## Orbiting Carbon Observatory-2 & 3 (OCO-2 & OCO-3)



# Data Product User's Guide, Operational Level 2 Lite Files

Version 2.0 Revision A July 5, 2022 Data Release: 11 (OCO-2), 10/10.4 (OCO-3)

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B – June 16, 2014	Update to prerelease, correcting MaxMS values	G. Osterman and team
C – December 30, 2014	Updated for release with L1B data	R. Granat and team
D – March 30, 2015	Updated for version 6 release with initial L2 data	R. Granat and team
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I – December 15, 2017	Updated to include missing BRDF Table	G. Osterman and team
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Version 2, Revision A – July 5, 2022	Updated for OCO-2 v11 and OCO-3 v10.4 data releases	G. Osterman and team

## **Document History**

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## 1 Introduction

#### 1.1 Document Overview

This document provides a brief overview of the Orbiting Carbon Observatory-2 (OCO-2) and Orbiting Carbon Observatory-3 (OCO-3) missions and then discusses the content of the publicly available Level 2 (L2) "Standard" data products. The data versions are the OCO-2 Level 2 (L2) release version 11 (v11) and the OCO-3 L2 data (v10).

The document also describes the data in the L2 "Lite" files, which are different from the L2 Standard products in that they are daily products with additional post processing data fields. They also include screened and bias corrected  $X_{CO2}$  values using the bias corrections described later in this document. The OCO-3 Lite data product is labeled as v10.4.

Much of the mission description and background information that was contained in previous versions has been removed in order to improve the utility of this document as a starting point for use of the data products. Some of the key references for background information are highlighted in Section 2.4 and the full list of references are in Section 15.

#### 1.2 Data Products

The primary product delivered by both OCO-2 and OCO-3 are the spatially resolved estimates of the column-averaged dry air mole fraction of carbon dioxide (CO<sub>2</sub>). This quantity, called  $X_{CO2}$  by members of the atmospheric carbon science community, quantifies the average concentration of carbon dioxide in a column of dry air extending from Earth's surface to the top of the atmosphere. Estimates of  $X_{CO2}$  are derived by taking the ratio of the column integrated number densities of carbon dioxide and molecular oxygen along the optical path between the Sun, the surface footprint, and the instrument, and then multiplying these results by the column-averaged oxygen concentration (0.20935). These carbon dioxide and oxygen number densities are estimated from high-resolution spectra of reflected sunlight, collected by the Observatory's instrument at wavelengths (colors) within the 0.765-micron molecular oxygen A band and two carbon dioxide bands centered at wavelengths near 1.61 and 2.06 microns. In addition, OCO-2 and OCO-3 are able to make measurements of steady-state Solar-Induced chlorophyll Fluorescence (SIF).

Both missions produce four different levels of data product for the user community that will provide comprehensive mission data results. These results can be summarized as:

- Level 1A full orbits or fractions of orbits of calibrated and geographically located science and calibration data with quality control flags set.
- Level 1B full orbits or fractions of orbits of calibrated and geographically located spectral radiances from the spectral channels centered on the 0.765-micron molecular oxygen A band and the carbon dioxide bands at wavelengths near 1.61 and 2.06 microns. This product contains a unique record of every sounding the instrument collects while viewing Earth during a single spacecraft orbit—approximately 74,000 soundings. Each sounding consists of collocated (observing the same location) spectra from the three spectrometer channels
- Level 2 full orbits or fractions of orbits of geographically located estimates of the column-averaged dry air mole fraction of carbon dioxide (also called  $X_{CO2}$ ) and several atmospheric and geophysical properties collected during each spacecraft orbit. This

product typically includes more than 4,000 retrievals of the concentration of atmospheric carbon dioxide in cloud-free scenes, as well as surface pressure, surface albedo, aerosol content and water vapor and temperature profiles. Estimates of the solar-induced chlorophyll fluorescence are provided in a preprocessor file (L2IDP).

The Level 1B and L2 are available at the NASA Goddard Earth Science Data and Information Services Center (GES DISC). More information on obtaining the data is provided in Sections 12 and 14.

#### 1.3 Data Usage Policy

These data have been produced by the OCO-2 and OCO-3 projects, and are provided freely to the public. In order to improve our products and have continued support for this work, we need user feedback and user acknowledgement of data usage. Therefore, we request that when publishing using OCO-2 and/or OCO-3 data, please acknowledge NASA and the individual projects.

- Include OCO-2 and/or OCO-3 as a keyword to facilitate subsequent searches of bibliographic databases if it is a significant part of the publication
- Include a bibliographic citation for OCO-3 and/or OCO-2 data. Some of the most relevant citations currently are listed in Section 2.4.
- Include the following acknowledgements:
  - "These data were produced by the OCO-2 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center."
  - "These data were produced by the OCO-3 project at the Jet Propulsion Laboratory, California Institute of Technology, and obtained from the OCO-2 data archive maintained at the NASA Goddard Earth Science Data and Information Services Center."
- We recommend sending courtesy copies of publications to the OCO-2 Project Scientist/OCO-3 Deputy Project Scientist, Vivienne Payne (Vivienne.H.Payne@jpl.nasa.gov), OCO-3 Project Scientist/OCO-2 Deputy Project Scientist, Abhishek Chatterjee (Abhishek.Chatterjee@jpl.nasa.gov).

#### 2 Mission Overviews

The Orbiting Carbon Observatory–2 (OCO-2) is NASA's first dedicated CO<sub>2</sub> monitoring satellite. OCO-2 is a "carbon copy" of the Orbiting Carbon Observatory (OCO), which was lost in 2009, when its launch vehicle malfunctioned and failed to reach orbit. A general description of the OCO mission is given in Crisp et al. [2004, 2008]. Most of the information is valid for OCO-2, but a few changes were needed to address known problems, replace obsolete hardware, or address operational changes. Changes that affect the OCO-2 data products are highlighted below.

The OCO-2 spacecraft carries and points a single instrument that incorporates 3, co-bore sighted, imaging, grating spectrometers. This instrument collects high-resolution spectra of reflected sunlight in the molecular oxygen (O<sub>2</sub>) A band, centered near 765 nm, and in the CO<sub>2</sub> bands centered near 1610 and 2060 nm. Each spectrometer collects 24 spectra per second, yielding about a million observations each day over the sunlit hemisphere. Coincident measurements from the three spectrometers are combined into "soundings" and analyzed with a "full-physics" retrieval algorithm to yield estimates of  $X_{CO2}$ . Clouds and optically thick aerosols preclude observations of the full atmospheric column in many regions, but this approach is expected to yield over 100,000 full-column  $X_{CO2}$  estimates each day.

OCO-2 was successfully launched from Vandenberg Air Force Base on a Delta-II 7320 launch vehicle at 2:56 AM PDT on July 2, 2014. The Observatory completed its in-orbit checkout phase in October 2014 and is now routinely collecting almost 1 million soundings over the sunlit hemisphere each day. More than 10% of these measurements are sufficiently cloud free to yield precise estimates of the column-averaged CO<sub>2</sub> dry air mole fraction,  $X_{CO2}$ .

The Orbiting Carbon Observatory-3 (OCO-3) continues NASA's carbon dioxide measurements from space, also measuring  $X_{CO2}$  and solar-induced fluorescence (SIF) from space. OCO-3 was launched from the Kennedy Space Center on May 4, 2019 via a Space-X Falcon 9 and Dragon capsule. The instrument was installed as an external payload on the Japanese Experimental Module Exposed Facility (JEM-EF) of the International Space Station (ISS) with a nominal mission lifetime of 3 years. The precessing orbit of the ISS allows for viewing of the Earth at all latitudes less than approximately 52 degrees, with a ground repeat cycle that is much more complicated than the polar-orbiting satellites that so far have carried all of the instruments capable of measuring carbon dioxide from space. The spectrometer used in OCO-3 is a direct copy of the OCO-2 spectrometer. As such, OCO-3 has similar instrument sensitivity and performance characteristics to OCO-2, making measurements of  $X_{CO2}$  with precision better than 1 ppm at 3 Hz, with each viewing frame containing eight footprints approximately 1.6 km by 2.2 km in size. However, the physical configuration of the instrument aboard the ISS, as well as the use of a new pointing mirror assembly (PMA), will alter some of the characteristics of the OCO-3 data compared to OCO-2. Specifically, there will be significant differences from day to day in the sampling locations and time of day. In addition, the flexible PMA system allows for a much more dynamic observation-mode schedule.

# Descriptions of the instrument properties and the data provided in this document for OCO-2 applies to OCO-3 except where noted otherwise.

#### 2.1 Scope of Document

This document is intended to get the user started with the OCO-2 and/or OCO-3 Level 2 data. The document contains information on using data for both instruments that are contained within the Level 2 (L2) Standard files (L2Std) and the Level 2 Lite files (Lite). The document contains

the full data tables for both files with brief descriptions of each variable in the data. A description is provided for the recommended data screening for both instruments and also a method for bias correcting the retrieved  $X_{CO2}$  data. The Lite data files provide both the retrieved value for  $X_{CO2}$  (called xco2 in the L2Std file and xco2\_raw in the Lite file) and an  $X_{CO2}$  value that has been through the recommended data screening and bias corrected (xco2 in the Lite files).

#### 2.2 Observing Modes for OCO-2

The OCO-2 spacecraft carries and points a 3-channel imaging grating spectrometer designed to record high-resolution spectra of reflected sunlight in O<sub>2</sub> and CO<sub>2</sub> bands as it flies over the sunlit hemisphere. It makes observations in three modes; nadir, glint and target. The nadir and glint observation cadence has evolved over the life of the mission. During the first year of observations the instrument observed 16 days in glint mode followed by 16 days of nadir observations (note the OCO-2 cycle for a near repeat of observations is 16 days or 233 orbits). After the first year, the observation strategy changed to glint only observations over the majority of the Pacific and Atlantic oceans and alternating nadir/glint observations on all other orbits.

Target mode observations are taken primarily for purposes of validating the instrument performance against ground-based observations from the Total Carbon Column Observation Network (TCCON) (Wunch et al., 2010). The validation strategy and findings have been described in Wunch et al. (2011 and 2017) and Kiel et al. (2019). Target mode observations are also used for evaluating the OCO-2 SIF products.

#### 2.3 Observing Modes for OCO-3

The nominal planned viewing strategy of OCO-3 is to take down-looking nadir viewing measurements over land to minimize the probability of cloud and aerosol contamination. Over water measurements will be taken near the specular reflection spot (glint viewing) to maximize the signal over the low reflectivity surface.

However, unlike OCO-2, which performs complex maneuvers of the entire satellite bus to observe ground targets, the OCO-3 instrument is fitted with an agile 2-D pointing mechanism, i.e., a pointing mirror assembly (PMA). This allows for rapid transitions between nadir and glint mode (less than 1 minute). The PMA also allows for target mode observations, similar to those taken by OCO-2; mostly TCCON ground sites for use in validation. The PMA provides the ability to scan large contiguous areas (order 80 km by 80 km), such as cities and forests, on a single overpass. These are known as "snapshot" mode and provide for fine scale spatial sampling of  $CO_2$  and SIF variations unlike any current satellite system. Together with OCO-2, the OCO-3 snapshot mode can be used to gather a significant fraction of overlapping data. More details are contained in Eldering et al. (2018).

#### 2.4 More Information on Missions

Mission background information is available in the OCO-2/OCO-3 Algorithm Theoretical Basis Documents (ATBD). There are separate ATBDs for the Level 1B algorithm and the Level 2 algorithm. A mission description is included in both documents. These documents are available at GES DISC (<u>https://disc.gsfc.nasa.gov/information/documents?keywords=OCO-2&title=OCO-2%20Documents</u>).

Listed below are some of the primary publications that provide information on different aspects of the missions. A full list of mission publications are available on the project web sites (<u>https://oco2.jpl.nasa.gov/publications/</u>) and (<u>https://oco3.jpl.nasa.gov/science/publications/</u>):

- OCO-2 Early Mission Performance:
  - D. Crisp et al. (2017), The on-orbit performance of the Orbiting Carbon Observatory-2 (OCO-2) instrument and its radiometrically calibrated products, *Atmos. Meas. Tech.*, 10, 59–81, 2017, <u>https://doi.org/doi:10.5194/amt-10-59-2017</u>
  - A. Eldering et al., (2017), The Orbiting Carbon Observatory-2 early science investigations of regional carbon dioxide fluxes, *Science*, 358, 2017, <u>http://dx.doi.org/10.1126/science.aam5745</u>.
- OCO-2 Validation:
  - Kiel M. et al. (2019), How bias correction goes wrong: measurement of X<sub>CO2</sub> affected by erroneous surface pressure estimates, 12, https://doi.org/10.5194/amt-12-2241-2019.
  - Wunch D. et al. (2011a), The Total Carbon Column Observing Network, *Phil. Trans. R. Soc. A*, 369, 2087–2112, 2011, <a href="https://doi.org/doi:10.1098/rsta.2010.0240">https://doi.org/doi</a>: 10.1098/rsta.2010.0240
  - Wunch D. et al. (2011b), A method for evaluating bias in global measurements of CO<sub>2</sub> total columns from Space, *Atmos. Chem. Phys. Discuss.*, *11*, 20899-20946, 2011, <u>https://doi.org/doi: 10.5194/acp-11-12317-2011</u>.
  - Wunch D. et al. (2017), Comparisons of the Orbiting Carbon Observatory-2 (OCO-2) X<sub>CO2</sub> Measurements with TCCON, Atmos. Meas. Tech. Discuss., 10, 2209-2238, 2017, <u>https://doi.org/doi:10.5194/amt-10-2209-2017</u>.
- OCO-3:
  - A. Eldering et al. (2019), The OCO-3 mission: measurement objectives and expected performance based on 1 year of simulated data, *Atmos. Meas. Tech.*, 12, 4, 2341-2370, 2019, <u>https://doi.org/doi:10.5194/amt-12-2341-2019</u>.
  - T.E. Taylor et al. (2020), OCO-3 early mission operations and initial (vEarly) X<sub>CO2</sub> and SIF retrievals, *Rem. Sens. Env.*, 251, 112032, <u>https://doi.org/10.1016/j.rse.2020.112032</u>.
- SIF:
  - Y. Sun et al. (2018), Overview of Solar-Induced chlorophyll Fluorescence (SIF) from the Orbiting Carbon Observatory-2: Retrieval, cross-mission comparison, and global monitoring for GPP, *Rem. Sens. Env.*, 209, 808-823, 2018, <a href="https://doi.org/10.1016/j.rse.2018.02.016">https://doi.org/10.1016/j.rse.2018.02.016</a>.
  - C. Frankenberg et al. (2014), Prospects for chlorophyll fluorescence remote sensing from the Orbiting Carbon Observatory-2, *Rem. Sens. Env.*, 147, 1-12, 2014, <u>https://doi.org/doi:10.1016/j.rse.2014.02.007</u>.

## 3 What is New in OCO-2 v11 and OCO-3 v10/v10.4

#### 3.1 OCO-2 Updates for v11

The version 11 of the OCO-2 L2 products includes several improvements and fixes when compared to previous versions. The most important updates in v11 include:

- Use of an updated Digital Elevation Map (DEM) in the L2 retrievals; this primarily affects retrievals above 60N latitude.
- Improvements in the L1B processing, including: gain degradation, dispersion trend, instrument line shape (ILS), noise model, footprint dependence
- Mitigation of previous issue with inadvertent flagging of majority of soundings over South Atlantic Anomaly
- Improvements to increase the throughput of the solar-induced chlorophyll fluorescence (SIF) retrievals
- Improvements to the IMAP-DOAS preprocessor, including updates to its spectroscopy to match that used by the L2 Full-Physics algorithm.
- Spectroscopy updates
- Updates to the absorption coefficient scaling factors used in the L2 retrievals that will help mitigate the overall X<sub>CO2</sub> bias and CO<sub>2</sub> profile shape issues
- Improvements to the ocean surface treatment that improve the linearity of retrievals over ocean
- Minor updates to land bidirectional reflectance distribution function (BRDF)
- New CO<sub>2</sub> *a priori* profiles
- Minor changes to the rules that govern sounding selection
- A fix for an issue with SIF availability for target mode observations (this will be seen in the L2 SIF lite files)

Users should note that the OCO-2 v11 level 2 standard and diagnostic data files (L2Std, L2Dia) will be smaller than in previous versions. This is due to new compression used in creating the files, as well as the removal of the albedo fields (Albedo folder in files).

#### **3.2 OCO-3 Updates for v10/v10.4**

#### 3.2.1 Radiometric errors

The radiometric calibration of v10 was significantly improved compared to vEarly. In contrast to vEarly, which contains a discontinuity at April 8, 2020, all lamp data across the entire mission is now processed with the same algorithms. The key improvement for v10 was to tie radiometric degradation to Lamp 1, which is used roughly once a week. Initially, Lamp 3 was being used with no correction for lamp aging. Additionally, v10 featured an updated stray light model which aims to account for spatial variability.



**Figure 3-1:** Lamp radiance trends relative to prelaunch over the course of the OCO-3 mission. The three panels are for the ABO2, WCO2, and SCO2 channels. Within each panel, different colors indicate different lamps. Lamp 3 is used roughly 12 times per day, Lamp 2 is used roughly 3 times per day, and Lamp 1 is used roughly 1 time per week.

Since the focal plane arrays are operated at cryogenic temperatures, ice accumulates over time, leading to increased stray light and decreased throughput. Several decontaminations have been performed to counteract this. The largest discontinuity in the gain degradation record (Figure 3-1) occurs following the decon from solar day 9720, which was nearly a year after the previous one.

A key indicator of calibration improvements was a reduction in time dependent and footprint dependent behavior in the L2 data in v10 compared to vEarly. The science team examined the behavior of dP, the difference between the retrieved and prior surface pressure, a parameter in the retrieval that is very sensitive to ABO2 radiometric calibration. We found that this parameter was more stable in v10 than in vEarly, although an increase in value correlated with detector icing remained. A clear increase is visible between June 2020 and Jan 2021. The dP test data record shown in Figure 3-2 ends in Dec 2020, just before a major decontamination event.

In addition to the time dependence, there is some variation in the dP values among footprints, which is consistent with our understanding that icing impacts are spatially nonuniform, but the magnitude in v10 is substantially reduced from vEarly. This is also seen in the throughput of data in L2 which worsened later in the vEarly record, especially for high numbered footprints. This pattern is not seen in v10.

Since the release of the OCO-3 v10 dataset, the team has continued to further characterize Level 1B calibration. The v10.4r Lite products incorporate an ad hoc correction to the Level 2  $X_{CO2}$  that aims to account for outstanding issues in the Level 1B calibration.



Figure 3-2: L2 dP values from OCO-3 v10 test data from Aug 2019 to Dec 2020.

#### 3.2.2 Geolocation errors

Geolocation errors were substantially improved for v10 compared to vEarly in three general areas. First, calibration of the Pointing Mirror Assembly (PMA) was completed and integrated directly into the gelocation algorithm. Second, an offset between the science detectors and the PMA camera was characterized and removed. Third, the OCO-3 project obtained a supplemental attitude source, derived from the CALET instrument which is near OCO-3 on the JEM-EF, for periods when the OCO-3 Stellar Reference Unit (SRU) is not available. The supplemental attitude data reduces geolocation errors associated with flexure between the ISS center, where the primary ISS ephemeris is reported, and the OCO-3 location on the JEM-EF. For periods when the OCO-3 SRU is available, geolocation errors are typically less than 500 m. For periods where the SRU is not available and CALET-derived attitude is available, errors are typically less than 1 km. Finally, a small percentage of the data remains when neither of the two primary attitude sources are available, and for these periods the errors are typically less than 2 km, with a small "tail" with errors up to 3 km. Starting with v10, the OCO-3 L2 products contain a field called /RetrievalGeometry/retrieval att data source. A value of 1 in this field represents the "no supplemental attitude" case, with the largest errors. Other values in the range 2-9, have good geolocation, with the errors listed above. The different numbers in the 2-9 range represent various permutations of SRU and CALET, accounting for nominal operations with the possibility of small gaps.

The improvements that rely on the CALET data are only available in the retrospective processing (v10r). In the forward stream processing, we rely solely on the OCO-3 SRU and ISS

BAD data, so geolocation performance may be poorer than in the retrospective data. The attitude source information that is included in the product can help the user to differentiate these cases.

#### 3.2.3 OCO-3 v10.4 Lite File Update

The v10.4r Lite file release addresses a problem with the v10r X<sub>CO2</sub> data. The new Lite file data version was necessary because it was noticed during routine validation of the v10r data product that a time dependent bias could be seen in the OCO-3 X<sub>CO2</sub> data compared to collocated OCO-2 observations  $(dX_{CO2})$ . The magnitude of the bias is correlated with the amount of time between instrument decontamination cycles, and so is assumed to be associated with icing on the OCO-3 detectors. One proxy for the build-up of ice on the detectors is an instrument calibration metric called the zero-level-offset (ZLO). For OCO-3, ZLO is measured for both the weak CO<sub>2</sub> and and the O<sub>2</sub> A-band, but the weak CO<sub>2</sub> band measurements of ZLO are less noisy, making them a more convenient metric than A-band ZLO. A bias correction term was calculated from a fit of  $dX_{CO2}$  to the ZLO from the weak CO<sub>2</sub> band. Comparisons between the new bias corrected  $X_{CO2}$ data and data from the Total Carbon Column Observation Network show that v10.4r Lite  $X_{CO2}$ data is minimally affected by the time dependence related to build up of ice on the detectors. Comparisons of OCO-3 data to OCO-2 X<sub>CO2</sub> also show that the effects of the ice build up have been resolved by the updated bias correction. The impact and magnitude of the correction can be seen in Figure 1-1. We have also completed validation of the OCO-3 v10.4r Lite products against TCCON and multimodel median, showing over all good agreement with these truth proxies – more details on these are available in Section 3

The OCO-3 v10.4r Lite data product should be used instead of the previous v10r Lite. Note that the time-dependent  $X_{CO2}$  correction for the v10.4r product comes in via the Level 2 bias correction. (Improvements between the previous OCO-3 v10r and vEarly data products were achieved via updates to the Level 1b radiometric calibration and geolocation.)

Users should be aware that the geolocation of the retrospective product in some cases will be superior to the forward stream of the data.

The L2 algorithms used to create the OCO-3 data are the same as those that are used for the current OCO-2 v10 L2 data release, to aid in the use of the two datasets together.



**Figure 3-3:** Showing the updated bias correction and the improvement in dXCO2. Compare the value of dXCO2 at the top of the figure (prior to the new bias correction) to that at the bottom (corrected). The middle of the figure shows the OCO-3 ZLO and the adjustment in XCO2 with time (orbit number).

## 4 OCO-2 v11 Lite Files: Description, Data Filtering and Bias Correction

In order to develop both the screening criteria and bias correction parameters, a set of "truth proxies" are defined:

- TCCON (compared to OCO-2 data acquired in nadir, glint and target modes)
- The "Small Area Analysis", in which  $X_{CO2}$  is assumed to be constant for OCO-2 observations taken over distances <~ 100 km within the same orbit.
- A multi-model mean of 4 models (Jena Carboscope, CarbonTracker, University of Edinburgh, and CAMS) that have all assimilated in-situ data, and only using soundings for which all the model values agree with each other to within a specified tolerance.

The process for using the truth proxies to develop screening and bias correction criteria and the full screening/bias correction process is available in O'Dell et al., (2018) with specifics for v11 provided below.

#### 4.1 Quality Filtering

Users of OCO-2 L2Std data can do a rough quality filtering of the soundings using the outcome\_flag variable, which is set to "1" or "2" for retrievals completed successfully.

When using the data contained in the Lite files, filtering can be done with xco2\_quality\_flag ("0" is good). This filter has been derived by comparing retrieved  $X_{CO2}$  for a subset of the data to the various truth proxies, and identifying thresholds for different variables that correlate with poor data quality. It applies quality filters based on a number of retrieved or auxiliary variables that correlate with excessive  $X_{CO2}$  scatter or bias (described below).

#### 4.2 Bias Correction

The bias correction (BC) maps the original  $X_{CO2}$  retrievals of the OCO-2 L2 algorithm to our best estimate of  $X_{CO2}$ . We used v11 data spanning November of 2014 through 2019. The BC approach implemented in the Lite files uses regional analysis to identify, within the OCO-2  $X_{CO2}$ data records themselves, which terms best predict bias (or Unexplained Variance (%UV)) in the retrievals. Our definition of %UV always uses a null-hypothesis denominator for ease of comparison. The full bias correction procedure was similar to that used in version V8, described in detail in O'Dell et al. (2018).

We have constructed several training datasets for our bias correction, such that the set provides an approximation of the  $X_{CO2}$  truth against which the retrievals are evaluated while attempting to ensure that real  $X_{CO2}$  atmospheric gradients are not removed by in the BC. The model-based training data set was the largest, with ~5.5 million soundings, and now, in v10 & v11 analyses, includes data over Greenland and Antarctica. The TCCON-based data set was also large, with ~1.9 million soundings. These were largely the same as the v10 training soundings, with additional soundings added after 2017. A new small area dataset was created with 3.9M soundings (this is much larger than for v8-v10). Figure 4-1shows the spatial distribution of these training data sets. We used v11 data spanning February 2015 through the end of 2019 for all cases, so roughly 5 years of OCO-2 data are included in the training data for filtering and bias correction.



Figure 4-1: Sounding density maps and time series of soundings for the three v11 training data sets.

The three steps to finalize the terms in the BC equation are as follows:

$$XCO_{2\ Corrected} = \frac{XCO_{2\ Raw} - \frac{FOOT[fp, mode]}{FOOT[fp, mode]} - FEATS[mode]}{TCCON\_AD[UST[mode]]}$$

#### **4.2.1** Step 1 – Removing Footprint Bias (term FOOT)

OCO-2 obtains 8 side-by-side, simultaneous, nearly-collocated measurement scenes called footprints. Although the  $X_{CO2}$  retrievals made from these soundings should, on average, be identical, there are small and highly statistically significant differences. These undoubtedly arise from imprecision in the L1 calibration.

For the v11 data set, we examined highly filtered data grouped into small areas. For each mode, the data set contained millions of soundings, so they were further filtered to only include the best data. Data were selected for the analysis when all 8 footprints in one sounding frame

(ID) converged. We computed the median  $X_{CO2}$  as the "ground truth" value, and subtracted this from the observed  $X_{CO2}$  to calculate the deviations for each footprint. The reported values are the average of the differences across all soundings per footprint. The footprint offsets are listed in Figure 4-2 under the term FOOT and shown in Table 4-1. One set of biases was obtained for land, and a different set for ocean glint. Land nadir, glint, and target observations had statistically indistinguishable biases and hence were set to the same values. Once obtained, these biases are subtracted from all sounding  $X_{CO2}$  in preparation for the next steps of BC.



**Figure 4-2:** Footprint Bias per viewing mode. The land nadir and glint biases were set to be the same in the end, as they were statistically indistinguishable, but the ocean glint footprint biases were statistically different and hence set to their own values.

#### 4.2.2 Step 2 – Remove *X*<sub>CO2</sub> Errors Correlated with Specific Variables (FEAT)

In this second step, we identify variables retrieved simultaneously with  $X_{CO2}$  that are correlated with unphysical  $X_{CO2}$  variability using a multivariate linear regression. This is the procedure followed by nearly all ACOS/GOSAT and OCO-2  $X_{CO2}$  bias corrections to date (e.g., Wunch et al. 2011, Guerlet et al. 2013). The procedure followed was very similar to that described in O'Dell et al. (2018).

**Table 4-1:** Features used in the Land Nadir (ND) + Glint (GL) bias correction, with reduction in unexplained variance in parentheses. Note SAA in this table is "Small Area Analysis". Coefficient uncertainties are  $1\sigma$ .

	Ν	Stddev	dPfrac	Co2_grad_del	logDWS	aod_fine	aod_ice	Albedo_qua
		(ppm)						d_wco2*1e6
TCCON: Ggg2014	377K	1.73 → 1.18	-0.82 (23%)	-0.0314 (27%)	-0.24 (2%)	6.2 (0.3%)	-36 (1.3%)	0.72 (0.5%)
Models:	1863K	1.65 → 1.12	-0.77 (23%)	-0.0318 (26%)	-0.23 (3%)	8.6 (0.9%)	-27 (0.9%)	0.59 (0.4%)
SAA:	1646K	1.53 →0.79	-0.816 (32%)	-0.0329 (33%)	-0.29 (5%)	7.4 (0.8%)	-37 (2.2%)	0.50 (0.3%)
B11			-0.83	-0.033	-0.27	6.7	-33	0.48
B11 need			-0.81	-0.032	-0.27	7.4	-33	0.60
B10	-	-	-0.855	-0.0335	-0.335	5.2	0	

The different analysis regions and modes have minor differences in the order of features chosen, but overall, the features selected and their slopes are remarkably consistent. Table 4-2 shows the bias correction parameters for Land Nadir & Glint soundings for the different training datasets, and

Table 4-3 shows the same for Ocean Glint. Each table shows the reduction in unexplained variance (UV in %) as features are added to the bias correction fit. Note that in each table, the  $X_{CO2}$  quality flag has been applied.

**Table 4-2:** Features used in the Land Target (TG) bias correction, with reduction in unexplained variance in parentheses. Coefficient uncertainties are  $1\sigma$ .

	Ν	Stddev	dPfrac	Co2_grad_del	logDWS	aod_fine	aod_ice	Albedo_qua
		(ppm)						d_wco2*1e6
TCCON:	1049K	1.42 → 0.98	-0.77 (24%)	-0.0246 (26%)	-0.25 (2%)	-	-	-
Ggg2014								
TCCON:	747K	$1.35 \rightarrow 0.95$	-0.75 (23%)	-0.0242 (27%)	-0.15 (1%)	-	-	-
ggg2020								
B11			-0.83	-0.033	-0.27	6.7	-33	0.48
B10	-	-	-0.855	-0.0335	-0.335	5.2	-	-

These terms are the differences between the retrieved and the *a priori* surface pressure evaluated at the geographic location of the strong CO band (dP\_sco2), the retrieved abundance of coarse aerosol (e.g., dust, sea salt, or water clouds), and (very large and unphysical) variation in the retrieved vertical profile of  $CO_2$  (parameter co2\_grad\_del) from that assumed in the prior. Also, note that over land, we have created a new quantity called "dPfrac". This term is similar to dP, but also takes into account that higher elevation surfaces have a smaller dry air column above them, and therefore over these locations, the dP correction must be proportionally stronger. A full derivation of this term is given in the appendix of Kiel et al. (2018). Here, we simply give the definition of dPfrac, which is:

$$dP frac = X_{CO2,raw} (1 - P_{ap,sco2}/P_{ret})$$

where  $P_{ap,sco2}$  is the prior surface pressure at the location of the strong CO<sub>2</sub> band, and  $P_{ret}$  is the surface pressure retrieved by the L2 algorithm. There are several additional terms in the land bias correction:

- logDWS : max(log( aod\_dust + aod\_water + aod\_seasalt ),-5)
- aod\_fine : aod\_oc + aod\_sulfate (where "oc"=organic carbon)
- albedo\_quad\_wco2 \* 1e6: This is the quadratic component of the retrieved amplitude of the surface BRDF in the weak CO<sub>2</sub> band. As it is naturally of order 1e-6, we scale it up by a factor of 1e6 for ease of use.

**Table 4-3:** Features used in the Ocean Glint (GL) bias correction, with reduction in unexplained variance in parentheses. Note SAA in this table is "Small Area Analysis". Coefficient uncertainties are  $1\sigma$ .

	Ν	Stddev	dP_sco2	Sqrt(Albe	Co2_grad_	Max_Declock	AOD	XCO2_unce
		(ppm)		do_wco2)	del	ing_wco2	Water	rtainty
TCCON:	119K	1.12 → 0.87	-0.262 (27%)	7.9 (8%)	-0.013 (2%)	-2.2 (1.2%)	-8 (0.4%)	1.5 (1.3%)
ggg2014								
TCCON:	81K	$1.04 \rightarrow 0.78$	-0.254 (30%)	7.2 (9%)	-0.016 (3%)	-2.2 (1.3%)	-6 (0.3%)	1.1 (0.8%)
ggg2020								
Models:	893K	1.11 → 0.74	-0.255 (36%)	8.3 (10%)	-0.019 (4%)	-2.3 (1.4%)	-15 (1.3%)	2.4 (3.1%)
SAA:	835K	0.92 →0.49	-0.241 (46%)	7.7 (13%)	-0.018 (6%)	-1.7 (1.1%)	-15 (1.7%)	2.0 (3.5%)
B11			-0.25	8.0	-0.0175	-2.0	-14	2.0
B10	-	-	-0.213	-	0.087	-	-	-

Because the ocean surface parameterization changed significantly in B11, this led to a large change in the bias correction for ocean glint. Instead of two terms in the parametric part of the bias correction. We now use six:

- $dP_{sco2} = (P_{ret} P_{ap,sco2})$  as discussed above, in units of hPa
- sqrt(albedo\_wco2) is the square root of the retrieved effective reflectivity (or surface albedo) in the weak CO<sub>2</sub> band.
- Co2\_grad\_del: As always, the retrieved CO<sub>2</sub> at the surface minus the same at pressure level 13 (~ 700 hPa), minus the a priori of the same, given in a priori.
- Max\_Declocking\_wco2: The term "max\_declocking\_wco2" is related to the subscene radiance variability in the weak CO<sub>2</sub> band as measured from the color slices. The original term in the L2Std files varies about unity. We therefore subtract off unity and take the absolute value, and multiply by 100 to express in %, to obtain the value used in the Lite files, as well as in the filtering and bias correction.
- AOD\_water is of course the retrieved optical depth of water cloud at 755 microns wavelength.
- XCO2\_uncertainty is the retrieval posterior uncertainty of XCO<sub>2</sub>, in ppm.

Figure 4-3, Figure 4-4 and 4-5 shows the bias correction plots for version 11 land Nadir+Glint, land Target, and Ocean Glint, respectively, all relative to TCCON (ggg2014).



Figure 4-3: Plot of XCO2 errors relative to TCCON (ggg2014) for B11 land nadir & glint observations. The regression coefficients for a simultaneous fit of all terms are given in blue ("ALL"), bottom left of each panel.



Figure 4-4: Same as Figure 4-4 but for Land Target Observations.

#### 4.2.3 Step 3 – Determine global offset from TCCON (TCCON\_Adjust)

The analyses described in Steps 1 and 2 provide no estimate of the overall global bias in  $X_{CO2}$ . To determine the offset over land, we used nadir, glint, and target mode observations obtained over the TCCON sites. The final numbers only used the recent ggg2020 data. A linear regression between TCCON  $X_{CO2}$  and the bias-corrected OCO-2 target mode  $X_{CO2}$  was performed, with the intercept forced to zero. Table 4-4 shows the process for TCCON target observations. Overall, this analysis scales the OCO-2 land nadir, glint, and target data to TCCON: OCO-2 = (0.9997 ± 0.003) TCCON. While the fit to individual modes have lower uncertainties, the fit across different modes and multiple time periods lead us to conclude that the real uncertainty is greater, on the order of 0.003.

To determine the global divisor for Ocean Glint, we exclusively used coastline crossings as discussed in O'Dell et al. (2018). The final global divisor adopted for ocean data was  $0.9997 \pm 0.003$ , identical to that of land soundings.



Figure 4-5: Same as Figure 4-4 but for Land Target Observations.



**Figure 4-6:** Linear Fit of OCO-2 v10 to TCCON XCO2 for a subset of target mode overpasses of TCCON sites. Both Quality Filtering as well as the feature and footprint biases have been applied.

		l able 4-4:	Bias Corre	ction formu	lation for v1	1		
		FOOTPRINT BIAS (FOOT) (ppm)						
Footprint (fp)	1	2	3	4	5	6	7	8
Land	-0.510	-0.220	-0.160	-0.120	0.090	0.370	0.150	0.400
Ocean	-0.500	-0.160	-0.160	-0.160	0.060	0.330	0.100	0.490
		FEATURE BIAS (FEATS) (ppm)						
LAND (ND,GL)	- 0.83*	$-0.83*(dPfrac) - 0.033*(co2_grad_del - 5) - 0.27*(max(logDWS,-5) + 5) + 6.7*(aod_fine - 0.03) - 33*(aod_ice - 0.006) + 0.48*(albedo guad wco2*1e6 + 0.06)$						
LAND (TG)	-0.77*	(dPfrac +	(0.3) - 0.02	5*( <b>co2_g</b> r	ad_del) -	0.25*(max	(log <b>DWS,-</b>	-5) + 5)
SEA GLINT	- 0.25*(d -2.0*(max	$-0.25*(dP_{sco2}) + 8.0*(sqrt(albedo_wco2) - 0.28) - 0.0175*(co2_grad_del + 15) -2.0*(max_declocking_wco2) - 14*(aod_water - 0.01) +2.0*(xco2_uncertainty - 0.46)$						
	0	VERALL TCCON_A	DIVISOR ADJUST)	1		Meth	od	
LAND GLINT LAND NADIF	0.9997			Comparison to TCCON ggg2020 (average of ND, GL, and TG modes)				

Table 4-4: Bias Correction formulatior	۱ for ۱	v11
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LAND TARGET					
SEA GLINT	0.9997 Coastline Crossings such that ocean matches land				
	Variable definitions us	sing full/HDF5/path for Lite files			
co2_grad_del	Retrie	val/co2_grad_del			
dP <sub>sco2</sub>	Retrieval/psurf – M	leteorology/psurf_apriori_sco2			
logDWS	Max( ln( aod_dust +aod_water + aod_seasalt ), -5)				
aod_fine	Retrieval/aod_sulfate + Retrieval/aod_oc				
aod_ice	Ret	rieval/aod_ice			
max_declocking_ co2	w Preprocessors	s/max_declocking_wco2			
xco2_uncertaint	xco2_uncertainty				
Albedo_quad_wc	02 Retrieval	/abedo_quad_wco2			

#### 4.2.4 *v11* Quality Flagging

After bias correction, additional outlier filtering is developed and applied. The xco2\_quality\_flag is set to "0" for good quality data and set to "1" for lower quality data. This allows users to remove the effects of one or more tests if they so choose.

Table 4-4 lists the details on the parameters that define the data quality flag. Table 4-5 illustrates these parameters as applied to land data.

Because this is a simple binary flag, we have created two additional bit-flag variables that give the user information as to which tests failed that leads to soundings marked as "bad" quality  $(xco2_quality_flag = 1)$ . There is variable  $xco2_qf_b$  bitflag which currently uses all 32 bits of a long integer to report the result of each individual test. A bit value of 0 means passed, and 1 means failed. If they all pass, the value of this variable will be 0, just as for the normal quality flag variable. The individual bits are given in Table 4-5. Furthermore, a new "simple bitflag",  $xco2_qf_simple_bitflag$ , has also been created. This 8-bit integer divides the tests into seven categories currently; each of the individual tests falls into exactly one of these categories. For instance, aerosol-related, surface-albedo related, etc. Table 4-6 gives the bit definitions for these variables.

For those unused to bit-flags, let us suppose a given sounding has a bitflag value of X. To get the value of bit b, which we call will B, simply do

IDL: 
$$B = (X AND 2^b) EQ 2^b$$
  
Python:  $B = (X and 2^b) == 2^b$   
Fortran:  $b2=2^{**b}$   
 $B = (X .AND. b2) == b2$ 

Table 4-5: OCO-2 B10 Quality Filter Thresholds and bit numbers for the associated bit-flags. Range
denotes allowed ranges for each variable. All variables must pass for a given sounding to be considered
"good" (xco2_quality_flag = 0).

Bit	Simple Bit	Field	Units	Land Range	Ocean Glint Range
0	2	Preprocessors/co2 ratio		0.999, 1.028	1.0, 1.018
1	2	Preprocessors/h2o ratio		0.75, 1.07	0.85, 1.08
2	0	Sounding/altitude stddev	m	0, 120 (0, 50)	
3	2	Preprocessors/max declocking wco2	%	0, 1.5	
4	6	Retrieval/dp o2a	hPa	-9,6	
5	6	Retrieval/dpfrac	ppm	-3.5, 3.0	
6	6	Retrieval/co2 grad del	ppm	-90, 90	-50, 35
7	3	Retrieval/albedo slope sco2	$1/cm^{-1}$	-15e-5, 100e-5	4e-6, 4e-5
8	4	Retrieval/aod total		0, 0.25	
9	4	Retrieval/aod_ice		8e-5, 0.04	0, 0.035
10	3	Retrieval/albedo_sco2		0.03, 0.60	
11	3	Retrieval/albedo_quad_wco2	$1/cm^{-2}$	-1e-6, 1e-6	
12	3	Retrieval/abledo_quad_sco2	$1/cm^{-2}$	-3.5e-6, 4e-6	
13	5	Retrieval/rms_rel_wco2	%	0, 0.35	
14	5	Retrieval/rms_rel_sco2	%	0, 0.80	
15	5	Retrieval/chi2_sco2		(0, 2.7) (0, 3.0)	0, 1.65
16	6	Retrieval/deltaT	Κ	-0.8, 1.5	
17	4	Retrieval/aod_sulfate + Retrieval/aod_oc		0, 0.15	
18	4	Retrieval/aod_water		0.0006, 0.07	0, 0.06
19	4	Retrieval/dust_height		0.85, 2.0	
20	4	Retrieval/aod_strataer		1e-4, 0.025	
21	4	Retrieval/aod_seasalt		0, 0.075	
22	6	Retrieval/fs_rel		-0.025, 0.03	
23	4	Retrieval/dws		0, 0.20	0, 0.30
24	2	Preprocessors/dp_abp	hPa	-15, 12 (-15, 50)	-10, 10
25	0	Retrieval/snow_flag		0, 0	
26	3	Retrieval/brdf_weight_slope_sco2			0, 4e-4
27	6	Retrieval/dp_sco2	hPa		-7, 9
28	5	Retrieval/chi2_wco2			0, 1.6
29	2	Preprocessors/max_declocking_sco2	%		0, 0.40
30	3	Retrieval/albedo_o2a-			0.002.0.027
		Retrieval/albedo_sco2			0.002, 0.027
31	3	Retrieval/brdf_weight_slope_wco2			-8.5e-5, 4.1e-5
32	3	Retrieval/albedo_o2a			0.04, 0.20
33	1	xco2_uncertainty			0.3, 1.0
34	6	Abs(Retrieval/eof3_1_rel)			0, 0.45
35	4	Retrieval/ice_height			-0.5, 0.5
36	0	Sounding/airmass			2, 4.2

Note: Numbers in (red) are used for target-mode soundings.

"Bit" denotes the bit number in  $xco2\_qf\_bitflag$ , a 32-bit integer in the v1 Lite files. (0=pass, 1=fail) "Simple Bit" denotes the bit number in  $xco2\_qf\_simple\_bitflag$ , an 8-bit integer in the v1 Lite files.

Bit	Category	Notes			
0	Direct Evolution	Directly excluded due to snow, uncharacterized modes (ocean			
0	Direct Exclusion	non-glint obs, etc), topography features			
1	Signal	Signal-related features (SNR or signal ratios out of bounds,			
1		posterior uncertainty too high)			
2	Preprocessors	Failed one or more preprocessor-related quality flags (co2 ratio,			
		h2o_ratio, max_declocking, dp_abp)			
2	Retrieved Surface	Failed a surface-reflectivity related quality flag (surface albedo,			
3	Reflectivity	surface albedo slope, retrieved wind speed)			
4	Detrieved Apresels	Failed a retrieved aerosol related quality flag (aerosol AOD or			
	Retrieved Aerosols	aerosol heights)			
5	Retrieval Fit Quality	L2FP fit quality too poor (in terms of rms_rel or chi^2)			
6	Other Retrieval Quantities	Failed other L2FP retrieval flags (SIF, dp quantities, etc)			
7	Unused Currently unused				

#### Table 4-6: Bit definitions in xco2\_qf\_simple\_bitflag.



b11-absco-scaling-test2-all.sav Sep 6, 2014 to Dec 30, 2020

**Figure 4-7:** Bias & Stddev of error as a function of selected outlier filtering variables for land observations. Here, the error is derived using the model comparison.

#### 4.2.5 Definition of Key Data Parameters

Some of the parameters used in the data screening or bias correction of the L2 data have different names in the L2Std and Lite files. There are also a few parameters which are calculated from terms in the L2Std or Lite files. The subsections below give the parameter names within the Lite file structure, their names in the L2Std files and a description. Note "Parent field refers to the field name in the L2Std file. The full listing of the OCO-2 and OCO-3 Lite file data fields are in the tables in Section 9.

#### 4.2.6 Assessment of potential spurious *X*<sub>CO2</sub> drift with time

Given that the OCO-2 data record is now  $\sim 8$  years long, there is always the possibility that there could be a small drift, related to priors or calibration, in our retrieved  $X_{CO2}$ . Therefore, for the truth datasets, we performed simple time-sensitivity analyses vs. TCCON and the model median. Specifically, we perform a linear least-squares fit of monthly mean of the  $X_{CO2}$  difference of OCO2 – Truth, accounting for averaging kernel effects. Only good quality soundings are included. To assign an uncertainty, each monthly mean  $X_{CO2}$  difference is assigned the same uncertainty, required to yield a fit reduced  $\chi^2$  value of unity. A sample time series and fit is shown in Figure 4-8, which shows the time series of OCO-2 minus TCCON  $X_{CO2}$ . The results for each fit are given in Table 4-7. Of the five slopes calculated, two (land ND+GL vs Models, and ocean Glint vs. TCCON) have drifts that are significant at 95% confidence; however, these drifts are of opposite sign. The first, landNG vs Models,  $-0.035 \pm 0.010$ , may easily be related to the models themselves, which seem inconsistent with TCCON in terms of growth rate at a level of about 0.04 ppm/yr. The other is oceanG vs. TCCON, at a level of  $0.052 \pm 0.024$  ppm/yr, or about 0.5 ppm/decade. To put this in context, these potentially spurious trend represents less than about 2% of the mean secular increase of 2.5 ppm/yr due to anthropogenic CO<sub>2</sub> emissions. Further, our errors are purely empirical as described above, and do not take into account the possible errors in TCCON or models in terms of drifts, which very well could be significant at this level. As the OCO-2 data record lengthens, spurious time trends should become easier to see (and remove). At this time, no time-dependent term is included in our bias correction.



**Figure 4-8** Sample linear Fit of OCO-2 v11 minus TCCON vs. time, to determine possible spurious time trend. Bias-corrected  $X_{CO2}$  differences are shown in (Blue); raw  $X_{CO2}$  differences are shown in (Red).

<b>Truth Source</b>	<b>Observation Mode</b>	Drift $\pm 1\sigma$ uncertainty	
Model Median	Land (Nadir+Glint)	$-0.035 \pm 0.010$ ppm/yr	
TCCON	Land (Nadir+Glint)	$0.011 \pm 0.023$ ppm/yr	
TCCON	Land Target	$0.044 \pm 0.027 \text{ ppm/yr}$	
Model Median	Ocean Glint	$0.013 \pm 0.011$ ppm/yr	
TCCON	Ocean Glint	$0.052 \pm 0.024$ ppm/yr	

Table 4-7: Time Drifts vs. Models & TCCON

#### 4.3 CO<sub>2</sub> scale change

Atmospheric CO<sub>2</sub> measurements are ultimately tied back to primary standards maintained by the NOAA Global Monitoring Laboratory. <u>Hall et al.</u> (2021) recently published a revision to the WMO CO<sub>2</sub> calibration scale that increases CO<sub>2</sub> mixing ratios by on the order of 0.2 ppm at 400 ppm. In situ CO<sub>2</sub> measurements have been undergoing recalibration to the new CO<sub>2</sub> scale, identified as WMO-CO<sub>2</sub>-X2019 (here referred to as X2019), since it was finalized.

The initial OCO-2 v11 release and the OCO-3 v10 releases remain tied to the X2007 CO<sub>2</sub> scale. This is because OCO-2 and -3 data are tied to the WMO CO<sub>2</sub> scale vicariously, using TCCON as a transfer standard, with TCCON scaled to match in situ measurements by comparing TCCON data with aircraft or balloon CO<sub>2</sub> profiles taken over TCCON sites (e.g. <u>Wunch et al.</u> 2010). The process of updating the TCCON scaling from the previous X2007 CO<sub>2</sub> scale to the new X2019 CO<sub>2</sub> scale was incomplete at the time of the initial OCO-2 v11 release, necessitating the temporary retention of the X2007 scale.

Any analysis using OCO-2 or -3 data in conjunction with other  $CO_2$  data (in situ, groundbased column, etc) should check which  $CO_2$  scale all the data used is calibrated or tied to, and convert the data to a consistent scale as needed. If OCO-2 or -3 data needs to be converted to the X2019 scale for proper comparison with other data sources, the ad hoc correction given by Eq. (6) of <u>Hall et al. (2021)</u> can be used to convert the lite file XCO<sub>2</sub>:

 $X2019 = 1.00079 \times X2007 - 0.142$  (ppm)

Please read section 9,1 of <u>Hall et al. (2021</u>) carefully to understand the errors introduced by this linear approximation before applying it to OCO-2 and -3 XCO<sub>2</sub> data. Also note that there may be some additional (unquantified but likely very small) error from applying this correction, developed for in situ data, to column  $CO_2$  data.

Future releases of v11 data may formally update the  $XCO_2$  data to tie to the X2019 scale. This will be indicated by the "comment" attribute of the "xco2" variable in the lite files. It is highly recommended that users check this attribute when downloading new versions of the lite files to verify which scale the  $XCO_2$  data is reported on.

## 5 OCO-3 v10: Description, Data Filtering and Bias Correction

#### 5.1 Quality Filtering and Bias Correction

Similar to  $X_{CO2}$  derived from OCO-2 measurements, for OCO-3 we apply a quality filtering procedure to remove soundings that show larger than expected scatter differences in  $X_{CO2}$  compared to a "truth" metric (O'Dell et al., 2018). Further, a large fraction of the error in  $X_{CO2}$  correlates with retrieved components of the state vector in the retrieval algorithm. It was shown that a linear correction demonstrably reduces such errors in  $X_{CO2}$  estimates from space-based measurements (Wunch et al., 2011a, Wunch et al., 2017, O'Dell et al., 2018, Kiel et al., 2019). In order to derive quality filters and bias correction terms for OCO-3, the same approach is followed as for OCO-2 (O'Dell et. al., 2018). The retrieved  $X_{CO2}$  values are compared to independent estimates, so-called truth proxies. For OCO-3 v10, we use three different truth proxy training data sets: TCCON, a small area approximation (SAA), and a truth proxy based on results from global carbon flux inverse models ("multi-model median").

#### 5.1.1 Truth Proxy Training Data Sets

The TCCON truth poxy includes data from 19 TCCON stations. We use the GGG2014 data set covering the time period between August 2019 and December 2020 and spanning from 55°N to 45°S in latitude. We use similar coincidence criteria as O'Dell et al. (2018) to match airmasses observed by TCCON and OCO-3. In total, we count ~101K coincident soundings between ground based TCCON measurements and OCO-3 in nadir mode over land, ~91K coincident soundings in SAM/target mode over land, and 18K soundings in glint mode over water.

The SAA truth proxy (for more details see O'Dell et al.,2018) makes use of the low spatial variability of XCO2 over small regions (up to 100 km) and short time spans (~10s). Here we define continuous segmentes of soundings that were collected along-track within ~10s as small areas. Between August 2019 and December 2020, the SAA truth proxy consists of ~656K soundings in nadir mode over land, ~219K sounding in SAM/target mode over land, and ~ 869K soundings in glint mode over water.

For the multi-model median truth proxy, a suite of four models sampled at the OCO-3 sounding locations and times was used (for more details see O'Dell et al.,2018). The models generally differ in their prior flux assumptions, prior flux uncertainty, transport model, initial conditions, spatial resolution, and inverse method. Each model assimilates either in-situ CO2 concentration data, GOSAT XCO2 data, OCO-2 XCO2 data, or a combination of the above. Between August 2019 and December 2020, the multi-model median truth proxy consists of ~1358K soundings in nadir mode over land, ~797K soundings in SAM/target mode over land, and ~ 1500K soundings in glint mode over water.

An overview of the different truth proxies is given in Table 5-1.

		Number of Obs		
Name	Observation Mode	$(x10^{3})$	Details	
TCCON	Nadir over land	~110	GGG2014	
TCCON	Target/SAM	~91	GGG2014	
TCCON	Glint over water	~18	GGG2014	

Table 5-1: Overview of the truth proxy training datasets for OCO-3 v10.

		Number of Obs	
Name	Observation Mode	$(x10^{3})$	Details
SAA	Nadir over land	~656	Areas < 100 km along track
SAA	Target/SAM	~219	Areas < 100 km along track
SAA	Glint over water	~869	Areas < 100 km along track
Multi Model Median	Nadir over land	~1358	
Multi Model Median	Target/SAM	~797	
Multi Model Median	Glint over water	~1500	

#### 5.1.2 Filter Variables and Limits

Soundings that show errors in  $X_{CO2}$  when compared to a truth proxy that are too large to provide reliable constraints on CO<sub>2</sub> fluxes are removed by threshold-based filters for multiple retrieval parameters. For v10, we apply two different sets of filter variables and limits for observations over land and water. The selection of filter variables and limits is based on Mandrake et al. (2015), Eldering et al. (2017) and O'Dell et al. (2018). The v10 quality filters are based on a number of retrieved or auxiliary variables that correlate with excessive  $X_{CO2}$  scatter or bias.

The selection of the variables was done sequentially by identifying individual variables responsible for the largest fraction of the variance in  $\delta$ XCO2 (defined as the retrieved – true XCO2). We then created a simple threshold-based filter for these variables. The selection of thresholds for particular filter variables followed the following procedure: both, scatter and bias, were considered with the latter being considered as more important. Variables were typically selected as filters if they were correlated with bias greater than ~0.5 ppm, or significant scatter (greater than 2 ppm). The filtering variables and thresholds were derived separately for land (nadir, Target/SAM) and ocean (glint) soundings. Filtering variables selected and their thresholds were the same or similar, regardless of the particular truth proxy used. On average, ~65% of all soundings in the truth proxy datasets pass the v10 quality filters over land (nadir, Target/SAM) and ~60% over water (glint).

Similar to the OCO-2 Lite Files, filtering can be done with xco2\_quality\_flag variable in the OCO-3 Lite Files ("0" is good). Table 4-2 lists the details on the parameters that define the data quality flag. In addition, we use the same bitflag convention as for OCO-2 to provide information as to which tests failed that leads to soundings marked as "bad" quality (see Table 4-2). For more details, see Section 3.1 and Section 3.2.4.

Bit	Simple Bit	Field	Units	Land Range	Ocean Glint Range
0	2	Preprocessors/co2_ratio		0.998, 1.035	0.998, 1.035
1	2	Preprocessors/h2o ratio		0.850, 1.035	0.850, 1.030
2	6	Retrieval/dp_o2a	hPa	-7, 7	
3	6	Retrieval/dpfrac	ppm	-3.0, 2.8	
4	5	Retrieval/rms rel o2a	%	0, 0.35	0, 1.0
5	5	Retrieval/chi2 wco2		0, 1.40	0, 1.25

**Table 5-2:** Filter variables and limits for the  $X_{CO2}$  quality flag definition in OCO-3 V10. For the definitions of the individual variables see Section 9 or O'Dell et al. (2018), Kiel et al. (2019). The "simple bits" use the same definitions as for OCO-2, given in Table 3-5.
Bit	Simple Bit	Field	Units	Land Range	Ocean Glint Range
6	3	Retrieval/albedo_wco2		0.12. 2.0	0, 0, 02
7	3	Retrieval/albedo slope o2a	1/cm <sup>-1</sup>	-1e-4, 1e-4	0,000
8	3	Retrieval/albedo slope sco2	1/cm <sup>-1</sup>	-2e-4, 5e-4	-5e-5, 7e-5
9	6	Retrieval/co2 grad del	ppm	-60, 85	-22, 5
10	0	Sounding/altitude stddev	m	0,120	
11	4	Retrieval/dust height		0.7, 10	
12	4	Retrieval/ice height		-0.15, 0.6	-10, 0.5
13	6	Retrieval/eof2 2 rel		-1.2, 1.2	
14	4	Retrieval/aod sulfate + Retrieval/aod oc		0, 0.20	
15	4	Retrieval/aod ice		8e-5, 0.035	0, 0.045
16	4	Retrieval/dws		0, 0.20	
17	5	Retrieval/ndiv		0,1	0,0
18	1	Retrieval/xco2_uncert	ppm	0, 1.25	0, 1.0
19	1	Retrieval/dof co2		1.5, 2.2	
20	6	Retrieval/Fs_rel		-0.020, 0.035	
21	5	Retrieval/rms_rel_sco2	%	0, 0.70	
22	6	Retrieval/dp	hPa		-4, 10
23	2	Preprocessors/dp_abp	hPa		-17, 10
24	3	Retrieval/windspeed	m/s		2, 25
25	1	Sounding/snr_o2a			200, 550
26	3	Retrieval/albedo_slope_wco2	1/cm <sup>-1</sup>		-2e-5, 2e-5
27	4	Retrieval/aod_total			0, 0.4
28	2	Preprocessor/11b_csstd_ratio_wco2			0,6
29	1	Sounding/s31			0.15, 0.25

"Bit" denotes the bit number in  $xco2\_qf\_bitflag$ , a 32-bit integer in the  $X_{CO2}$  Lite files. (0=pass, 1=fail) "Simple Bit" denotes the bit number in  $xco2\_qf$  simple bitflag, an 8-bit integer in the  $X_{CO2}$  Lite files.

#### 5.1.3 Footprint Bias Correction

OCO-3 obtains eight side-by-side, simultaneous, nearly-collocated measurement scenes called footprints. Similar to OCO-2, there are small and highly statistically significant differences between these eight footprints which likely arise from imprecision in the L1 calibration. To derive the v10 footprint biases for OCO-3, we follow the same procedure as for OCO-2 v10 (for more details see Section 3.2.1). For that, we used the SAA truth proxy. Data were selected for the analysis when all 8 footprints in one sounding frame (ID) converged. We computed the median  $X_{CO2}$  as the "ground truth" value, and subtracted this from the observed  $X_{CO2}$  to calculate the deviations for each footprint. The reported values are the average of the differences across all soundings per footprint. The footprint offsets are listed in Table 4-3 under the term FOOT. One set of biases was obtained for land (nadir, Target/SAM), and a different set for ocean glint. These biases are subtracted from all sounding  $X_{CO2}$  in preparation for the next steps of the bias correction. For both, land and water soundings, the largest bias is estimated for footprint seven (-0.35 ppm over land, -0.18 ppm over water) which is consistent with the pre-flight tests.

	FOOTPRINT BIAS (FOOT) (ppm)							
Footprint (fp)	1	2	3	4	5	6	7	8
Land	-0.09	0.13	-0.04	-0.33	0.33	0.19	-0.35	0.16

 Table 5-3: Bias Correction Parameters for OCO-3 v10.

Ocean Glint	0.00	0.09	-0.03	-0.16	0.12	0.10	-0.18	0.06	
		FEATURE BIAS (FEATS) (ppm)							
LAND (ALL)	- 0.62	$-0.62*(dPfrac) - 0.30*(max(logDWS,-5) + 5) - 0.011*(co2_grad_del - 5)) - 2.5*(albedo wco2 - 0.25)$							
OCEAN GLINT		_	0.16*max	( <b>dP</b> ,0) +	0.13*( <b>co2_g</b>	grad_del +	6.0)		
		OVERALL DIVISOR (TCCON ADJUST) Method				od			
LAND GLINT LAND NADIE LAND TARGE LAND SAM	r k /T	0.9963			Direct Comparison to TCCON (using Targe & Nadir observations only)				
OCEAN GLIN	T	0.9	9961		Coastline bootstrap & bootstrap				
		Variable definitions using full/HDF5/path for Lite files							
co2_grad_de	l	Retrieval/co2_grad_del							
dP		Retrieval/dp							
dPfrac		Retrieval/dpfrac							
logDWS		MAX( ln(Retrieval/dws), -5)							
albedo_wco2	,	Retrieval/albedo_wco2							

## 5.1.4 Parametric Bias Correction

The procedure to derive the Parametric Bias Correction is very similar to that described in O'Dell et al. (2018) and Section 3.2.2 above. This is the procedure followed by nearly all ACOS/GOSAT and OCO-2  $X_{CO2}$  bias corrections to date (e.g., Wunch et al. 2011, Guerlet et al. 2013). As previous versions of the OCO-2 data product, the OCO-3 v10 analysis found that over land, the different viewing modes (nadir, target, SAM) all had similar biases. The different analysis regions and modes have minor differences in the order of features chosen, but overall the features selected and their slopes are consistent with the exception of the SAA truth proxy. By definition, the SAA truth proxy is not able to provide information about spurious variations in  $X_{CO2}$  on large (>500km) scales (e.g. changing surface albedo over land). Therefore, coefficients derived from the SAA over land were not considered in the derivation of the final parametric bias correction coefficients. Table 4-4 shows the bias correction parameters for land soundings for the different training datasets, and Table 4-5 shows the same for glint observations over water. Each table shows the reduction in unexplained variance as features are added to the bias correction fit. Note that in each table, the  $X_{CO2}$  quality flag has been applied.

**Table 5-4:** Features used in land bias correction, with reduction in unexplained variance in parentheses. Coefficient uncertainties are  $1\sigma$ .

	N	Stddev (ppm)	dPfrac	Co2_grad_del	logDWS	albedo_wco2
TCCON (nadir)	77K	1.53 → 1.33	-0.646 (16%)	-0.0094 (2.1%)	-0.325 (2.8%)	-3.66 (3.7%)

	N	Stddev (ppm)	dPfrac	Co2_grad_del	logDWS	albedo_wco2
TCCON (TG/SAM)	61K	1.50 → 1.31	-0.629 (20%)	-0.0077 (1.7%)	-0.248 (1.2%)	-1.79 (1.0%)
Models (nadir)	673K	1.51 → 1.23	-0.627 (18%)	-0.0165 (6%)	-0.348 (6%)	-2.48 (3.9%)
Models (TG/SAM)	518K	1.46 → 1.22	-0.595 (19%)	-0.0121 (4%)	-0.244 (3%)	-2.88 (4.0%)
SAA (nadir)	414K	1.07 → 0.81	-0.516 (27%)	-0.0107 (6%)	-0.373 (9%)	-0.14 (0%)
SAA (TG/SAM)	151K	1.16 → 0.95	-0.542 (25%)	-0.0081 (2.7%)	-0.264 (3.4%)	-1.03 (0.8%)
B10 (adapted, all modes)	-	-	$\textbf{-0.62} \pm \textbf{0.02}$	$-0.011 \pm 0.004$	$-0.29 \pm 0.05$	$-2.7\pm0.8$

Table 5-5: Same as Table 4-4 but for glint measurements over water.

	Ν	Stddev (ppm)	$dP_sco2 > 0$	co2_grad_del
TCCON	10K	1.18 → 0.98	-0.202 (15%)	0.098 (16%)
Models	795K	1.21 → 0.77	-0.190 (23%)	0.145 (37%)
SAA	621K	0.97 <b>→</b> 0.37	-0.090 (22%)	0.158 (63%)
B10 (adapted)	-	-	$0.161 \pm 0.061$	$0.134\pm0.032$

For v10 observations over land in nadir and Target/SAM mode, four different parameters account for the largest fraction of the variability in  $X_{CO2}$ : dPfrac, co2\_grad\_del, logDWS, and albedo\_wco2. The definition of these variables is given in Section 9 and 11. The reduction in unexplained variance due to dPfrac and co2\_grad\_del is smaller for OCO-3 v10 than for all previous OCO-2 data versions. It appears that due to the more complex viewing geometry of the OCO-3 instrument, the unexplained variance is distributed across multiple retrieval variables, with each variable accounting for a small fraction of the variance. This is in contrast to the OCO-2 v10 parametric bias correction, where a large part of the unexplained variance can be explained by two variables (dPfrac and co2\_grad\_del).

For measurements over water in glint mode, the v10 parametric bias correction includes two variables: dP\_sco2 and co2\_grad\_del. Here, the dP\_sco2 term accounts for roughly ~20% of the unexplained variance and is only applied where dP\_sco2 > 0 hPa. The co2\_grad\_del term, on average, accounts for ~ 40% of the unexplained variance. The contribution of each parametric bias correction term to the raw XCO2 is shown in Figure 4-2 for land observations and in Figure 4-3 for observations over water.

# 5.1.5 Global Scaling Factor

The global scaling factor corrects for an overall bias in  $X_{CO2}$  and ties it to the WMO trace gas standard scale. TCCON serves as a link between the WMO trace gas standard scale and satellite measurements. Over land, this factor is derived by comparing OCO-3 nadir and target mode observations to ground-based TCCON measurements over several sites globally. We use similar coincidence criteria as O'Dell et al. (2018). A linear regression between TCCON  $X_{CO2}$  and the bias-corrected OCO-3  $X_{CO2}$  was performed, with the intercept forced to zero. For v10, we use the TCCON GGG2014 dataset to derive the global scaling factor. Overall, this analysis scales the OCO-3 land data to TCCON in the following way: OCO-3 = (0.9963 ± 0.003) TCCON.

# 6 Overview of OCO-2 v11 and OCO-3 v10 Data Products

With the exception of the Lite files, all OCO-2 and OCO-3 product files are in Hierarchical Data Format-5 (HDF), developed at the National Center for Supercomputing Applications (http://www.hdfgroup.org). This format facilitates the creation of logical data structures by organizing the data product into folders and subfolders. Each file corresponds to one orbit contiguous mode set of data. Spectral radiances are contained in the SoundingMeasurements folder of the L1BSc product; retrieved  $X_{CO2}$  values are contained in the RetrievalResults folder of the L2Std product. Official data products are stored at the NASA GES DISC https://disc.gsfc.nasa.gov/datasets?keywords=0c02&page=1.

The OCO-2 and OCO-3 L2 data files are consistent in format to the degree possible, the primary differences having to do with how each instruments points and differences in the orbits of OCO-2 and the ISS.

OCO-2 provides multiple L2Std data files per day, generally one per orbit. However, OCO-2 data will be further separated into separate files for nadir, glint and target. As a result, for orbits with a target observation, there could be a file for the target data and another for the nadir/glint data. OCO-3 also breaks the data into separate files per orbit, but because OCO-3 could possible observe in different modes in a single orbit, the data is not further separated by observation mode.

As with past releases, the OCO-2 team has produced lite files for both  $X_{CO2}$  and the Solar Induced Fluorescence (SIF) product. The OCO-3 team has done this as well.

The OCO-2 L2 Lite files contain a subset of the information in the standard OCO-2 L2 product. They are meant to be significantly smaller but still contain all necessary information for typical science analyses. In addition, they have some value added:

- Only contain L2 soundings that converged
- They include a nominal recommended filtering flag (xco2\_quality\_flag)
- They include the recommended bias correction already applied to  $X_{CO2}$  (the  $X_{CO2}$  without bias correction is also contained in the Lite files)

There is one file per day, for each day that had at least one retrieved sounding.

The OCO-2 Lite files are in the NetCDF-4 format. Because NetCDF -4 is a subset of HDF-5, the files may be read with both NetCDF and HDF software.

#### 6.1 File Naming Conventions

The OCO-3 data follow the OCO-2 file naming convention with one difference. The data from all modes in combined into one file for OCO-3, and the Mode element is specified as 'SC in the file name. Otherwise, the convention noted below applies.

• The OCO-2 L1BSc files follow this convention:

oco2\_L1bSc[Mode]\_[Orbit][ModeCounter]\_[AcquisitionDate]\_[ShortBuildId]\_[Production DateTime][Source].h5

• The OCO-2 L2Std files follow this convention:

oco2\_L2Std[Mode]\_[Orbit][ModeCounter]\_[AcquisitionDate]\_[ShortBuildId]\_[Production DateTime] [Source].h5

• The OCO-2 L2Dia files follow this convention:

oco2\_L2Dia[Mode]\_[Orbit][ModeCounter]\_[AcquisitionDate]\_[ShortBuildId]\_[Production DateTime] [Source].h5

- The OCO-2 L2IDP files follow this convention:
- oco2\_L2IDP[Mode]\_[Orbit][ModeCounter]\_[AcquisitionDate]\_[ShortBuildId]\_[Production DateTime][Source].h5
- The OCO-2 LtCO2 files follow this convention (note that these are NetCDF, not HDF): oco2\_LtCO2\_[AcquisitionDate]\_[ShortBuildId]\_[ProductionDateTime][Source].nc4

There is no Orbit or Mode, as one day of data is aggregated.

Similarly,

• The OCO-2 LtSIF files follow this convention (note that these are NetCDF, not HDF): oco2\_LtSIF\_[AcquisitionDate]\_[ShortBuildId]\_[ProductionDateTime][Source].nc4

For all files, the fields are defined as below.

- [Mode] is the acquisition mode as a two-character string:
  - GL—Sample Glint
  - ND—Sample Nadir
  - TG—Sample Target
  - DS—Sample Dark Calibration
  - LS—Sample Lamp Calibration
  - SS—Sample Solar Calibration
  - BS—Sample Limb Calibration
  - NP—Single-Pixel Nadir
  - GP—Single-Pixel Glint
  - TP—Single-Pixel Target
  - DP—Single-Pixel Dark Calibration
  - LP—Single-Pixel Lamp Calibration
  - SP—Single-Pixel Solar Calibration
  - BP—Single-Pixel Limb Calibration
  - XS—Sample Transition
  - XP—Single-Pixel Transition
  - MS—Sample Lunar Calibration
  - MP—Single-Pixel Lunar Calibration
- [Orbit] is the five-digit orbit number
- [ModeCounter] is a letter (a, b, c, d) denoting the times an acquisition mode occurred in an orbit. If a mode occurs only once, ModeCounter is set to "a"
- [AcquisitionDate] is the UTC date (yymmdd) the data were acquired
- [ShortBuildId] identifies the L1B build version used (Bn.m.uu) where n is the major version, m is subversion number, and the uu is the incremental/patch number
- [ProductionDateTime] is the date and time the file was produced (yymmddhhmmss)

• [Source] (if present) identifies production sources different from the standard operations pipeline. This field will be missing from normal pipeline data

A note regarding the short build ID. All data with the same build version can be used together for science, regardless of the subversion and patch number.

For both OCO-2 and OCO-3 there is the retrospective processing (10r), which we recommend for science. The forward processing stream (10), has predicted calibration, and 10r has interpolated calibration. In addition, the forward stream has only 6% of the data, the 10r collection has all data that was deemed to be cloud free enough for processing.

Example filenames for both L2Std and Lite files can be found in Table 6-1.

Filename	Instrument	Туре	Orbit	Date	Mode
oco2_L2StdND_301 14a_200229_B10007 r_200404203338.h5	OCO-2	L2 Standard	30114	Feb 29, 2020 (200229)	Nadir (ND)
oco2_L2StdGL_3011 3a_200229_B10007r _200404181241.h5	OCO-2	L2 Standard	30113	200229	Glint (GL)
oco2_L2StdTG_3011 3a_200229_B10007r _200404201105.h5	OCO-2	L2 Standard	30113	200229	Target (TG)
oco3_L2StdSC_0541 6a_200417_B10200_ 200419001142.h5	OCO-3	L2 Standard	5416	April 17, 2020 (200417)	All
oco2_LtCO2_191018 _B10_v0.nc4	OCO-2	L2 Lite	N/A	Oct 18, 2019 (191018)	All
oco3_LtCO2_200219 B10_vearly.nc4	OCO-3	L2 Lite	N/A	200219	All

 Table 6-1: Example L2 filenames for OCO-2 and OCO-3

#### 6.1.1 File Format and Structure

The OCO-2 product files contain data structures indexed by sounding (1 to N soundings/file) and are associated by the sounding\_id variable in all products.

Variables are combined into groups by type (e.g., SoundingGeometry). Within each type, a variable has one or more values per sounding. Variables may be single-valued (e.g., sounding altitude) or multi-valued (e.g., co2 profile).

The metadata of each variable describes the variable's attributes, such as dimensions, data representation, and units.

Note that many variables in the L2 products use \_fph to denote full physics algorithm, \_idp for IMAP-DOAS, and \_abp for the  $O_2$  A band preprocessor. For example, surface pressure is calculated in each of the algorithms, so it is reported with a tag on the variable to differentiate them.

#### 6.1.2 Data Definition

The OCO-2 data products contain many variables with a variety of dimensions. The following list describes only the most important of the dimensions. Dimensions and data shapes are fully described within the HDF files.

- Retrieval—the number of retrievals reported (those soundings for which retrievals converged or were converging when the maximum number of iterations was reached)
- Band—the three bands of OCO-2 are O<sub>2</sub> A, weak CO<sub>2</sub>, and strong CO<sub>2</sub>
- Footprint—the eight footprints across the swatch are identified as 1 to 8
- Sample—the spectral element. Each band has 1016 spectral elements, although some are masked out in the L2 retrieval
- Sounding—one set of measurements (one footprint across three bands) that is the primary unit for retrievals

## 6.1.3 Global Attributes

In addition to variables and arrays of variables, global metadata is stored in the files. The granule-level metadata is described in Table 11-2. ECHO metadata and other metadata related to HDF version and production location can be found in the HDF file but are not discussed here.

#### 6.2 Data Files Content

#### 6.2.1 L2Std

Geolocated retrieved CO<sub>2</sub> column-averaged dry air mole fraction - physical model. This file contains the retrieved values for the state vector as well as geolocation information. A number of fields from the iterative maximum *a posteriori* differential optical absorption spectroscopy (IMAP-DOAS) and O<sub>2</sub> A-band (ABO2) cloud preprocessors are brought forward to the L2 products.

#### 6.2.2 L2Dia

This file has the data that is in the L2Std, as well as averaging kernels, *a priori* covariance matrices, posterior covariance matrices, and measured and model radiances.

#### 6.2.3 L2IDP

There are the results from the IMAP-DOAS process. The IMAP-DOAS process is used in cloud screening, but also provides solar induced fluorescence (SIF) measurements for a much larger set of data than contained in L2.

#### 6.2.4 L1BSc

These are the radiance spectra that are the input to the L2 retrievals.

# 7 OCO-2 and OCO-3 L2 Standard Data Products

#### 7.1 Data Description and User Alerts

The primary data products for both missions are the L2 Standard files. Figure 7-1 shows the folders in a L2Std folder of OCO-2. The folders are the same for the OCO-3 folders. A complete list of all the variables in each of the folders are contained in the tables in Section 11.

Figure 7-1: Data folders in the L2Std file.

#### 7.2 The RetrievalHeader Folder

Figure 7-2 shows the variables contained in the RetrievalHeader folder for an OCO-2 L2Std file. The list of variables is identical for the OCO-3 RetrievalHeader folder.

🔻 💆 RetrievalHeader
🗢 frame_index
😔 retrieval_time_string
🗢 retrieval_time_tai93
🗢 sounding_id
sounding_index
sounding_operation_mode

Figure 7-2: Variables in the Retrieval Header folder.

- **Sounding\_ID** This is the label for the sounding that will let you link the data across all of the product files. The sounding\_id is the primary identification number for soundings Figure 7-3Figure 7-3acquired and the footprint number (f) in the form yyyymmddhhmmsssf.
- *Retrieval\_time\_string* This is the time as a string. An example of this field is 2010-09-23T18:36:04.334Z.
- *Retrieval\_time\_tai93* This field is the time of the measurement, in seconds since Jan. 1, 1993. The TAI time corresponding to the example above is 559.420571E6.

## 7.3 RetrievalGeometry Folder

Figure 7-3 shows the variables contained in the RetrievalGeometry folder for an OCO-2 file and Figure 7-4 shows the variables for an OCO-3 folder. The OCO-3 files have additional variables related to the PMA and PCS.

- Retrieval\_latitude This is the latitude of the sounding. These values range from –90 to +90.
- Retrieval\_longitude This is the longitude. We use the convention of –180 to +180 longitude, with fractional degrees.
- Retrieval\_zenith The satellite zenith angle (in degrees) at the target.
- Retrieval altitude Altitude of the sounding based on Earth topography.
- Retrieval\_pma\_azimuth The OCO-3 Pointing Mirror Assembly azimuth rotation angle in science reference.
- Retrieval\_pma\_elevation The OCO-3 PMA elevation rotation angle in science reference.

🔻 🛃 RetrievalGeometry	
🗢 retrieval_altitude	
😔 retrieval_altitude_per_band	
🗢 retrieval_altitude_uncert	
🗢 retrieval_aspect	
🗢 retrieval_azimuth	
retrieval_center_offset_o2_weak_co2	
retrieval_center_offset_strong_co2_o2	
retrieval_center_offset_weak_co2_strong_co2	
retrieval_land_fraction	
retrieval_land_water_indicator	
🗢 retrieval_latitude	
🗢 retrieval_latitude_geoid	
🗢 retrieval_longitude	
🗢 retrieval_longitude_geoid	
retrieval_los_surface_bidirectional_angle	
🗢 retrieval_num_topo_points	
🗢 retrieval_overlap	
🗢 retrieval_overlap_o2_weak_co2	
retrieval_overlap_strong_co2_o2	
retrieval_overlap_weak_co2_strong_co2	
🗢 retrieval_plane_fit_quality	
🗢 retrieval_polarization_angle	
🗢 retrieval_relative_velocity	
🗢 retrieval_slant_path_diff_02_weak_co2	
retrieval_slant_path_diff_strong_co2_o2	
🗢 retrieval_slant_path_diff_weak_co2_strong_co2	
🗢 retrieval_slope	
ᅌ retrieval_solar_azimuth	
retrieval_solar_distance	
retrieval_solar_relative_velocity	
retrieval_solar_surface_bidirectional_angle	
🗢 retrieval_solar_zenith	
🗢 retrieval_surface_roughness	
retrieval_vertex_latitude	
🗢 retrieval_vertex_longitude	
🗢 retrieval_zenith	

Figure 7-3: Variables in the Retrieval Geometry folder for an OCO-2 file.

10

<ul> <li>RetrievalGeometry</li> </ul>
🗢 retrieval_altitude
ᅌ retrieval_altitude_per_band
retrieval_altitude_uncert
🗢 retrieval_aspect
🗢 retrieval_azimuth
retrieval_center_offset_o2_weak_co2
retrieval_center_offset_strong_co2_o2
retrieval_center_offset_weak_co2_strong_co2
retrieval_land_fraction
retrieval_land_water_indicator
🗢 retrieval_latitude
ᅌ retrieval_latitude_geoid
🗢 retrieval_longitude
retrieval_longitude_geoid
retrieval_los_surface_bidirectional_angle
ᅌ retrieval_overlap
retrieval_overlap_o2_weak_co2
retrieval_overlap_strong_co2_o2
retrieval_overlap_weak_co2_strong_co2
retrieval_pcs_data_source
retrieval_pcs_mode
retrieval_plane_fit_quality
ᅌ retrieval_pma_azimuth
retrieval_pma_elevation
retrieval_pma_motion_flag
retrieval_polarization_angle
retrieval_relative_velocity
retrieval_slant_path_diff_o2_weak_co2
retrieval_slant_path_diff_strong_co2_o2
retrieval_slant_path_diff_weak_co2_strong_co2
🗢 retrieval_slope
ᅌ retrieval_solar_azimuth
retrieval_solar_distance
retrieval_solar_relative_velocity
retrieval_solar_surface_bidirectional_angle
ᅌ retrieval_solar_zenith
retrieval_surface_roughness
retrieval_vertex_latitude
retrieval_vertex_longitude
🗢 retrieval_zenith

Figure 7-4: Variables in the Retrieval Geometry folder for an OCO-3 file.

## 7.4 RetrievalResults

The retrieval results folder contains all of the elements of the state vector in the L2 full physics retrieval. The list of fields in this folder is the same for both OCO-2 and OCO-3.

- xco2 This variable expresses the column-averaged CO2 dry air mole fraction for a sounding. Those soundings that did not converge will not be present. These values have units of mol/mol. This can easily be converted to ppm by multiplying by 10<sup>6</sup>.
- $xco2\_uncert This is an estimate of the uncertainty on the reported <math>X_{CO2}$ . These values have units of mol/mol.
- $xco2_apriori This$  is the initial guess for the  $X_{CO2}$ , in mol/mol.
- xco2\_avg\_kernel This is the averaging kernel. Note that the normalized averaging kernel (RetrievalResults/xco2\_avg\_kernel\_norm) for a given pressure level is equal to the non-normalized value (retrieval-results/xco2\_avg\_kernel) divided by the pressure weighting function at that level. Note that levels are "layer boundaries" and have no thickness. See Appendix A of O'Dell et al. [2012] for details on how these quantities are defined.

🔻 💆 Retrieval Results	fluorescence_at_reference	🗢 xco2
🗢 apriori_o2_column	fluorescence_at_reference_apriori	xco2_apriori
co2_profile	fluorescence_at_reference_uncert	xco2_avg_kernel
co2_profile_apriori	fluorescence_slope	xco2_avg_kernel_norm
co2_profile_averaging_kernel_matrix	fluorescence_slope_apriori	xco2_pressure_weighting_function
co2_profile_covariance_matrix	fluorescence_slope_uncert	xco2_uncert
co2_profile_uncert	h2o_scale_factor	xco2_uncert_interf
co2 vertical gradient delta	h2o_scale_factor_apriori	xco2_uncert_noise
diverging_steps	h2o_scale_factor_uncert	xco2_uncert_smooth
dof_co2_profile	<ul> <li>iterations</li> </ul>	
dof full vector	last_step_levenberg_marquardt_parameter	
eof 1 scale apriori o2	v num_active_levels	
eof 1 scale apriori strong co2	outcome_flag	
eof 1 scale apriori weak co2	v retrieved_co2_column	
e of 1 scale o2	<pre>v retrieved_dry_air_column_layer_thickness</pre>	
e eof 1 scale strong co2	retrieved_n20_column	
e e e e e e e e e e e e e e e e e e e	retrieved_n2o_column_layer_thickness	
e eof_1_scale_uncert_strong_co2	retrieved_oz_column	
a of 1 scale uncert weak co2	<pre>retrieved_wet_air_column_layer_thickness</pre>	
eof 1 scale weak co2	surface pressure apriori fph	
a eof 2 scale apriori o2	surface_pressure_aprion_rpn	
a est 2 scale apriori strong co2	surface_pressure_uprest fob	
<pre> eol_2_scale_apriori_scrong_coz  c eol_2_scale_apriori_week_co2 </pre>	surface_pressure_uncert_ipin	
<pre> eoi_2_scale_apriori_weak_coz  f acf 2 scale_a2 </pre>	temperature offset apriori fph	
eor_2_scale_oz	temperature_offset_ph	
eof_2_scale_strong_co2	temperature offset uncert fph	
eof_2_scale_uncert_oz	temperature profile met	
eof_2_scale_uncert_strong_co2	tropopause altitude	
eof_2_scale_uncert_weak_co2	tropopause pressure	
eof_2_scale_weak_co2	vector_altitude_levels	
eof_3_scale_apriori_o2	vector_altitude_levels_apriori	
eof_3_scale_apriori_strong_co2	vector_pressure_levels	
eof_3_scale_apriori_weak_co2	vector_pressure_levels_apriori	
eof_3_scale_o2	vector_pressure_levels_met	
eof_3_scale_strong_co2	wind_speed	
eof_3_scale_uncert_o2	wind_speed_apriori	
eof_3_scale_uncert_strong_co2	wind_speed_u_met	
eof_3_scale_uncert_weak_co2	wind_speed_uncert	
eof_3_scale_weak_co2	wind_speed_v_met	

Figure 7-5: Variable in the Retrieval Results folder of the L2Std file.

#### 7.5 Aerosols

The aerosol retrieval for uses eight aerosol types. These are the same types used in previous data releases. The L2 ATBD contains a complete description of the aerosols. For any particular sounding, 5 types are included. Ice clouds, water clouds, and a stratospheric aerosol are included in all soundings, and the other two types change, depending on the dominant aerosols in the GMAO *a priori* fields.

To simplify the use of data and identification of the types used, we store the aerosol results in arrays that are at least number of soundings by 8 (the total number of aerosol types).



Figure 7-6: Variables in the AerosolResults folder.

The fields and brief descriptions:

- aerosol\_aod- This field is N soundings x 8 x 4. This contains retrieved column-integrated aerosol optical depth for column segment: [Total, Low, Med, High]. The data are fill values where that aerosol type was not retrieved, and contains a value where it was included.
- aerosol\_model This string field is N soundings x 8, and contains the aerosol model used, if retrieved. The options are [profile\_linear, profile\_log, linear\_aod, gaussian\_linear, gaussian\_log]. For v10, all retrievals are in gaussian log.
- aerosol\_param This N sounding by 8 by 3 field contains the retrieved aerosol parameter values. For the Gaussian log set up, these parameters are the natural log of total aod, center pressure/surf-pressure, pressure sigma/surf-pressure. If a fill value is present (-999999.0), the aerosol type was not included for that retrieval. There are similar fields for the apriori and the uncertainty.
- aerosol\_total\_aod This field in a vector with N sounding elements and contains the retrieved total column-integrated aerosol optical depth for all aerosol types. It can be useful for data screening.
- aerosol\_type\_retrieved This N soundings x 8 field is a flag that indicates whether aerosol type was retrieved or not (1 yes, 0 no). You can multiply the aerosol\_aod field by this to get the data you are interested.
- Note that Metadata/AllAerosolTypes contains the list of the 8 aerosol types. They are DU, SS, BC, OC, SO, Ice, water, and ST. This stands for dust, sea salt, black carbon, organic carbon, sulfate, ice, water, and stratospheric aerosol.

#### 7.6 L1B Spectral Parameters

This folder contains selected L1B parameters that could be useful in L2 data analysis. In particular there are variable related to the declocking algorithm that has been implemented to correct for the slight misalignment of the focal plane arrays (FPAs) (for more information see the L1B ATBD). The algorithm uses spatial information from selected color slices to estimate a correction factor by which L1B spectra are multiplied to eliminate discontinuities. The selected color slices are first aggregated into "groups" for statistical purposes. For each group an estimate is made of a correction factor needed at each clocking boundary. Then, a correction function is determined from averages of these estimates, weighted by a column's distance to a group. A much more detailed description can be found in the Level 1B Algorithm Theoretical Basis Document (L1B ATBD).

🔻 🔄 L1bScSpectralParameters
max_declocking_factor_o2
max_declocking_factor_strong_co2
max_declocking_factor_weak_co2
ᅌ rad_continuum_o2
rad_continuum_strong_co2
ᅌ rad_continuum_weak_co2
ᅌ rad_mean_spectra_o2
rad_mean_spectra_strong_co2
ᅌ rad_mean_spectra_weak_co2
rad_stddev_spectra_o2
rad_stddev_spectra_strong_co2
rad_stddev_spectra_weak_co2
ᅌ snr_02_l1b
snr_strong_co2_l1b
ᅌ snr_weak_co2_l1b
sounding_color_slice_mean_o2
sounding_color_slice_mean_strong_co2
sounding_color_slice_mean_weak_co2
sounding_color_slice_noise_ratio_o2
sounding_color_slice_noise_ratio_strong_co2
sounding_color_slice_noise_ratio_weak_co2
sounding_color_slice_o2_qual_flag
sounding_color_slice_quadratic_o2
sounding_color_slice_quadratic_strong_co2
sounding_color_slice_quadratic_weak_co2
sounding_color_slice_slope_o2
sounding_color_slice_slope_strong_co2
sounding_color_slice_slope_weak_co2
sounding_color_slice_stddev_o2
sounding_color_slice_stddev_strong_co2
sounding_color_slice_stddev_weak_co2
sounding_color_slice_strong_co2_qual_flag
sounding_color_slice_weak_co2_qual_flag
spike_eof_bad_colors_o2
spike_eof_bad_colors_strong_co2
🗢 spike_eof_bad_colors_weak_co2

Figure 7-7: Variables in the L1BSCSpectralParameters folder.

# 8 ABO2 Preprocessor

The O<sub>2</sub>-A band cloud screening algorithm was developed at Colorado State University (CSU) under the ACOS program. It employs a fast Bayesian retrieval to estimate surface pressure and surface albedo, assuming clear-sky conditions with only molecular Rayleigh scattering, from high-resolution spectra of the O<sub>2</sub>-A band near 765 nm. The estimated surface pressure, surface albedo and the chi-squared goodness-of-fit statistic are used to flag scenes as cloudy, clear, or indeterminate [Taylor et al., 2012].

The basic method is that, absent clouds or aerosols, the surface pressure of a clear scene can be determined to within 2-5 hPa accuracy using the O<sub>2</sub>-A band spectrum of reflected sunlight. This is because of the strong oxygen absorption features that are present in this band. When surface pressure is higher, the absorption features are deeper for a given observation geometry. When clouds or aerosols are present, they change the path lengths for most photons, either via shortening or lengthening, such that the retrieved surface pressure can be very different from the expected value based on a meteorological forecast, and also the O<sub>2</sub>-A spectrum itself cannot be well-fit with a clear-sky assumption.

#### 8.1 Prescreening of OCO-2 Soundings for Cloud and Aerosol

The primary objective of the ABO2 algorithm is to remove from the OCO-2 operational processing streams the soundings that are deemed too contaminated by clouds and /or aerosol for reliable  $X_{CO2}$  retrieval in the computationally expensive L2 algorithm. The key screening parameters are interpreted internally via thresholds to provide a simple cloud flag. Furthermore, the key screening parameters can be used as inputs to a genetic algorithm used for individual sounding selection [Mandrake et al., 2013]. Details of the technique will be described in the Level 2 Algorithm Theoretical Basis Document (L2 ATBD) as well as an upcoming publication [Taylor et al., 2016]. As this is used as a preprocessor, the primary objective is to flag as cloudy scenes that are obviously cloudy or aerosol-contaminated. Therefore, thresholds are set rather loosely so scenes that have some cloud or aerosol contamination will sometimes pass the filter. This is by design. These scenes are sometimes useful for science, or may be rejected by additional pre- or postprocessor flags. The prescreening also checks for observations are impacted by cosmic rays. Starting with V8, soundings that might have been affected by the South Atlantic Anomaly are screened by the ABO2 preprocessor. New for b10, the ABO2 preprocessor contains in the state vector a zero level offset to the calculated top of the atmosphere radiances to account for uncalibrated instrument stray light and SIF. ABP b10 also uses gas absorption cross-section tables (ABSCO) v5.1, consistent with those used by the b10 L2FP.

#### 8.2 Key ABO2 Preprocessor Data Fields in Preprocessing Results Folder

The ABO2 data fields can be found in the standard L2 product (L2Std) PreprocessingResults folder, labeled with the \_abp data field designation.

Figure 8-1 shows a screenshot of an example OCO-2 L2Sc product file as viewed by HDFView. The ABO2 data fields within the PreprocessingResults folder are highlighted and will be described in detail below.

PreprocessingResults
🗢 albedo_o2_abp
cloud_flag_abp
🗢 cloud_flag_idp
co2_column_strong_band_apriori_idp
co2_column_strong_band_idp
co2_column_strong_band_uncert_idp
🗢 co2_column_weak_band_apriori_idp
🗢 co2_column_weak_band_idp
co2_column_weak_band_uncert_idp
🗢 co2_ratio_idp
co2_strong_band_processing_flag_idp
co2_weak_band_processing_flag_idp
🗢 dispersion_multiplier_abp
dry_air_column_apriori_idp
fluorescence_offset_relative_757nm_idp
fluorescence_offset_relative_771nm_idp
🗢 fluorescence_qual_flag_idp
fluorescence_radiance_757nm_idp
🗢 fluorescence_radiance_757nm_uncert_idp
fluorescence_radiance_771nm_idp
ᅌ fluorescence_radiance_771nm_uncert_idp
🗢 h2o_ratio_idp
h2o_ratio_uncert_idp
🗢 noise_o2_abp
🗢 o2_ratio_idp
reduced_chi_squared_o2_abp
reduced_chi_squared_o2_threshold_abp
sea_ice_flag_abp
selection_priority
signal_o2_abp
snr_o2_abp
surface_pressure_abp
surface_pressure_apriori_abp
surface_pressure_delta_abp
surface_pressure_offset_abp
temperature_offset_abp

Figure 8-1: Screenshot of an HDFView look at the ABO2 preprocessor file.

• surface\_pressure\_delta\_abp - The delta surface pressure is calculated as meteorological forecast surface pressure – retrieved pressure – offset:

surface pressure apriori abp – surface pressure abp – surface pressure offset abp

in SI units (Pascals). This is the primary screening criterion for the ABO2 preprocessor, and represents the difference between the retrieved and meteorologically estimated surface pressure in the target field of view. Because the algorithm uses imperfect spectroscopy to retrieve surface pressure, there is a path length dependent offset term that is determined by analyzing clear scenes and subtracted from the retrieved value. This yields an unbiased estimate of the retrieved surface pressure. A threshold value can be set independently for nadir, glint, and target viewing modes. At the time of this writing, scenes with a difference greater than 25 hPa (2500 Pa) are flagged as cloudy, for all OCO-2 viewing modes.

- albedo\_o2\_abp The retrieved surface albedo at 0.755 μm and 0.785 μm. Note that the retrieval assumes a perfect Lambertian surface albedo that varies linearly with wavelength. This assumption is currently made for all viewing modes; in glint mode, this means that the retrieved surface albedo can sometimes exceed unity. Over a dark ocean surface, the retrieved surface albedo is a good way to tell the presence of cloud: if the retrieved surface albedo is too large, a cloud or reflective aerosol layer is likely present. This test is not useful in glint mode or over land, and therefore is generally not used for OCO-2 prescreening.
- reduced\_chi\_squared\_o2\_abp The reduced  $\chi^2$  value of the spectral fit of the fast retrieval. Values greater than a specified threshold value are also indicative of clouds or aerosols present; as they are not accounted for in the retrieval, spectra containing them cannot be well fit. The threshold  $\chi^2$  value is a parameterized function of SNR, as there are persistent spectral features (due to imperfect spectroscopy or instrument calibration) that scale with the signal level.
- dispersion\_multiplier\_abp This parameter is also fit in the retrieval, and accounts for wavelength shifts in the spectra due primarily to the Earth-instrument Doppler shift. This is typically a maximum of ±7 km/sec, which corresponds roughly to shifts of ±0.3 cm-1 or ±0.018 nm (at maximum). This Doppler shift is easily fit for in the retrieval. Because the Doppler shift is formally a wavelength scaling, the ABO2 algorithm fits it as a scaling rather than a simple shift, though because of the narrowness of the fitted spectral region, it amounts to roughly the same thing.
- noise\_o2\_abp The determined radiance noise value in the continuum based on the preflight calibration.
- reduced\_chi\_squared\_o2\_threshold\_abp The threshold reduced  $\chi^2$  as described above. The logarithm of the reduced  $\chi^2$  in clear scenes is assumed to be a piecewise linear function of SNR. This relationship is determined from clear scenes separately for nadir and glint modes.
- signal\_o2\_abp The determined radiance mean value in the continuum.
- snr\_o2\_abp The ratio of signal\_o2\_abp to noise\_o2\_abp.
- surface\_pressure\_abp The retrieved value of surface pressure by the ABO2 algorithm, in units of Pa.
- surface\_pressure\_apriori\_abp The prior estimate of surface pressure in the target field of view, as determined from short-term meteorological forecasts, and adjusted based on the mean elevation in the target field of view.
- surface\_pressure\_offset\_abp The empirically determined offset of the retrieved surface pressure for clear sky scenes. This offset is determined as a piecewise linear function of solar zenith angle, separately for nadir and glint modes, and is based on soundings that are determined to be approximately clear based on other methods (which include output from the IMAP-DOAS preprocessor as well as soundings collocated with the MODIS sensor aboard Aqua).
- temperature\_offset\_abp The retrieved temperature offset, a simple additive offset to the meteorological estimate of the temperature profile. At the time of this writing this parameter is included in the state vector, but may be taken out to increase processing speed.
- cloud\_flag\_abp The result of the surface pressure,  $\chi^2$ , and albedo tests to determine if a scene is likely cloudy (or heavily aerosol-laden). If a single test is failed, the cloud flag is set equal to 1, indicating the likely presence of cloud and/or aerosol. If all threshold

checks are successfully passed, then the cloud flag is assigned a value of 0, indicating a sufficiently clear-sky scene. The cloud flag can also be set to 2 for "undetermined" cases. These are chiefly caused by solar zenith angle out of bounds or when viewing water surfaces in nadir observation mode (insufficient SNR).

# 9 IMAP-DOAS Preprocessor

The iterative maximum a posteriori differential optical absorption spectroscopy preprocessor is a non-scattering fast retrieval algorithm for optically thick absorbers [Frankenberg et al., 2005]. The preprocessor now serves two purposes for OCO 2: (1) retrieve vertical columns of trace gases in all bands individually for advanced cloud and aerosol screening and (2) retrieve solar induced chlorophyll fluorescence (SIF) using an algorithm described in Frankenberg et al. [2011]. The IMAP-DOAS Preprocessor code is essentially unchanged for the b10 software build.

The SIF data from IMAP is also available in the SIF lite files. These are described in more detail in a separate SIF Lite File User's Guide.

#### 9.1 Advanced Cloud and Aerosol Screening

For OCO-2, it is being used to derive vertical column densities of  $H_2O$  and  $CO_2$  independently in both  $CO_2$  bands (1.6 and 2.0  $\mu$ m) with the assumption of a non-scattering atmosphere. Given that Rayleigh scattering is very low in the near-infrared, this assumption holds true if neither aerosols nor clouds are present. In this case, both bands should yield an accurate and consistent result, i.e., the ratio of retrieved quantities in both  $CO_2$  bands is approaching unity in clear sky conditions.

We found that the ratio of both  $CO_2$  and  $H_2O$  vertical column densities is deviating significantly from unity in the presence of aerosols and clouds [e.g., Mandrake et al., 2013]. The details of this technique will be described in the algorithm theoretical basis document as well as an upcoming publication.

#### 9.2 Retrievals of Solar-Induced Chlorophyll Fluorescence

The possibility of retrieving solar induced chlorophyll fluorescence from high-resolution spectra in the vicinity of the O<sub>2</sub>-A band have been shown in Frankenberg et al. [2011] and Joiner et al. [2011]. Here, we apply the retrieval algorithm described in Frankenberg et al. [2011], embedded in the IMAP-DOAS retrieval code. It is important to note that this is the dedicated fluorescence retrieval, as opposed to the fluorescence retrieval within the full-physics L2 code. Interference with scattering properties in this retrieval is thus minimized [e.g., Frankenberg et al., 2012].

#### 9.3 Key Science Data Fields

#### The Preprocessing folder (

Figure 8-1) includes many of the key IDP variables from the preprocessing step.

- co2\_column\_strong\_band\_apriori\_idp A priori vertical column density of CO<sub>2</sub> in the strong (2.0 μm) band in molecules/m<sup>2</sup>. Note that a constant volume mixing ratio (VMR) is assumed across the globe in this IMAP-DOAS version and that the *a priori* thus mostly depends on surface pressure.
- co2\_column\_weak\_band\_apriori\_idp See above but for weak band (both are identical).
- co2\_column\_strong\_band\_idp Retrieved vertical column density of CO<sub>2</sub> in the strong (2.0 μm) band in molecules/m<sup>2</sup>. Note that this is different from the FP L2 CO<sub>2</sub> vertical column as this variable here is only retrieved in one band and ignores scattering.
- co2 column weak band idp See above but for the weak band.

- co2\_column\_strong\_band\_uncert\_idp Uncertainty in retrieved vertical column density of  $CO_2$  in the strong (2.0  $\mu$ m) band in molecules/m<sup>2</sup>.
- co2\_column\_weak\_band\_uncert\_idp See above but for weak band.
- co2\_column\_strong\_band\_processing\_flag\_idp Processing flag for the strong CO<sub>2</sub> band retrieval. Every sounding will have a value: 0 (successfully processed), 1 (not converged) or 2 (not processed).
- co2\_column\_weak\_band\_processing\_flag\_idp See above but for weak band.
- dry\_air\_column\_apriori\_idp *A priori* total dry air column (mol/m<sup>2</sup>) of the respective sounding (based purely on meteorological input data and topography).
- cloud\_flag\_idp Tentative cloud flag based purely used on the IMAP preprocessor. Values can be:
  - -2 = unusable (not processed)
  - -1 =not all retrievals converged
  - 0 = clearly cloudy
  - 1 = probably cloudy
  - 2 =probably clear

3 = very clear

The values are based on simple threshold criteria and based on the ratios defined in the same folder. This flag is *not* being used as input for FP L2 sounding selection and is also not being validated.

- co2\_ratio\_idp Ratio of retrieved CO<sub>2</sub> vertical column density (VCD) in weak and strong band (VCD<sub>1.6µm</sub>/VCD<sub>2.0µm</sub>). Please note that there might be a footprint dependence of this ratio, i.e., each OCO-2 footprint may have a different optimal ratio value. Eventually, we will document these subtleties but the users of early mission data should be aware of this fact, which applies to all variables discussed here.
- h2o\_ratio\_idp Ratio of retrieved H<sub>2</sub>O vertical columns in weak and strong band (VCD<sub>1.6µm</sub>/VCD<sub>2.0µm</sub>).
- h2o\_ratio\_uncert\_idp 1-sigma uncertainty of the ratio of retrieved H<sub>2</sub>O vertical columns in weak and strong band (VCD<sub>1.6µm</sub>/VCD<sub>2.0µm</sub>).
- o2\_ratio\_idp Ratio of retrieved vs. expected O<sub>2</sub> column density based on the fluorescence 771 nm retrieval window, which includes some weak O<sub>2</sub> line used to derive an O<sub>2</sub> column. Values substantially lower than 1 indicated the presence of clouds.
- fluorescence\_offset\_relative\_757nm\_idp Fraction of continuum level radiance explained by an additive offset term in the 757 nm spectral window (unitless). In the absence of instrumental errors, this will be only caused by fluorescence. Rotational Raman scattering should be negligible over typical vegetated surface and moderate solar zenith angles (<65 degrees).
- fluorescence\_offset\_relative\_771nm\_idp Same as above but for the 771 nm window.
- fluorescence\_radiance\_757nm\_idp Fluorescence term expressed in absolute radiance units (ph/s/m<sup>2</sup>/sr/ $\mu$ m) in the 757 nm fit window. This is a derived quantity based on the fit of the relative contribution multiplied with the overall continuum level radiance.
- fluorescence\_radiance\_771nm\_idp Same as above but for the 771 nm window.
- fluorescence\_radiance\_757nm\_uncert\_idp Estimated uncertainty (1-sigma) of the fluorescence term expressed in absolute radiance units (ph/s/m<sup>2</sup>/sr/µm) in the 757 nm fit window.

- fluorescence\_radiance\_771nm\_uncert\_idp Same as above but for the 771 nm window.
- fluorescence\_qual\_flag\_idp Quality flag for the fluorescence retrieval (0 = ok, 1 = did not pass quality filter or unprocessed).

# 10 Format Specification for OCO-2 v11 and OCO-3 v10 Lite Files

#### 10.1 Overview

The OCO-2 and OCO-3 L2 Lite files contain a subset of the information in the standard OCO-2 L2 product. They are meant to be significantly smaller but still contain all necessary information for typical science analyses. In addition, they have some value added:

- Only contain L2 soundings that converged
- They include a nominal recommended filtering flag (xco2\_quality\_flag)
- For this release, they do NOT contain warn levels. This is a difference from previous releases such as V8.
- They include the recommended bias correction already applied to  $X_{CO2}$  (the  $X_{CO2}$  without bias correction is also contained in the Lite files)

There is one file per day, for each day that had at least one retrieved sounding.

The OCO-2 Lite files are in the NetCDF-4 format

(http://www.unidata.ucar.edu/software/netcdf/docs/netcdf/NetCDF\_002d4-Format.html).

Because NetCDF-4 is a subset of HDF-5, the files may be read with both NetCDF and HDF software.

Generally speaking, each field in the file is described in the Attributes of that field within the file itself. Descriptions for selected fields are given below, but please be sure to read the Attributes of each used field within the actual Lite file. A few fields are present in OCO-2 files but not OCO-3, and vice versa, as indicated.

## 10.2 File Structure & Fields

The primary variables that most users will need exist at the main level. In addition, there are some additional variables that certain users might want, contained in three groups within the file: Preprocessors, Retrieval, and Sounding. Some NetCDF readers may not see these groups; if this happens, please update your NetCDF reader or use an HDF-5 reader.

## 10.2.1 Main Level Variables

- *latitude* The latitude at the center of the sounding field-of-view. *Parent Field: L2Std/RetrievalGeometry/retrieval\_latitude*
- *longitude* The longitude at the center of the sounding field-of-view. *Parent Field: L2Std/RetrievalGeometry/retrieval longitude*
- *vertex\_latitude* The latitude at each of the corners of the parallelogram that defines the field-of-view. *Parent Field: L2Std/RetrievalGeometry/retrieval vertex latitude*
- *vertex\_longitude* The longitude at each of the corners of the parallelogram that defines the field-of-view. *Parent Field: L2Std/RetrievalGeometry/retrieval vertex longitude*
- *time* The time of the sounding in seconds since 1970-01-01 00:00:00 UTC. *Parent Field: None (computed from RetrievalHeader/retrieval\_time\_string)*

- *date* The full date and time of the sounding in UTC, organized as [year,month,day,hour,minute,second,milliseconds]. This information is redundant with that from the *time* variable. *Parent Field: None (computed from RetrievalHeader/retrieval time string)*
- *solar\_zenith\_angle* The solar zenith angle (in degrees) at the target. *Parent Field: L2Std/RetrievalGeometry/retrieval solar zenith*
- *sensor\_zenith\_angle* The satellite zenith angle (in degrees) at the target. *Parent Field: L2Std/RetrievalGeometry/retrieval\_zenith*
- *xco2* The bias-corrected *X*<sub>CO2</sub> (in units of ppm). This *should be used for science analysis*. The bias correction formulae are contained in the metadata of the file. *Parent Field: None (derived using bias-correction formula)*
- *xco2\_apriori* The prior *X*<sub>CO2</sub> assumed by the L2 retrieval, in ppm. *Parent Field: L2Std/RetrievalResults/xco2\_apriori \* 1e6*
- $xco2\_uncertainty$  The posterior uncertainty in  $X_{CO2}$  calculated by the L2 algorithm, in ppm. This is generally 30-50% smaller than the true retrieval uncertainty. *Parent Field: L2Std/RetrievalResults/xco2\\_uncert \* 1e6*
- *xco2\_quality\_flag* A simple quality flag denoting science quality data. 0=higher quality, 1=lower quality. *Parent Field: None* [Note, the "warn level" field has been removed from version 10].
- *xco2\_qf\_bitflag* Similar to xco2\_quality\_flag, but each bit is meaningful. The different bits of this 32-bit integer tells whether a given threshold test passed (0) or failed (1). See Section 4.2.4 and Table 4-5 in the quality flagging section for detail. *Parent Field: None*
- *xco2\_qf\_simple\_bitflag* An 8-bit version of xco2\_qf\_bitflag, but the various quality flag tests are grouped into eight simpler test categories, as described Table 4-6. OCO-2 only. *Parent Field: None*
- *co2\_profile\_apriori* The prior profile of co2 in ppm. *Parent Group: L2Std/RetrievalResults/co2\_profile\_apriori \* 1e6*
- *xco2\_averaging\_kernel* The normalized column averaging kernel for the retrieved *X*<sub>CO2</sub> (dimensionless). *Parent Group: L2Std/RetrievalResults/xco2 avg kernel*
- *pressure\_levels* The retrieval pressure level grid for each sounding in hPa. Note that is simply equal to SigmaB multiplied by the surface pressure. *Parent Group: L2Std/RetrievalResults/vector\_pressure\_levels* \* 0.01
- *pressure\_weight* The pressure weighting function *on levels* used in the retrieval. It has the same dimensions as both "pressure levels" and "co2\_profile\_apriori". *Parent Group: L2Std/RetrievalResults/pressure\_weighting\_function*
- *sounding\_id* The sounding\_id of the sounding. For GOSAT, this is a 14-digit number defined as YYYYMMDDhhmmss. {YYYY=year, MM=month 1-12, DD=day 1-31,

hh=hour 0-23, mm=minute 0-59, ss=seconds 0-59, m=hundreds of milliseconds 0-9, f=footprint number 1-8}. For OCO, it is a 16-digit number defined as YYYYMMDDhhmmssmf. {YYYY=year, MM=month 1-12, DD=day 1-31, hh=hour 0-23, mm=minute 0-59, ss=seconds 0-59, m=hundreds of milliseconds 0-9, f=footprint number 1-8}. *Parent Field: L2Std/RetrievalHeader/sounding\_id* 

- *source\_files* The L2Std files used to generate this file. *Parent Group: None*
- *file\_index* The 1-based index used to identify which source file each sounding was drawn from. I.e., file\_index=2 for a particular sounding means that sounding was drawn from the 2<sup>nd</sup> element of *source\_files*. *Parent Group: None*

## Main-Level Dimension Variables

(these variables are part of the netcdf-4 definition and will not be needed by most users)

- *bands*: The three OCO-2 bands.
- *levels:* The twenty vertical levels in the OCO-2 level-2 full-physics retrieval.
- *epoch\_dimension:* Variable used for dimensioning the 7-integer *date* variable.
- *vertices*: The 4 vertex indices for vertex\_latitude and vertex\_longitude.
- *footprints:* The 8 footprint indices for footprint-dimensioned variables such as *Preprocessors/co2\_ratio\_offset\_per\_footprint.*

# **10.2.2** Preprocessors Group

This group contains information for the two OCO-2 preprocessor algorithms: The A-Band Preprocessor (ABP) and the IMAP-DOAS Preprocessor (IDP).

- co2\_ratio: Contains the ratio of the retrieved CO2 column from the weak Co2 band relative to that from the strong CO2 band. This ratio should be near unity. Significant departure from unity is currently used as a way to flag bad soundings (usually cloud or aerosol-contaminated). This value has also been footprint corrected using co2\_ratio\_offset\_per\_footprint, and further it has been bias corrected to remove a small feature-dependent bias. Parent Field: L2Std/PreprocessingResults/co2\_ratio\_idp (and then footprint-corrected).
- *co2\_ratio\_offset\_per\_footprint:* Contains the approximate offset in *co2\_ratio* from the mean value across all footprints, used in the construction of *co2\_ratio*. OCO-2 only. *Parent Field: none*.
- h2o\_ratio: Contains the ratio of the retrieved H<sub>2</sub>O column from the weak CO2 band relative to that from the strong CO2 band. This ratio should be near unity. Significant departure from unity is currently used as a way to flag bad soundings (usually cloud or aerosol-contaminated). This value has also been footprint corrected using h2o\_ratio\_offset\_per\_footprint. Parent Field: L2Std/PreprocessingResults/h2o\_ratio\_idp (and then footprint-corrected).

- *h2o\_ratio\_offset\_per\_footprint:* Contains the approximate offset in *h2o\_ratio* from the mean value across all footprints, used in the construction of *h2o\_ratio*. OCO-2 only. *Parent Field: none*.
- *dp\_abp*: This is the retrieved surface pressure minus the "best-guess" surface pressure from the meteorological forecast model. This has been adjusted for a clear-sky bias as well as the local surface elevation of the observed footprint. A value of this greater than about 50 hPa absolute value typically indicates cloud or aerosol contamination. *Parent Field: L2Std/PreprocessingResults/surface pressure delta abp \* 1e-2*
- $xco2\_strong\_idp$ : Estimate of  $X_{CO2}$  using only the IMAP-DOAS strong CO2 band retrieval at 2.06 µm. The dry air column is taken from the prior. It is constructed as the ratio of the co2 column from the strong CO2 band, divided by the dry air column. Units are ppm.

Parent Fields: L2Std/PreprocessingResults/co2\_column\_strong\_band\_idp, L2Std/PreprocessingResults/dry\_air\_column\_apriori\_idp

- xco2\_weak\_idp: Estimate of X<sub>CO2</sub> using only the IMAP-DOAS weak CO2 band retrieval at 1.61 µm. The dry air column is taken from the prior. It is constructed as the ratio of the co2 column from the weak CO2 band, divided by the dry air column. Units are ppm. Parent Fields: L2Std/PreprocessingResults/co2\_column\_weak\_band\_idp, L2Std/PreprocessingResults/dry\_air\_column\_apriori\_idp
- max\_declocking\_{o2a,wco2,sco2}: An estimate of the absolute value of the clocking error in the O2-A, Weak CO2, and Strong CO2 bands (used in the clocking correction algorithm that attempts to correct the L1b radiances for clocking errors). Expressed in percent. Typical values range from 0 to 10%.
   Parent Field: abs(L2Std/L1bSpectralParameters/max\_declocking\_factor\_{o2,weak\_co2,strong\_co2}-1)\*100
- *color\_slice\_noise\_ratio\_{o2a,wco2,sco2}:* An estimate of the sub-FOV variability in continuum radiance as estimated from the color slices for each of the three spectral bands. This is a calculation done only for the Lite Files, but it uses information from L1bScSpectralParameters/sounding\_color\_slice\_noise\_ratio\_{o2,weak\_co2,strong\_co2}.
- h\_continuum\_{o2a,wco2,sco2}: This is the standard deviation of the continuum for all soundings in the the frame in which a desired sounding is located, divided by the continuum of that sounding. This is a calculation only done for the lite files. It uses L1bScSpectralPararameters/radiance\_continuum\_{o2,weak\_co2,strong\_co2} as input. This is a measure of the fov-scale variability of the continuum radiance in each band.

## 10.2.3 Retrieval Group

This group contains information from the OCO-2 level-2 retrieval algorithm. It contains many fields that will only briefly be summarized here. These are other fields that may be useful to users. Some were used for quality filtering, some for bias correction, and others for neither.

• *xco2\_raw* is the "raw" *X*<sub>CO2</sub> retrieved by the L2 code *without bias correction*. It should not be used for science analysis. *Parent Field: L2Std/RetrievalResults/xco2\*1e6* 

• surface type Surface type used in the retrieval: 0=ocean and corresponds to a Coxmunk+Lambertian surface; 1=land and corresponds to a non-Lambertian surface with a fixed BRDF shape (this is applied to land surfaces). The BRDF is described in the L2 ATBD.

Parent Group: L2Std/RetrievalResults/surface type (changing Coxmunk,Lambertian->0, *Non-Lambertian->1*)

snow flag Flag to denote the presence of snow on the ground. For snow to be indicated, ٠ this requires albedo  $o_{2a} \ge 0.55$  AND albedo  $s_{co} \le 0.35$ . Land soundings only. OCO-2 only.

Parent Group: None.

psurf Retrieved surface pressure (in hPa) from the L2 algorithm. Note: this can be ٠ multiplied with the variable *SigmaB* to determine the profile of pressures for any sounding.

Parent Group: L2Std/RetrievalResults/surface pressure fph

- *psurf apriori* A priori surface pressure (in hPa) assumed by the L2 algorithm, taken originally from GEOS5-FP-IT analysis. Calculated from the band-averaged pointing location on the ground. Note: this should be used in conjunction with the variable SigmaB Coefficient to determine the a priori profile of pressures. Parent Group: L2Std/RetrievalResults/surface pressure apriori fph
- $dp \ o2a$  The difference psurf psurf apriori o2a, in hPa. Parent Group: None.
- *dp* sco2 The difference *psurf psurf* apriori sco2, in hPa. This variable is used in the  $X_{CO2}$  bias correction over both land and water surfaces. Parent Group: None.
- *tcwv* Retrieved Total Column Water Vapor (TWCV) in units of kg m<sup>-2</sup>. Parent Group: L2Std/RetrievalResults/retrieved h2o column \* (0.0180153/6.0221415e23). The latter is required to convert from molecules of H<sub>2</sub>O per  $m^2$  to kg H<sub>2</sub>O per m<sup>2</sup>.
- tcwv apriori A priori value of the TCWV derived from the prior H<sub>2</sub>O profile in units of • kg m<sup>-2</sup>. Obtained by dividing the retrieved *tcwv* by the retrieved *h2o* scale factor. Parent Group: RetrievalResults/h2o scale factor (along with tcwv).
- *tcwv uncertainty* Noise-driven uncertainty on the retrieved TWCV in kg m<sup>-2</sup>. Obtained from the product of *tcwv apriori* times the posterior uncertainty on the *h2o scale* factor. Parent Group: RetrievalResults/h2o scale factor uncert
- albedo o2a Over-land retrievals: Surface reflectance at a reference wavelength in band 1 (0.77 µm) in the primary scattering geometry (sun->ground->sensor) derived from the retrieved BRDF. Over-water retrievals: Retrieved Lambertian albedo at the band 1 reference wavelength. Parent Group: L2Std/AlbedoResults/albedo o2 fph (b10: water), L2Std/BRDFResults/brdf reflectance o2 (land).
- albedo wco2 Over-land retrievals: Surface reflectance at a reference wavelength in band ٠ 2 (1.615 µm) in the primary scattering geometry (sun->ground->sensor) derived from the

retrieved BRDF. Over-water retrievals: Retrieved Lambertian albedo at the band 2 reference wavelength.

Parent Group: L2Std/AlbedoResults/albedo\_weak\_co2\_fph (b10: water), L2Std/BRDFResults/brdf\_reflectance\_weak\_co2 (land).

• *albedo\_sco2* Over-land retrievals: Surface reflectance at a reference wavelength in band 3 (2.06 µm) in the primary scattering geometry (sun->ground->sensor) derived from the retrieved BRDF. Over-water retrievals: Retrieved Lambertian albedo at the band 3 reference wavelength.

Parent Group: L2Std/AlbedoResults/albedo\_strong\_co2\_fph (b10: water), L2Std/BRDFResults/brdf\_reflectance\_strong\_co2 (land).

- *albedo\_slope\_o2a* Slope of the albedo\_o2a term with respect to wavenumber. *Parent Group: L2Std/AlbedoResults/albedo\_slope\_o2\_fph (b10: water), L2Std/BRDFResults/brdf\_reflectance\_slope\_o2 (land).*
- *albedo\_slope\_wco2* Slope of the albedo\_wco2 term with respect to wavenumber. Parent Group: L2Std/AlbedoResults/albedo\_slope\_weak\_co2\_fph (b10: water), L2Std/BRDFResults/brdf\_reflectance\_slope\_weak\_co2 (land).
- *albedo\_slope\_sco2* Slope of the albedo\_sco2 term with respect to wavenumber. Parent Group: L2Std/AlbedoResults/albedo\_slope\_strong\_co2\_fph (b10: water), L2Std/BRDFResults/brdf\_reflectance\_slope\_strong\_co2 (land).
- *albedo\_quad\_o2a* Quadratic coefficient of the albedo\_o2a term with respect to wavenumber (land only). *Parent Group: L2Std/BRDFResults/brdf reflectance quadratic o2 (land).*
- *albedo\_quad\_wco2* Quadratic coefficient of the albedo\_wco2 term with respect to wavenumber (land only). *Parent Group: L2Std/BRDFResults/brdf reflectance quadratic weak co2.*
- *albedo\_quad\_sco2* Quadratic coefficient of the albedo\_sco2 term with respect to wavenumber (land only). *Parent Group: L2Std/BRDFResults/brdf reflectance quadratic strong co2 (land).*
- *aod\_ice* Retrieved Extinction Optical Depth of cloud ice at 0.755 μm. Parent Group: L2Std/AerosolResults/aerosol\_aod[\*,6,1] (1-based counting)
- *aod\_water* Retrieved Extinction Optical Depth of cloud water at 0.755 μm. Parent Group: L2Std/AerosolResults/aerosol aod[\*,7,1] (1-based counting)
- *aod\_dust* Retrieved Extinction Optical Depth of dust aerosol at 0.755 μm. Parent Group: L2Std/AerosolResults/aerosol aod[\*,1,1] (1-based counting)
- *aod\_seasalt* Retrieved Extinction Optical Depth of sea salt aerosol at 0.755 μm. *Parent Group: L2Std/AerosolResults/aerosol aod[\*,2,1] (1-based counting)*
- *aod\_bc* Retrieved Extinction Optical Depth of black carbon at 0.755 μm. Parent Group: L2Std/AerosolResults/aerosol\_aod[\*,3,1] (1-based counting)
- *aod\_oc* Retrieved Extinction Optical Depth of organic carbon at 0.755 μm. Parent Group: L2Std/AerosolResults/aerosol aod[\*,4,1] (1-based counting)

- *aod\_strataer* Retrieved Extinction Optical Depth of stratospheric aerosol at 0.755 μm. *Parent Group: L2Std/ AerosolResults/aerosol\_aod[\*,8,1] (1-based counting)*
- *aod\_sulfate* Retrieved Extinction Optical Depth of sulfate aerosol at 0.755 μm. *Parent Group: L2Std/ AerosolResults/aerosol\_aod[\*,5,1] (1-based counting)*
- *aod\_total* Retrieved Extinction Optical Depth of cloud+aerosol at 0.755 μm. *Parent Group: L2Std/AerosolResults/aerosol\_total\_aod*
- *brdf\_weight\_slope\_{wco2,sco2}* Retrieved slope across the band of the weight of the parent BRDF function (soil over land, cox-munk over ocean) in the weak & strong CO2 band. *L2Std/BRDFResults/brdf\_weight\_slope\_{weak,strong}\_co2*
- *dws* Retrieved aod's of the large aerosols, given by *aod\_dust + aod\_water + aod\_seasalt*. This is used in the *X*<sub>CO2</sub> bias correction for soundings over land. *Parent Group: none*
- dust\_height Retrieved central pressure of the dust aerosol layer, relative to the retrieved surface pressure. OCO-2 only. Parent Group: L2Std/AerosolResults/aerosol\_param[1,\*]
- *ice\_height* Retrieved central pressure of the cloud ice layer, relative to the retrieved surface pressure.
   *Parent Group: L2Std/AerosolResults/aerosol\_param[1,\*]*
- water\_height Retrieved central pressure of the cloud water layer, relative to the retrieved surface pressure. OCO-2 only.
   Parent Group: L2Std/AerosolResults/aerosol\_param[1,\*]
- *deltaT* Retrieved offset (in Kelvin) to a priori temperature profile. *Parent Group: L2Std/RetrievalResults/temperature\_offset\_fph*
- *h2o\_scale* Retrieved water vapor scale factor. *Parent Group: L2Std/RetrievalResults/h2o\_scale\_factor*
- co2\_grad\_del Change (between the retrieved profile and the prior profile) of the co2 dry air mole fraction difference from the surface minus that at level 13, measured in ppm. Level 13 is at a pressure P = 0.631579 Psurf. This variable is used in the X<sub>CO2</sub> bias correction over both land and water surfaces.
   Derived from L2Std/RetrievalResults/co2\_profile and co2\_profile\_apriori. If c=co2\_profile and a=co2\_profile\_apriori, then delta\_grad\_co2 = (c[20]-c[13])\*1e6 (a[20]-a[13])\*1e6
- *fs* Retrieved fluorescence in units of W m<sup>-2</sup> μm<sup>-1</sup> sr<sup>-1</sup> at 757 nm. *Derived from: L2Std/RetrievalResults/fluorescence\_at\_reference.*
- *fs\_rel* Retrieved fluorescence relative to Band 1 continuum signal. OCO-2 only. *Derived from: L2Std/RetrievalResults/fluorescence\_at\_reference.*
- *chi2\_02a* Reduced chi-squared value of the L2 fit residuals for band 1. *Parent Group: L2Std/SpectralParameters/reduced chi squared o2 fph*
- *chi2\_wco2* Reduced chi-squared value of the L2 fit residuals for band 2. *Parent Group: L2Std/SpectralParameters/reduced\_chi\_squared\_weak\_co2\_fph*

- *chi2\_sco2* Reduced chi-squared value of the L2 fit residuals for band 3. *Parent Group: L2Std/SpectralParameters/reduced\_chi\_squared\_strong\_co2\_fph*
- *rms\_rel\_o2a* RMS of the L2 fit residuals for band 1, relative to the continuum signal, in percent.
   *Parent Group: L2Std/SpectralParameters/relative residual mean square o2\*100*
- rms\_rel\_wco2 RMS of the L2 fit residuals for band 2, relative to the continuum signal, in percent.
   Parent Group: L2Std/SpectralParameters/relative\_residual\_mean\_square\_weak\_co2\*100
- *rms\_rel\_sco2* RMS of the L2 fit residuals for band 3, relative to the continuum signal, in percent.
   *Parent Group:* L2Std/SpectralParameters/relative residual mean square strong co2\*100
- windspeed Retrieved surface wind speed (in m/s) from the L2 algorithm, over water surfaces only. Parent Group: L2Std/RetrievalResults/wind speed
- *windspeed\_apriori* Prior surface wind speed (in m/s) used in the L2 algorithm, over water surfaces only. Taken from the GEOS5-FP-IT analysis. *Parent Group: L2Std/RetrievalResults/wind\_speed\_apriori*
- *t700* The estimated temperature at 700 hPa for each sounding, taken from the GEOS5-FP-IT forecast and estimated using linear interpolation. Invalid for soundings in which the surface pressure is lower than 700 hPa. *Parent Group: None.*
- s31 Ratio of continuum signal in the strong co2 band to that of the o2a band. Derived from: L2Std/SpectralParameters/signal\_strong\_co2\_fph (divided by) L2Std/SpectralParameters/signal\_o2\_fph
- *s32* Ratio of continuum signal in the strong co2 band to that of the weak co2 band. Derived from: L2Std/SpectralParameters/signal\_strong\_co2\_fph (divided by)

L2Std/SpectralParameters/signal\_weak\_co2\_fph

- *iterations* Number of iterations taken by the retrieval. *Parent Group: L2Std/RetrievalResults/iterations*
- *diverging\_steps* Number of diverging steps taken by the retrieval. *Parent Group: L2Std/RetrievalResults/diverging\_steps*
- *eof3\_1\_rel* Relative amplitude of the 1<sup>st</sup> EOF in the strong CO2 band. OCO-2 only. *Parent Group: (L2Std/RetrievalResults/eof\_3\_scale\_strong\_co2) / (L2Std/SpectralParameters/signal\_strong\_co2\_fph) \* 1.7e19 \* 100*
- *SigmaB* The coefficients by which to multiply *psurf* to determine the pressure at each vertical level in the profile. Note this is a single list of numbers, rather than repeated for each sounding (as all the other quantities are).

## 10.2.4 Sounding Group

Contains all the geolocation and time information for each sounding. For GOSAT, these contain the corrected geolocation information.

- *altitude* The mean surface elevation in the target field of view, in meters. *Parent Field: L2Std/RetrievalGeometry /retrieval altitude*
- *altitude\_stddev* The standard deviation of the surface elevation in the target field of view, in meters. *Parent Field: L2Std/RetrievalGeometry /retrieval surface roughness*
- *orbit* is the orbit number within the current repeat cycle. *Parent Field: L2Std/Metadata/StartOrbitNumber*
- *path* The WRS path number of the current orbit. 1-233. *Parent Field: L2Std/Metadata/StartPathNumber*
- *footprint* The footprint number of each sounding (1-8). *Parent Field: L2Std/RetrievalHeader/sounding\_index*
- *land\_water\_indicator* determines the land surface properties at the field of view. 0: land; 1: water; 2: inland water; 3: mixed. *Parent Field: L2Std/RetrievalGeometry/retrieval\_land\_water\_indicator*
- *land\_fraction* The fraction of land contained in the field-of-view for each sounding. *Parent Field: L2Std/RetrievalGeometry /retrieval\_land\_fraction.*
- *IIb\_type* gives the version number of the input level-1B data. (e.g., "5000", which means B5.0.00)
   *Parent Field: Derived from parent file name.*
- operation\_mode Nadir (0), Glint (1), Target (2), Transition (3), or Snapshot Area Mode (4).
  - Parent Field: Derived from L2Std/RetrievalGeometry/retrieval\_operation\_mode
- *solar\_azimuth\_angle* The solar azimuth angle (in degrees) at the target, measured east of north from the point of view of an observer on the ground at the target. *Parent Field: L2Std/RetrievalGeometry/retrieval\_solar\_azimuth*
- *sensor\_azimuth\_angle* The satellite azimuth angle (in degrees) at the target, measured east of north from the point of view of an observer on the ground at the target. *Parent Field: L2Std/RetrievalGeometry/retrieval\_sensor\_azimuth*
- *polarization\_angle* The angle (in degrees) between the polarization axis of the sensor and the local meridian plane (as defined by the plane made between the local normal at the target location and the ray from the satellite to the target). *Parent Field: L2Std/RetrievalGeometry/retrieval\_polarization\_angle*
- *glint\_angle* The angle (in degrees) between the local direction to the sensor, and the direction for pure glint observation (i.e., the outgoing direction from the surface for specularly reflected solar rays).
- *airmass* The relative airmass of the sounding, defined as 1/cos(solar\_zenith\_angle) + 1/cos(sensor\_zenith\_angle).

- *snr\_o2a* The estimated signal-to-noise ratio in the continuum of the O2A-band. *Parent Field: L2Std/L1bScSpectralParameters/snr o2 11b*
- *snr\_wco2* The estimated signal-to-noise ratio in the continuum of the weak CO<sub>2</sub> band. *Parent Field: L2Std/L1bScSpectralParameters/snr weak co2 l1b*
- *snr\_sco2* The estimated signal-to-noise ratio in the continuum of the strong CO<sub>2</sub> band. *Parent Field: L2Std/L1bScSpectralParameters/snr\_strong\_co2\_l1b*
- pcs\_data\_source The data source used by PCS in determining sounding times. OCO-3 only.
   Parent Field: L2Std/RetrievalGeometry/retrieval\_pcs\_data\_source
- *pma\_zenith\_angle* The zenith angle of the pointing mechanism assembly, in degrees. OCO-3 only. *Parent Field: L2Std/RetrievalGeometry/retrieval pma zenith angle*
- *pma\_azimuth\_angle* The azimuth angle of the pointing mechanism assembly, in degrees. OCO-3 only. *Parent Field: L2Std/RetrievalGeometry/retrieval pma azimuth angle*
- *targed\_id* For target or SAM-mode data, the id of the target. OCO-3 only. *Parent Field: Derived from an offline file.*
- *target\_name* For target or SAM-mode data, the name of the target. OCO-3 only. *Parent Field: Derived from an offline file.*

## **10.2.5** Meteorology Group

Contains updated meteorological information specific to version 9, using the updated GEOS5-FP-IT meteorological resampler code, as well as the updated pointing information. The resampler is run for both per-band pointing information, as well as the band-averaged location.

- *psurf\_apriori\_o2a* The estimated a priori surface pressure (hPa), for the O2A-band pointing location. *Parent Field: Met/FootprintMeteorology/footprint surface pressure met[0]* \* 0.01
- *psurf\_apriori\_wco2* The estimated a priori surface pressure (hPa), for the WCO2-band pointing location. *Parent Field: Met/FootprintMeteorology/footprint\_surface\_pressure\_met[1] \* 0.01*
- *psurf\_apriori\_sco2* The estimated a priori surface pressure (hPa), for the SCO2-band pointing location. *Parent Field: Met/FootprintMeteorology/footprint surface pressure met[2]* \* 0.01
- windspeed\_u\_met Prior surface wind speed (in m/s) in the horizontal U (North-South) direction. Positive u means the N-S wind component is flowing to the north (is from the south). Taken from the GEOS5-FP-IT analysis. Can be used along with windspeed\_v\_met to calculate the prior wind direction. Parent Group: Met/RetrievalResults/wind\_speed\_u\_met
- *windspeed\_v\_met* Prior surface wind speed (in m/s) in the horizontal V (East-West) direction. Positive v means the E-W wind component is flowing to the east (is from the west). Taken from the GEOS5-FP-IT analysis. Can be used along with *windspeed\_u\_met*

to calculate the prior wind direction. Parent Group: Met/RetrievalResults/wind\_speed\_v\_met

# 11 Full Data Tables for OCO-2 and OCO-3 Level 2 Standard Files (L2Std)

The tables below give a full listing of the variables in each folder/group and a short description including the data type. We suggest that users familiarize themselves with the data dimensions by browsing with HDFview or a similar tool.

The L2 data products in these tables are from the v10 L2Std and Lite files.

#### 11.1 OCO-2 and OCO-3 L2Std Metadata Group

The Metadata group (see Table 11-2 below) contains detailed information about the metadata fields from the L2 retrievals. The values in the table apply to both OCO-2 and OCO-3 data products.

Element	Storage	Comment
AbscoCO2Scale	Float32	Empirical scaling factors for CO2 ABSCO tables. Values should be different for the 1.6 micron and 2.06 micron bands and were chosen to provide agreement of retrieved $X_{CO2}$ with TCCON $X_{CO2}$ .
AbscoH2OScale	Float32	Empirical scaling factor for H <sub>2</sub> O ABSCO tables. Currently should be 1.0.
AbscoO2Scale	Float32	Empirical scaling factor for O2 ABSCO tables. Values chosen to improve agreement between retrieved surface pressure and independent estimates from a numerical weather prediction model.
AcquisitionMode	VarLenStr	The instrument mode in which the data in the product were collected. Valid values are: \'Glint\', \'Nadir\', \'Target\', \'Sample Dark Calibration\', \'Sample Lamp Calibration\', \'Sample Solar/limb Calibration\', \'Single-Pixel Dark Calibration\', \'Single-Pixel Lamp Calibration\', \'Single-Pixel Solar/limb Calibration\'
ActualFrames	Signed32	Actual number of frames reported in this product
ActualGoodRetrievals	Signed32	Number of retrievals with outcome flag that passed convergence/divergence criteria
ActualRetrievals	Signed32	Actual number of retrievals reported in the product
AllAerosolTypes	VarLenStr	List of aerosol types available for use in retrieval";
AncillaryDataDescriptors	VarLenStr	An array of file names that specifies all of the ancillary data files that were used to generate this output product. Ancillary data sets include all input except for the primary input files.
ARPAncillaryDatasetDescripto r	VarLenStr	The name of the Ancillary Radiometric Product file used to calibrate this file

Table 11-1: Metadata in Level 2 Standard Data file (L2Std).

Element	Storage	Comment
AscendingEquatorCrossingDat e (OCO-2 Only)	FixLenStr	The date of the equator crossing of the spacecraft ground track in the ascending direction
AscendingEquatorCrossingLon gitude (OCO-2 Only)	FixLenStr	The longitude of the equator crossing of the spacecraft ground track in the ascending direction
AscendingEquatorCrossingTim e (OCO-2 Only)	FixLenStr	The time of the equator crossing of the spacecraft ground track in the ascending direction
BuildId	VarLenStr	The identifier of the build containing the software that created the product.
CollectionLabel	VarLenStr	Label associating files in a collection
ColorSlicePositionO2	Signed16	Absolute spectral position of each ABO2 color slice.
ColorSlicePositionStrongCO2	Signed16	Absolute spectral position of each SCO2 color slice.
ColorSlicePositionWeakCO2	Signed16	Absolute spectral position of each WCO2 color slice.
DataFormatType	FixLenStr	'NCSA HDF' - A character string that describes the internal format of the data product.
EphemerisType (OCO-2 Only)	VarLenStr	The source of the spacecraft ephemeris data that were utilized to generate this data file
EquatorCrossingDate (OCO-2 Only)	FixLenStr	The date of the equator crossing of the spacecraft ground track in the descending direction
EquatorCrossingLongitude (OCO-2 Only)	Float32	The longitude of the equator crossing of the spacecraft ground track in the descending direction
EquatorCrossingTime (OCO-2 Only)	FixLenStr	The time of the equator crossing of the spacecraft ground track in the descending direction
ExpectedFrames	Signed32	Nominal number of frames in this product
FirstSoundingId	Signed64	The ID of the first sounding in this file
GapStartTime	FixLenStr	The timestamp after which a nonexistent, unnecessary, spurious, questionable, or erroneous data segment begins
GapStopTime	FixLenStr	The timestamp before which a nonexistent, unnecessary, spurious, questionable, or erroneous data segment ends
GranulePointer	VarLenStr	The filename of this product
HDFVersionId	VarLenStr	'5.x\' - A character string that identifies the version of the HDF (Hierarchical Data Format) software that was used to generate this data file
InputPointer	VarLenStr	A pointer to one or more data granules that provide the major input that was used to generate this product.
InstrumentShortName	VarLenStr	"OCO-2\' - The name of the instrument that collected the telemetry data

Element	Storage	Comment
L2FullPhysicsAlgorithmDescri ptor	VarLenStr	Identification of the algorithm and/or version used to generate this product
L2FullPhysicsDataVersion	VarLenStr	The source of the data used by the Full-physics algorithm: \'r01\' - initial processing; \'r02\', \'r03\', etc reprocessed data
L2FullPhysicsExeVersion	VarLenStr	The build version number of the Full-physics algorithm used to generate this product
L2FullPhysicsInputPointer	VarLenStr	Pointer to one or more data granules and auxilliary files that provide the major input that was used to generate this product
L2FullPhysicsProductionLocat ion	VarLenStr	Facility in which Full Physics code was run, typically: \'JPL\', \'Pleiades\'
LastSoundingId	Int64	he ID of the last sounding in this file
LongName	VarLenStr	A complete descriptive name for the data type of this product
ModeCounter	FixLenStr	The Nth occurrence of this particular mode for this orbit, indicated by letter (\'a\', \'b\', \'c\', \'d\', etc.)
OperationMode	FixLenStr	The two-letter abbreviation of the AcquisitionMode: GL, ND, TG, DS, LS, SS, BS, NP, GP, TP, DP, LP, SP, BP, XS, XP, MS, MP, SB
OrbitEccentricity (OCO-2 Only)	Float32	The eccentricity of the spacecraft orbital path
OrbitInclination (OCO-2 Only)	Float32	The angle between the plane of the spacecraft orbital path and the Earth equatorial plane
OrbitParametersPointer (OCO- 2 Only)	VarLenStr	The data files that provided the orbit parameters used to generate this product
OrbitPeriod (OCO-2 Only)	Float32	The time span between two consecutive descending node crossings
OrbitSemiMajorAxis (OCO-2 Only)	Float32	The length of the semimajor axis of the spacecraft orbit
OrbitStartDate (OCO-2 Only)	FixLenStr	The date of the equator crossing of the spacecraft nadir track in the descending direction
OrbitStartLongitude (OCO-2 Only)	Float32	The longitude of the equator crossing of the spacecraft ground track in the descending direction
OrbitStartTime (OCO-2 Only)	FixLenStr	The time of the equator crossing of the spacecraft ground track in the descending direction
PlatformLongName	VarLenStr	'Orbiting Carbon Observatory 2'
PlatformShortName	VarLenStr	'OCO-2'
PlatformType	VarLenStr	'spacecraft' - The type of platform associated with the instrument which acquires the accompanying data
ProcessingLevel	VarLenStr	Indicates data level (Level 0, Level 1A, Level 1B, Level 2) in this product

Element	Storage	Comment
ProducerAgency	VarLenStr	'NASA' - Identification of the agency that provides the project funding
ProducerInstitution	VarLenStr	'JPL' - Identification of the institution that provides project management.
ProductionDateTime	VarLenStr	The date and time at which the product was created (yyyy-mm-ddThh:mm:ss.mmmZ)
ProductionLocation	VarLenStr	Facility in which this file was produced, typically:'Operations Pipeline', 'Operations Pipeline 2', 'Science Computing Facility', 'Test Pipeline', Test Pipeline 2'
ProductionLocationCode	VarLenStr	One-letter code indicating the ProductionLocation, typically: ' ' - Operations Pipelines (1) or 2, 's' - Science Computing Facility, 't' - Test Pipelines (1) or 2
ProjectId	VarLenStr	'OCO-2' - The project identification string
QAGranulePointer	VarLenStr	A pointer to the quality assessment product that was generated with this product
RadianceConversionFactor	Float32	Multiplicative factor used to convert W m $^{-2}$ sr $^{-1}$ um $^{-1}$ to Ph sec $^{-1}$ m $^{-2}$ sr $^{-1}$ um $^{-1}$ at 760 nm (38.228x10^{17})
RangeBeginningDate	FixLenStr	The date on which the earliest data contained in the product were acquired (yyyy-mm-dd)
RangeBeginningTime	FixLenStr	The time at which the earliest data contained in the product were acquired (hh:mm:ss.mmmZ)
RangeEndingDate	FixLenStr	The date on which the latest data contained in the product were acquired (yyyy-mm-dd)
RangeEndingTime	FixLenStr	The time at which the latest data contained in the product were acquired (hh:mm:ss.mmmZ)
ReportedSoundings	Signed8	Indicates the inclusion of each footprint in the data: 0 - not included, 1 - included
RetrievalIterationLimit	String	Maximum number of iterations allowed before the algorithm gives up and sets the outcome_flag to 3
ShortName	VarLenStr	The short name identifying the data type of this product
SISName	VarLenStr	The name of the document describing the contents of the product
SISVersion	VarLenStr	The version of the document describing the contents of the product
SizeMBECSDataGranule	Float32	The size of this data granule in Megabytes
SpectralChannel	String	A description of the spectral channels used for the measurements
StartOrbitNumber (OCO-2 Only)	Signed32	The first orbit on which data contained in the product were acquired
StartPathNumber (OCO-2 Only)	Signed32	The first WRS path on which data contained in the product was collected
Element	Storage	Comment
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StopOrbitNumber (OCO-2 Only)	Signed32	The last orbit on which data contained in the product were acquired
StopPathNumber (OCO-2 Only)	Signed32	The last WRS path on which data contained in the product was collected
StartMissionSolarDay (OCO-3 Only)	Signed32	The first local solar day of the mission on which data contained in the product were acquired
StopMissionSolarDay(OCO-3 Only)	Signed32	The last local solar day of the mission on which data contained in the product were acquired
VMRO2	Float32	The volume mixing ratio of atmospheric O2

#### 11.2 Aerosol Results Group

The AerosolResults group (see Table 11-2 below) contains detailed information about the data fields from the L2 retrievals. The values in the table apply to both OCO-2 and OCO-3 data products.

Data Element	Туре	Comments
aerosol_aod	Float32	Retrieved column-integrated aerosol optical depth for column segment: [Total, Low, Med, High]
aerosol_model	FixLenStr	Aerosol model used, if retrieved, one of: [profile_linear, profile_log, linear_aod, gaussian_linear, gaussian_log]
aerosol_param	Float32	Retrieved aerosol parameter value
aerosol_param_apriori	Float32	A priori of retrieved aerosol parameter
aerosol_param_uncert	Float32	Uncertainty of retrieved aerosol parameter
aerosol_total_aod	Float32	Retrieved total column-integrated aerosol optical depth for all aerosol types
aerosol_type_retrieved	Signed8	Flag that indicates whether aerosol type was retrieved or not (1 yes, 0 no)

Table 11-2: Aerosol Results data in Level 2 Standard Data file (L2Std).

### 11.3 Albedo Results Group

The AlbedoResults group (see Table 11-3 below) contains detailed information about the albedo properties in the L2 retrievals. The values in the table apply only to OCO-3 v10 data products. These tables have been removed from the OCO-2 v11 data products.

Table TF-5. Albedo Results data in Level 2 Standard Data ine (L2Sta).		
Data Element	Туре	Comments
albedo_apriori_o2_fph	Float32	<i>a priori</i> of retrieved Lambertian component of albedo at 0.77 microns
albedo_apriori_strong_co2_fph	Float32	<i>a priori</i> of retrieved Lambertian component of albedo at 2.06 microns
albedo_apriori_weak_co2_fph	Float32	<i>a priori</i> of retrieved Lambertian component of albedo at 1.615 microns

 Table 11-3: Albedo Results data in Level 2 Standard Data file (L2Std).

Data Element	Туре	Comments
albedo_o2_fph	Float32	Retrieved Lambertian component of albedo at 0.77 microns
albedo_slope_apriori_o2	Float32	<i>a priori</i> of retrieved spectral dependence of Lambertian component of albedo within ABO2 band
albedo_slope_apriori_strong_co2	Float32	<i>a priori</i> of spectral dependence of Lambertian component of albedo within SCO2 band
albedo_slope_apriori_weak_co2	Float32	<i>a priori</i> of retrieved spectral dependence of Lambertian component of albedo within WCO2 band
albedo_slope_o2	Float32	Retrieved spectral dependence of Lambertian component of albedo within ABO2 band
albedo_slope_strong_co2	Float32	Retrieved spectral dependence of Lambertian component of albedo within SCO2 band
albedo_slope_uncert_o2	Float32	Uncertainty of retrieved spectral dependence of Lambertian component of albedo within ABO2 band
albedo_slope_uncert_strong_co2	Float32	Uncertainty of spectral dependence of Lambertian component of albedo within SCO2 band
albedo_slope_uncert_weak_co2	Float32	Uncertainty of retrieved spectral dependence of Lambertian component of albedo within WCO2 band
albedo_slope_weak_co2	Float32	Retrieved spectral dependence of Lambertian component of albedo within WCO2 band
albedo_strong_co2_fph	Float32	Retrieved Lambertian component of albedo at 2.06 microns
albedo_uncert_o2_fph	Float32	Uncertainty of retrieved Lambertian component of albedo 0.77 microns
albedo_uncert_strong_co2_fph	Float32	Uncertainty of retrieved Lambertian component of albedo at 2.06 microns
albedo_uncert_weak_co2_fph	Float32	Uncertainty of retrieved Lambertian component of albedo at 1.615 microns
albedo_weak_co2_fph	Float32	Retrieved Lambertian component of albedo at 1.615 microns

### 11.4 BRDF Results

The BRDFResults group (see Table 11-4 below) contains detailed information about the Bidirectional reflectance distribution function in L2 retrievals.

Table 11-4: BRDF Results data in Level 2 Standard Data file (L2S)	td) and Diagnostic file (L2Dia)	1.
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Data Element	Туре	Comments
brdf_anisotropy_parameter_o2	Float32	RPV kernel anisotropy parameter for ABO2 band (set to 0.75)

Data Element	Туре	Comments
brdf_anisotropy_parameter_stron g_co2	Float32	RPV kernel anisotropy parameter for SCO2 band (set to 0.75)
brdf_anisotropy_parameter_wea k_co2	Float32	RPV kernel anisotropy parameter for WCO2 band (set to 0.75)
brdf_asymmetry_parameter_o2	Float32	RPV kernel asymmetry parameter for ABO2 band (set to -0.1)
brdf_asymmetry_parameter_stro ng_co2	Float32	RPV kernel asymmetry parameter for SCO2 band (set to -0.1)
brdf_asymmetry_parameter_wea k_co2	Float32	RPV kernel asymmetry parameter for WCO2 band (set to -0.1)
brdf_breon_factor_o2	Float32	Amplitude factor applied for Breon part of BRDF for ABO2 band (set to 1e-20)
brdf_breon_factor_strong_co2	Float32	Amplitude factor applied for Breon part of BRDF for SCO2 band (set to 1e-20)
brdf_breon_factor_weak_co2	Float32	Amplitude factor applied for Breon part of BRDF for WCO2 band (set to 1e-20)
brdf_hotspot_parameter_o2	Float32	RPV kernel hotspot parameter for ABO2 band (set to 0.05)
brdf_hotspot_parameter_strong_ co2	Float32	RPV kernel hotspot parameter for SCO2 band (set to 0.05)
brdf_hotspot_parameter_weak_c o2	Float32	RPV kernel hotspot parameter for WCO2 band (set to 0.05)
brdf_rahman_factor_o2	Float32	Amplitude factor for Rahman (RPV) part of BRDF for ABO2 band (set to 1.0)
brdf_rahman_factor_strong_co2	Float32	Amplitude factor for Rahman (RPV) part of BRDF for SCO2 band (set to 1.0)
brdf_rahman_factor_weak_co2	Float32	Amplitude factor for Rahman (RPV) part of BRDF for WCO2 band (set to 1.0)
brdf_reflectance_apriori_o2	Float32	A priori of retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 0.77 micron wavelength
brdf_reflectance_apriori_strong_ co2	Float32	A priori of retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 2.06 micron wavelength
brdf_reflectance_apriori_weak_c o2	Float32	A priori of retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 1.615 micron wavelength
brdf_reflectance_o2	Float32	Retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 0.77 micron wavelength
brdf_reflectance_quadratic_aprio ri_o2	Float32	A priori of retrieved quadtratic spectral dependence of reflectance in ABO2 band
brdf_reflectance_quadratic_aprio ri_strong_co2	Float32	A priori of retrieved quadratic spectral dependence of reflectance in SCO2 band
brdf_reflectance_quadratic_aprio ri_weak_co2	Float32	A priori of retrieved quadratic spectral dependence of reflectance in WCO2 band

Data Element	Туре	Comments
brdf_reflectance_quadratic_o2	Float32	Retrieved quadratic spectral dependence of reflectance in ABO2 band
brdf_reflectance_quadratic_stron g_co2	Float32	Retrieved quadratic spectral dependence of reflectance in SCO2 band
brdf_reflectance_quadratic_unce rt_o2	Float32	Uncertainty of retrieved quadratic spectral dependence of reflectance in ABO2 band
brdf_reflectance_quadratic_unce rt_strong_co2	Float32	Uncertainty of retrieved quadratic spectral dependence of reflectance in SCO2 band
brdf_reflectance_quadratic_unce rt_weak_co2	Float32	Uncertainty of retrieved quadratic spectral dependence of reflectance in WCO2 band
brdf_reflectance_quadratic_weak _co2	Float32	Retrieved quadratic spectral dependence of reflectance in WCO2 band
brdf_reflectance_slope_apriori_o 2	Float32	A priori of retrieved linear spectral dependence of reflectance in ABO2 band
brdf_reflectance_slope_apriori_s trong_co2	Float32	A priori of retrieved linear spectral dependence of reflectance in SCO2 band
brdf_reflectance_slope_apriori_ weak_co2	Float32	A priori of retrieved linear spectral dependence of reflectance in WCO2 band
brdf_reflectance_slope_o2	Float32	Retrieved linear spectral dependence of reflectance in ABO2 band
brdf_reflectance_slope_strong_c o2	Float32	Retrieved linear spectral dependence of reflectance in SCO2 band
brdf_reflectance_slope_uncert_o 2	Float32	Uncertainty of retrieved linear spectral dependence of reflectance in ABO2 band
brdf_reflectance_slope_uncert_st rong_co2	Float32	Uncertainty of retrieved linear spectral dependence of reflectance in SCO2 band
brdf_reflectance_slope_uncert_w eak_co2	Float32	Uncertainty of retrieved linear spectral dependence of reflectance in WCO2 band
brdf_reflectance_slope_weak_co 2	Float32	Retrieved linear spectral dependence of reflectance in WCO2 band
brdf_reflectance_strong_co2	Float32	Retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 2.06 micron wavelength
brdf_reflectance_uncert_o2	Float32	Uncertainty of retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 0.77 micron wavelength
brdf_reflectance_uncert_strong_ co2	Float32	Uncertainty of retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 2.06 micron wavelength
brdf_reflectance_uncert_weak_c o2	Float32	Uncertainty of retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 1.615 micron wavelength
brdf_reflectance_weak_co2	Float32	Retrieved reflectance, computed from BRDF evaluated at the observation geometry, at 1.615 micron wavelength

Data Element	Туре	Comments
brdf_weight_apriori_o2	Float32	A priori of overall retrieved weight for the composite BRDF, at reference wavelength, for ABO2 band
brdf_weight_apriori_strong_co2	Float32	A priori of overall retrieved weight for the composite BRDF, at reference wavelength, for SCO2 band
brdf_weight_apriori_weak_co2	Float32	A priori of overall retrieved weight for the composite BRDF, at reference wavelength, for WCO2 band
brdf_weight_o2	Float32	Overall retrieved weight for the composite BRDF, at reference wavelength, for ABO2 band
brdf_weight_quadratic_apriori_o 2	Float32	A priori of overall retrieved in-band quadratic of the weight for the composite BRDF for ABO2 band
brdf_weight_quadratic_apriori_st rong_co2	Float32	A priori of overall retrieved in-band quadratic of the weight for the composite BRDF for SCO2 band
brdf_weight_quadratic_apriori_ weak_co2	Float32	A priori of overall retrieved in-band quadratic of the weight for the composite BRDF for WCO2 band
brdf_weight_quadratic_o2	Float32	Overall retrieved in-band quadratic of the weight for the composite BRDF for ABO2 band
brdf_weight_quadratic_strong_c o2	Float32	Overall retrieved in-band quadratic of the weight for the composite BRDF for SCO2 band
brdf_weight_quadratic_uncert_o	Float32	Uncertainty of overall retrieved in-band quadratic of the weight for the composite BRDF for ABO2 band
brdf_weight_quadratic_uncert_st rong_co2	Float32	Uncertainty of overall retrieved in-band quadratic of the weight for the composite BRDF for SCO2 band
brdf_weight_quadratic_uncert_w eak_co2	Float32	Uncertainty of overall retrieved in-band quadratic of the weight for the composite BRDF for SCO2 band
brdf_weight_quadratic_weak_co 2	Float32	Overall retrieved in-band quadratic of the weight for the composite BRDF for WCO2 band
brdf_weight_slope_apriori_o2	Float32	A priori of overall retrieved in-band slope of the weight for the composite BRDF for ABO2 band
brdf_weight_slope_apriori_stron g_co2	Float32	A priori of overall retrieved in-band slope of the weight for the composite BRDF for SCO2 band
brdf_weight_slope_apriori_weak _co2	Float32	A priori of overall retrieved in-band slope of the weight for the composite BRDF for WCO2 band
brdf_weight_slope_o2	Float32	Overall retrieved in-band slope of the weight for the composite BRDF for ABO2 band
brdf_weight_slope_strong_co2	Float32	Overall retrieved in-band slope of the weight for the composite BRDF for SCO2 band

Data Element	Туре	Comments
brdf_weight_slope_uncert_o2	Float32	Uncertainty of overall retrieved in-band slope of the weight for the composite BRDF for ABO2 band
brdf_weight_slope_uncert_stron g_co2	Float32	Uncertainty of overall retrieved in-band slope of the weight for the composite BRDF for SCO2 band
brdf_weight_slope_uncert_weak _co2	Float32	Uncertainty of overall retrieved in-band slope of the weight for the composite BRDF for SCO2 band
brdf_weight_slope_weak_co2	Float32	Overall retrieved in-band slope of the weight for the composite BRDF for WCO2 band
brdf_weight_strong_co2	Float32	Overall retrieved weight for the composite BRDF, at reference wavelength, for SCO2 band
brdf_weight_uncert_o2	Float32	Uncertainty of overall retrieved weight for the composite BRDF, at reference wavelength, for ABO2 band
brdf_weight_uncert_strong_co2	Float32	Uncertainty of overall retrieved weight for the composite BRDF, at reference wavelength, for SCO2 band
brdf_weight_uncert_weak_co2	Float32	Uncertainty of overall retrieved weight for the composite BRDF, at reference wavelength, for WCO2 band
brdf_weight_weak_co2	Float32	Overall retrieved weight for the composite BRDF, at reference wavelength, for WCO2 band

### 11.5 Dispersion Results

The DispersionResults group (see Table 11-5 below) contains detailed information about the dispersion properties in the L2 retrievals.

Data Element	Туре	Comments
dispersion_offset_apriori_o2	Float64	a priori of retrieved dispersion offset term in ABO2 band
dispersion_offset_apriori_strong _co2	Float64	a priori of retrieved dispersion offset term in SCO2 band
dispersion_offset_apriori_weak_ co2	Float64	a priori of retrieved dispersion offset term in WCO2 band
dispersion_offset_o2	Float64	Retrieved dispersion offset term in ABO2 band
dispersion_offset_strong_co2	Float64	Retrieved dispersion offset term in SCO2 band
dispersion_offset_uncert_o2	Float32	Uncertainty of retrieved dispersion offset term in ABO2 band
dispersion_offset_uncert_strong_ co2	Float32	Uncertainty of retrieved dispersion offset term in SCO2 band
dispersion_offset_uncert_weak_c o2	Float32	Uncertainty of retrieved dispersion offset term in WCO2 band

Table 11-5: Dispersion Results fields in Level 2 Standard Data file (L2Std) and Diagnostic file (L2Dia)

Data Element	Туре	Comments
dispersion_offset_weak_co2	Float64	Retrieved dispersion offset term in WCO2 band
dispersion_spacing_apriori_o2	Float32	a priori of retrieved dispersion spacing in ABO2 band
dispersion_spacing_apriori_stron g_co2	Float32	a priori of retrieved dispersion spacing in SCO2 band
dispersion_spacing_apriori_weak _co2	Float32	a priori of retrieved dispersion spacing in WCO2 band
dispersion_spacing_o2	Float32	Retrieved dispersion spacing in ABO2 band
dispersion_spacing_strong_co2	Float32	Retrieved dispersion spacing in SCO2 band
dispersion_spacing_uncert_o2	Float32	Uncertainty of retrieved dispersion spacing in ABO2 band
dispersion_spacing_uncert_stron g_co2	Float32	Uncertainty of retrieved dispersion spacing in SCO2 band
dispersion_spacing_uncert_weak _co2	Float32	Uncertainty of retrieved dispersion spacing in WCO2 band
dispersion_spacing_weak_co2	Float32	Retrieved dispersion spacing in WCO2 band

### 11.6 L1BSc Sounding Reference Fields

The L1bScSoundingReference group (see Table 11-6 below) contains certain fields from the L1BSc data files.

Data Element	Туре	Comments
packaging_qual_flag	UInt8	Bit flags recording errors during packaging of L2 full physics and preprocessing output into retrieval arrays: • 0—Good • Non-zero—See documentation
retrieval_index	Int32	The index into the Retrieval dimension of arrays in the RetrievalResults, RetrievedStateVector, and SpectralParameters groups for soundings associated with retrievals
selection_flag_sel (OCO-2 v11 only)	IntBitfield 8	Bitfield qual flag (selected = all bits 0), bit pos: 0: preconditions not met, 1: exceeded max warn level, 2: exceeded warn level cutoff, 3: randomly deselected, 4: matched to 0 size bin, 5: invalid geolocation, 6: no matching bin, 7: no matching enhanced mode.
sounding_id_11b	Int64	Unique identifier for each sounding
sounding_qual_flag	UInt64	Bit flags indicating the quality of the data in sounding: • 0—Good • Non-zero—See documentation

Table 11-6:         L1BSc sounding reference in Level 2	Standard Data file (L2Std	) and Diagnostic file (L2Dia).
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### 11.7 L1BSc Spectral Parameter Fields

The L1BScSpectralParameters group (see Table 11-7Table 11-7 below) contains certain fields regarding spectral properties of OCO-2 from the L1BSc data files.

Data Element	Туре	Comments
max_declocking_factor_o2	Float32	Maximum clocking correction factor of the ABO2 spectrum
max_declocking_factor_strong_c o2	Float32	Maximum clocking correction factor of the SCO2 spectrum
max_declocking_factor_weak_c o2	Float32	Maximum clocking correction factor of the WCO2 spectrum
rad_continuum_o2	Float32	The mean signal of the good samples in ABO2 falling between the 98th and 99th percentile for signal level
rad_continuum_strong_co2	Float32	The mean signal of the good samples in SCO2 falling between the 98th and 99th percentile for signal level
rad_continuum_weak_co2	Float32	The mean signal of the good samples in WCO2 falling between the 98th and 99th percentile for signal level
rad_mean_spectra_o2	Float32	The mean radiance of the ABO2 spectrum
rad_mean_spectra_strong_co2	Float32	The mean radiance of the SCO2 spectrum
rad_mean_spectra_weak_co2	Float32	The mean radiance of the WCO2 spectrum
rad_stddev_spectra_o2	Float32	The standard deviation of the radiance of the ABO2 spectrum
rad_stddev_spectra_strong_co2	Float32	The standard deviation of the radiance of the SCO2 spectrum
rad_stddev_spectra_weak_co2	Float32	The standard deviation of the radiance of the WCO2 spectrum
snr_o2_11b	Float32	The mean signal-to-noise ratio of the good samples in the band falling between the 98th and 99th percentile for signal level
snr_strong_co2_l1b	Float32	The mean signal-to-noise ratio of the good samples in the band falling between the 98th and 99th percentile for signal level
snr_weak_co2_l1b	Float32	The mean signal-to-noise ratio of the good samples in the band falling between the 98th and 99th percentile for signal level
sounding_color_slice_mean_o2	Float32	Mean radiance of the valid color slice pixels within the ABO2 footprint.
sounding_color_slice_mean_stro ng_co2	Float32	Mean radiance of the valid color slice pixels within the SCO2 footprint.
sounding_color_slice_mean_wea k_co2	Float32	Mean radiance of the valid color slice pixels within the WCO2 footprint.

Table 11-7: L1BSc SpectralParameters in Level 2 Standard Data file (L2Std) and Diagnostic file (L2Dia).

Data Element	Туре	Comments
sounding_color_slice_noise_r atio_o2 (OCO-2 only)	Float32	Ratio between the ABO2 footprint color slice radiance standard deviation, and the expected radiance noise level.
sounding_color_slice_noise_r atio_strong_co2 (OCO-2 only)	Float32	Ratio between the SCO2 footprint color slice radiance standard deviation, and the expected radiance noise level.
sounding_color_slice_noise_r atio_weak_co2 (OCO-2 only)	Float32	Ratio between the WCO2 footprint color slice radiance standard deviation, and the expected radiance noise level.
sounding_color_slice_o2_qual _flag (OCO-2 only)	IntBitfield 16	Bitfield qual flag, bit pos: 0: has no valid ABO2 color slice radiance.
sounding_color_slice_quadrati c_o2 (OCO-2 only)	Float32	Quadratic coefficient of a quadratic fit of the radiances of the valid color slice pixels as a function of the 0-based pixel row number within the ABO2 footprint.
sounding_color_slice_quadrati c_strong_co2 (OCO-2 only)	Float32	Quadratic coefficient of a quadratic fit of the radiances of the valid color slice pixels as a function of the 0-based pixel row number within the SCO2 footprint.
sounding_color_slice_quadrati c_weak_co2 (OCO-2 only)	Float32	Quadratic coefficient of a quadratic fit of the radiances of the valid color slice pixels as a function of the 0-based pixel row number within the WCO2 footprint.
sounding_color_slice_slope_o 2 (OCO-2 only)	Float32	Slope coefficient of a linear fit of the radiances of the valid color slice pixels as a function of the 0- based pixel row number within the ABO2 footprint.
sounding_color_slice_slope_st rong_co2 (OCO-2 only)	Float32	Slope coefficient of a linear fit of the radiances of the valid color slice pixels as a function of the 0- based pixel row number within the SCO2 footprint
sounding_color_slice_slope_ weak_co2 (OCO-2 only)	Float32	Slope coefficient of a linear fit of the radiances of the valid color slice pixels as a function of the 0-based pixel row number within the WCO2 footprint.
sounding_color_slice_stddev_ o2 (OCO-2 only)	Float32	Radiance standard deviation of the valid color slice pixels within the ABO2 footprint.
sounding_color_slice_stddev_ strong_co2 (OCO-2 only)	Float32	Radiance standard deviation of the valid color slice pixels within the SCO2 footprint.
sounding_color_slice_stddev_ weak_co2 (OCO-2 only)	Float32	Radiance standard deviation of the valid color slice pixels within the WCO2 footprint.
sounding_color_slice_strong_ co2_qual_flag (OCO-2 only)	IntBitfield 16	Bitfield qual flag, bit pos: 0: has no valid SCO2 color slice radiance.
sounding_color_slice_weak_c o2_qual_flag (OCO-2 only)	IntBitfield 16	Bitfield qual flag, bit pos: 0: has no valid WCO2 color slice radiance.
spike_eof_bad_colors_o2	Int16	Number of bad colors in the ABO2 spectrum

Data Element	Туре	Comments
spike_eof_bad_colors_strong_ co2	Int16	Number of bad colors in the SCO2 spectrum
spike_eof_bad_colors_weak_c o2	Int16	Number of bad colors in the WCO2 spectrum

### **11.8 L2 Preprocessing Fields**

The PreprocessingResults group (see Table 11-8 below) contains fields from the Level 2 preprocessing results.

Data Element	Туре	Comments
albedo_o2_abp	Float32	O2 albedo at 785 and 755 nm
cloud_flag_abp	Signed8	Indicator of whether the sounding contained clouds: 0—'Classified clear' 1—'Processing failed' 2—'Not classified' All other values undefined
cloud_flag_idp	Signed8	Cloud flag derived from IMAP-DOAS algorithm: -2—'Measurement unusable' -1—'Did not converge' 0—'Definitely cloudy' 1—'Probably cloudy' 2—'Probably clear' 3—'Very clear' All other values undefined.
co2_column_strong_band _apriori_idp	Float32	A priori CO2 vertical column density from meteorological data
co2_column_strong_band_idp	Float32	CO2 vertical column density (from SCO2 band)
co2_column_strong_band _uncert_idp	Float32	1-sigma error in the CO2 vertical column density (from SCO2 band)
co2_column_weak_band _apriori_idp	Float32	A priori CO2 vertical column density from meteorological data
co2_column_weak_band_idp	Float32	CO2 vertical column density (from WCO2 band)
co2_column_weak_band _uncert_idp	Float32	1-sigma error in the CO2 vertical column density (from WCO2 band)
co2_ratio_idp	Float32	Ratio of retrieved CO2 column (no scattering code) in WCO2 and SCO2 bands
co2_strong_band _processing_flag_idp	Int8	Indicator of whether the SCO2 analysis succeeded: 0—'Processing succeeded' 1—'Processing failed' 2—'Processing skipped' All other values undefined

<b>Table 11-8:</b> Preprocessing Results data in Level	2 Standard Data file (L2Std	) and Diagnostic file (L	_2Dia).
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Data Element	Туре	Comments
co2_weak_band_ processing_flag_idp	Int8	Indicator of whether the WCO2 analysis succeeded: 0—'Processing succeeded' 1—'Processing failed' 2—'Processing skipped' All other values undefined
dispersion_multiplier_abp	Float64	A number retrieved by the ABO2 algorithm that multiplies the dispersion coefficients as given in the L1B input file to get the effective wavelength of each channel to correct for the spacecraft-to- Earth Doppler shift.
dry_air_column_apriori_idp	Float32	Integrated vertical column of dry airmass derived from meteorological data
fluorescence_offset_relative _757nm_idp	Float32	Fraction of continuum level radiance explained by an additive offset term in the 757 nm spectral window (unitless). In the absence of instrumental errors, this will be only caused by fluorescence. Rotational Raman scattering should be negligible over typical vegetated surface and moderate solar zenith angles (<65 degrees).
fluorescence_offset_relative _771nm_idp	Float32	Fraction of continuum level radiance explained by an additive offset term in the 771 nm spectral window (unitless). In the absence of instrumental errors, this will be only caused by fluorescence. Rotational Raman scattering should be negligible over typical vegetated surface and moderate solar zenith angles (<65 degrees).
fluorescence_qual_flag_idp	UInt8	Indicator of the quality of the IMAP DOAS fluorescence retrieval for each sounding: 0—good 1—bad
fluorescence_radiance 757nm idp	Float32	Radiance generated by fluorescence at 757 nm
fluorescence_radiance _757nm_uncert_idp	Float32	Standard deviation of the radiance generated by fluorescence at 757 nm
fluorescence_radiance _771nm_idp	Float32	Radiance generated by fluorescence at 771 nm
fluorescence_radiance 771nm_uncert_idp	Float32	Standard deviation of the radiance generated by fluorescence at 771 nm
h2o_ratio_idp	Float32	Ratio of retrieved H <sub>2</sub> O column (no scattering code) in WCO2 and SCO2 bands
h2o_ratio_uncert_idp	Float32	1-sigma error in the ratio of retrieved H <sub>2</sub> O column (no scattering code) in WCO2 and SCO2 bands
noise_o2_abp	Float32	O2 measurement noise retrieved by the ABO2 algorithm
o2_ratio_idp	Float32	Ratio of retrieved and meteorological O2 column
reduced_chi_squared _o2_abp	Float32	O2 reduced chi squared retrieved by ABO2 preprocessing

Data Element	Туре	Comments
reduced_chi_squared _o2_threshold_abp	Float32	Threshold of O2 reduced chi squared used to set cloud_flag
sea_ice_flag_abp	Signed8	Simple, unvalidated parameterization for determination of sea ice presence over a water surface based on continuum signals in bands 1 and 3; use with caution. 0=no sea ice, 1=sea ice, 2=undetermined
selection_priority	Signed8	Indicator of the likelihood of generating a good retrieval from the sounding: 0 = most likely 20 = least likely
signal_o2_abp	Float32	O2 measurement signal level retrieved by the ABO2 algorithm
snr_o2_abp	Float32	O2 measurement SNR retrieved by the ABO2 algorithm
surface_pressure_abp	Float32	Surface pressure retrieved by the ABO2 algorithm
surface_pressure_apriori_abp	Float32	<i>a priori</i> surface pressure used by the ABO2 algorithm
surface_pressure_delta_abp	Float32	The value of surface_pressure_abp minus surface_pressure_apriori_abp and surface_pressure_offset_abp
surface_pressure_offset_abp	Float32	Empirically determined value to be added to the A band retrieved surface pressure, such that their sum is unbiased in clear scenes. It is modeled as a piecewise linear function of solar zenith angle; separate functions are used for land vs. ocean pixels.
temperature_offset_abp	Float32	The offset to the prior meteorological temperature profile as retrieved by the ABO2 algorithm

### **11.9 L2 Retrieval Geometry Fields**

The RetrievalGeometry group (see Table 11-9 below) contains fields geographic properties of the OCO-2 and OCO-3 observations.

Data Element	Туре	Comments
retrieval_altitude	Float32	Altitude of the sounding based on Earth topography
retrieval_altitude_per_band	Float32	Altitude of the per-spectrum footprint based on Earth topography
retrieval_altitude_uncert	Float32	Uncertainty of the source Earth topography data
retrieval_aspect	Float32	Orientation of the surface slope relative to the local North
retrieval_azimuth	Float32	Angle between the LOS as defined from the sounding location to the spacecraft, and the sounding location local north direction

Table 11-9: Retrieval Geometry in Level 2 Standard Data file (L2Std).

Data Element	Туре	Comments
retrieval_center_offset _o2_weak_co2	Float32	Distance between the ABO2 band footprint center and the WCO2 band footprint center
retrieval_center_offset _strong_co2_o2	Float32	Distance between the SCO2 band footprint center and the ABO2 band footprint center
retrieval_center_offset _weak_co2_strong_co2	Float32	Distance between the WCO2 band footprint center and the SCO2 band footprint center
retrieval_land_fraction	Float32	Percentage of land surface type within the sounding
retrieval_land_water_indicator	Int8	Surface type at the sounding location: 0—Land 1—Water 2—Unused 3—Mixed land water
retrieval_latitude	Float32	Geodetic latitude of the sounding based on Earth topography
retrieval_latitude_geoid	Float32	Geodetic latitude of the sounding based on standard geoid
retrieval_longitude	Float32	Longitude of the sounding based on Earth topography
retrieval_longitude_geoid	Float32	Longitude of the sounding based on standard geoid
retrieval_los_surface_bidirection al_angle	Float32	Angle between the LOS as defined from the sounding location to the spacecraft, and the sounding surface normal
retrieval_overlap	Float32	Area of intersection of all three band footprints relative to average area of all three band footprints
retrieval_overlap _o2_weak_co2	Float32	Area of intersection of the footprints of ABO2 and WCO2 relative to the average area of the two footprint
retrieval_overlap _strong_co2_o2	Float32	Area of intersection of the footprints of ABO2 and SCO2 relative to the average area of the two footprints
retrieval_overlap _weak_co2_strong_co2	Float32	Area of intersection of the footprints of WCO2 and SCO2 relative to the average area of the two footprints
retrieval_pcs_data_source (OCO- 3 only)	Signed8	0 = Estimator uses SRU, IMU, and GPS, 1 = Estimator uses SRU, and GPS, 2 = Estimator uses IMU, and GPS, 3 = Estimator uses SRU, IMU, and BAD position, 4 = Estimator uses SRU, and BAD position, 5 = Estimator uses IMU, and BAD position, 6 = Estimator uses BAD attitude, and GPS position, 7 = Estimator uses ISS BAD data only Else = no data available
retrieval_pcs_mode (OCO-3 only)	FixLenStr	The two-letter abbreviation of the Pointing Control System mode: PS, PA, PR, PC, PJ, PT, RN, ND, RG, GL, RT, TG, RA, AM

Data Element	Туре	Comments
retrieval_plane_fit_quality	Float32	Goodness-of-fit of surface slope: the standard deviation of the points, to which the plane is fitted, with the expected values taken as the orthogonal projection of the points onto the plane
retrieval_pma_azimuth (OCO-3 only)	Float32	Pointing Mirror Assembly azimuth rotation angle in science reference
retrieval_pma_elevation (OCO-3 only)	Float32	Pointing Mirror Assembly elevation rotation angle in science reference
retrieval_pma_motion_flag (OCO-3 only)	Signed8	Motion flag for Pointing Mirror Assembly $(0 = not moving, 1 = in motion, -1 = unknown)$
retrieval_polarization_angle	Float32	The angle between the accepted polarization axis of the instrument and the instrument reference plane for polarization, defined as the plane formed by the LOS and the ray from the sounding location to the local zenith
retrieval_relative_velocity	Float32	Velocity of the spacecraft along the LOS: positive indicates spacecraft moving toward sounding location
retrieval_slant_path_diff _o2_weak_co2	Float32	Difference in slant path between ABO2 and WCO2 footprints
retrieval_slant_path_diff _strong_co2_o2	Float32	Difference in slant path between SCO2 and ABO2 footprints
retrieval_slant_path_diff _weak_co2_strong_co2	Float32	Difference in slant path between WCO2 and SCO2 footprints
retrieval_slope	Float32	Slope of a plane fit to points within the sounding
retrieval_solar_azimuth	Float32	Angle between the solar direction as defined from the sounding location to the Sun, and the sounding location local North direction
retrieval_solar_distance	Float64	Distance between sounding location and the Sun
retrieval_solar_relative_velocity	Float32	Velocity of the Sun along the sounding location/Sun vector: negative indicates Sun moving toward sounding location
retrieval_solar_surface_bidirecti onal_angle	Float32	Angle between the solar direction as defined from the sounding location to the sun, and the sounding surface normal
retrieval_solar_zenith	Float32	Angle between the solar direction as defined from the sounding location to the Sun, and the sounding location local zenith direction
retrieval_surface_roughness	Float32	Standard deviation of the altitude within the sounding
retrieval_vertex_latitude	Float32	Geodetic latitude of the footprint vertices using Earth topography
retrieval_vertex_longitude	Float32	Longitude of the footprint vertices using Earth topography

Data Element	Туре	Comments
retrieval_zenith	Float32	Angle between the LOS as defined from the sounding location to the spacecraft, and the sounding location local zenith direction

#### 11.10 L2 Retrieval Header Fields

The Retrieval Header group (see Table 11-10 below) contains fields information about the time and date of the OCO-2 observations.

Data Element	Туре	Comments
frame_index	Signed32	Index of the frame dimension of the corresponding sounding in L1bScSoundingReference data elements
retrieval_time_string	FixLenStr	Data acquisition time for the retrieval based upon the three footprint times (yyyy-mm- ddThh:mm:ss.mmmZ)
retrieval_time_tai93	Float64	Data acquisition time for the retrieval based upon the three footprint times in seconds since Jan. 1, 1993
sounding_id	Signed64	The sounding_id of the sounding containing the spectra used to perform the retrieval
sounding_index	Signed32	Index of the sounding dimension of the corresponding sounding in the L1bScSoundingReference data elements
sounding_operation_mode	FixLenStr	The two-letter abbreviation of the science AcquisitionMode: GL, ND, TG, XS

Table 11-10: Retrieval Header data in Level 2 Standard Data file (L2Std).

### 11.11 L2 Retrieval Results

The RetrievalResults group (see Table 11-11Table 11-11 below) contains the retrieval results from the OCO-2 Level 2 data products.

Data Element	Туре	Comments
apriori_o2_column	Float32	a priori vertical column of O2
co2_profile	Float32	Vertical profile of CO2
co2_profile _averaging_kernel_matrix	Float32	Averaging kernel for CO2 profile
co2_profile_apriori	Float32	Vertical a priori profile of CO2
co2_profile_covariance_matrix	Float32	Covariance matrix for CO2 profile
co2_profile_uncert	Float32	Vertical profile of CO2 uncertainty

Table 11-11: Retrieval Results data in Level 2 Standard Data file (L2Std).

Data Element	Туре	Comments
co2_vertical_gradient_delta	Float32	The change from apriori to retrieved value of the vertical gradient in the co2 profile. Indicates that the apriori co2 profile was substantially different than that which was retrieved.
diverging_steps	Int16	Number of iterations in which solution diverged
dof_co2_profile	Float32	Degrees of freedom (X <sub>CO2</sub> only)
dof_full_vector	Float32	Degrees of freedom (Full state vector)
eof_1_scale_apriori_o2	Float32	a priori of retrieved scale factor of first empirical orthogonal residual function in ABO2 band
eof_1_scale_apriori_strong_co2	Float32	a priori of retrieved scale factor of first empirical orthogonal residual function in SCO2 band
eof_1_scale_apriori_weak_co2	Float32	a priori of retrieved scale factor of first empirical orthogonal residual function in WCO2 band
eof_1_scale_o2	Float32	Retrieved scale factor of first empirical orthogonal residual function in ABO2 band
eof_1_scale_strong_co2	Float32	Retrieved scale factor of first empirical orthogonal residual function in SCO2 band
eof_1_scale_uncert_o2	Float32	Uncertainty of retrieved scale factor of first empirical orthogonal residual function in ABO2 band
eof_1_scale_uncert_strong_co2	Float32	Uncertainty of retrieved scale factor of first empirical orthogonal residual function in SCO2 band
eof_1_scale_uncert_weak_co2	Float32	Uncertainty of retrieved scale factor of first empirical orthogonal residual function in WCO2 band
eof_1_scale_weak_co2	Float32	Retrieved scale factor of first empirical orthogonal residual function in WCO2 band
eof_2_scale_apriori_o2	Float32	a priori of retrieved scale factor of second empirical orthogonal residual function in ABO2 band
eof_2_scale_apriori_strong_co2	Float32	a priori of retrieved scale factor of second empirical orthogonal residual function in SCO2 band
eof_2_scale_apriori_weak_co2	Float32	a priori of retrieved scale factor of second empirical orthogonal residual function in WCO2 band
eof_2_scale_o2	Float32	Retrieved scale factor of second empirical orthogonal residual function in ABO2 band
eof_2_scale_strong_co2	Float32	Retrieved scale factor of second empirical orthogonal residual function in SCO2 band
eof_2_scale_uncert_o2	Float32	Uncertainty of retrieved scale factor of second empirical orthogonal residual function in ABO2 band

Data Element	Туре	Comments
eof_2_scale_uncert_strong_co2	Float32	Uncertainty of retrieved scale factor of second empirical orthogonal residual function in SCO2 band
eof_2_scale_uncert_weak_co2	Float32	Uncertainty of retrieved scale factor of second empirical orthogonal residual function in WCO2 band
eof_2_scale_weak_co2	Float32	Retrieved scale factor of second empirical orthogonal residual function in WCO2 band
eof_3_scale_apriori_o2	Float32	a priori of retrieved scale factor of third empirical orthogonal residual function in ABO2 band
eof_3_scale_apriori_strong_co2	Float32	a priori of retrieved scale factor of third empirical orthogonal residual function in SCO2 band
eof_3_scale_apriori_weak_co2	Float32	a priori of retrieved scale factor of third empirical orthogonal residual function in WCO2 band
eof_3_scale_o2	Float32	Retrieved scale factor of third empirical orthogonal residual function in ABO2 band
eof_3_scale_strong_co2	Float32	Retrieved scale factor of third empirical orthogonal residual function in SCO2 band
eof_3_scale_uncert_o2	Float32	Uncertainty of retrieved scale factor of third empirical orthogonal residual function in ABO2 band
eof_3_scale_uncert_strong_co2	Float32	Uncertainty of retrieved scale factor of third empirical orthogonal residual function in SCO2 band
eof_3_scale_uncert_weak_co2	Float32	Uncertainty of retrieved scale factor of third empirical orthogonal residual function in WCO2 band
eof_3_scale_weak_co2	Float32	Retrieved scale factor of third empirical orthogonal residual function in WCO2 band
fluorescence_at_reference	Float32	Retrieved fluorescence at 0.757 microns
fluorescence_at_reference _apriori	Float32	a priori of retrieved fluorescence at 0.757 microns
fluorescence_at_reference _uncert	Float32	Uncertainty of retrieved fluorescence at 0.757 microns
fluorescence_slope	Float32	Retrieved fluorescence slope at 0.757 microns
fluorescence_slope_apriori	Float32	<i>a priori</i> of retrieved fluorescence slope at 0.757 microns
fluorescence_slope_uncert	Float32	Uncertainty of retrieved fluorescence slope at 0.757 microns
h2o_scale_factor	Float32	Retrieved scale factor for H <sub>2</sub> O profile
h2o_scale_factor_apriori	Float32	<i>a priori</i> of retrieved scale factor for H <sub>2</sub> O profile
h2o_scale_factor_uncert	Float32	Uncertainty of retrieved scale factor for H <sub>2</sub> O profile
iterations	Int16	Number of iterations

Data Element	Туре	Comments
last_step_levenberg_marquardt parameter	Float32	Levenberg Marquardt parameter corresponding to last iteration
num_active_levels	Int16	Number of levels in atmospheric model
outcome_flag	Int8	Indicator of retrieval results: 1—'Passed internal quality check' 2—'Failed internal quality check' 3—'Reached maximum allowed iterations' 4—'Reached maximum allowed divergences'
retrieved_co2_column	Float32	Retrieved vertical column of CO2
retrieved_dry_air_column_layer_ thickness	Float32	Retrieved vertical column of dry air per atmospheric layer
retrieved_h2o_column	Float32	Retrieved vertical column of H2O
retrieved_h2o_column_layer_thi ckness	Float32	Retrieved vertical column of H <sub>2</sub> O per atmospheric layer
retrieved_o2_column	Float32	Retrieved vertical column of O2
retrieved_wet_air_column_layer _thickness	Float32	Retrieved vertical column of wet air per atmospheric layer
specific_humidity_profile_met	Float32	Meteorological specific humidity profile interpolated to observation location, time
surface_pressure_apriori_fph	Float32	a priori surface pressure retrieved by full-physics algorithm
surface_pressure_fph	Float32	Surface pressure retrieved by full-physics algorithm
surface_pressure_uncert_fph	Float32	Uncertainty in the surface pressure retrieved by the full-physics algorithm
surface_type	String	Type of model used for the Earth's surface: 'Lambertian' 'Coxmumk,Lambertian'
temperature_offset_apriori_fph	Float32	a priori of retrieved offset of temperature profile
temperature_offset_fph	Float32	Retrieved offset of temperature profile
temperature_offset_uncert_fph	Float32	Uncertainty of retrieved offset of temperature profile
temperature_profile_met	Float32	Meteorological temperature profile interpolated to observation location, time
tropopause_altitude	Float32	Inferred tropopause altitude based on lapse rate
tropopause_pressure	Float32	Inferred tropopause pressure altitude based on lapse rate
vector_altitude_levels	Float32	Altitude corresponding to each atmospheric level
vector_altitude_levels_apriori	Float32	A priori altitude corresponding to each atmospheric level
vector_pressure_levels	Float32	Pressure altitude corresponding to each atmospheric level
vector_pressure_levels_apriori	Float32	a priori pressure altitude corresponding to each atmospheric level

Data Element	Туре	Comments
vector_pressure_levels_met	Float32	Pressure altitude corresponding to each meteorological atmospheric level
wind_speed	Float32	Retrieved Cox-Munk wind speed
wind_speed_apriori	Float32	a priori of retrieved Cox-Munk wind speed
wind_speed_u_met	Float32	Meteorological eastward wind interpolated to observation location, time
wind_speed_uncert	Float32	Uncertainty of retrieved Cox-Munk wind speed
wind_speed_v_met	Float32	Meteorological northward wind interpolated to observation location, time
xco2	Float32	Column-averaged CO2 dry air mole fraction
xco2_apriori	Float32	a priori of column-averaged CO2 dry air mole fraction
xco2_avg_kernel	Float32	Column averaging kernel
xco2_avg_kernel_norm	Float32	Normalized column averaging kernel
xco2_pressure _weighting_function	Float32	Pressure weighting function used to form $X_{CO2}$
xco2_uncert	Float32	Uncertainty in column averaged CO2 dry air mole fraction
xco2_uncert_interf	Float32	Variance of $X_{CO2}$ due to interference
xco2_uncert_noise	Float32	Variance of X <sub>CO2</sub> due to noise
xco2_uncert_smooth	Float32	Variance of $X_{CO2}$ due to smoothing

### 11.12 L2 Spectral Parameters Group

The SpectralParameters group (see Table 11-12 below) contains the retrieval results from the OCO-2 Level 2 data products.

Data Element	Туре	Comments
noise_o2_fph	Float32	Aggregate noise in the ABO2 band
noise_strong_co2_fph	Float32	Aggregate noise in the SCO2 band
noise_weak_co2_fph	Float32	Aggregate noise in the WCO2 band
reduced_chi_squared_o2_fph	Float32	Reduced chi squared of spectral fit of the ABO2 band
reduced_chi_squared_strong_co2 _fph	Float32	Reduced chi squared of spectral fit of the SCO2 band
reduced_chi_squared_weak_co2 _fph	Float32	Reduced chi squared of spectral fit of the WCO2 band
relative_residual_mean_square_o 2	Float32	Mean square of the residuals divided by the signal for the ABO2 band
relative_residual_mean_square _strong_co2	Float32	Mean square of the residuals divided by the signal for the SCO2 band
relative_residual_mean_square _weak_co2	Float32	Mean square of the residuals divided by the signal for the WCO2 band

 Table 11-12: Spectral Parameters data in Level 2 Standard Data file (L2Std).

Data Element	Туре	Comments
residual_mean_square_o2	Float32	Mean of the squares of the residuals for the ABO2 band
residual_mean_square_strong_co 2	Float32	Mean of the squares of the residuals for the SCO2 band
residual_mean_square_weak_co 2	Float32	Mean of the squares of the residuals for the WCO2 band
signal_o2_fph	Float32	Aggregate signal in the ABO2 band
signal_strong_co2_fph	Float32	Aggregate signal in the SCO2 band
signal_weak_co2_fph	Float32	Aggregate signal in the WCO2 band

# 12 Full Data Tables for OCO-2 and OCO-3 Level 2 Lite Files (LtCO2)

With the v10 delivery of the OCO-2 and OCO-3 data products, we have released a version of the Lite data files similar to the OCO-2 Lite files from V9. The main differences between the Lite data file are that the files are aggregated on a daily basis, the files contain a streamlined set of output parameters (a subset of the full L2 data products) and they contain screened and bias corrected values for  $X_{CO2}$  (see Section 3 for OCO-2 screening/bias corrected values are included as well.

Table 12-1 Table 12-2, Table 12-3 and Table 12-4 provide a description of the variables available in the Lite data files. They are designed to be somewhat easier to use (smaller files, aggregated daily). The data included in these files are consistent with the Level 2 data products.

#### 12.1 OCO-2 and OCO-3 Lite File Main Group Fields

The main group (see Table 12-1 below) contains the many of the geographic and retrieval related fields from the OCO-2 and OCO-3 Level 2 Lite data products

Element	Туре	Comment
co2_profile_apriori	Float32	Prior CO2 Prior assumed by L2 code; Defined on layer boundaries. These are oriented space-to- surface so the first element defines the TOA the
		last element defines the surface.
date	Float32	Observation date and time matching sounding id.
File_index	Float32	1-Based Index of L2 File for each sounding
latitude	Float32	Center latitude of the measurement
longitude	Float32	Center longitude of the measurement
levels	Long	Level counter
pressure_levels	Float32	Pressure at each level; Defined on layer boundaries. These are oriented space-to-surface, so the first element defines the TOA, the last element defines the surface
pressure_weight	Float32	Pressure weighting function for each level; Defined on layer boundaries. These are oriented space-to-surface, so the first element defines the TOA, the last element defines the surface
sensor_zenith_angle	Float32	Zenith angle of the satellite at the time of the measurement
solar_zenith_angle	Float32	Solar zenith angle at the time of the measurement
sounding_id	Long	From scan start time in UTC
source_files		Source L2 File Names for these soundings
time	Long	Seconds since 1970-01-01 00:00:00
vertex_latitude	Float32	Corner latitudes of the measurement FOV
vertex_longitude	Float32	Corner longitudes of the measurement FOV

 Table 12-1: Provides a description of the fields in the OCO-2 and OCO-3 Lite Data Product files.

Element	Туре	Comment
xco2	Float32	Column-averaged dry-air mole fraction of CO2
		(Bias corrected as described in Section 3 for
		OCO-2 and Section 4 for OCO-3)
xco2_apriori	Float32	A priori $X_{CO2}$ value
xco2_averaging_kernel	Float32	$X_{CO2}$ column averaging kernel
xco2_qf_bitflag	Byte	xco2_quality_flag bit flag
xco2_quality_flag	Byte	<i>X<sub>CO2</sub></i> quality flag ( "0=Good Retreival, 1=Bad Retrieval)
xco2_uncertainty	Float32	$X_{CO2}$ posterior error estimate

#### 12.2 OCO-2 and OCO-3 Lite File Preprocessor Group Fields

The Preprocessor group (see Table 12-2 below) contains the many of the key fields from the different preprocessing steps of the retrievals.

Element	Туре	Comment
co2_ratio	Float32	Band 3 / Band 2 Ratio of retrieved Single-band <i>X</i> <sub>CO2</sub> using IMAP-DOAS algorithm
co2_ratio_offset_per_footprint (OCO-2 only)	Float32	Per footprint offset subtracted from co2_ratio in the L2Std files to form co2_ratio in the lite files
dp_abp	Float32	Retrieved-Prior Pressure from the fast O2A-band only preprocessor retrieval
h2o_ratio	Float32	H <sub>2</sub> O Ratio
h2o_ratio_offset_per_footprint (OCO-2 only)	Float32	Per footprint offset subtracted from h2o_ratio in the L2Std files to form co2_ratio in the lite files
max_declocking_o2a	Float32	ABS(MaxDeclockingFactor_O2A_Band - 1)*100
max_declocking_sco2 (OCO-2 only)	Float32	ABS(MaxDeclockingFactor_StrongCO2_Band - 1)*100
max_declocking_wco2 (OCO-2 only)	Float32	ABS(MaxDeclockingFactor_WeakCO2_Band - 1)*100
xco2_strong_idp	Float32	$X_{CO2}$ from Strong CO2 Band only, IMAP-DOAS algorithm
xco2_weak_idp	Float32	<i>X</i> <sub>CO2</sub> from Weak CO2 Band only, IMAP-DOAS algorithm

 Table 12-2: Contains description of the fields in the "Preprocessor" folder of the Lite files.

### 12.3 OCO-2 and OCO-3 Lite File Retrieval Group Fields

The Retrievals group (see Table 12-3 below) contains the many of the key fields from the L2 retrievals.

Table 12-3: Contains description of the fields in the "Retrievals" folder of the Lite files.

Element	Туре	Comment
albedo_o2a	Float32	Retrieved Band 1 reflectance (land), or lambertian albedo component of BRDF (ocean)

Element	Туре	Comment
albedo sco?	Float32	Retrieved Band 3 reflectance (land), or lambertian
	1100052	albedo component of BRDF (ocean)
albedo quad o?a	Float32	Retrieved Band 1 reflectance quadratic component
		(land), n/a (ocean)
albedo quad sco2	Float32	Retrieved Band 3 reflectance quadratic component
		(land), n/a (ocean)
albedo_quad_wco2	Float32	(land) $n/a$ (ocean)
		Retrieved Band 1 reflectance slope (land), or slope of
albedo_slope_o2a	Float32	lambertian albedo component of BRDF (ocean)
albada alana aaa?	Elect22	Retrieved Band 3 reflectance slope (land), or slope of
	F10at52	lambertian albedo component of BRDF (ocean)
albedo slope wco?	Float32	Retrieved Band 2 reflectance slope (land), or slope of
	11000.52	lambertian albedo component of BRDF (ocean)
albedo wco2	Float32	Retrieved Band 2 reflectance (land), or lambertian
	Elect22	albedo component of BRDF (ocean)
aod_bc	Float32	Retrieved Black Carbon Optical Depth at 0.755 microns
aod_ice	Float32	Retrieved Ice Cloud Optical Depth at 0.755 microns
aod_oc	Float32	Retrieved Organic Carbon Optical Depth at 0.755 microns
aod seasalt	Float32	Retrieved Sea Salt Carbon Optical Depth at 0.755 microns
	F1 (22	Retrieved Upper Trop+Stratospheric Aerosol Optical
aod_strataer	Float32	Depth at 0.755 microns
aod_sulfate	Float32	Retrieved Sulfate Aerosol Optical Depth at 0.755 microns
aod total	Float32	Retrieved Total Cloud+Aerosol Optical Depth at 0.755
	T100002	microns
aod_water	Float32	Retrieved Water Cloud Optical Depth at 0.755 microns
chi2_o2a	Float32	spectral fit
		Reduced Chi-Squared for Band 3 (Strong CO2 band)
chi2_sco2	Float32	of L2 spectral fit
1:2	E1	Reduced Chi-Squared for Band 2 (Weak CO2 band)
ch12_wco2	Float32	of L2 spectral fit
co2_grad_del	Float32	level 13 is at P/Psurf=0.631579
defined mode (OCO-2 only)	Byte	Prior surface pressure used in the retrieval, as determined
	E)	by GEOS5-FP-IT short-term (0-9 hour) forecast
delta l	Float32	Retrieved Offset to Prior Temperature Profile in Kelvin
diverging_steps	Eloat32	No. of diverging steps taken in retrieval
dp dp o?a	Float32	Delta Psurf from L 2 O2A-hand Prior
$dp_{02a}$	Float32	Delta Psurf from L2, SCO2-band Prior
dpfrac	F1 (22	$xco2 raw^{*}(1-$
1	Float32	{Meteorology/psurf apriori band3}/{Retrieval/psurf}
dwa	Float22	Retrieved AOD_dust+AOD_water+AOD_seasalt at
dws	F10at52	0.755 microns
eof3_3_rel (OCO-2 only)	Float32	3rd EOF of Band 3, relative to Signal
	Float32	Simultaneous Fluorescence retrieval (at 757 nm) by L2
IS		code; note this is different than the dedicated retrieval using
h20 scale	Float32	Retrieved scale factor to Prior Water Vapor Profile
ice height	Float32	Retrieved Ice Cloud Height

Element	Туре	Comment
iterations	Byte	No. of iterations used in retrieval
psurf	Float32	Surface pressure retrieved by the Level-2 retrieval
psurf_apriori	Float32	Prior surface pressure used in the retrieval, as determined by ECMWF short-term (0-9 hour) forecast
rms_rel_o2a	Float32	RMS of the L2 fit residuals in the o2a band, relative to the continuum signal, times 100 [so it is in percent]
rms_rel_sco2	Float32	RMS of the L2 fit residuals in the strong co2 band, relative to the continuum signal, times 100 [so it is in percent]
rms_rel_wco2	Float32	RMS of the L2 fit residuals in the weak co2 band, relative to the continuum signal, times 100 [so it is in percent]
s31	Float32	Ratio of Band 3 to Band 1 signal level
s32	Float32	Ratio of Band 3 to Band 2 signal level
SigmaB	Float32	Multiply Psurf by these values to get the pressure layer boundaries (= pressure levels)
surface_type	Byte	Surface type used in the retrieval: 0=ocean and corresponds to a Coxmunk+Lambertian surface; 1=land and corresponds to a pure Lambertian surface
T700	Float32	Temperature at 700 hPa (from ECMWF)
tcwv	Float32	Retrieved TCWV obtained by multiplying retrieved h2o scale factor to prior (ECMWF) TCWV
tcwv_apriori	Float32	Prior TCWV (from ECMWF prior profile)
tcwv_uncertainty	Float32	Retrieved TCWV Posterior Uncertainty
water_height	Float32	Retrieved Water Cloud Height
windspeed	Float32	Surface wind speed retrieved by the Level-2 retrieval
windspeed_apriori	Float32	Surface wind speed retrieved by the Level-2 retrieval
xco2_raw	Float32	Raw value of Retrieved $X_{CO2}$ (not bias corrected)

### 12.4 OCO-2 and OCO-3 Lite File Sounding Group Fields

The Sounding group (see Table 12-4Table 12-3 below) contains the many of the geographic fields from the L2 retrievals.

Element	Туре	Comment
airmass	Elect22	Airmass, computed as 1/cos(solar_zenith_angle)
anmass	110at32	+ 1/cos(sensor_zenith_angle)
altitude	Float32	Surface Altitude in meters above sea level
altituda atdday	Elect22	Standard deviation of surface elevation within the
annude_studev	F10at52	FOV
footprint	Byte	Index of OCO-2 (OCO-3) Sounding 1-8
alint anala	Elect22	Angular distance from viewing along the perfect
gint_angle	F10at52	glint direction
land_fraction	Int8	Fraction of the footprint that contains land in
		percent
land water indicator	Int8	0=Land;1=Ocean;2=Inland Water;3=Mixed
operation_mode	Int8	OCO-2 Operation Mode: 0=Nadir, 1=Glint,
		2=Target, 3=Transition
orbit	Int8	OCO-2 orbit number since mission start

Table	12-4:	Contains	description	of the	fields in	the	"Soundina"	' folder	of the	Lite files.
1 4 5 1 5		Containe	accomption	01 010			oounung	101001		EILO 11100.

Element	Туре	Comment
Path (OCO-2 Only)	Int8	OCO-2 fixed orbit path number ranging from 1- 233
polarization_angle (OCO-2 Only)	Float32	Polarization angle
pcs_data_source (OCO-3 Only)	Byte	Sounding_pcs_data_source
pma_azimuth_angle (OCO-3 Only)	Float32	Azimuth angle PMA
pma_elevation_angle (OCO-3 Only)	Float32	Elevation angle PMA
polarization_angle (OCO-3 Only)	Float32	Sounding_polarization_angle
sensor_azimuth_angle	Float32	azimuth angle of the satellite at the time of the measurement
snr_o2	Float32	O2A-Band Continuum Signal-to-Noise Ratio
snr_strong_co2	Float32	Strong CO2-Band Continuum Signal-to-Noise Ratio
snr_weak_co2	Float32	Weak CO2-Band Continuum Signal-to-Noise Ratio
solar_azimuth_angle	Float32	solar azimuth angle at the time of the measurement
target_id (OCO-3 Only)	Int8	OCO-3 Target (or SAM) ID
target_name (OCO-3 Only)	VarLenStr	OCO-3 Target (or SAM) Name

### 12.5 OCO-2 and OCO-3 Lite File Meteorology Group Fields

The Sounding group (see Table 12-5 below) contains the meteorology fields from the L2 retrievals.

		Jy Toldel of the OCO-2, OCO-3 Lite lifes.		
Element	Туре	Comment		
psurf_apriori_o2a	Float32	Prior surface pressure for Band 1 location, as determined by GEOS5-FP-IT short-term (0-9 hour) forecast		
psurf_apriori_sco2	Float32	Prior surface pressure for Band 3 location, as determined by GEOS5-FP-IT short-term (0-9 hour) forecast		
psurf_apriori_wco2	Float32	Band 2 Prior Surface Pressure		
windspeed_u_met	Float32	Apriori Surface Wind Speed, U Component from GEOS-5 FPIT in the N-S direction, m/s		
windspeed_v_met	Float32	Apriori Surface Wind Speed, V Component from GEOS-5 FPIT in the E-W direction, m/s		

Table 12-5: Fields in the "Meteorology" folder of the OCO-2, OCO-3 Lite files.

# 13 Tools and Data Services

### 13.1 HDFView

HDFView is a Java based graphical user interface created by the HDF Group that can be used to browse all ACOS HDF products. The utility allows users to view all objects in an HDF file hierarchy, which is represented as a tree structure. HDFView can be downloaded or support found at: <u>https://portal.hdfgroup.org/display/support/Download+HDFView</u>

### 13.2 Panoply

Panoply is a tool from the Goddard Institute for Space Studies (GISS). It plots geo-referenced and other arrays from NetCDF, HDF, GRIB, and other datasets. Panoply is a cross-platform application that runs on Macintosh, Windows, Linux and other desktop computers. A particularly convenient feature of Panoply is its ability to communicate with remote Hyrax (xml) catalogues and thus plotting datasets without the need to download the data files. Apart from the on-line archive, Goddard DAAC serves ACOS and OCO data through Hyrax (OPeNDAP) as well, and this path to data can be discovered in the ACOS and OCO dataset landing pages (see below). Panoply is available for free download from the <u>GISS website</u>.

### 13.3 Goddard DAAC user interface.

The NASA Goddard Earth Sciences Data and Information Services Center (GES DISC) provides temporal and spatial searches, as well as variable and spatial subsets, through its <u>user interface</u>. Dataset landing pages provide basic summary and data access points for all datasets curated by the GES DISC. A simple keyword search would suffice to discover all OCO-2 or OCO-3 datasets:

https://disc.gsfc.nasa.gov/datasets?keywords=OCO-2&page=1 https://disc.gsfc.nasa.gov/datasets?keywords=OCO-3&page=1

Apart from the direct access to the online archive and Hyrax (OPeNDAP) directories, the interface ultimately provides the search results as lists of data links. Goddard DAAC requires **user registration** before any data can be downloaded. Detailed instructions on how to register and how to use wget and curl with the data download links, as well as other advanced methods, are provided on the interface:

https://disc.gsfc.nasa.gov/data-access#

### 13.4 NASA Earth Data Search Client

In a similar manner, information and data access can be found from the NASA Earth Data Search Client:

 $\underline{https://search.earthdata.nasa.gov/search?q=oco-2}$ 

https://search.earthdata.nasa.gov/search?q=oco-3

All NASA data centers from the Earth Science Data Information System (ESDIS) report their data collections to this system. It is a convenient one-stop shop for discovery of all NASA Earth Science Missions data. JPL CO2 Virtual Science Data Environment.

# **14 Contact Information**

For the most up-to-date contact information, please refer to the JPL mission sites (which provides a link to the official mission sites:

OCO-2: https://www.jpl.nasa.gov/missions/orbiting-carbon-observatory-2-oco-2

OCO-3: https://www.jpl.nasa.gov/missions/orbiting-carbon-observatory-3-oco-3.

## 15 Acknowledgements and References

#### 15.1 Acknowledgements

This research was carried out at the Jet Propulsion Laboratory, California Institute of Technology, under a contract with the National Aeronautics and Space Administration.

#### 15.2 Additional Resources

There are a number of other project documents that the user should refer to as they work with the data

- 1. Solar Induced Chlorophyll Fluorescence Data User's Guide provide guidance for using the OCO-2 and OCO-3 SIF data products.
- 2. L1B ATBD this algorithm theoretical basis document describes the process used to take the uncalibrated spectrum to calibrated radiance spectra
- 3. L2 ATBD this ATBD steps through the physics and implementation of the Level 2 algorithm
- 4. ATBDs for IMAP-DOAS and ABO2 these ATBD documents describe the two methods of identifying potentially cloudy footprints, in what we refer to as the prescreening step. These data are then used for setting data quality and data selection levels
- 5. Published papers—in addition to the references in the next section, there are a number of published papers describing the algorithm, application to GOSAT, prescreening steps, etc. Please see the most up to date list of publications on oco2.jpl.nasa.gov

### 15.2.1 Links

- OCO-2 Mission <u>site</u>
- OCO-3 Mission <u>site</u>
- <u>OCO-2 data summary</u> page at the Goddard DISC
- OCO-3 data summary page at the Goodard DISC
- JPL retrievals using the radiances from the Japanese GOSAT satellite, known as the Atmospheric CO2 Observations from Space (ACOS) data at the Goddard DISC summary page: <u>https://disc.gsfc.nasa.gov/datasets/ACOS\_L2S\_9r/summary</u>

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# 17 Acronyms

ABO2	O <sub>2</sub> -A band cloud screening algorithm
ACOS	Atmospheric CO <sub>2</sub> observations from space
AFE	Analog front-end electronics
aod	Aerosol optical depth
ARP	Ancillary radiometric product
ATBD	Algorithm theoretical basis document
$CO_2$	Carbon dioxide
CSU	Colorado State University
DN	Data number
DOAS	Differential optical absorption spectroscopy
ECMWF	European Centre for Medium-Range Weather Forecasts
EOS	Earth Observing System
EOS A-Train	EOS Afternoon Constellation
FP	Full physics (algorithm)
FPA	Focal plane array (or assembly)
FWHM	Full width at half maximum
GES DISC	Goddard Earth Sciences Data and Information Services Center
GOSAT	Greenhouse Gases Observing Satellite
GSFC	Goddard Space Flight Center
H <sub>2</sub> O	Water
HDF	Hierarchical data format
ILS	Instrument line shape
IMAP-DOAS	Iterative maximum <i>a posteriori</i> differential optical absorption spectroscopy
JPL	Jet Propulsion Laboratory
L (0,1,)	Level 0, 1, etc. data product
LOS	Line of sight
NASA	National Aeronautics and Space Administration
O <sub>2</sub>	Oxygen
OCO	Orbiting Carbon Observatory
OCO-2	Orbiting Carbon Observatory-2
OCO-3	Orbiting Carbon Observatory-3
SAA	South Atlantic Anomaly
SCO2	Strong CO <sub>2</sub> band
SIF	Solar-induced chlorophyll fluorescence
SNR	Signal-to-noise ratio
TAI	International atomic time
TCCON	Total Carbon Column Observing Network
UTC	Coordinated universal time
VCD	Vertical column density
VMR	Volume mixing ratio
WCO2	Weak CO <sub>2</sub> band
WMO	World Meteorological Organization

X<sub>CH4</sub>Column-averaged dry air mole fraction of atmospheric methaneX<sub>CO2</sub>Column-averaged dry air mole fraction of atmospheric carbon dioxide