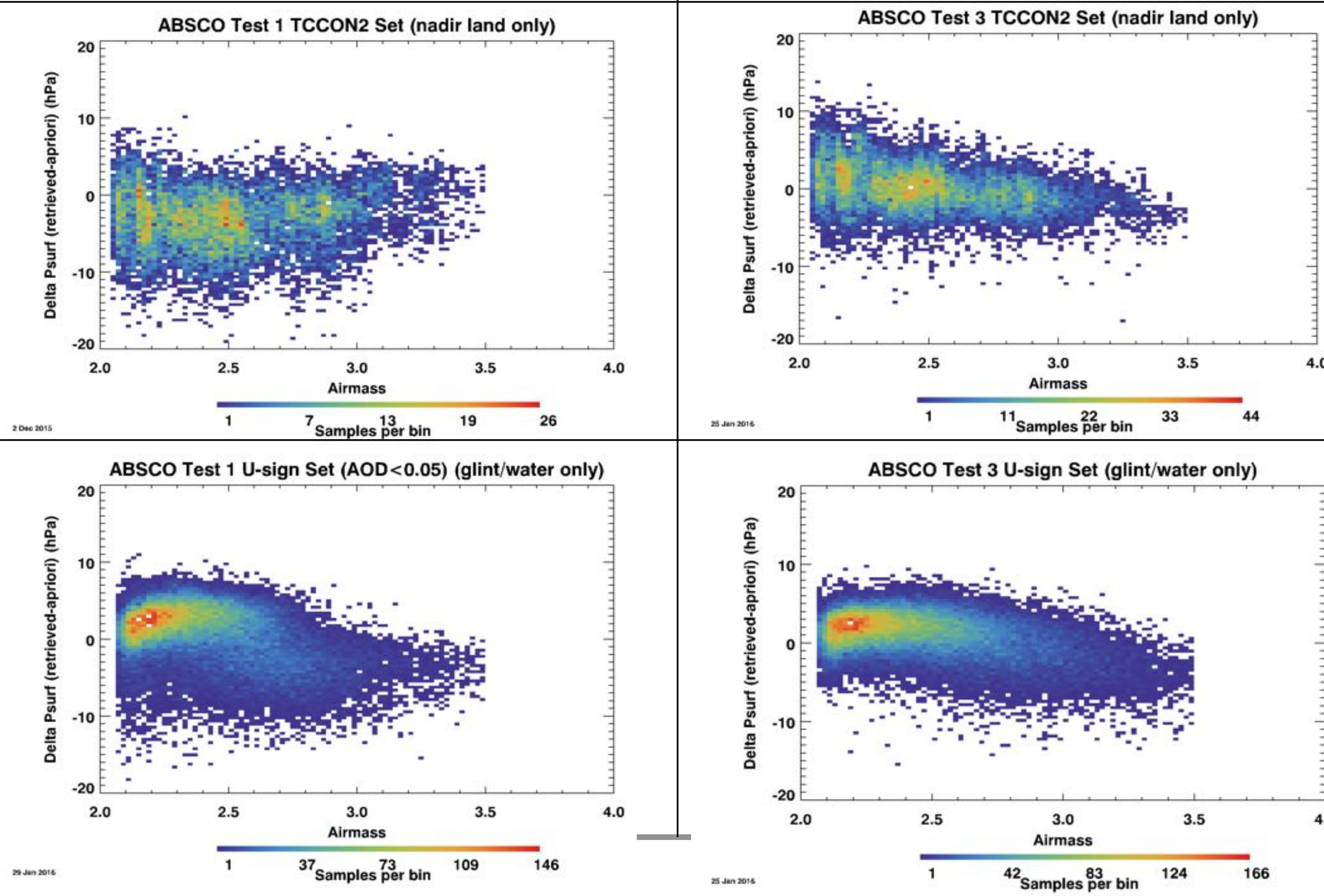
- Peak closer to zero
- Std. dev. reduced
- Distribution more symmetric
- Negative tail still obvious

Impact of O_2 A-band ABSCO update on airmass dependence of PSUR retrieval

B7 No-EOF baseline (ABSCO v4.2) | ABSCO v5.0

Land nadir ("TCCON2")

Ocean glint ("u-sign")

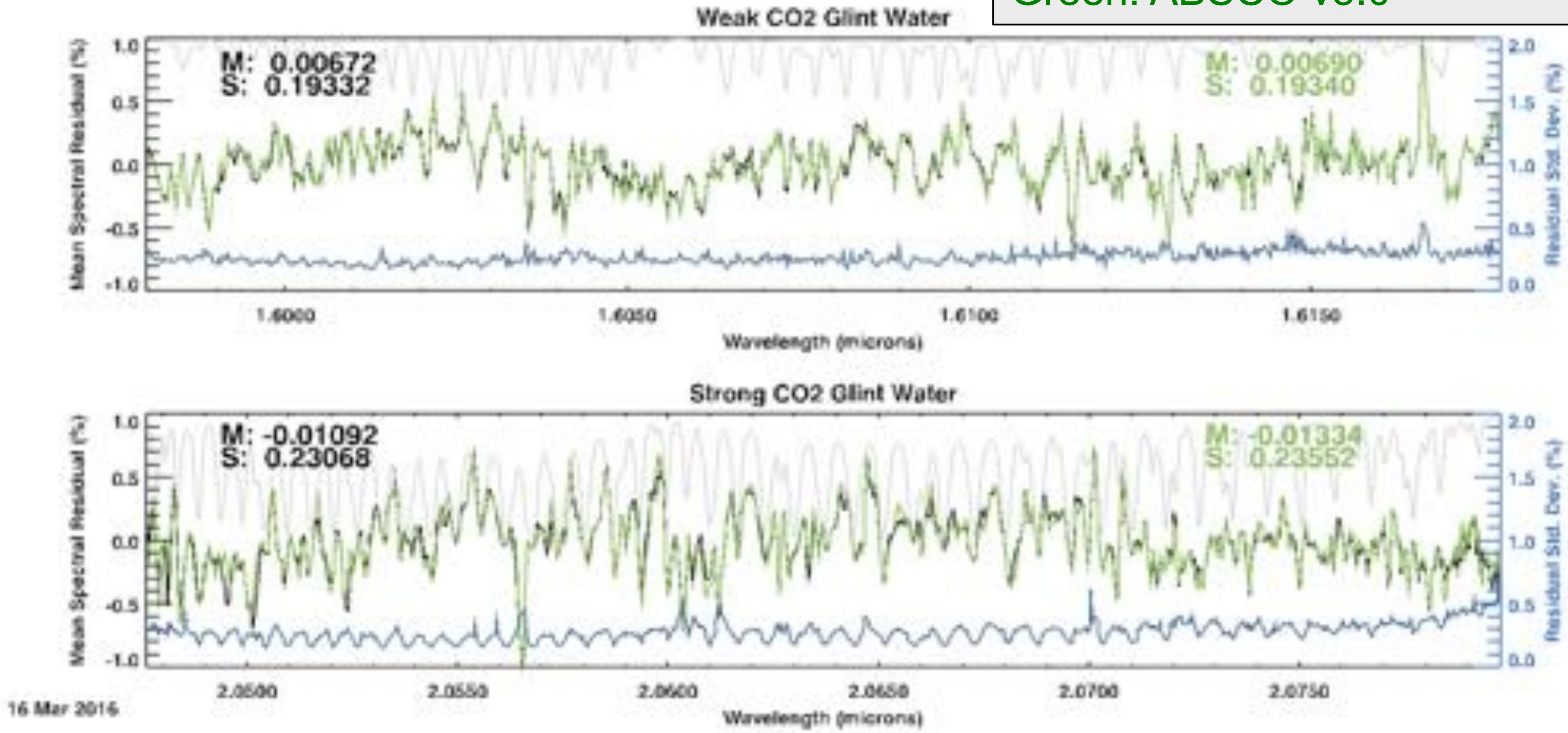


Inter-band scaling

- **1.6 μm (weak) CO_2 band**
  - Weak band fits to atmospheric measurements are reasonable
  - **Apply constant scaling to ABSCO table** as calculated from Devi et al. [2016] fits
  - Scaling factor: **1.014**
    - **Scaling factor is currently baked into the WCO2 table**
    - Rationale: Aim for consistency with NIST-measured intensities in Polyansky et al. [2015]
    - ABSCO-based single-band ground-based XCO2 retrievals (from TCCON spectra) show very good agreement with official TCCON XCO2 after this scaling
- **2.06 μm (strong) CO_2 band**
  - Strong band fits to atmospheric measurements remain problematic
    - ***Line shape / line mixing / airmass dependence remain a concern***
    - Ad-hoc "CIA" (not based on physics) is still in the ABSCO v5.0 tables
  - Apply constant scaling factor to ABSCO table: **1.006**
    - **Scaling factor not currently baked into the SCO2 table**
    - Happens to be ratio between Benner et al. and Zak et al. (2016) ab initio intensities
    - Brings single-band ground-based XCO2 retrievals into agreement with official TCCON XCO2 (at least at low airmass)

Spectral residuals: CO_2 bands

Black: ABSCO v4.2 (no EOF)
Green: ABSCO v5.0



- Residuals do not change much going from ABSCO v4.2 to v5.0.
- Residuals very similar for different observation modes and test sets.
- Largest residual features are H_2O lines (minimal impact on XCO_2)
- (Scaling does not significantly affect the residuals.)

CO_2 bands

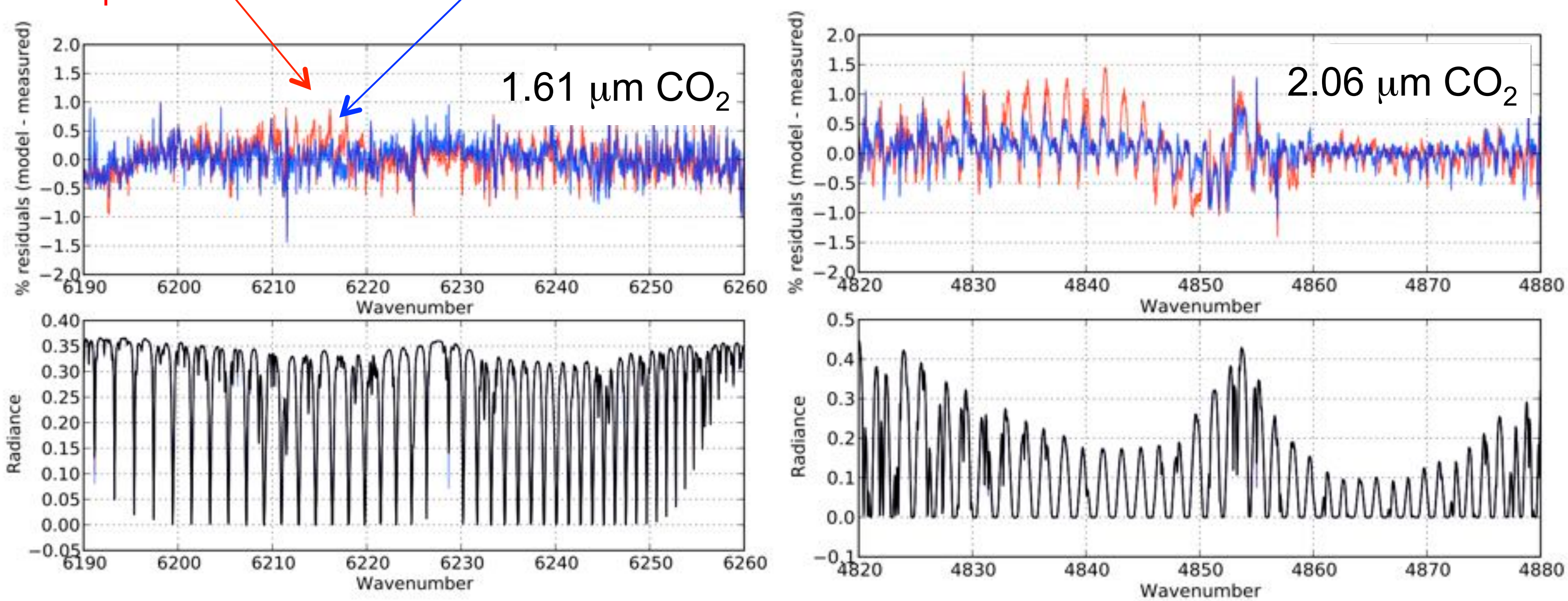
- Moving to nearest-neighbor line mixing brought marked improvement
- Time to move beyond nearest-neighbor line mixing?

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

First-order line mixing, Voigt shapes

Nearest-neighbor line mixing
Speed dependent profile

Thompson et al., *JQRST* [2012]



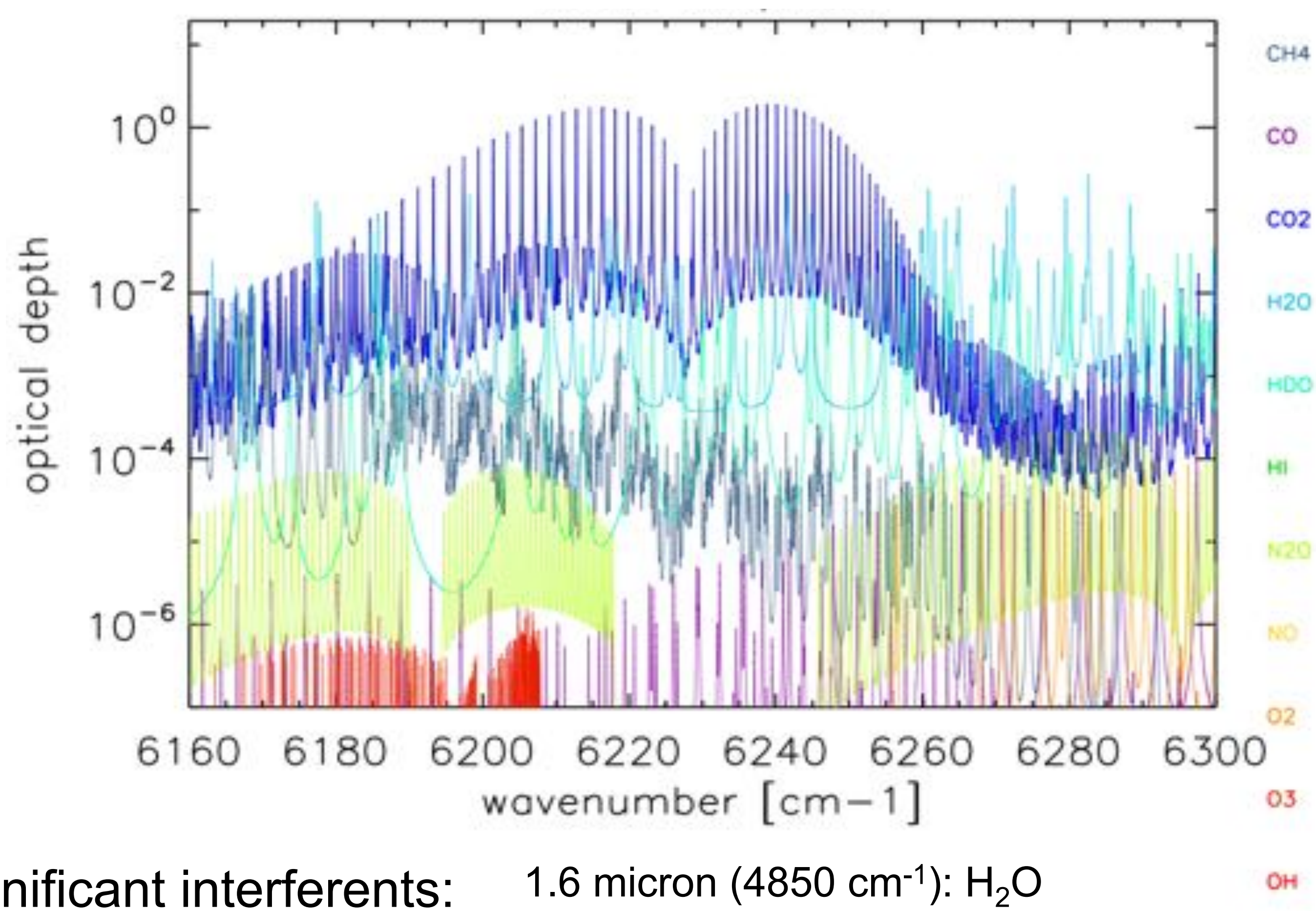
Clarifications on retrievals

- **Official TCCON XCO2 product (Wunch et al., 2010)**
  - Surface pressure is measured at the ground site
  - XCO2 retrievals performed using the 1.6 μm CO2 band
  - Retrievals involve scaling of an a priori CO2 profile
  - Official TCCON XCO2 retrievals do not use our ABSCO tables
  - Retrieval results calibrated for consistency with aircraft/AirCore measurements
  - Consistency with reference measurements
    - Without stringent requirements on spectroscopic accuracy

- **Retrievals from TCCON FTS for ABSCO validation**
  - Single-band XCO2 retrievals using the 1.6 or 2.06 μm bands
  - Retrievals involve scaling of an a priori CO_2 profile
  - Can also jointly retrieve an H2O scaling factor and T offset
  - Retrieve XCO_2 using OCO-2 ABSCO tables/spectroscopy
  - Compare result to official TCCON XCO2 product

- **OCO-2 L2 retrieval algorithm**
  - 3 band joint retrieval
  - PSUR, CO2 profile on 20 levels, H2O scaling, T offset, aerosol parameters
  - XCO2 calculated afterwards from retrieved profile
  - Retrievals use OCO-2 ABSCO tables

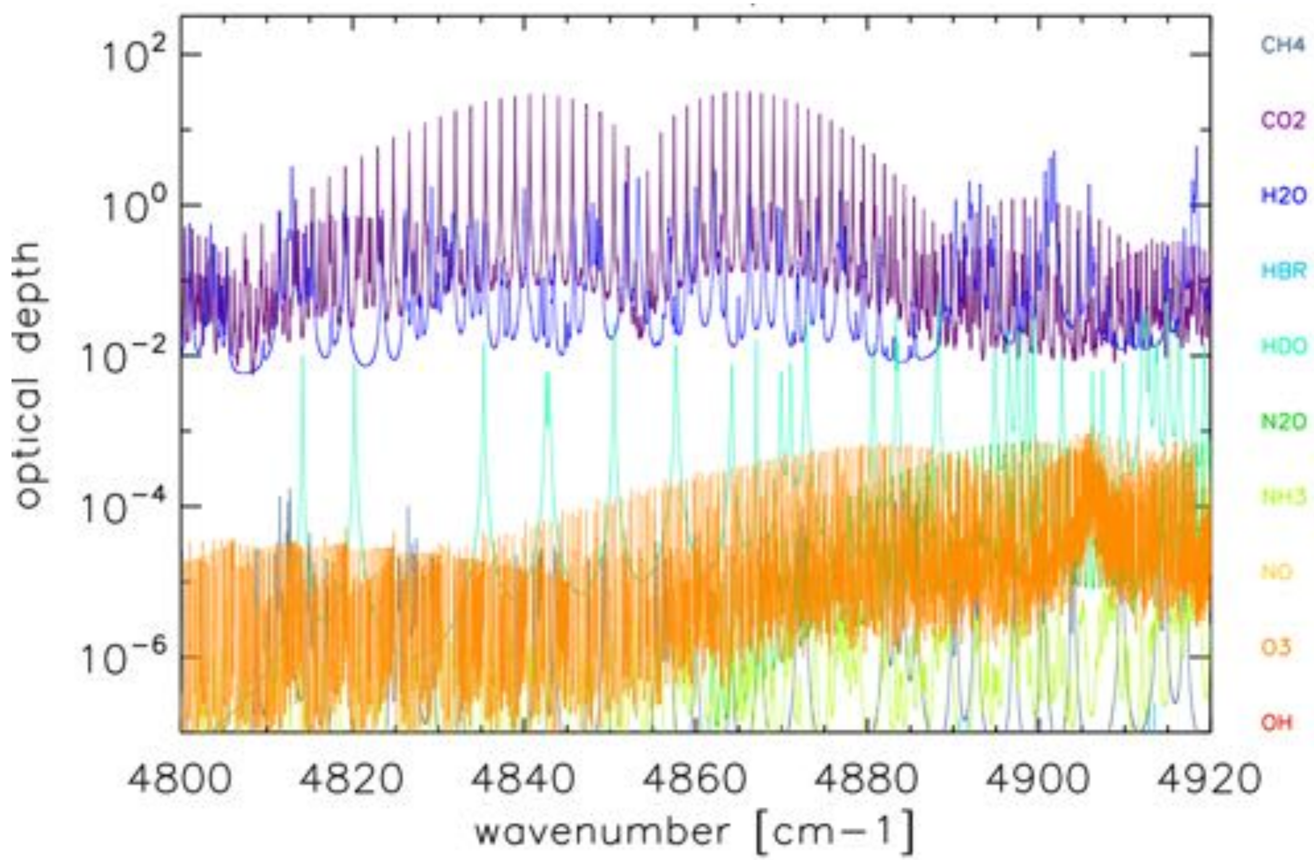
Interferents



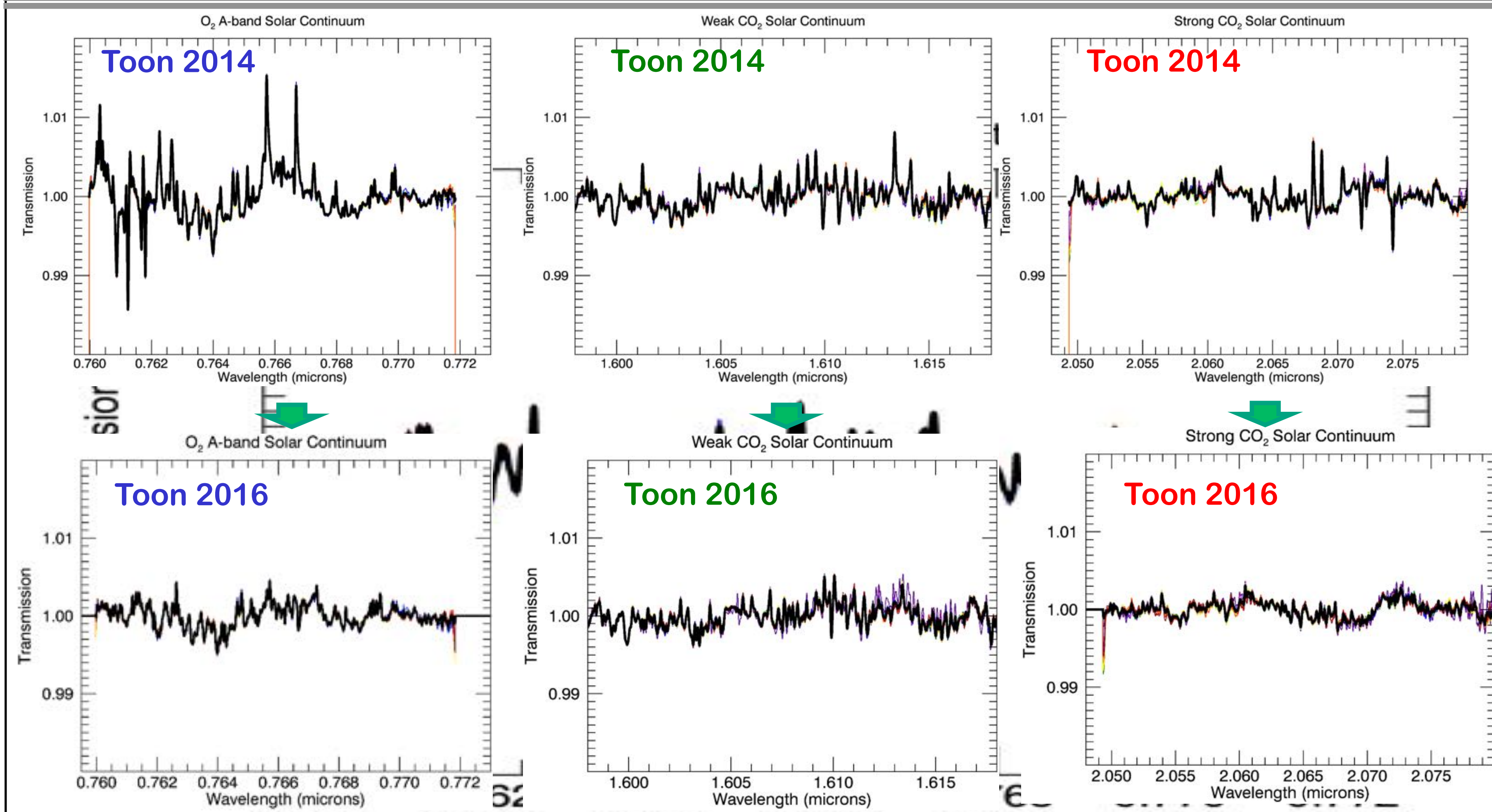
Significant interferents:

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

Interferents

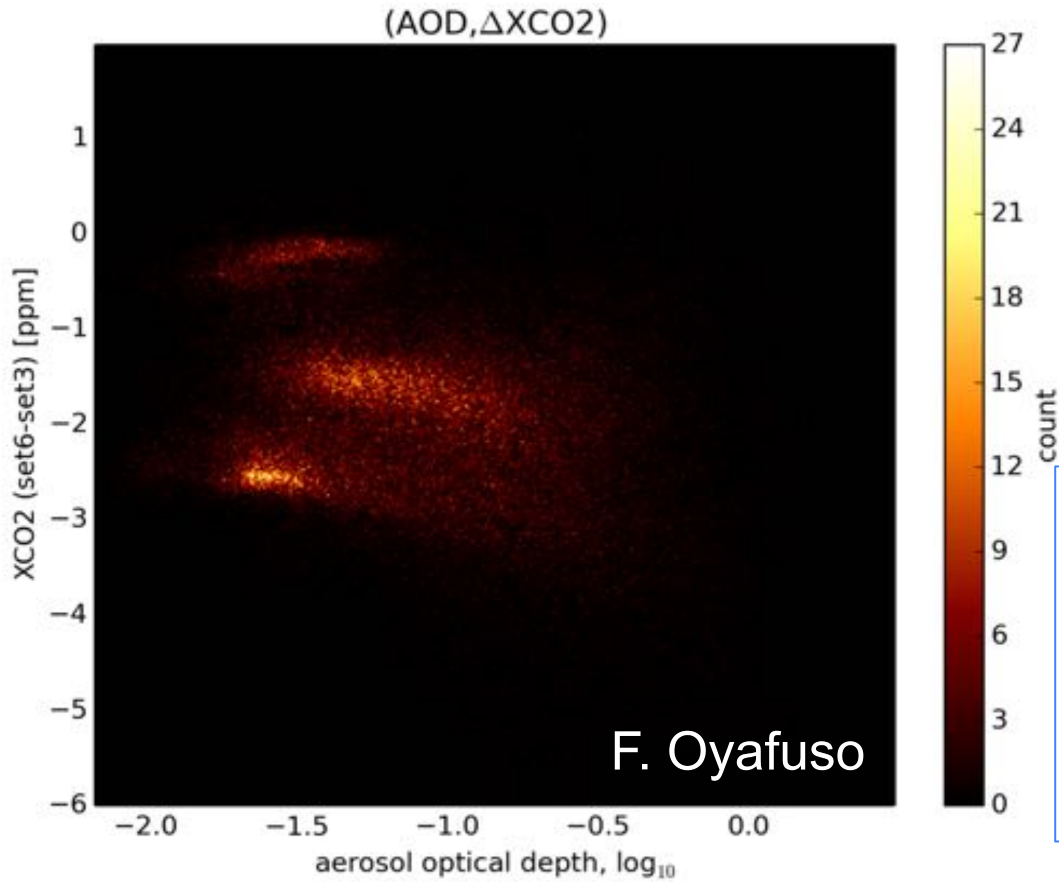


Reduced Solar Doppler Residuals for Updated Solar Line List (D. Crisp, R. Lee)



Continuum corrections are smaller for Toon (2016) than those for Toon (2014), reflecting improvements in the synthetic solar spectrum.

Impact of CO_2 ABSCO updates: Different populations



Disclaimer:
This plot is results from ABSCO test 6 rather than test 5.
The main point of showing this is the 3 different populations in the ΔXCO2 rather than the absolute ΔXCO2 values shown.

Impact of CO_2 spectroscopy is not globally uniform.
Distribution of differences is not mono-gaussian.