GGG/IPP Update

Main topics:

- Continuum Fitting
- Errors Scale factor
- Spectroscopy
- FVSI from DC interferogram
- Future Plans

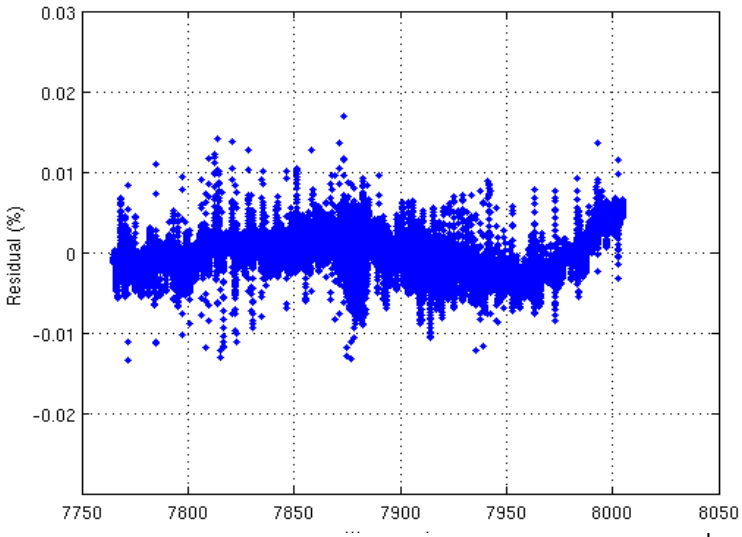
GFIT Continuum Fitting

"Continuum" is spectrum that would be measured above atmosphere. It is defined by the instrumental spectral response and the solar Planck function.

Previously GFIT would fit the continuum across a window as a straight line.

In 2012 we introduced the (hidden) option of also fitting a curvature to allow accurate fitting of wider windows

But some instruments have more complex structures in their continuum (right)



2013 GGG release provides capability for fitting up to 30 Continuum Basis Functions.

INTERNATIONAL JOURNAL FOR NUMERICAL METHODS

DISCRETE (LEGENDRE) ORTHOGONAL POLYNOMIALS—A SURVEY

C. P. NEUMAN† AND D. I. SCHONBACH‡

Carnegie–Mellon University, Department of Electrical Engineering, Pittsburgh, Pennsylvania, U.S.A.

Discrete Legendre Polynomial -- Theory

Generalized continuum fitting by using the equations from Neuman & Schonbach:

$$P_m(K,N) = \sum_{j=0}^{m} (-1)^j \binom{m}{j} \binom{m+j}{j} \frac{K^{(j)}}{N^{(j)}} = \sum_{j=0}^{m} l(m,j) \frac{K^{(j)}}{N^{(j)}}$$

for $m = 0, 1, 2, \ldots, N$. In particular, the first five DLOP's are:

Continuum Level $\quad P_0(K,N) = 1$

Continuum Tilt $\quad P_1(K,N) = 1 - 2\frac{K}{N}$

Curvature $\quad P_2(K,N) = 1 - 6\frac{K}{N} + 6\frac{K^{(2)}}{N^{(2)}}$

..... $\quad P_3(K,N) = 1 - 12\frac{K}{N} + 30\frac{K^{(2)}}{N^{(2)}} - 20\frac{K^{(3)}}{N^{(3)}}$

..... $\quad P_4(K,N) = 1 - 20\frac{K}{N} + 90\frac{K^{(2)}}{N^{(2)}} - 140\frac{K^{(3)}}{N^{(3)}} + 70\frac{K^{(4)}}{N^{(4)}}$

where K=0,N represent the spectral points across the window

Continuum Fitting -- Implementation

How to select the Number of Continuum Basis Functions (NCBF) to be fitted

Specified in the window (and last line of .ggg) file in two different ways, e.g.,

6339.50 85.00 15 1 1 0 cl ct cc fs so : co2 h2o hdo [Old way]

6339.50 85.00 15 1 1 0 ncbf=3 fs so : co2 h2o hdo [New way]

For instruments with continuum structure, increasing NCBF will improve RMS fits, but not necessarily retrieval accuracy.

Although the DLPBFs are orthogonal to each other, they may be similar to other fitted parameters (e.g. O_2 CIA), which can cause gas absorption to be fitted as continuum. For O2_7885, this starts already at NCBF=3 because the O_2 CIA absorption resembles the quadratic continuum term.

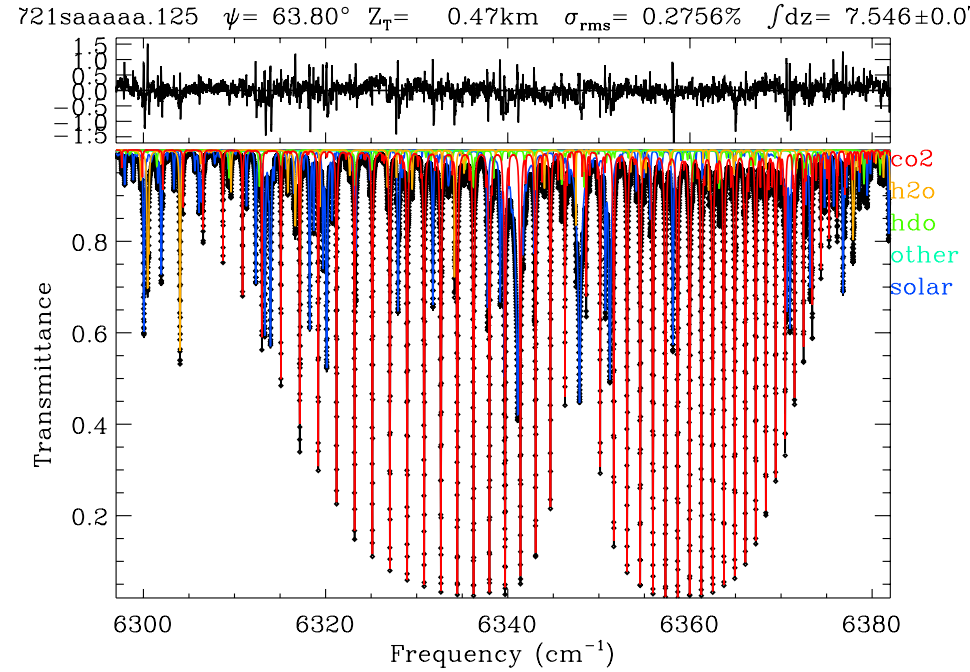
Optimum number of DLPBFs is instrument-dependent.

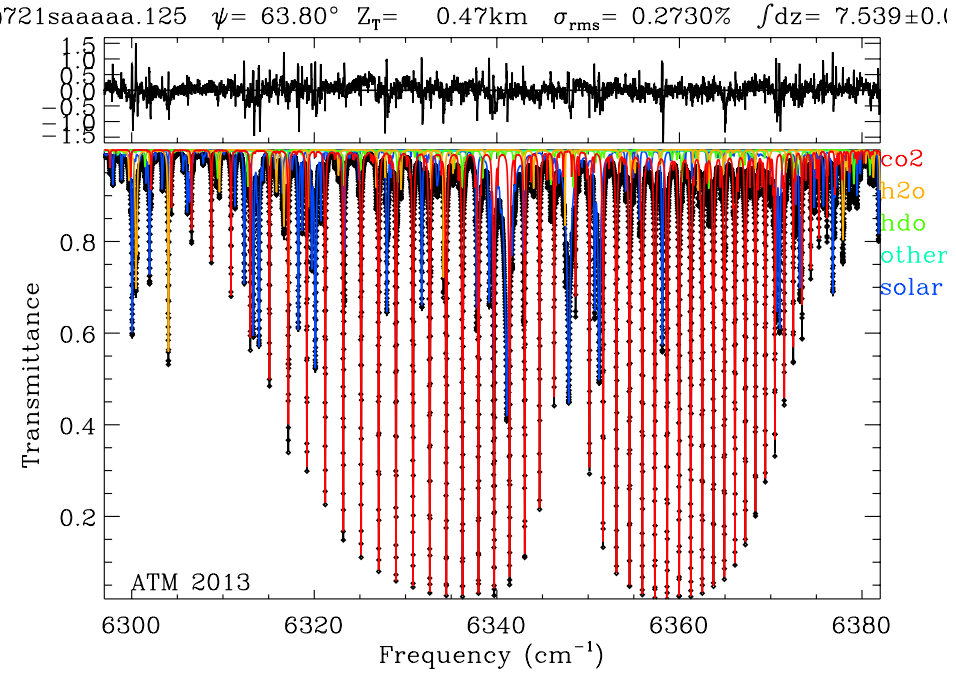
How to reconcile with TCCON approach of standardized windows?

Example of fitting Continuum Curvature

Left panel fitted with CL and CT only (ncbf=2). Slight concavity in the residuals.

Right panel also fits CC (ncbf=3). RMS residual reduced from 0.2756% to 0.2730%. Retrieved CC coefficient of +0.8, corresponds to a peak-to-peak curvature of ~0.08%
CO_2 column reduced by 0.1%





GFIT Error Scale Factor

The column uncertainties from GFIT assumes random spectral fitting residuals.

Typically the residuals are dominated by systematic errors (spectroscopy) so the GFIT-provided error bars will be larger than the true measurement precision.

GFIT error bars are realistic, but we don't want the TCCON error bars to include contributions (e.g. spectroscopic) that are constant over time or between sites. So the GFIT-reported uncertainties are empirically re-scaled.

The program error_scale factor.f compares spectrum-to-spectrum variability in XGAS, with XGAS_error values computed using the GFIT-reported uncertainties.

$$ESF_{GAS} = \Sigma_i w_i (XG_i - XG_{i-1})^2 / (XG\_error_i^2 + XG\_error_{i-1}^2) / \Sigma_i w_i$$

Typical re-scaling factors for ESF are:

- XCH4: 0.12
- XCO2: 0.13
- XN2O: 0.3
- XCO: 0.4
- XHF: 0.7

For weak absorbers (e.g. HF) with nearly random residuals, ESF approaches 1.0

For strong absorbers (e.g. CO_2 & CH_4) ESF << 1

New ESF Implementation

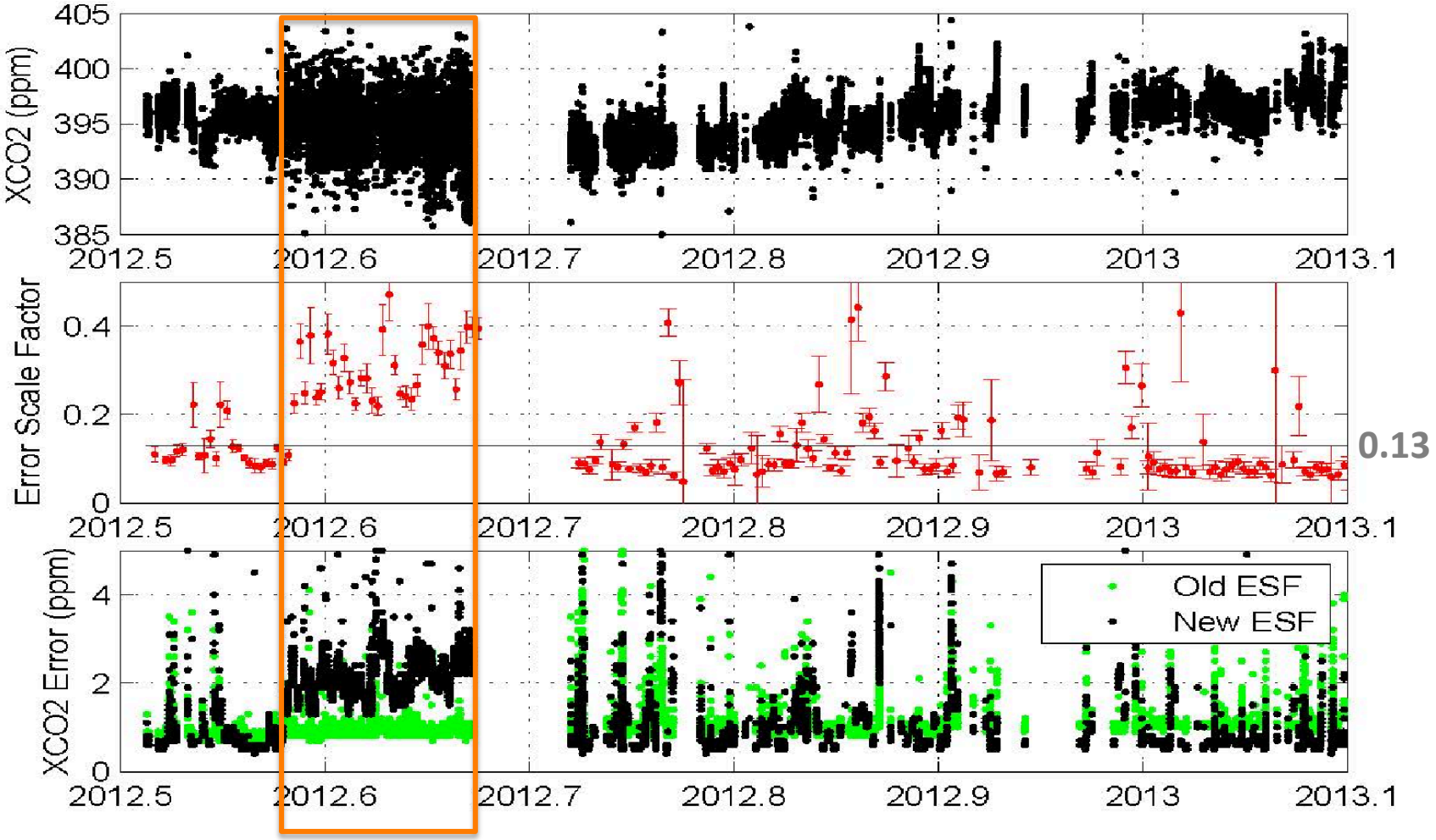
Previously, the same gas-dependent ESF values were used for every day within a given runlog.

This was inconvenient when there was a change in the noise performance of the instrument. For example, during malfunctions (laser failure, loss of signal) or when analyzing single spectra instead of averages.

New approach is to derive an independent ESF value for each day, and use the tabulated values in the xx_qc.dat file only as a priori estimates.

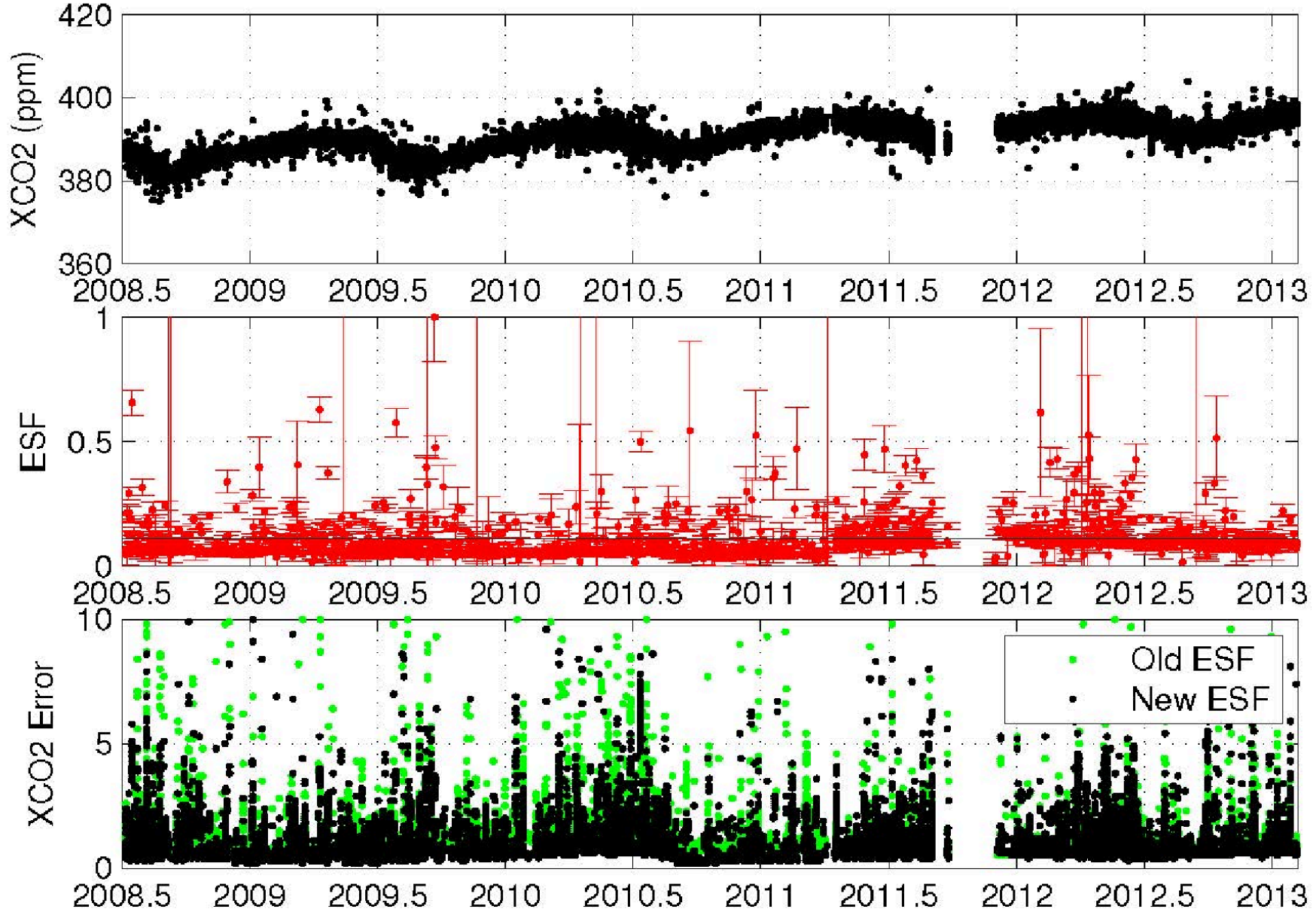
This requires error_scale_factor program be run as part of the post-processing pipeline (previously it was run off-line). The post-processing script will handle this transparently.

Caltech ESFs



During laser failure, XCO2 became much more variable, but RMS spectral fits didn't worsen much because they were still dominated by spectroscopic errors. So GFIT-computed uncertainties, using a constant ESF=0.13, remained ~1ppm (Green). New daily ESFs (red) increase CO2 uncertainties to 2-3 ppm during laser failure period.

Lamont, Oklahoma ESFs



ESF Update Summary

Doesn't change the retrieved column amounts, only the reported uncertainties.

This change should be completely transparent to TCCON GGG-users. It is mentioned here only to alert you to the fact that your reported uncertainties in the official output file (.oof) will change in GGG 2013.

Easier to handle situations where the instrument noise characteristics change (e.g. laser failing; analyzing average spectra instead of single spectra)

ESF will also change when spectroscopic parameters are updated, becoming closer to 1.0 when the fits are improved.

Eventually, when the spectroscopy is sufficiently perfect that systematic fitting errors fall below noise level in every window, the whole ESF artifice will be discarded.

Comparison of HITRAN 2008 & 2012

Compare spectral fits and retrieved gas amounts with three different linelists:

1. HIT08 (HITRAN 2008)
2. HIT12 (beta release received Jun 5, 2013, from Iouli Gordon)
3. ATM (the linelist used by MkIV & TCCON)

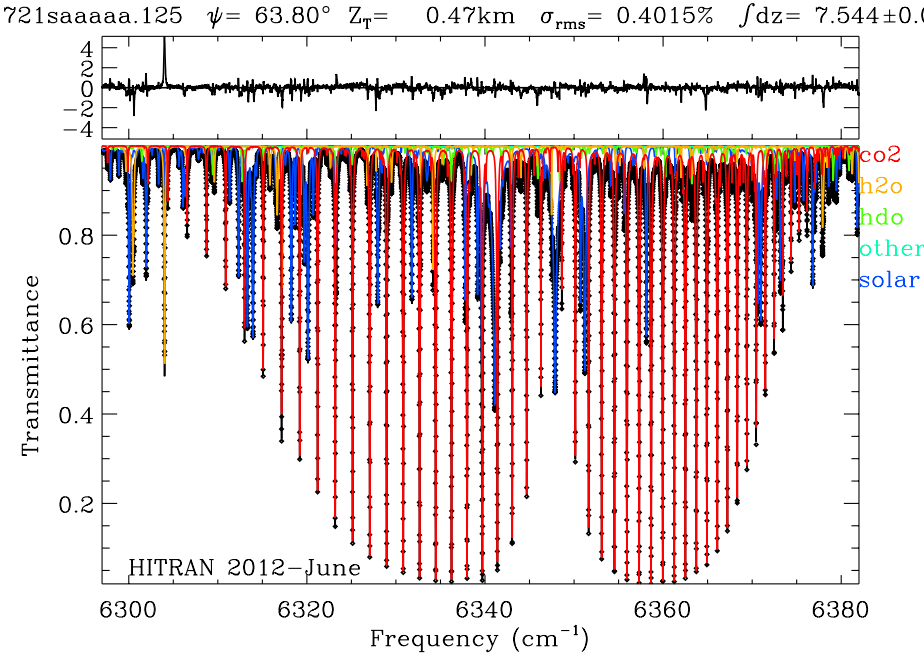
The ATM is similar to HITRAN 2008 but with several improvements:

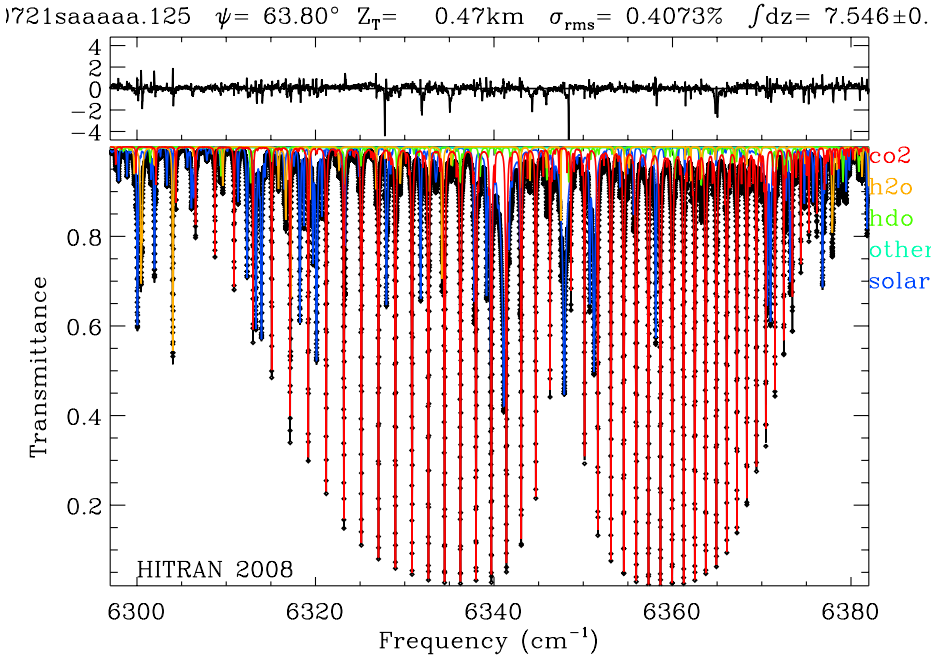
- Empirical fixes representing missing $^{13}CH4$ lines
- Changing instances of E”=-1 to E”=555.555 cm-1
- Setting HDO pressure shifts of 0.0 to a more sensible value (e.g. -0.01)
- Adding weak H_2O lines (over 700) located in TCCON windows
- Fits to Kitt Peak laboratory spectra.

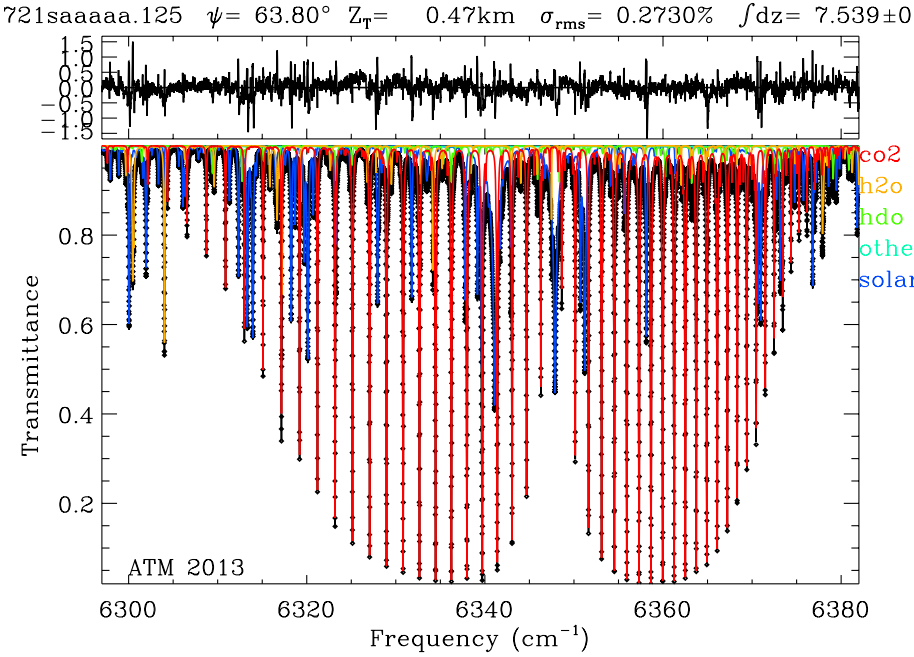
Linelist Comparison CO_2 6340 cm^{-1}

HITRAN 2012 is slightly better than 2008 but worse than ATM 2013 linelist used by TCCON.

Main problem here is H_2O (not CO_2 itself)
ATM 2013 uses empirically adjusted H_2O.

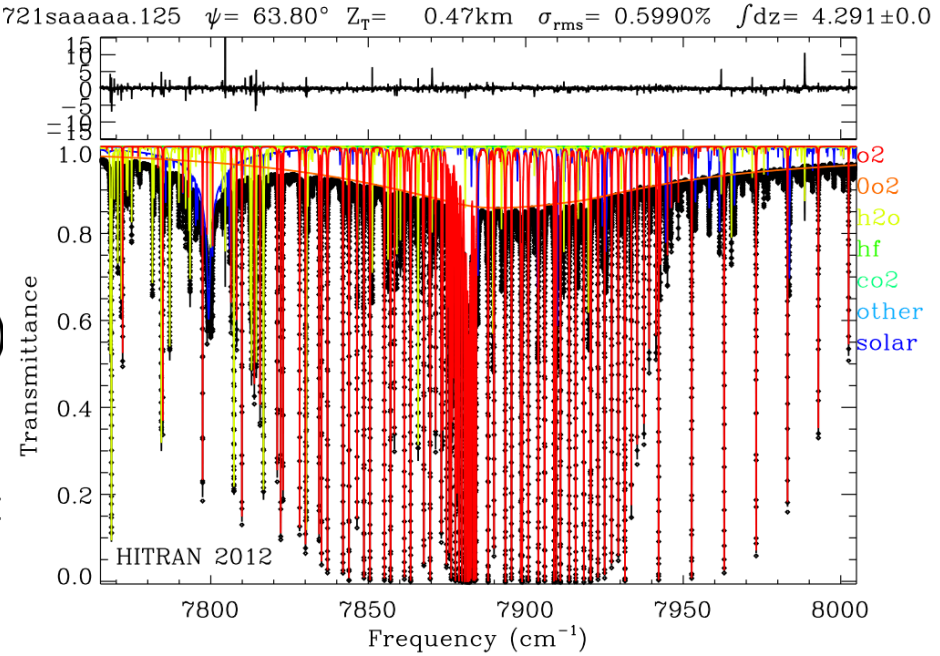


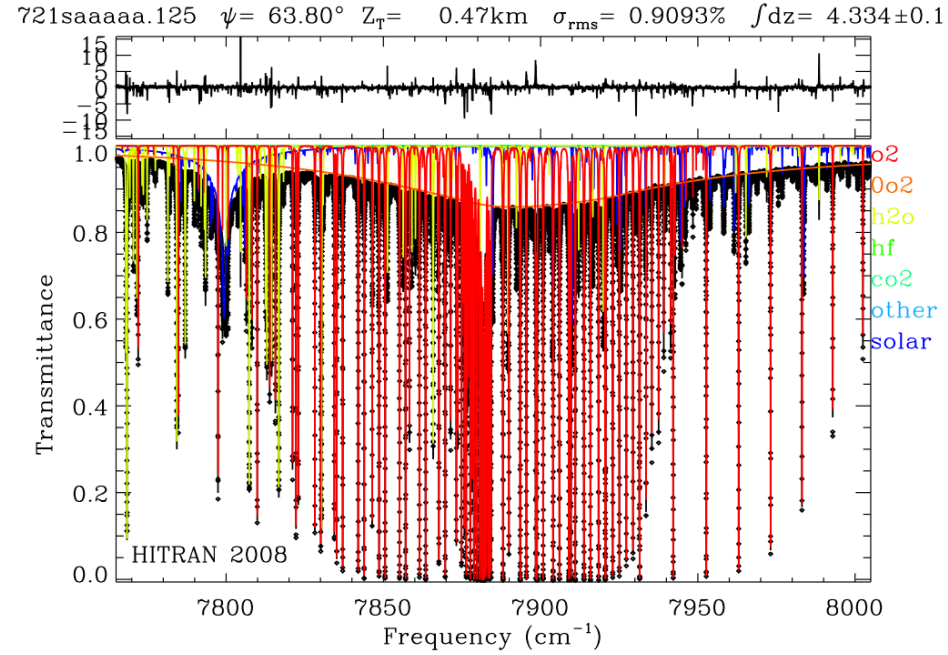


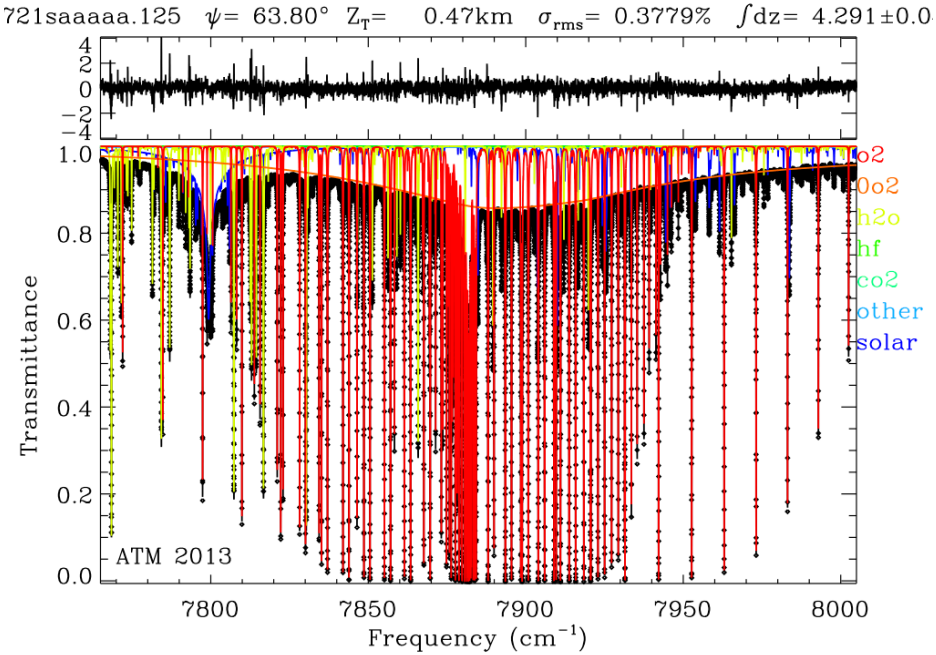


Linelist Comparison O_2 7890 cm^{-1}

"2.7.2. a1Δg - X3Σg- transitions (around 1.27 μm) In 2009 an update to the HITRAN2008 oxygen file was issued featuring substantial improvements based on the work of Newman et al. [2000] and Washenfelder et al. [2006]."
Rothman et al., [JQSRT, 2013]





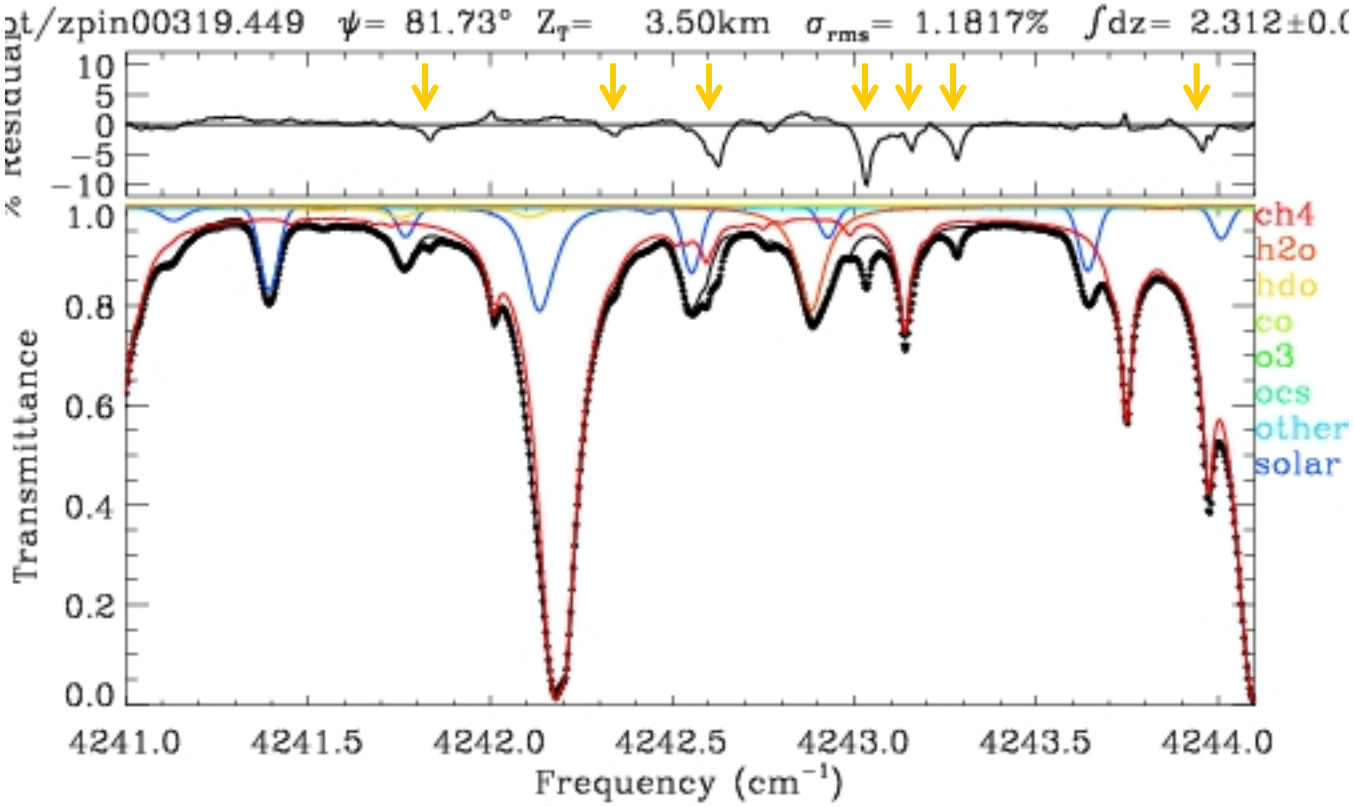


Case Study: Missing $^{13}CH_4$ lines

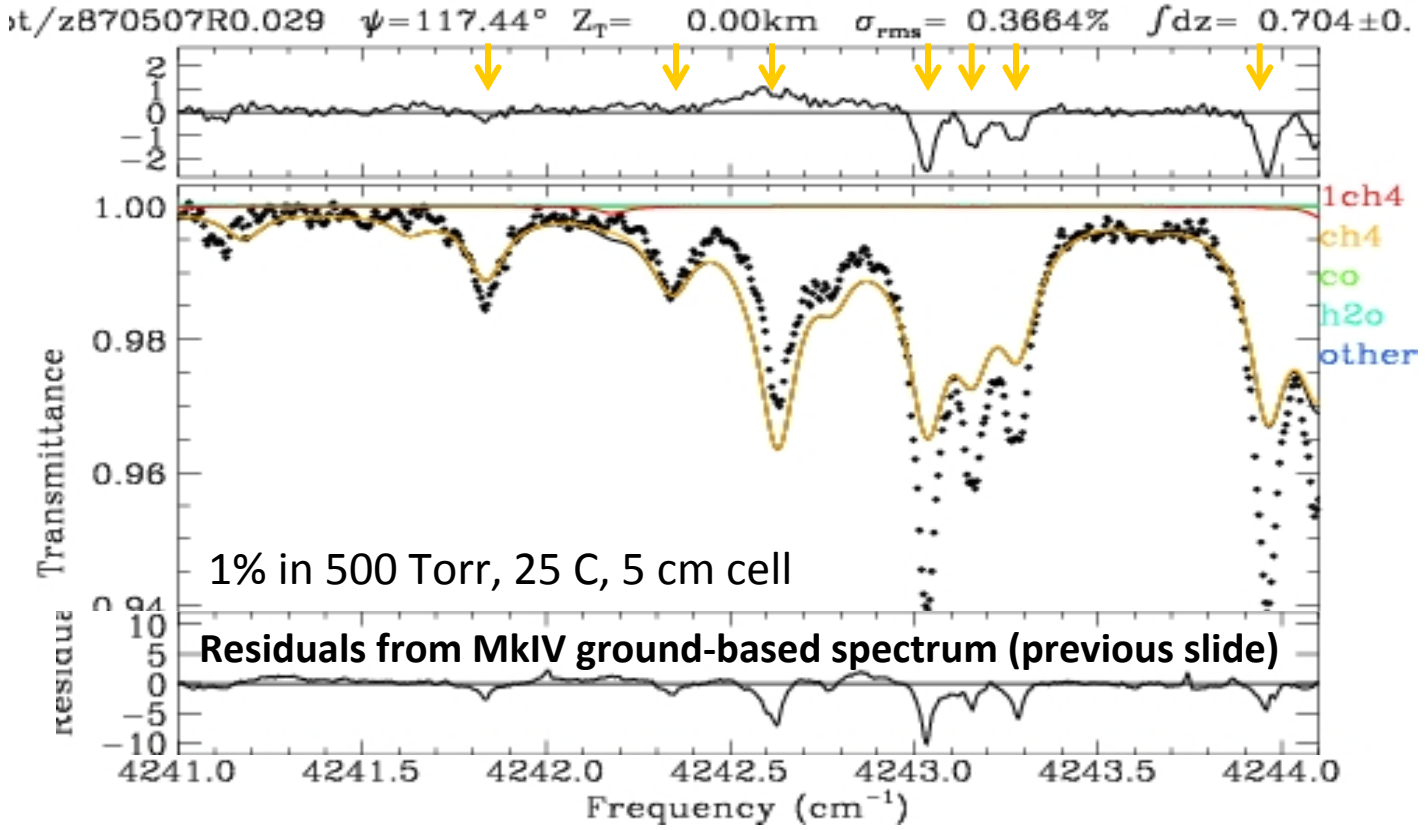
HITRAN 2008 contains no $^{13}CH_4$ lines between 3364 and 5898 cm^{-1}

Below is a fit to a high-airmass, high altitude, MkIV ground-based

Could $^{13}CH_4$ be causing the dips in the residuals which reach 10% ?



Fit to Kitt Peak $^{13}CH_4$ lab spectrum



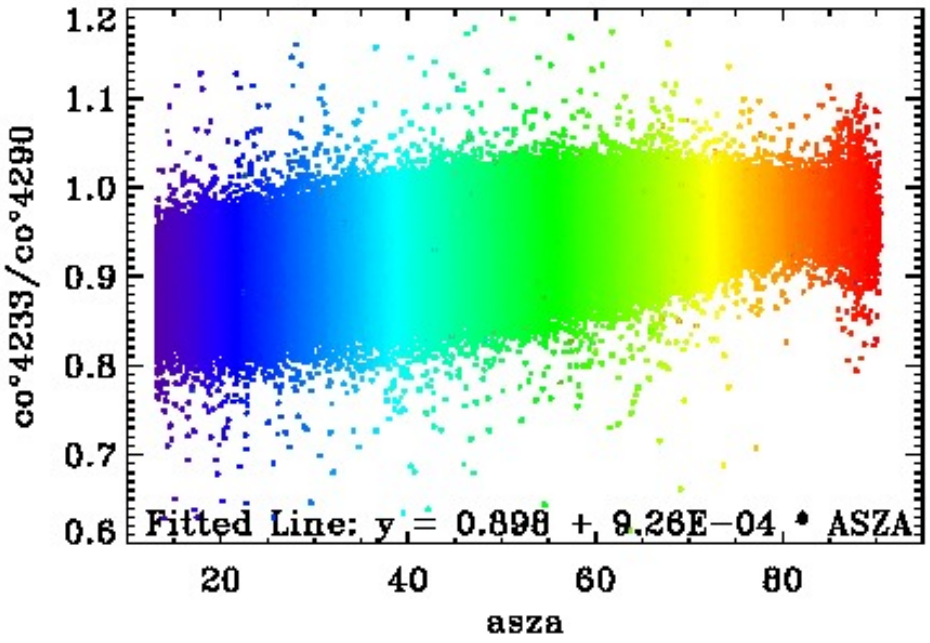
Almost perfect correlation between the MkIV fitting residuals from the previous slide and the ^{13}CH4 absorption features in the Kitt Peak spectrum (black dots).
Yellow line is $^{13}CH_4$ calculation using linelist downloaded from "Methane@Titan" website: http://www.icb.cnrs.fr/titan/

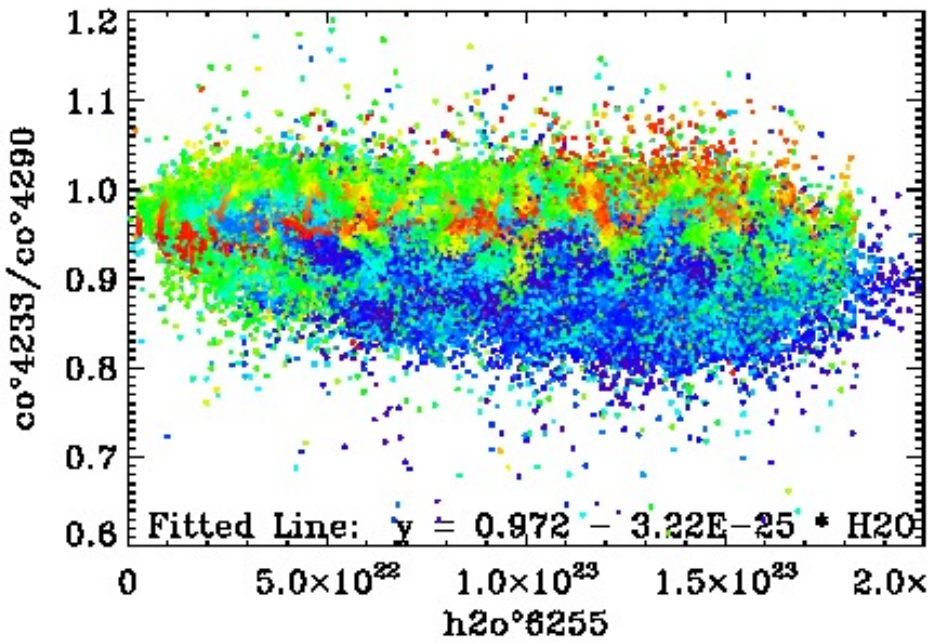
CO P/R branch Comparison

TCCON measures CO in the 4200-4320 cm^{-1} region using the overtone band. There is a systematic bias (~10%) in the CO retrieved from the P-branch window centered at 4233 cm^{-1} and from the R-branch window centered at 4290 cm^{-1}.

Since this bias is not seen in balloon spectra, it Is likely related to the spectroscopy of the strongly interfering H_2O or CH_4 absorption lines, which strongly overlap the CO absorptions in ground-based spectra.

Below 239,400 Lamont observations of the ratio: P-branch_CO / R-branch_CO

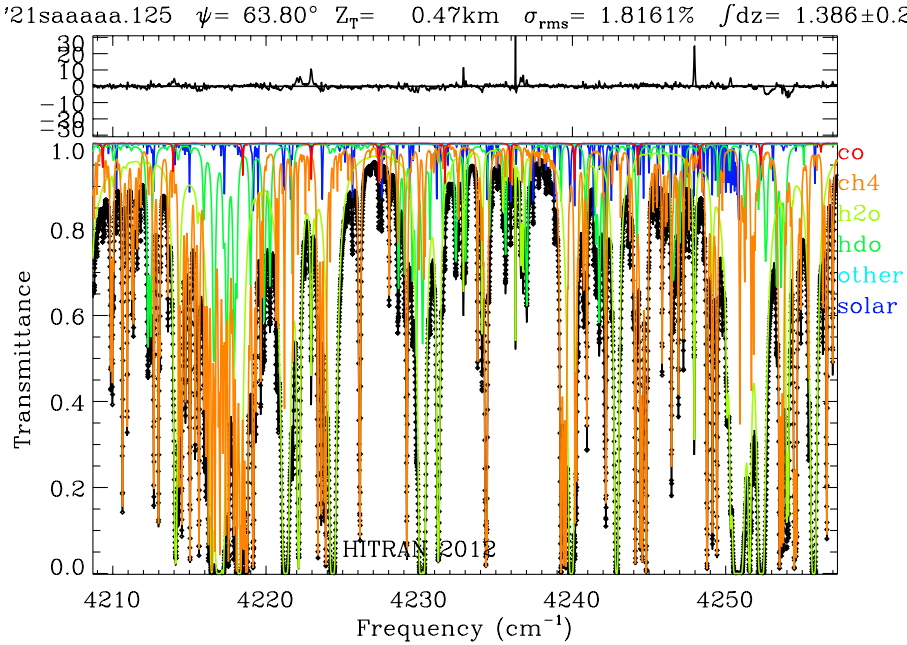


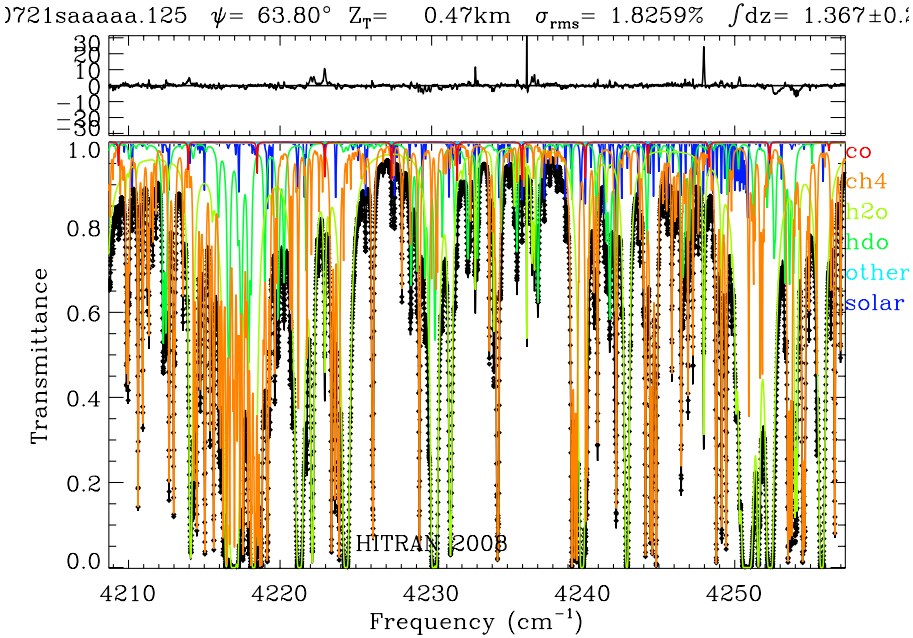


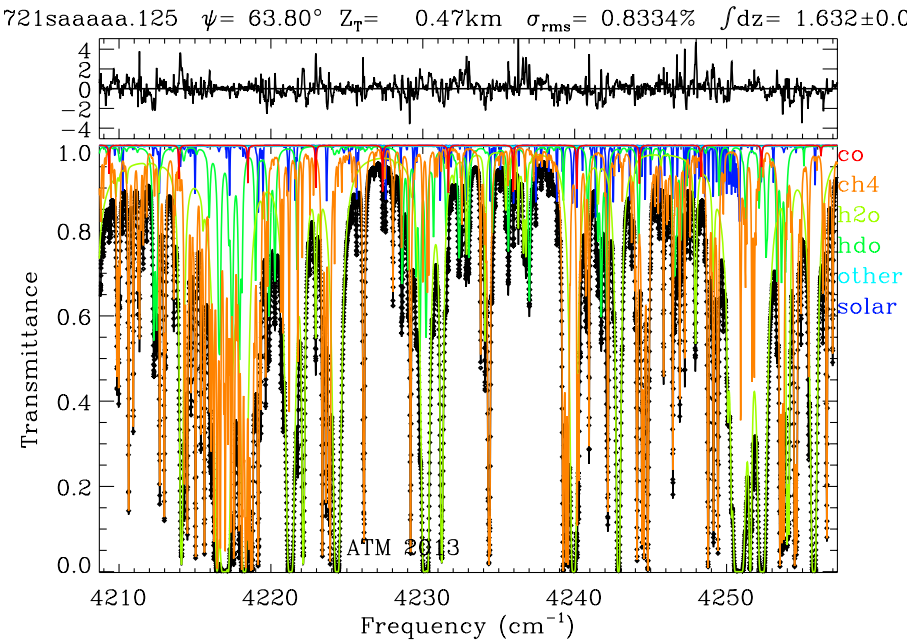
CO_4233 Window

Warm humid Park Falls spectrum.
Large H_2O-related residuals
Only minor improvement in HIT 2012

ATM linelist reduces RMS residual by factor 2.5, and increases retrieved CO by up to 20% under humid conditions.



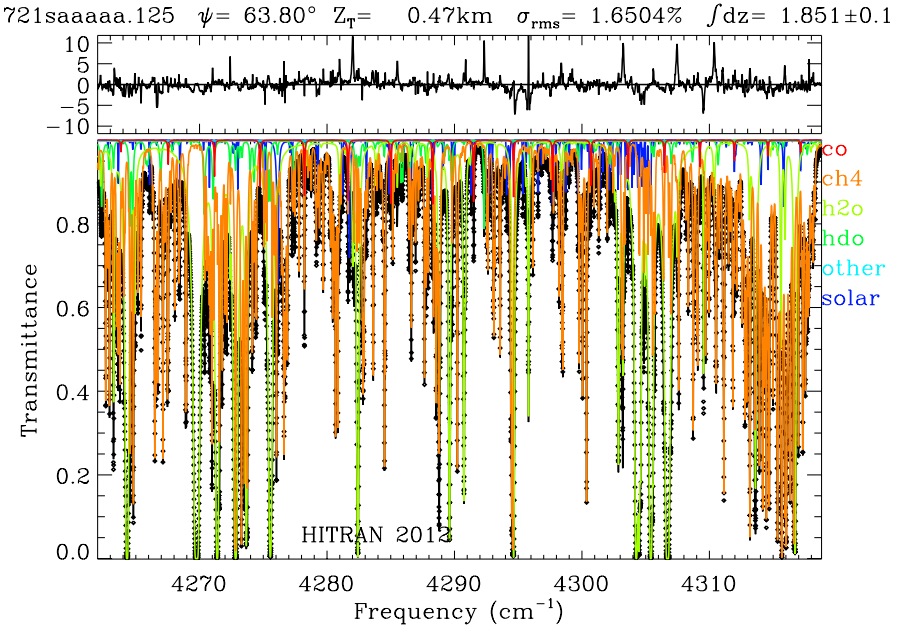


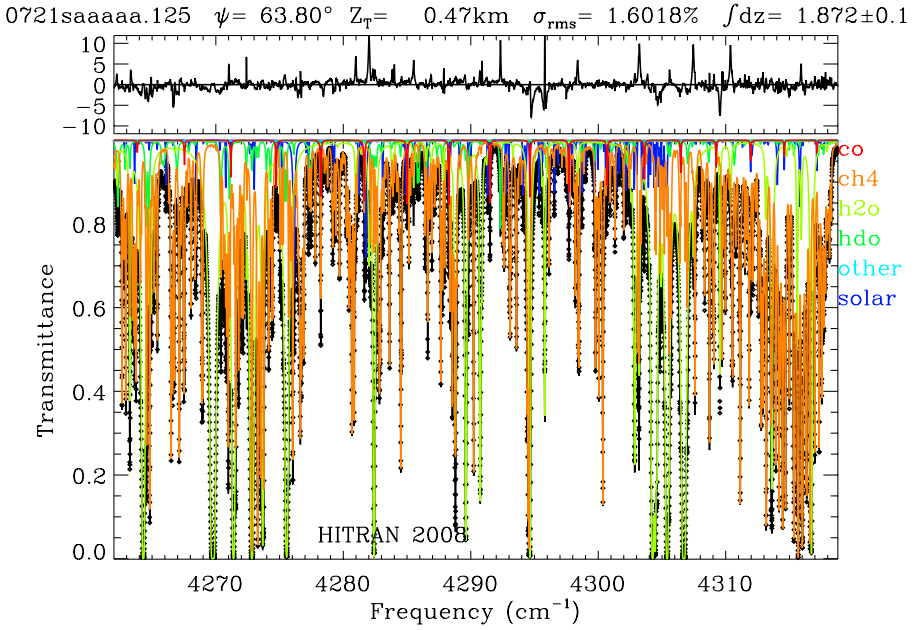


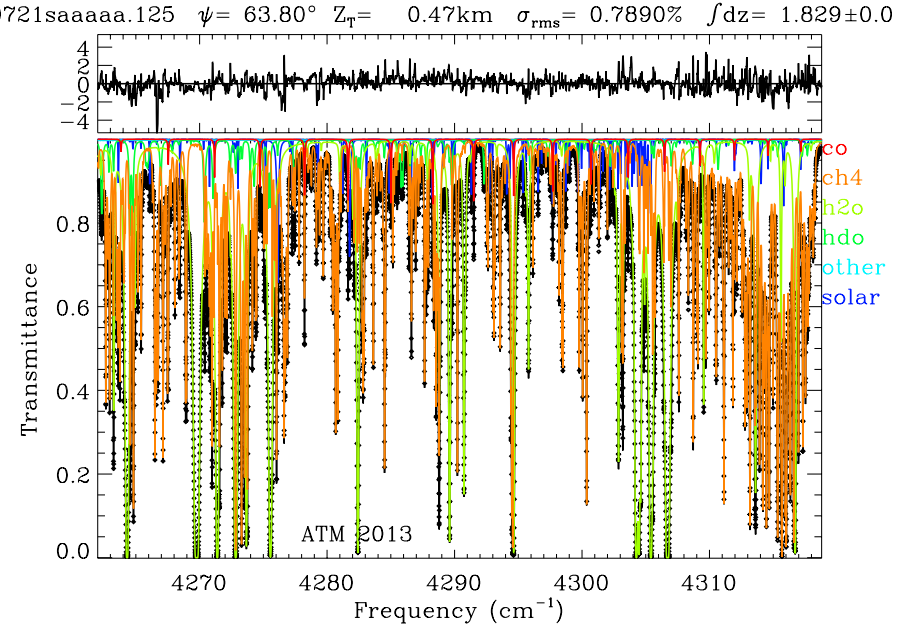
CO_4290 Window

R-branch in same warm humid spectrum

HITRAN 2012 provides slightly poorer fits than HITRAN 2008







Results of fitting Atmospheric spectra

Window / Linelist	CO_4233 cm-1 RMS	CO_4233 cm-1 VSF	CO_4290 cm-1 RMS	CO_4290 cm-1 VSF
HITRAN 2008	1.577%	0.944	1.35%	1.049
HITRAN 2012 (beta)	1.387	0.979	1.48%	1.044
ATM	0.885%	0.985	0.860%	1.062

RMS is the average RMS spectral fit using all the spectra in the pa_ggg_benchmark.grl runlog. VSF is the average CO vmr scale factor

HITRAN 2008 causes 10.5% bias

The HITRAN 2012 linelist includes $^{13}CH_4$ and makes the two windows more consistent (6.5% bias)

ATM 13 linelist produces smallest residuals but still an 7.7% bias.

Bias seems to be airmass dependent implying spectroscopy. Very likely interfering CH_4 or H_2O.

Atmos. Meas. Tech., 6, 879–894, 2013
www.atmos-meas-tech.net/6/879/2013/
doi:10.5194/amt-6-879-2013

Atmospheric Measurement Techniques Open Access

Improved water vapour spectroscopy in the 4174–4300 cm^{-1} region and its impact on SCIAMACHY HDO/H_2O measurements

R. A. Scheepmaker[1], C. Frankenberg[2], A. Galli[1], A. Butz[3], H. Schrijver[1], N. M. Deutscher[4,5], D. Wunch[6], T. Warneke[4], S. Fally[7], and I. Aben[1]

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[4]Institute for Environmental Physics, University of Bremen, Bremen, Germany
[5]Centre for Atmospheric Chemistry, University of Wollongong, Wollongong, Australia
[6]Department of Earth Science and Engineering, California Institute of Technology, Pasadena, CA, USA
[7]Formerly at: Institut d'Aéronomie Spatiale de Belgique (IASB-BIRA), Brussels, Belgium

This new paper was recently brought to my attentions.
Will evaluate the H_2O spectroscopy therein when I return to JPL.

Linelist Status Summary

In most windows of interest to TCCON, HITRAN 2012 provides better spectral fits than HITRAN 2008.

In nearly all windows, ATM 2013 already provides better fits than either

This is because ATM linelist (used by TCCON) has been hand-edited to adjust lines that give rise to large residuals in fits to atmospheric spectra.

These adjustments may be **triggered** by outliers in fits to atmospheric spectra, but are **based on** fits to Laboratory spectra.

In least squares fitting, large residual outliers have a disproportionate impact on the retrieval, so it is important that they be dealt with in some way.

In my opinion, the linelist is not sacred – it is okay to empirically adjust provided the adjustments have defensible basis (e.g. are supported by lab measurements).

But this approach does create difficulty in citing the linelist used for TCCON analyses.

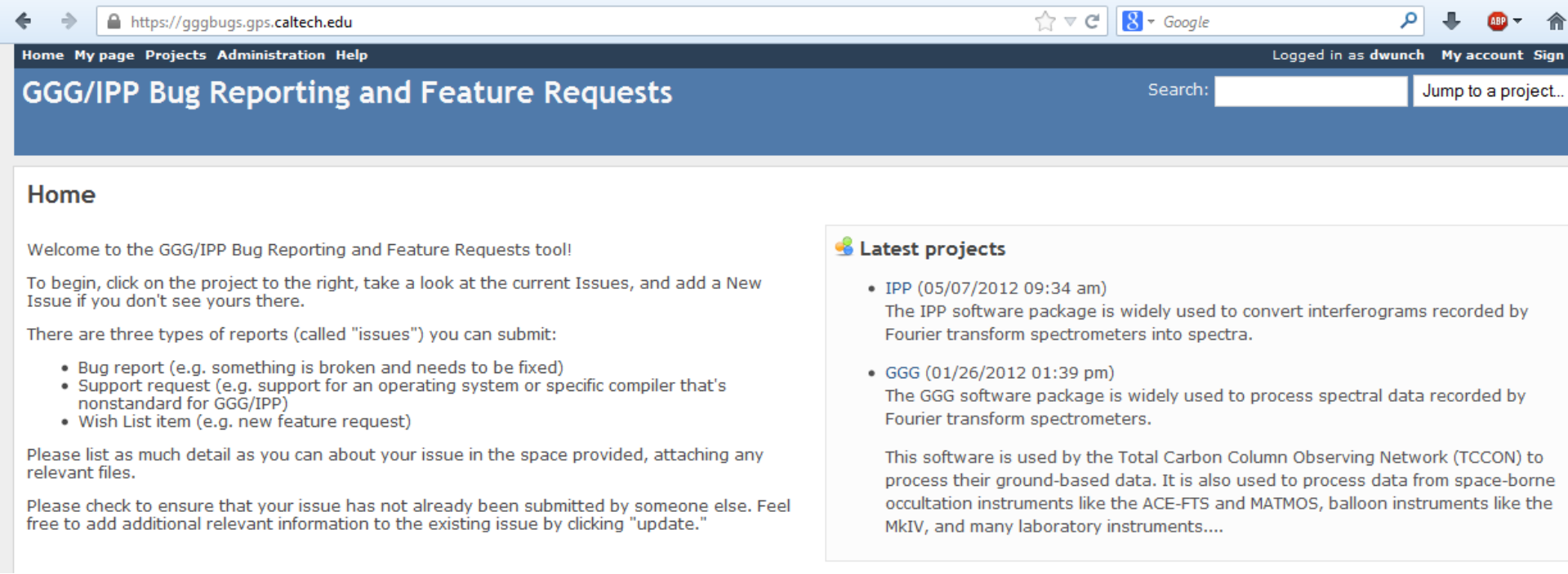
Linelist Summary/Plans

Evaluate HITRAN 2012 in TCCON windows.
Adopt the gases/bands that are improved.
Assess new linelists as they become available (e.g. Sheepmaker et al., 2013)

HITRAN 2012 represents:

- Two steps forward
- One step backwards
- A long way to go

Reporting Bugs/Requests in IPP/GGG



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#	Project	Tracker	Status	Priority	Subject	Author	Assignee	Updated
99	GGG	Wish List	New	Low	Add delimiter to all file headers.	Geoffrey Toon	Geoffrey Toon	06/02/2013 03:30 pm
98	GGG	Bug	Resolved	Normal	file_size_in_bytes.f appears not to work on files larger than 1GB	Geoffrey Toon	Geoffrey Toon	05/21/2013 11:40 am
97	GGG	Bug	New	Normal	collate_results and December 31 of leap years	Nicholas Deutscher		05/07/2013 08:50 am
96	GGG	Wish List	New	Low	Merge fm3.f into fm.f	Geoffrey Toon	Geoffrey Toon	05/02/2013 07:20 pm
95	GGG	Wish List	New	Low	Modularize .col file I/O	Geoffrey Toon	Debra Wunch	04/26/2013 05:50 pm
94	GGG	Wish List	New	Low	Add scan duration to runlog	Geoffrey Toon	Geoffrey Toon	04/26/2013 05:34 pm
93	GGG	Bug	Resolved	Normal	gfortran version 4.4.7 producing NaNs	Debra Wunch		04/09/2013 02:39 pm
92	GGG	Bug	Resolved	Normal	map files do not contain HF	Debra Wunch	Debra Wunch	03/14/2013 11:30 am
91	GGG	Wish List	In Progress	Normal	calculate time-dependent error scale factor	Debra Wunch		02/28/2013 12:11 pm
90	GGG	Wish List	New	Low	rewrite mod_maker in fortran	Debra Wunch		02/14/2013 05:38 pm
89	GGG	Wish List	New	Normal	mrow consolidation	Debra Wunch		02/14/2013 09:40 am
87	GGG	Bug	New	Normal	extremely large tcorr values	Nicholas Deutscher		01/17/2013 10:23 am
85	GGG	Wish List	New	Normal	Fix inconsistency in wet/dry vmrs in GFIT	Debra Wunch		12/24/2012 09:19 am
84	GGG	Bug	New	Low	apply_ghost_correction.f	Geoffrey Toon	Nicholas Deutscher	01/15/2013 09:10 am

99 GGG bugs/requests logged so far.
Whoever submits 100’th bug wins trip to next TCCON meeting.

Wish List #52

Compute FVSI from lowpass filtered DC interferogram

Added by Debra Wunch 12 months ago. Updated 8 months ago.

Status:	Resolved	**Start date:**	06/21/2012
Priority:	Normal	**Due date:**	
Assignee:	Debra Wunch	**% Done:**	0%
Category:	-	**Spent time:**	-
Target version:	IPP-2013		

Description

Several sites (Eureka, Caltech, etc.) do not use the Bruker tracker and may not have an FVSI value from the tracker quadrant diodes to use as a pre- or post-processing filter on the TCCON data. This filter turns out to be important to assess the quality of the TCCON data.

The low-pass filtered DC interferogram used to perform the SIV correction contains similar information to the FVSI from the quadrant sensor, and could be used to compute a SIV field that could be written into the header. This would then be available for all TCCON sites, regardless of the solar tracker they use.

This would require reporting the standard deviation (or other statistical variability measure) of the smoothed DC interferogram, and would probably require a (hopefully minor) modification to the siv_correction.f program.

calculated_vs_measured_FVSI.png - Comparison between FVSI from the tracker and a calculated FVSI from the smoothed interferogram. (9 kB) Debra Wunch, 10/15/2012 06:07 pm

fvsi_vs_fvsi_calc_AC_DC.png - Tracker FVSI versus AC and DC calculations of VDC. (8.8 kB) Debra Wunch, 10/18/2012 11:24 am

Subtasks

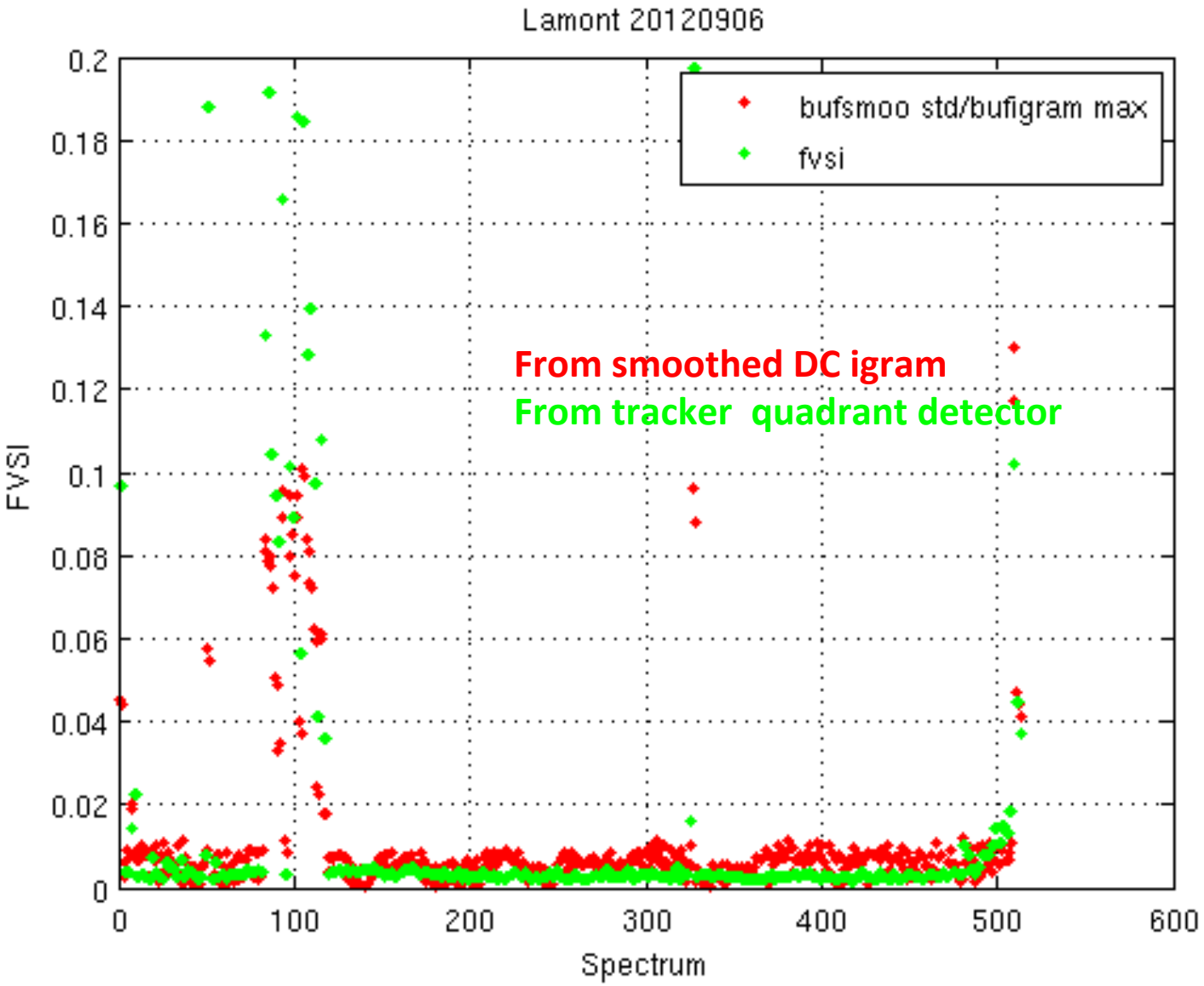
Related issues

History

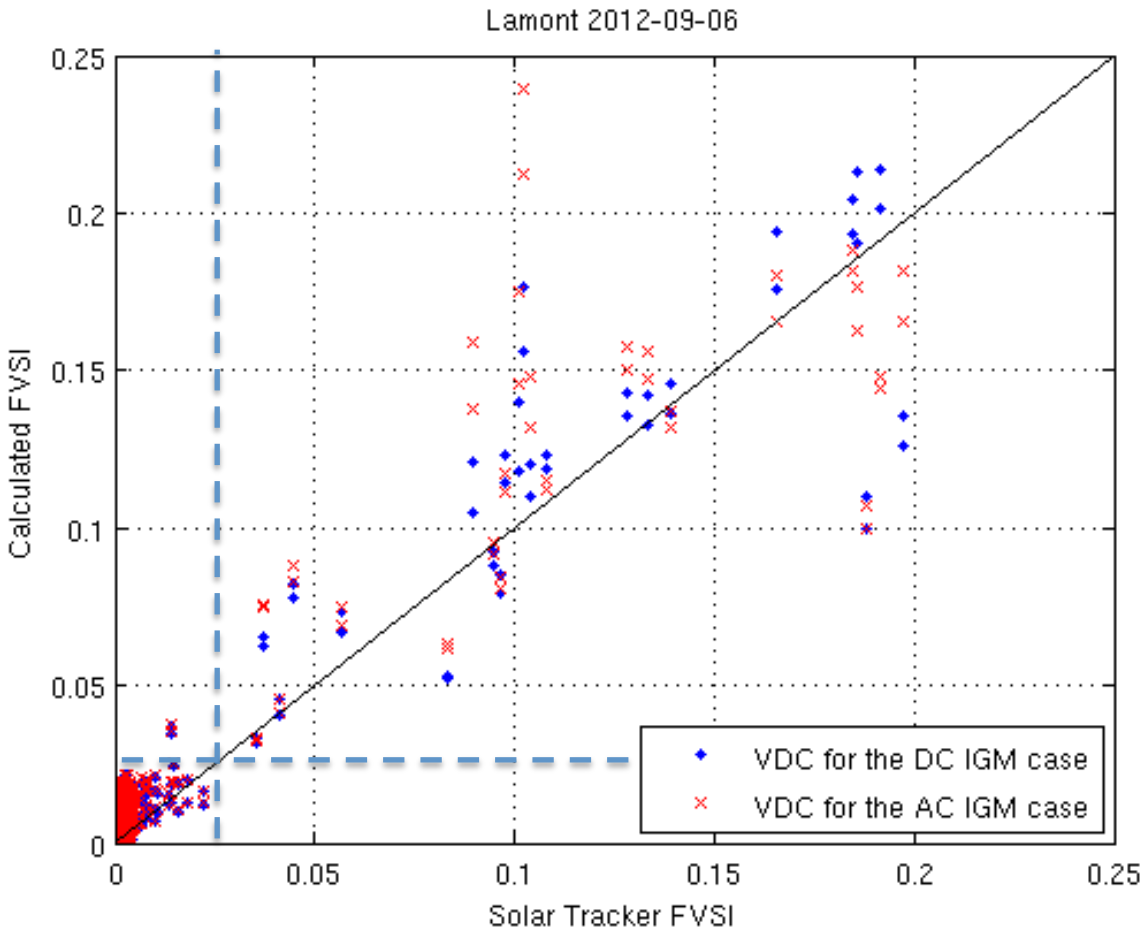
Updated by Geoffrey Toon 11 months ago #1

Debra, I think that this is a good idea, but foresee two complications:
1) When people record AC interferograms, the info needed to derive an igram-based FVSI is lost. What to do in this case?
2) For dual channel acquisition in DC mode, there will be two igram-derived FVSI values, plus the regular FVSI from the tracker. Which one of the three do we report?
Geoff

Fractional Variation in Solar Intensity (FVSI)



FVSI



Filtering the FVSI based on the solar tracker quadrant intensity versus the smoothed DC igram will produce very similar results. In the particular case shown above, filtering for FVSI < 2.5% will yield the exact same subset of spectra in either case.

Short side of Interferogram ZPD

Short side of ZPD is not wasted. It is used for:

- Phase correction
- Interferogram smoothing (for SIV correction)
- ZPD dip removal (SIV correction)

4 years ago, the limit was 4000 points on shorts side of ZPD.

Then a site was accepted to TCCON recording <4000 points, so the minimum operator length was reduced to 3600 points.

This affects **all sites (**to keep IPP processing identical for all sites).

Now a new instrument has recorded data with only 3100 points on the short side of ZPD. What to do? Decrease limit to 3000?

The time saved by recording only 3000 points versus 4000 points on short side is only 0.05s per scan, or 0.07% for 45 cm OPD

Strongly encourage at least 4000 points on short side of ZPD.

Park Falls, Lamont, Darwin record 140,000 points on short side of ZPD

Future TCCON Plans

GGG

- Profile Retrieval (Connor, Sherlock)
- Frequency Calibration of spectra
- Improved P/T (ECMWF, intra-day model variation)
- Use model PV to improve a priori vmr profiles
- Empirical ILS
- Improved ray tracing at high airmass (tlpath)

IPP

- Ghost Correction implementation
- Short side of ZPD (minimum length)
- FWD/REV bias in A-band results (ZPD-dependent)