Updates to the Spectroscopic Model for the OCO-2 Retrieval Algorithm: ABSCO v5.2 for Level 2 v11

3-P06

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0. Introduction

Accurate retrievals of absorbing gases in remote sensing missions such as the Orbiting Carbon Observatory 2 (OCO-2) require an accurate characterization of absorption cross sections. Systematic errors in the spectroscopic model can lead to both spatial and temporal errors in retrieved atmospheric composition and consequently to biases in derived flux estimates. The exacting error budget demanded by OCO-2 necessitates a degree of accuracy in the spectroscopy that has not yet been attained. Nevertheless, continual improvements are being made. This work highlights the latest update to the spectroscopy models used in version 11 of the OCO-2 algorithm. These models are ingested by the algorithm in the form of absorption cross section (ABSCO) tables covering two CO_2 bands at 1.61 μm ("weak band") and 2.06 μm ("strong band") and the O_2 A-band (0.76 μm). This latest update (v5.2) comprises two main changes: the adoption of a HITRAN-based H_2O line list developed by Geoff Toon and a new parameterization of the CO_2 cross sections in the strong band which utilizes a full relaxation matrix representation of line mixing developed by Lamouroux. Previous ABSCO versions for this band assumed a nearest neighbor line mixing formulation that required an *ad hoc* correction to account for "missing" absorption between the P and R branches observed in ground-based retrievals.

This work compares retrieval fits using ABSCO v5.2 with other models, including the previous version, v5.1, using both ground-based TCCON spectra as well as satellite OCO-2 data. We demonstrate that the revised water tables significantly reduce residuals, particularly in the TCCON retrievals, and show that the updated CO_2 cross sections yield residuals comparable to those obtained previously but without the need for an *ad hoc* correction.

1. Absco tables and testing methodology

The ACOS/OCO-2/OCO-3 ABSCO tables are "lookup tables" that supply cross section values for absorbing gases in the Level 2 algorithm (L2) retrieval process. They record molecular absorption cross sections in units of cm^2/mol for the gases O_2, H_2O, and CO_2 over a four dimensional grid of relevant wavelengths, temperatures, pressures, and water vapor mixing ratios, over which cross sections are linearly interpolated during the L2 generation process. Successive versions have refined these tables by incorporating new laboratory results and theoretical results for increasingly accurate absorption coefficients. ABSCO tables are released together with each major build of the OCO-2 Level 2 algorithm, and the update (v5.2) described here is used in version 11. Currently, publicly available Level 2 products for the duration of the OCO-2 and OCO-3 missions are derived using the version 10 algorithm, which employs ABSCO v5.1. However, beginning in March 2022, OCO-2 forward data processing switched over to version 11, and the entire OCO-2 Level 2 record will eventually be reprocessed using version 11 as well.

The results shown here rely on retrievals using both ground-based TCCON and satellite OCO-2 spectra. When candidate ABSCO tables are generated, they are typically first tested using TCCON spectra. The finer spectral resolution and fewer confounding effects (e.g. aerosol scattering, BRDF) offered by the ground-based measurements enable easier identification of issues related to spectroscopy. Once candidate tables have been validated with TCCON, testing on a much larger set (~10^6) of OCO-2 measurements is done. The ground-based results shown here are single band retrievals of a small set of measurements using the Bruker FTS at Lamont as described in [1].
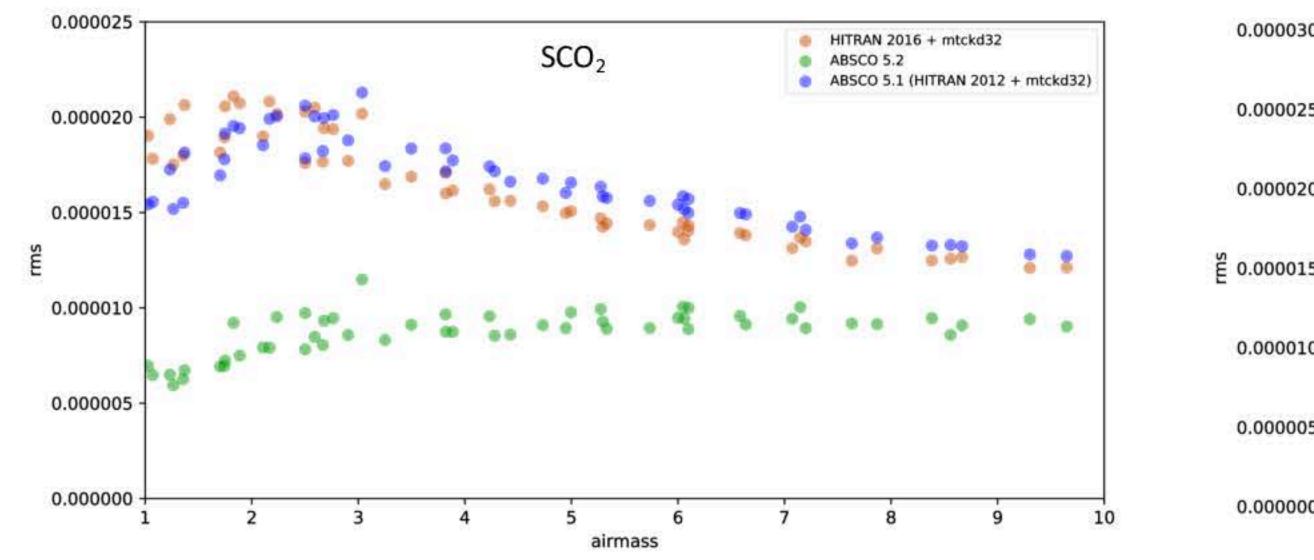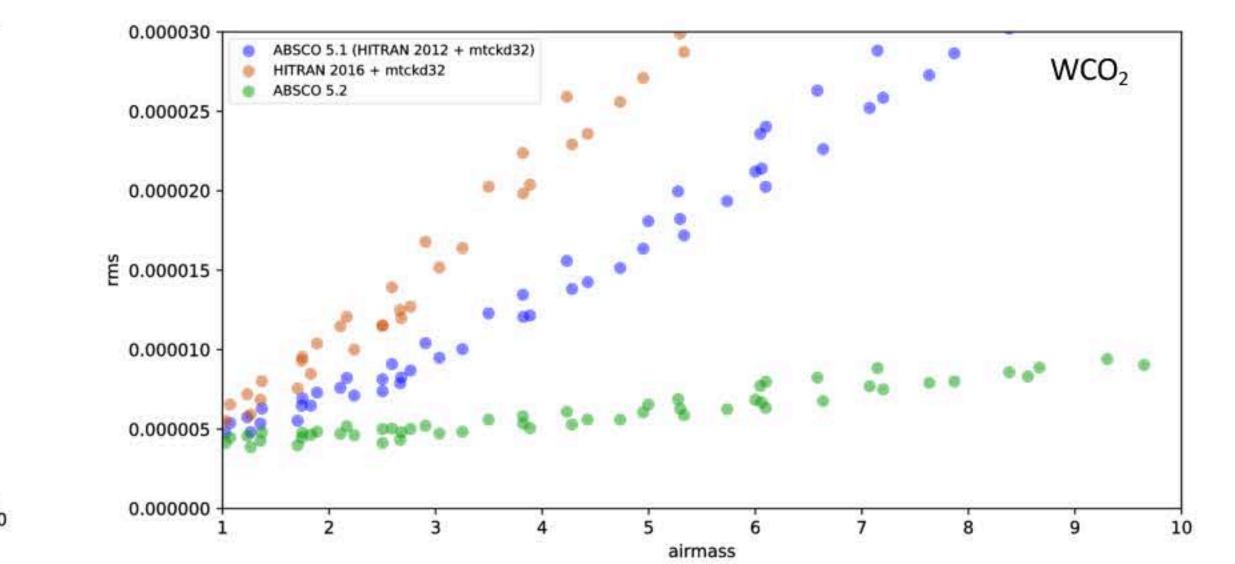
References

[1] Oyafuso, F, Payne, VP, Drouin, BJ, et al. (2017). High accuracy absorption coefficients for the Orbiting Carbon Observatory-2 (OCO-2) mission: Validation of updated carbon dioxide cross-sections using atmospheric spectra. JQSRT, 203. https://doi.org/10.1016/j.jqsrt.2017.06.012

[2] https://mark4sun.jpl.nasa.gov/toon/atm18/atm18.html

[3] Mlawer, E.J., V.H. Payne, J.-L. Moncet, J.S. Delamere, M.J. Alvarado, D.D. Tobin, Development and recent evaluation of the MT_CKD model of continuum absorption, *Phil. Trans. Roy. Soc.A*, June 13, 2012 370 1968 2520-2556.

[4] D. C. Benner, V. M. Devi, K. Sung, L. R. Brown, C. E. Miller, V. H. Payne, B. J. Drouin, S. Yu, T. J. Crawford, A. W. Mantz, M. A. H. Smith, R. R. Gamache, Line parameters including temperature dependences of air- and self-broadened line shapes of 12C16O2: 2.06 micron region, J. Mol. Spec., 2016

[5] J Lamouroux, L. Régalia b, X. Thomas b, J. Vander Auwera c, R.R. Gamache d, J.-M. Hartmann, "CO2 line-mixing database and software update and its tests in the 2.1 μm and 4.3 μm regions", JQSRT, 151, 88-96 (2015), http://dx.doi.org/10.1016/j.jqsrt.2014.09.017

[6] H Fleurbaey, H Yi, EM Adkins, AJ Fleisher, JT Hodges, Cavity ring-down spectroscopy of CO2 near λ = 2.06 μm: Accurate transition intensities for the Orbiting Carbon Observatory-2 (OCO-2) "strong band", JQSRT, 252 107104 (2020), https://doi.org/10.1016/j.jqsrt.2020.107104.
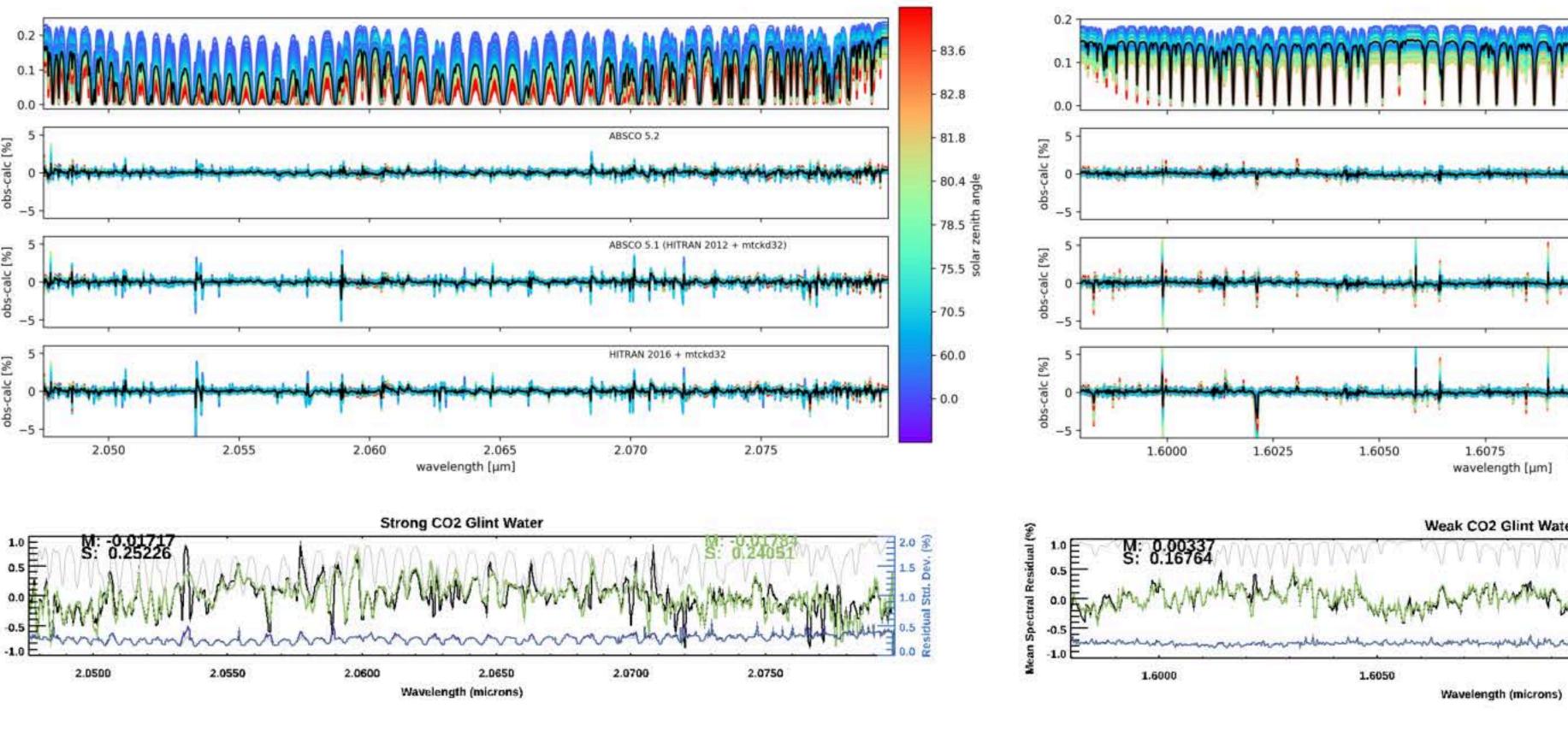
2. H2O update

Recent versions of ABSCO (v5.0 and v5.1) had used the HITRAN 2012 line list to characterize resonant absorption of water lines. The transition to HITRAN 2016 had demonstrated a degradation in quality of fit in the weak (1.61 μm) CO_2 band and was therefore not adopted. Instead, version 5.2 of ABSCO has adopted a line list developed by Geoff Toon based on a modification of his ATM18 line list [2]. The continuum model remains MT-CKD v3.2 [3]. Unlike in previous versions of ABSCO, retrieved column abundances of water vapor using TCCON spectra were consistent between the two OCO-2 bands that are sensitive to water. However, it was found that both ground-based and satellite-based retrievals underestimated truth values (based on GGG 2014) by ~2%. In order to align mean satellite-retrieved water column values with their prior, a scaling factor of 0.981 is applied to water cross sections in ABSCO v5.2.
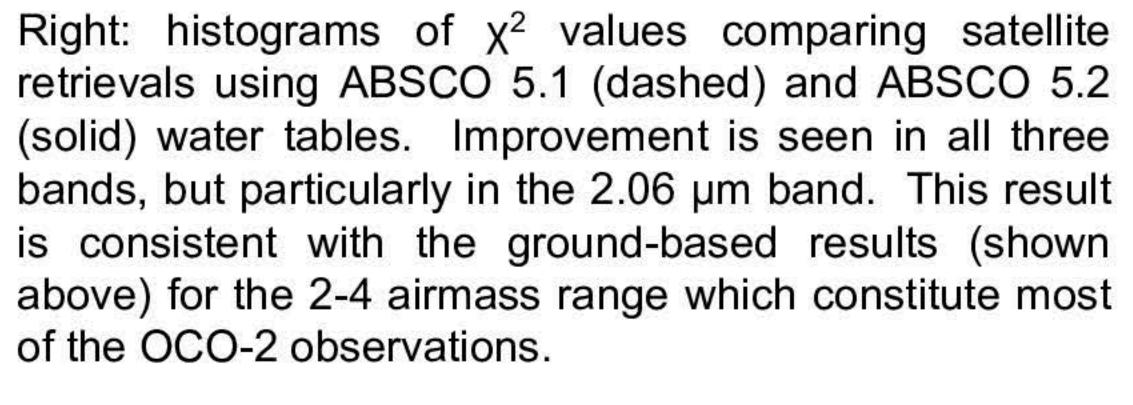
The figure below shows the rms of residuals for a small set of TCCON spectra as functions of airmass. ABSCO v5.2 shows considerable improvement over both ABSCO v5.1 (HITRAN 2012) and HITRAN 2016 for both the strong and weak CO_2 bands. Note, however, that the improvement in the strong band is most pronounced at lower airmasses.
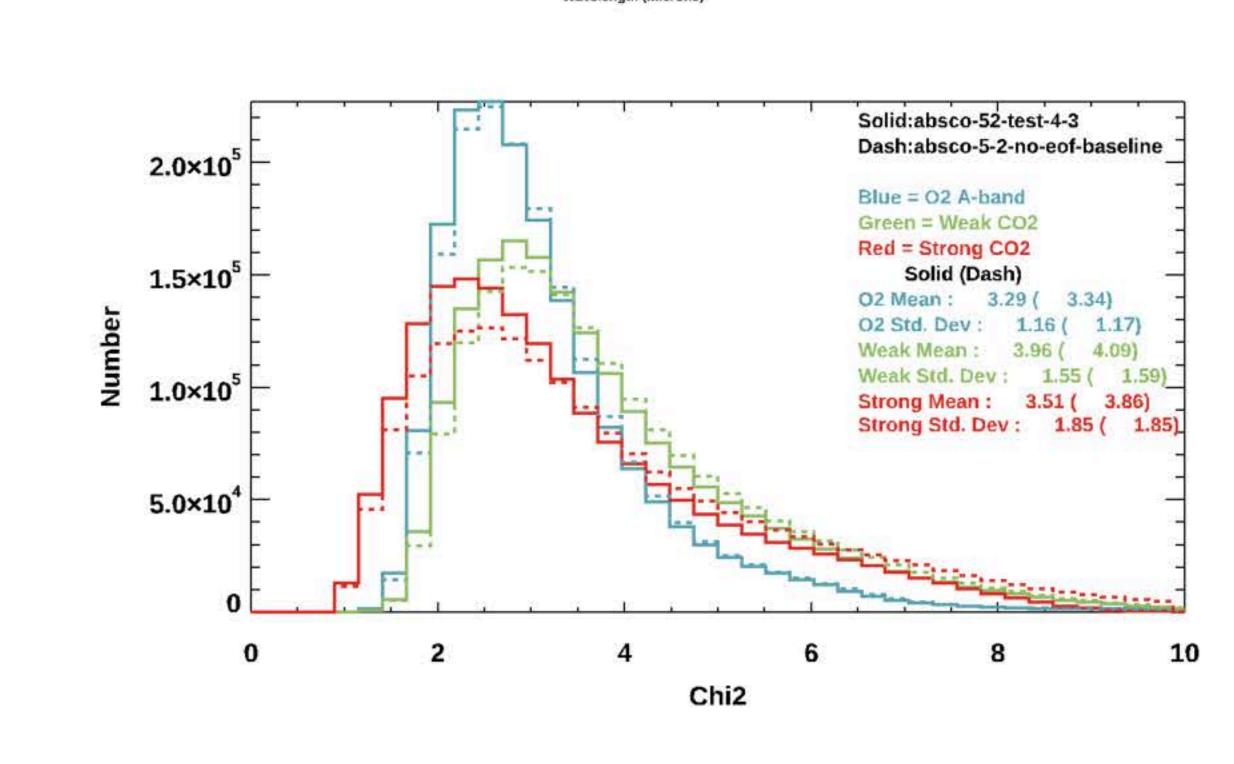

In the figures below, the top panels below plot residuals of retrievals of summer (a proxy for higher water content) TCCON spectra where color indicates solar zenith angle. The mean is shown in black. The same three sets of water line lists are compared, and many features evident in the older versions of HITRAN are substantially reduced in ATM 18. The bottom panel shows mean residuals from a set of OCO-2 ocean glint retrievals, where ABSCO 5.1/5.2 are in black/green. Regions where black and green lines differ correlate well with differences between ABSCO v5.2 and v5.1 in the top panel.
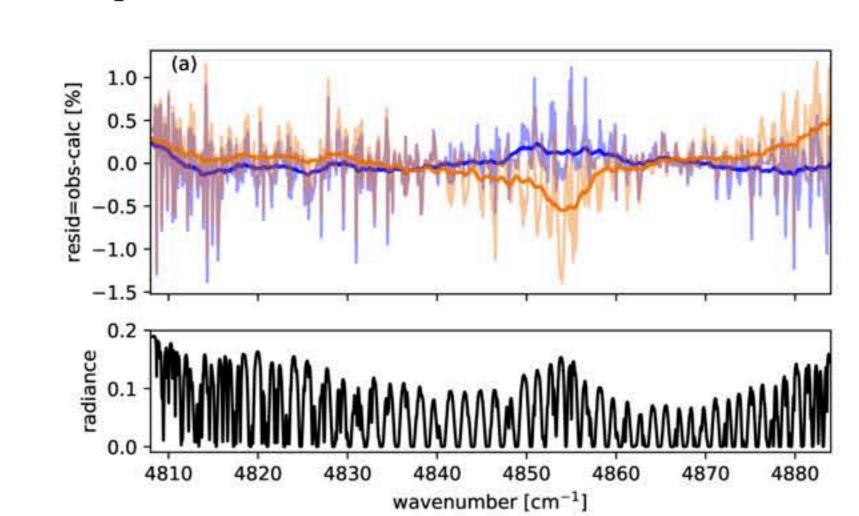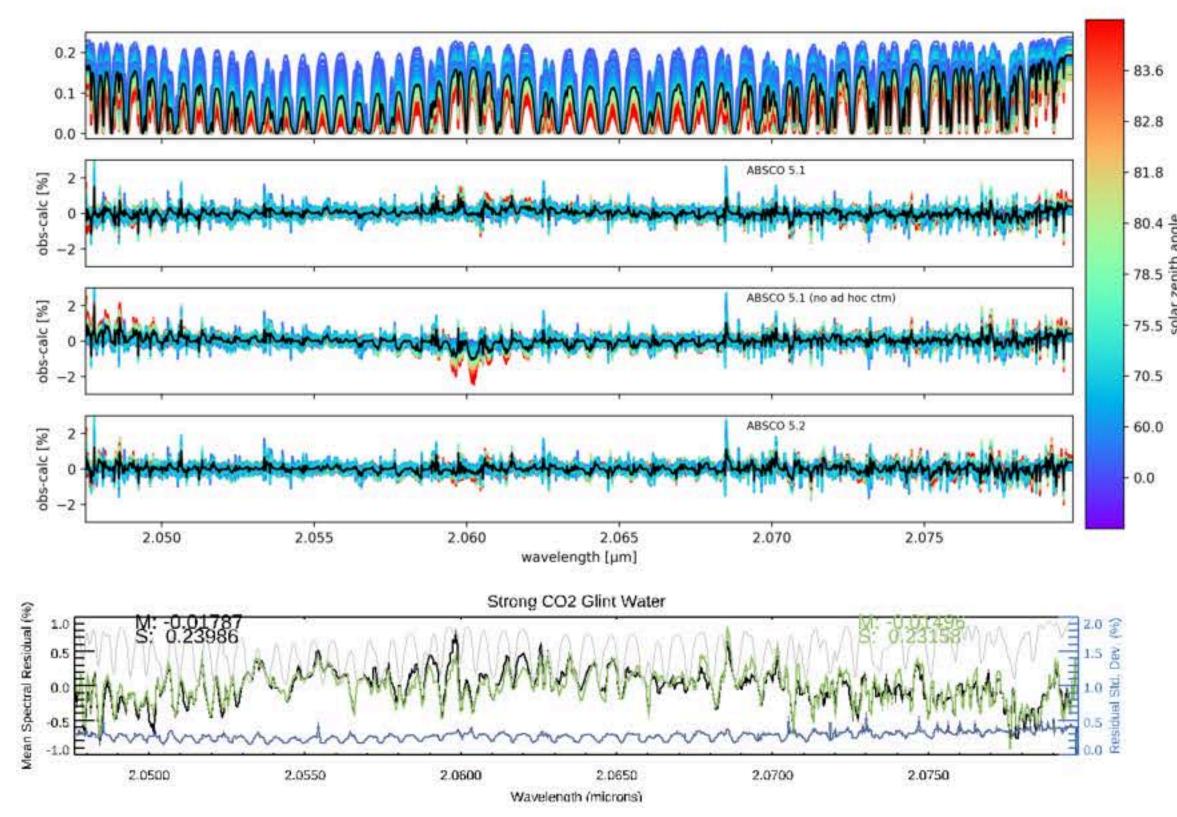

Right: histograms of χ^2 values comparing satellite retrievals using ABSCO 5.1 (dashed) and ABSCO 5.2 (solid) water tables. Improvement is seen in all three bands, but particularly in the 2.06 μm band. This result is consistent with the ground-based results (shown above) for the 2-4 airmass range which constitute most of the OCO-2 observations.

3. CO2 update to the "strong" 2.06 μm band

The CO_2 cross sections provided in ABSCO v5.0 and v5.1 in the 2.06 μm band were generated using a speed-dependent Voigt profile and a line mixing model that allowed for only nearest-neighbor relaxation matrix elements as described in Benner [4]. Additionally, the P and R branches were assumed to be uncoupled. This model was unable to account for the observed absorption between the P and R branches in atmospheric spectra. To correct this deficiency, an empirically determined *ad hoc* continuum-like absorption was added in previous versions of ABSCO.
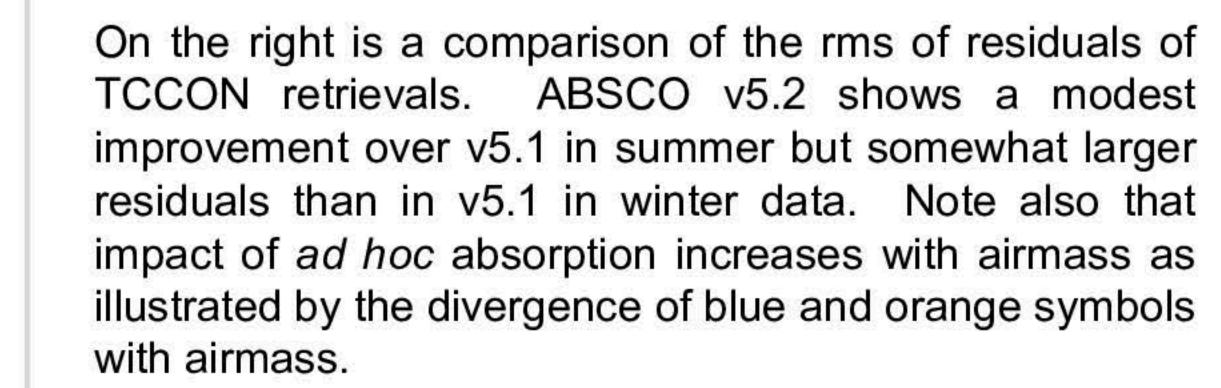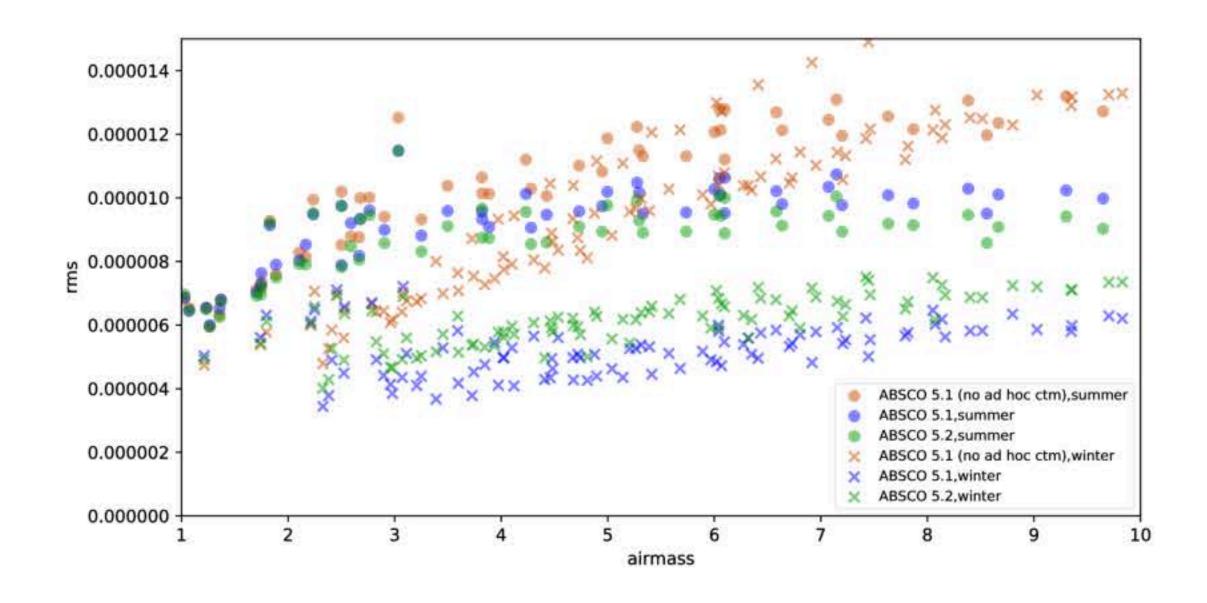

The figure above shows mean residuals for retrievals of a set of high (>4) airmass TCCON spectra. The blue/orange curves correspond to retrievals with/without the *ad hoc* absorption, and the darker shaded curves are moving averages using a boxcar width of 4 cm-1. Missing absorption is evident between the P and R branches (near 4584 cm^{-1}).

ABSCO v5.2 fits to the same set of laboratory measurements as in the previous version but sets non-nearest-neighbor off-diagonals of the relaxation matrix to values determined by Lamouroux [5]. Several scalings of these off-diagonals were attempted, but value of 1.0 was found to be most consistent with ground-based retrievals. The additional coupling between non-adjacent lines results in enhanced absorption between the P and R branches and obviates the need for an *ad hoc* absorption.
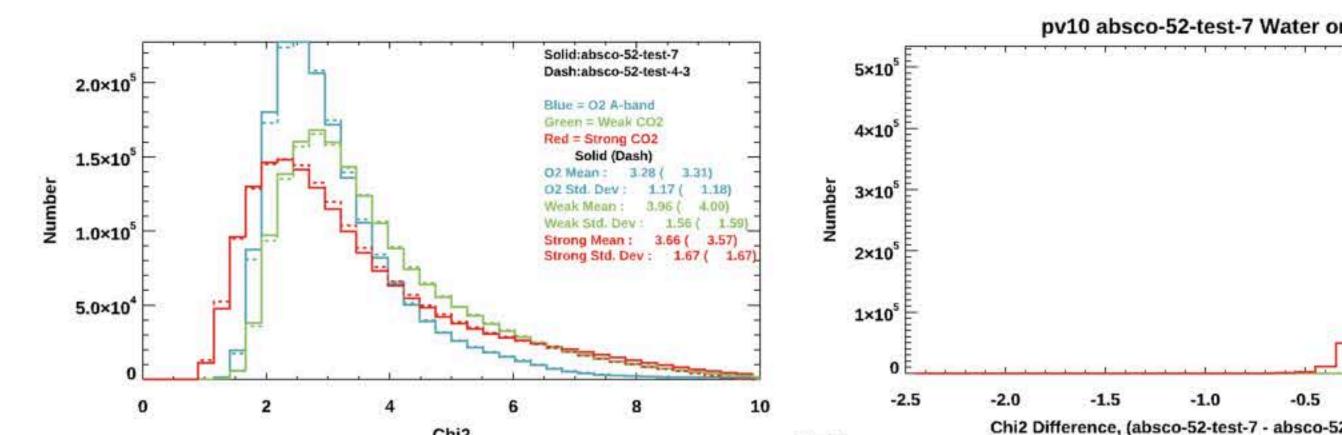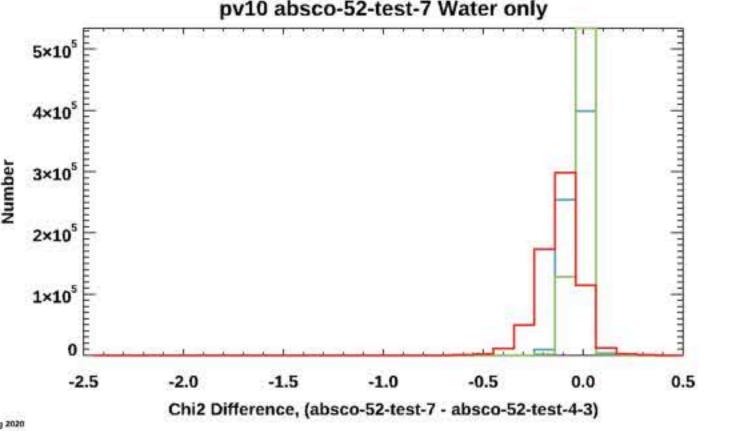

The top four panels on the left compare residuals of single band retrievals of TCCON spectra using three different absorption CO_2 models: ABSCO v5.1 with and without the *ad hoc* absorption and ABSCO v5.2. "Missing" absorption is evident at 2.060 μm at high solar zenith angles in the model without the *ad hoc* absorption. The bottom panel overlays mean residuals from ocean glint OCO-2 retrievals using v5.2 (green) over those using v5.1 (black). Residuals for these two cases are quite similar.
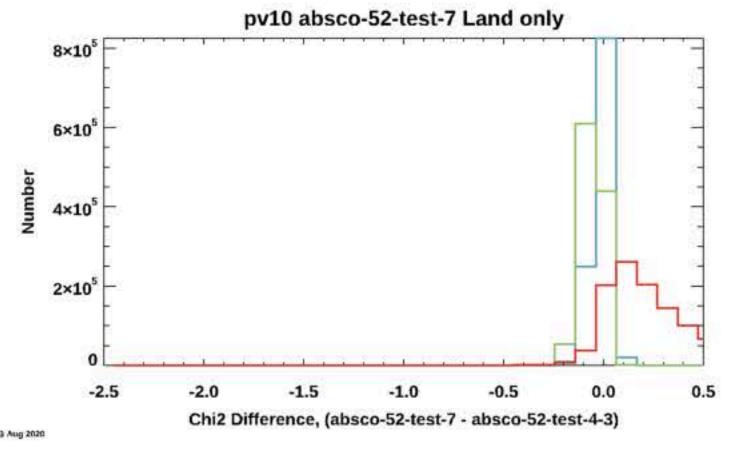
On the right is a comparison of the rms of residuals of TCCON retrievals. ABSCO v5.2 shows a modest improvement over v5.1 in summer but somewhat larger residuals than in v5.1 in winter data. Note also that impact of *ad hoc* absorption increases with airmass as illustrated by the divergence of blue and orange symbols with airmass.

Below are histograms of χ^2 values for each spectrometer comparing OCO-2 retrievals using ABSCO 5.2 (solid) and ABSCO 5.1 (dashed) CO_2 tables. The overall distributions are not significantly changed, but a reduction is seen in χ^2 over ocean and an increase over land:

One source of systematic uncertainty in the derivation of a spectroscopic model is the absolute intensity of a band. The ABSCO v5.2 tables for the SCO_2 scaled its line intensities in accordance with preliminary results that were subsequently published in Fleurbaey [6]. Final results in [6] were 0.05 - 0.10% smaller than the values used in v5.2. However, direct use of v5.2 in both single band TCCON and OCO-2 retrievals yielded X_{CO2} values consistently lower than those obtained using the 1.61 μm band (by 0.25-0.65%, depending on airmass). To enforce band consistency, the L2 algorithm applies a -0.65% scaling to the strong band relative to the scaling it applies to the weak band. Thus, in v11 of the L2 algorithm, scaling factors of 0.994 and 0.9875 are applied to ABSCO tables of the strong and weak bands, respectively.

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