AIRS Version 5 Release Tropospheric CO_2 Products

by:

Edward T. Olsen
Jet Propulsion Laboratory, California Institute of Technology

December, 2009
Version 1

Jet Propulsion Laboratory
California Institute of Technology
Pasadena, CA

Submit Questions to:
http://airs.jpl.nasa.gov/AskAirs

Table of Contents

Table of Contents 2

Table of Figures 3

Introduction 4

Access to AIRS Tropospheric CO_2 Product Files 5

AIRS Mid-Tropospheric CO2 Products 6

CO2 Product File Names, Shortnames and Sizes 7

Content of L2 CO2 Standard Product Files and Support Product Files 9

Level 2 Dimension Fields 9

Level 2 Attribute Fields 9

Level 2 Data Fields 10

Contents of Level 3 CO2 Product Files 11

Level 3 Dimension Fields 11

Level 3 Attribute Fields 12

Level 3 Data Fields 13

Quality Indicators 13

Caveats 14

Recommended Supplemental User Documentation 14

Data Processing 14

VPD Retrieval of Tropospheric CO2 15

Auxiliary AIRS CO2 Weighting Function Data File 23

ACKNOWLEDGMENT 26

ACRONYMS 26

REFERENCES 27

Table of Figures

FIGURE 1: AVERAGE WEIGHTING FUNCTIONS FOR CO_2 IR CHANNELS USED BY VPD ALGORITHM. 18
FIGURE 2: BLOCK DIAGRAM OF VPD POST-PROCESSING RETRIEVAL OF TROPOSPHERIC CO_2. 19
FIGURE 3: INDEPENDENCE OF VPD SOLUTION FROM STARTING VALUE FOR CO_2. 22
FIGURE 4: LACK OF CORRELATION OF CO2 SOLUTION WITH TEMPERATURE, WATER VAPOR AND OZONE. 23
FIGURE 5: CO2 WEIGHTING FUNCTIONS AND AVERAGING KERNELS FOR THREE MODEL ATMOSPHERES. 25

Introduction

The Atmospheric Infrared Sounder (AIRS) is mounted on the sun-synchronous, near-polar orbiting NASA Aqua satellite with equator local ascending crossing time of 13:38 local solar time; it is a cross-track scanning grating spectrometer covering the 3.74 μm to 15.4 μm spectral range with 2378 channels having a nominal spectral resolving power, $\lambda/\delta\lambda$, of 1200. Data from AIRS and its companion instrument, the Advanced Microwave Sounding Unit (AMSU), are combined to eliminate the effects of clouds. The resulting AIRS Level 2 products include these cloud-cleared infrared radiances and retrieved profiles of atmospheric temperature T(p), water vapor $H_2O(p)$, and ozone $O_3(p)$ at a nominal spatial resolution of 45 km at nadir. The Version 5 Level 2 retrieval algorithm (V5) used to retrieve these products assumes a global average linear time-variable CO_2 climatology throughout the atmosphere. This time-variable climatology is necessary to assure that the rapid transmittance algorithm employed to forward calculate radiances from the atmospheric physical state during the retrieval process remains in the linear regime for the lifetime of the mission [Maddy et al., 2008]. It is worth noting that this is the simplest possible climatology that achieves this desired result and it does not impose a seasonal or geospatial signal upon the measurements or retrievals. The linear relation is:

$$\mathbf{Climatology_CO_2(t) = A + B \times (t - t_0)}$$

Where **Climatology_CO_2** is the concentration of CO_2 everywhere in the atmosphere at date/time, **t**, in ppm, **A** = 371.92429, **B** = 1.840618, $\mathbf{t_0}$ = 1/1/2002 @ 0 UT, and the date/time is expressed in year and fraction of year i.e., t_0 = 2002.0 and 7/1/09 @ 12 UT is t = 2009.5). Although a CO_2 profile is now part of V5, all elements are set to this climatology CO_2 value for the date and time of the AIRS Level 1B radiance measurements used for the Level 2 retrieval. The V5 algorithm does not retrieve CO_2. That is left to a post-processing stage employing the Vanishing Partial Derivative (VPD) algorithm described later in this document.

Access to AIRS Tropospheric CO_2 Product Files

The AIRS CO_2 product files may be freely downloaded from the Goddard Earth Sciences (GES) Data and Information Services Center (DISC). The URL providing links to all methods of access to AIRS data products is

http://disc.sci.gsfc.nasa.gov/AIRS/data-holdings

Links on this web page may be used to search for and subset all AIRS data products by type, geospatial location, and time and to download them via ftp or directly via links on web pages.

URLs for access via Mirador to the Level 2 (standard, support) CO_2 Data Products:

http://mirador.gsfc.nasa.gov/cgi-bin/mirador/collectionlist.pl?keyword=airx2stc
http://mirador.gsfc.nasa.gov/cgi-bin/mirador/collectionlist.pl?keyword=airx2spc

URLs for access via Mirador to the Level 3 CO_2 (daily, 8-day, monthly) Data Products:

http://mirador.gsfc.nasa.gov/cgi-bin/mirador/collectionlist.pl?keyword=airx3c2d
http://mirador.gsfc.nasa.gov/cgi-bin/mirador/collectionlist.pl?keyword=airx3c28
http://mirador.gsfc.nasa.gov/cgi-bin/mirador/collectionlist.pl?keyword=airx3c2m

Corresponding URLs for access via the Web Portals:

http://disc.sci.gsfc.nasa.gov/AIRS/data-holdings/by-data-product/airsL2_Stc
http://disc.sci.gsfc.nasa.gov/AIRS/data-holdings/by-data-product/airsL2_Spc
http://disc.sci.gsfc.nasa.gov/AIRS/data-holdings/by-data-product/AIRX3C2D
http://disc.sci.gsfc.nasa.gov/AIRS/data-holdings/by-data-product/AIRX3C28
http://disc.sci.gsfc.nasa.gov/AIRS/data-holdings/by-data-product/AIRX3C2M

The sample swath and grid data readers provided with the AIRS V5 documentation package is available at the URL:

http://disc.sci.gsfc.nasa.gov/AIRS/documentation

provide access to the AIRS CO_2 products as well as to the other AIRS products. The swath readers are for the Level 2 products and the grid readers are for the Level 3 products.

AIRS Mid-Tropospheric CO2 Products

The V5 Level 2 products and climatology CO_2 are assumed as the initial state for the VPD retrieval algorithm that separately determines the tropospheric CO_2 mixing ratio. The nominal spatial resolution of the VPD Level 2 CO_2 product at nadir is 90 km x 90 km, or approximately 1° x 1° on the Earth's surface. A spatial coherence quality assurance (QA) test is applied and the retrievals that satisfy the acceptance criterion are written to the Level 2 CO_2 standard product. Those that fail the QA are written to the Level 2 CO_2 support product.

There are three VPD Level 3 CO_2 products derived from the VPD Level 2 CO_2 standard product: daily, 8-day (one-half of the Aqua orbit repeat cycle), and calendar monthly (i.e., Jan, Feb, …, Dec). The multi-day products are simply the arithmetic mean weighted by the counts of the daily data combined in each grid box, whose resolution is 2.5° in longitude and 2° in latitude.

The Level 3 CO_2 daily product contains information for a temporal period of 24 hours rather than midnight-to-midnight. The data included in the gridding on a particular day start at the international dateline and progress westward (as do the subsequent orbits of the Aqua satellite) so that neighboring gridded cells of data are no more than a swath of time apart (about 90 minutes). In the event that a scan line crosses the dateline, the data on either side are included in separate data sets, according to the appropriate date and UT. This ensures that data points in a grid box are always coincident in time. If the data were gridded using the midnight-to-midnight time-span, the start of the day and the end of the day could be in the same grid cell, producing an artificial time discontinuity. The edge of the Level 3 gridded cells is at the date line (the 180° E/W longitude boundary). When plotted, this produces a map with 0° longitude in the center of the image unless the bins are reordered. This method is preferred because the left (West) side of the image and the right (East) side of the image contain data farthest apart in time. The gridding scheme used to produce the Level 3 CO_2 products as well as all other AIRS Level 3 products is the same as used by TOVS Pathfinder.

CO2 Product File Names, Shortnames and Sizes

The Level 2 and Level 3 CO_2 product files share the naming convention of all other AIRS data product files. The templates for file names are:

Level 2: AIRS.YYYY.MM.DD.GGG.CO2_ppp.VER.PROCTAG.hdf
Level 3: AIRS.YYYY.MM.DD.CO2pppNNN.VER.PROCTAG.hdf

IDEN	Level 2 Product	Level 3 Product
YYYY	Date year (i.e. 2009) of the measurement	Initial date year of time period
MM	Date month (i.e. 01->12) of the measurement	Initial date month of time period
DD	Date day of month (i.e. 01->31) of measurement	Initial date day of month of time period
GGG	Granule (001->240)	N/A
ppp	Standard or Support Product (Std or Sup)	Product (only Std)
NNN	N/A	Number of sequential days for multiday; number of days in month for monthly
VER	Version of software used to create product	Version of S/W used to create product
PROCTAG	Processing tag	Processing tag

The following are examples of the product file names, shortnames and file sizes. The “X” in the shortnames indicates that the V5 Level 2 retrieval products input to the VPD algorithm were derived using the AIRS and AMSU observed radiances.

Level 2 CO_2 Standard Product file naming for granule 229 of September 6, 2002:
Name: AIRS.2002.09.06.229.L2.CO2_Std.v5.4.11.0.CO2.T09210175254.hdf
Shortname: AIRX2STC
Size: 312 KB
Data Span: Granule 229 of September 6, 2002

Level 2 CO_2 Support Product file naming for granule 229 of September 6, 2002:
Name: AIRS.2002.09.06.229.L2.CO2_Sup.v5.4.11.0.CO2.T09210175254.hdf
Shortname: AIRX2STP
Size: 312 KB
Data Span: Granule 229 of September 6, 2006

Level 3 CO_2 Daily Product file:
Name: AIRS.2002.09.05.L3.CO2Std001.v5.4.12.67.X09261111805.hdf
Shortname: AIRX3C2D
Size: 412 KB
Data Span: September 5, 2002

Level 3 CO_2 8-Day Product file:
Name: AIRS.2002.09.01.L3.CO2Std008.v5.4.12.65.X09260131026.hdf
Shortname: AIRX3C28
Size: 616 KB
Data Span: September 1, 2002 through September 8, 2002

Level 3 CO_2 Monthly Product file:
Name: AIRS.2002.09.01.L3.CO2Std030.v5.4.12.65.X09260130847.hdf
Shortname: AIRX3C2M
Size: 596 KB
Data Span: Calendar month September 2002

Content of L2 CO2 Standard Product Files and Support Product Files

A total of 240 Level 2 CO_2 Standard Product Files and Level 2 CO_2 Support Product Files are produced each day, just as for the AIRS Level 2 physical retrieval products. They contain dimension fields, attribute fields and data fields. The data field is comprised of a single swath named **CO2**.

Level 2 Dimension Fields

Name	Type	Value	Description
Track	32-bit INT	22	Dimension along track for retrieval positions
XTrack	32-bit INT	15	Dimension across track for retrieval positions
AvgKernDim	32-bit INT	100	Dimension of averaging kernel array for each retrieval

Level 2 Attribute Fields

Name	Type	Dimensions	Description
PresLvls	32-bit FLT	[101]	Pressure levels, ordered from TOA to surface (hPa)
PresLyrs	32-bit FLT	[100]	Pressure layers, equal to geometrical mean of the pressure levels bounding the layer (hPa)
CO2retType	STRING	[15,22]	Final QA applied to separate standard from support product **Standard**: “CO2 stddev >= 0 and <= 2” **Support**: “CO2 stddev > 2”
CO2retNum	32-bit INT	[1]	# of CO2 retrievals in granule (maximum possible = 330)

Level 2 Data Fields

Name	Type	Dimensions	Description
Latitude	32-bit FLT	[15,22]	Latitude (deg)
Longitude	32-bit FLT	[15,22]	Longitude (deg, +E/-W)
Time	32-bit FLT	[15,22]	UT (hr, 0.0 -> 23.99)
Year	32-bit INT	[15,22]	Year (i.e., 2009)
Month	32-bit INT	[15,22]	Month (1 -> 12)
Day	32-bit INT	[15,22]	Day of month (1 -> 31)
Hour	32-bit INT	[15,22]	UT HR (0 -> 23)
Minute	32-bit INT	[15,22]	UT MIN (0 -> 59)
Seconds	32-bit FLT	[15,22]	UT SEC (0.0 -> 59.9999)
LandFrac	32-bit FLT	[15,22]	Fraction FOV not water (unitless, 0.0 -> 1.0)
CO2ret	32-bit FLT	[15,22]	Retrieved CO2 (mole fraction)
CO2std	32-bit FLT	[15,22]	CO2 error measure by spatial coherence QA (mole fraction)
Solzen	32-bit FLT	[15,22]	Solar zenith angle (deg, 0.0 -> 180.0)
AvgKern	32-bit FLT	[100,15,22]	Averaging kernel, ordered from TOA to surface at preslyrs (unitless)

Contents of Level 3 CO2 Product Files

The L2 CO2 Standard Product Files are binned on 2 deg latitude x 2.5 deg longitude grids to create daily, 8-day and calendar monthly L3 products. Users can combine the contents of multiple daily files to create multi-day averages over any desired period. The data field is comprised of a single grid named **CO2**.

Level 3 Dimension Fields

Name	Type	Value	Description
LatDim	32-bit INT	91	Number of latitude intervals (width of bins is 2 deg in latitude, save for one bin nearest to each pole, where they are 1°)
LonDim	32-bit INT	144	Number of longitude intervals (width of bins is 2.5 deg in longitude)

Level 3 Attribute Fields

Name	Type	Dimensions	Description
Year	32-bit INT	[4]	First element is integer year of initial day for data included in the product file(i.e., 2009)
Month	32-bit INT	[4]	First element is integer month of initial day for data included in the product file (1 -> 12)
Day	32-bit INT	[1]	The day of month of the initial day for data included in the product file (1 -> 31)
NumDays	32-bit INT	[1]	The number of consecutive days over which data are averaged in the product
PresLvls	32-bit FLT	[101]	Pressure levels, ordered from TOA to surface (hPa)
PresLyrs	32-bit FLT	[100]	Pressure layers, equal to geometrical mean of the pressure levels bounding the layer (hPa)
CO2retType	STRING	[15,22]	Final QA applied to separate standard from support product **Standard**: “CO2 stddev >= 0 and <= 2” **Support**: “CO2 stddev > 2”
CO2retNum	32-bit INT	[1]	# of CO2 retrievals in granule (maximum possible = 330)

Level 3 Data Fields

Name	Type	Dimensions	Description
Latitude	32-bit FLT	[144,91]	Latitude of center of bin (deg)
Longitude	32-bit FLT	[144,91]	Longitude of center of bin (deg, +E/-W)
mole_fraction_of_carbon_dioxide_in_free_troposphere	32-bit FLT	[144,91]	VMR (unitless)
mole_fraction_of_carbon_dioxide_in_free_troposphere_sdev	32-bit FLT	[144,91]	VMR (unitless)
mole_fraction_of_carbon_dioxide_in_free_troposphere_count	32-bit INT	[144,91]	(unitless)

Quality Indicators

There are no specific quality indicators for the Level 2 CO2 products other than **CO2std**, the QA error measure for spatial coherence over the 2x2 array of AMSU FOVs over which individual retrievals were combined to arrive at the final product. The Level 2 CO_2 Standard Product contains the retrievals meeting the criterion that CO2std ≤ 2 ppm, and retrievals not satisfying that threshold are placed in the Level 2 CO_2 Support Product. The Level 3 CO_2 Product is derived from the Level 2 Standard Product.

As described in the following section on data processing, the AIRS V5 Level 2 retrievals are filtered according to one of their internal quality factors, **PGood**, as well as the retrieved tropopause pressure, **PTrop**. Only AMSU FOVs satisfying the condition

$$(PGood-PTrop) > 200 \text{ hPa}$$

are passed to the CO_2 retrieval post-processing algorithm. This test ensures that the temperature profile is of sufficient quality from the TOA to a height at least 200 hPa below the tropopause.

Caveats

Guards against effects of surface emission have been built into the CO_2 retrieval post-processing algorithm, but it is likely that some adverse impact may remain for extreme topographies, e.g. the Andes mountain range, the Himalayan mountain range and highlands, and the Greenland ice sheet. Caution should be exercised when using retrievals over those areas.

Recommended Supplemental User Documentation

V5_Data_Release_UG.pdf
V5_l2_Standard_Product_QuickStart.pdf
V5_Level2_Cloud-Cleared_Radiances.pdf
V5_L2_Standard_Pressure_Levels.pdf
V5_L2_Support_Pressure_Levels.pdf
V5_L2_Quality_Control_and_Error_Estimation.pdf
V5_CalVal_Status_Summary.pdf
V5_Retrieval_Channel_Sets.pdf

Data Processing

The VPD retrieval is a post-processing algorithm applied after the AIRS Level 2 products have been generated. In brief, the VPD CO_2 solution for an AIRS Level 2 retrieval spot is obtained by an iterative process that minimizes the RMS difference (i.e., residuals) between the Level 2 cloud-cleared radiances and radiances computed from the retrieved Level 2 profiles for a number of selected CO_2 channels in the 15 µm band. The process begins with the AIRS derived Level 2 atmospheric state and then proceeds to separately perturb the T(p), $H_2O(p)$, $O_3(p)$, and CO_2 . The solution is obtained when the residuals are individually minimized.

The AIRS Level 2 tropospheric CO_2 product is the average of the solutions for a 2 x 2 array of adjacent AIRS Level 2 retrieval spots, covering a 90 km x 90 km area at nadir. Retrievals for which the solutions for the 2 x 2 arrays satisfy a spatial coherence QA that requires agreement of the separate retrievals to be within 2 ppm in an RMS sense are included in the standard product (AIRX2STC). Retrievals that fail this QA test are included in the support product (AIRX2STP).

The AIRS Level 3 tropospheric CO_2 products are derived by binning the Level 2 standard product retrievals in a grid that is 2° in latitude by 2.5° in longitude over a daily, an 8-day and a calendar monthly time span. The user may easily generate custom time spans by combining one or more of these products.

VPD Retrieval of Tropospheric CO2

Researchers have applied various methods to retrieve CO_2 using AIRS data [Chahine et al., 2005 and 2008; Engelen et al., 2005 and 2009; Maddy et al., 2008; Strow et al., 2008]. The tropospheric CO_2 products released by the AIRS Project through the GES DISC are derived by means of the VPD method of Chahine et al. [2005]. The VPD retrieval is a post-processing algorithm applied to an AIRS Level 2 retrieval satisfying the criterion, (PGood-PTrop) > 200 hPa.

We have constrained the VPD solution by minimizing the variance, reducing the amplitude of oscillations vs. latitude, of the annual rates of growth between ± 60° latitudes, for the period from 1/2003-12/2008. This is achieved by adjusting the Level 2 cloud-cleared radiances by -15.24 x (t-t_0) mK where $\mathbf{t_0}$ is January 1, 2003 (i.e. 2003.0) and **t** is the date of measurement expressed as a fractional year.

The VPD CO_2 solution is obtained by an iterative process that minimizes the RMS difference (i.e., residuals) between the Level 2 cloud-cleared radiances and forward-computed radiances from the retrieved Level 2 profiles for selected CO_2 channels in the 15 µm band. The process begins with the AIRS V5 retrieved Level 2 atmospheric state and CO_2 climatology and then separately perturbs the T(p), H_2O(p), O_3(p), and CO_2. The solution is obtained at the point where the partial derivatives of the CO_2 channels with respect to T(p), H_2O(p), O_3(p), and CO_2 are individually equal to zero (minimized). The auxiliary T(p), H_2O(p), O_3(p) channels are used to accelerate the iteration process, i.e., reducing the number of iterations required. The solution is obtained when the residuals are individually minimized. Table I summarizes the IR channels whose cloud-cleared radiances are used in the VPD retrieval of tropospheric CO_2.

T(p)		$H_2O(p)$		$O_3(p)$		CO_2	
Chan	ν (cm^{-1})	Chan	ν (cm^{-1})	Chan	ν (cm^{-1})	Chan	ν (cm^{-1})
145	691.391	1616	1420.874	203	707.562	192	704.436
151	693.029	1621	1423.756	208	708.992	198	706.137
155	694.125	1646	1438.342	219	712.160	209	709.279
157	694.674	1673	1471.292	222	713.029	210	709.566
172	698.823	1711	1495.124	225	713.900	212	710.141
183	701.899	1744	1516.448	240	718.288	214	710.716
188	703.306	1745	1517.104	319	741.599	215	711.005
244	719.467	1797	1565.797	321	742.227	216	711.293
		1802	1569.288			217	711.582
		1808	1573.498			218	711.871
		1813	1577.022			228	714.773
		1825	1585.544			239	717.994
		1842	1597.769			250	721.244
		1854	1606.509				

Table I - List of channels used for the VPD iterative solution

Evaluation of the relative sensitivity of channels to T(p), $H_2O(p)$, $O_3(p)$, and CO_2 lead to the choice of two spectral ranges for use in the VPD retrieval. The range 690-742 cm^{-1} is well suited for selecting the channel set to retrieve the CO_2 mixing ratio and the two auxiliary channel sets for temperature and ozone. The range 1420-1607 cm^{-1} is best suited for selecting the auxiliary channel set for water vapor. The three auxiliary sets are required to separate the interdependence of temperature, water vapor and ozone on each other and on CO_2. Specifically, since all IR channels depend upon temperature, we select the CO_2 channels to have a strong dependence on CO_2 and a weak dependence upon O_3 and H_2O. Similarly, we choose the H_2O and O_3 channels to have a weak dependence on CO_2 and upon each other. For instance a change of 10% in either the water vapor or ozone profiles results in a radiance change that is less than that due to a change of 1 ppm in CO_2 volume mixing ratio. The auxiliary set for temperature is selected to have a weak dependence upon CO_2.

Figure 1 depicts representative AIRS vertical weighting functions for the 1976 US standard atmosphere [Anderson et al., 1986]. The figure shows the average of the weighting functions for the CO_2 channel set assuming CO_2 volume mixing ratios of 330, 370 and 390 ppm. The weighting function is the derivative of the atmospheric transmission function with respect to the natural logarithm of the pressure, $\frac{\partial \tau(\nu, p)}{\partial \ln p}$, and quantifies the fraction of the emitted radiation arising from the various layers in the atmosphere. It is an essential parameter in the physical inverse solution of the radiative transfer equation.

The V5 implementation of the VPD algorithm does not solve for contribution to the radiances from and steps have been taken to avoid complications due to variable surface emissivity and surface temperature. As can be seen in Figure 1, the infrared channels used in the retrieval have been chosen to minimize sensitivity to the surface temperature and surface emissivity. The implementation of the VPD algorithm avoids contamination by surface emissions by calculating the radiance contribution from the surface to each channel at each iteration step and rejecting channels in which the surface contribution to the outgoing radiance is larger than 50 mK. The net error in the surface emission as determined from AIRS Level 2 products is less than 2%, which is equivalent to 0.001 K. Channels for which the surface contribution is found to exceed 0.05 K are discarded. If less than three of the thirteen CO_2 channels used by the VPD algorithm survive, the retrieval is terminated and results discarded.

Average weighting functions for CO_2 channels assuming 330, 370 and 390 ppm CO_2 volume mixing ratio

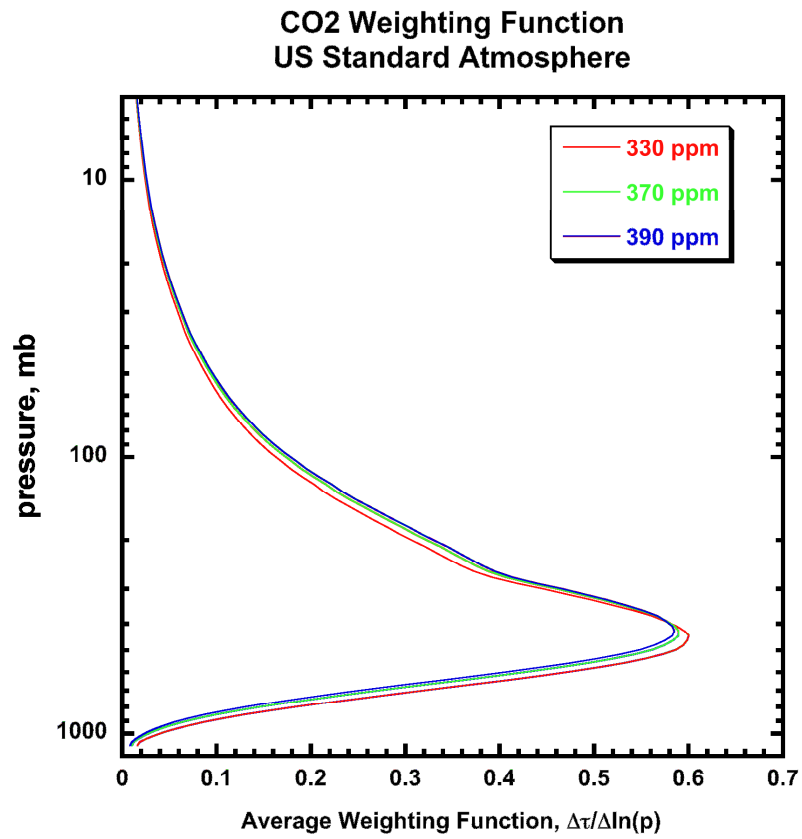

Figure 1: Average weighting functions for CO_2 IR channels used by VPD algorithm.

The altitude dependence of the sensitivity is a weak function of the CO_2 mixing ratio.

The AIRS weighting functions have a tail that intrudes into the stratosphere, more so in the polar regions where the tropopause height is lower. The stratospheric air is older than that of the troposphere by an amount that varies with latitude [Boering et al., 1996; Waugh and Hall, 2002; Morgan et al., 2004; Shia et al., 2006]. We have investigated the impact on the AIRS CO_2 tropospheric product and found that incorporation of a correction would result in a latitudinally dependent increase, varying from zero at the equator and approaching 3 ppm polarward of ~ 80°. This effect is seasonally dependent and we have elected not to include a correction in the V5 released CO_2 products. Our current estimate of the correction is based on the fraction of the radiance originating above the tropopause with respect to the total radiance.

Figure 2 is a block diagram of the processing flow for the VPD algorithm. Figure 2a depicts the steps in the retrieval of CO2 within a single AMSU FOV, whereas Figure 2b depicts the averaging of retrievals in the 2x2 array of AMSU FOVs to arrive at a reported product and the final QA step to place the report in the Level 2 CO_2 Standard Product or the Level 2 CO_2 Support Product.

a) CO_2 retrieval for an AIRS Level 2 retrieval which satisfies the criterion, (PGood-PTrop) > 200 hPa	b) Assemble of 2x2 array; apply spatial coherence QA; report product

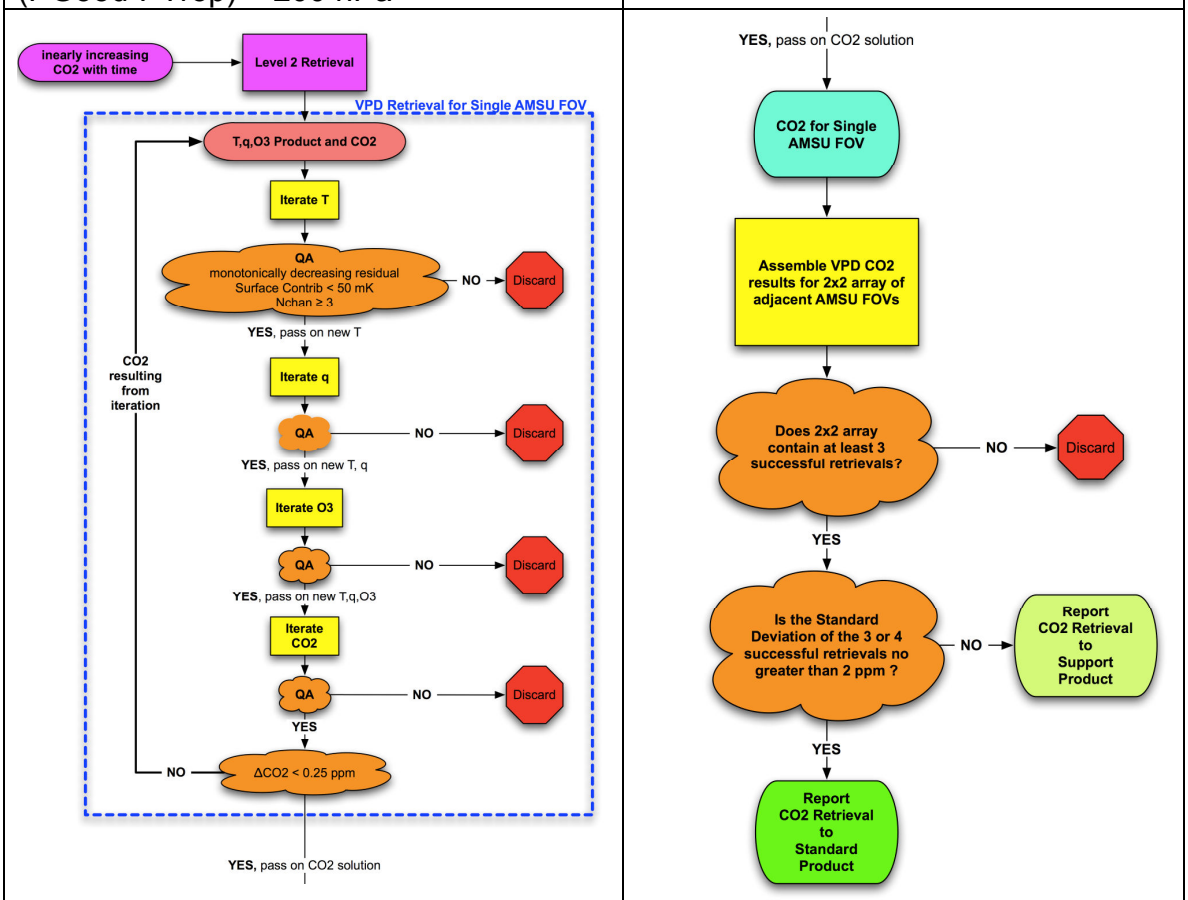

Figure 2: Block diagram of VPD post-processing retrieval of tropospheric CO_2.

Iterative solution is calculated for each AIRS Level 2 retrieval at a spatial resolution of an AMSU FOV; reported retrieval is over a field comprised of a 2x2 array of AMSU FOVs. Radiance residuals must monotonically decrease at each iteration step or the solution is discarded.

The VPD method is based on Gauss' method for finding the local minimum on an n-dimensional surface. It is based on a general property of the total differential of multi-variable functions: at the point of local minimum (or maximum) the first partial derivatives of the function with respect to each unknown must individually vanish. Since the goal of all retrieval methods is to minimize the residual difference in a least squares sense between measured and computed spectra, we write

$$G^{(n)} = \sum_{\nu} [\Theta_M(\nu) - \Theta_C^{(n)}(\nu)]^2 \qquad (1)$$

where G^n is a multi-variable function of temperature, ozone, water vapor, carbon dioxide, and surface emission, $\Theta_M(\nu)$is the measured brightness temperature at frequency ν (after eliminating the effects of clouds), $\Theta_C^{(n)}(\nu)$ is the computed brightness temperature and n is the order of iteration.

To minimize the residual function G we express its total differential as

$$dG = \frac{\partial G}{\partial X_1} dX_1 + \frac{\partial G}{\partial X_2} dX_2 + \frac{\partial G}{\partial X_3} dX_3 + \frac{\partial G}{\partial X_4} dX_4 \qquad (2)$$

Where X = $[X_1, X_2, X_3 X_4]$ is the solution vector and require dG to be minimized.

Equation (2) is necessary for a minimum to exist but not sufficient for retrieving a unique solution.

To achieve uniqueness we determine the local minimum point where each of the first partial derivatives vanishes individually. Note that variables $[\mathrm{X}_1, \mathrm{X}_2, \mathrm{X}_3, \mathrm{X}_4]$ are linearly independent in the AIRS Radiative Transfer Algorithm used to compute $\Theta_C^{(n)}(\nu)$.

$$\frac{\partial G}{\partial X_1} = 0, \quad \frac{\partial G}{\partial X_2} = 0, \quad \frac{\partial G}{\partial X_3} = 0, \quad \frac{\partial G}{\partial X_4} = 0 \qquad (3)$$

where X_1 may represent CO_2, X_2 =T(p), X_3 =O_3 , and X_4=H_2O.
Condition (3) is both necessary and (ideally) sufficient to retrieve a local minimum (or maximum) for the solution of CO_2.

The current VPD algorithm is described in Chahine et al. [2005]. Because of noise and other uncertainties in the various component of the G function, the necessary condition, (3), may not be sufficient. Consequently, in order to seek uniqueness the VPD algorithm tracks the variations of residuals with iterations and discards solutions whose residuals do not decrease monotonically with successive iterations down to the termination threshold of ΔCO_2 = 0.25 ppm. The result is that accepted solutions have a single minimum. Furthermore, the algorithm requires that at least three out of four adjacent CO_2 retrievals (making a cluster, or 2 x 2 array covering a 90 km x 90 km area at nadir) have solutions. Finally, a spatial coherence QA test is applied. If the surviving three or four solutions in the cluster agree to within 2 ppm in an RMS sense, a threshold chosen consistent with our goal of retrieving CO_2 within a data variability of 2 ppm, the retrieval is placed in the Level 2 CO_2 Standard Product. Retrievals failing this QA test are placed in the Level 2 CO_2 Support Product.

After retrieving the CO_2, we compute the averaging kernel by sequentially perturbing each of the 100 layers of the atmospheric profile. The averaging kernels are not used in the VPD retrieval, but are provided in the product to aid in the assimilation of AIRS CO_2 data and for comparison with TCCON observations. The averaging kernels represent the change of the apparent mixing ratio that results from a perturbation at each atmospheric level and is used in assimilation studies.

The VPD algorithm has been tested using different initial CO_2 mixing ratios from that used for the Level 2 retrievals, ranging between 330 ppm and 390 ppm in the polar regions and between 365 ppm and 405 ppm in the tropics, to determine whether the solution depends upon the initial value for CO_2 used in the iterative process as illustrated in Figure 3. The granule used in Figure 3 covers far Eastern Siberia, from the shoreline of the Sea of Okhotsk to deep into the East Siberian Sea and just North of the Arctic Circle. This is a challenging area for AIRS Level 2 retrievals and a good area to stress test the stability of the VPD CO_2 retrieval. The results show that the CO_2 solution arrived at is stable with respect to the starting values of CO_2. Despite a 25 ppm range of solutions, in almost all cases the same solution (within 1 ppm) is arrived regardless of whether the starting value used for CO_2 in the VPD algorithm is 373, 380 or 390 ppm.

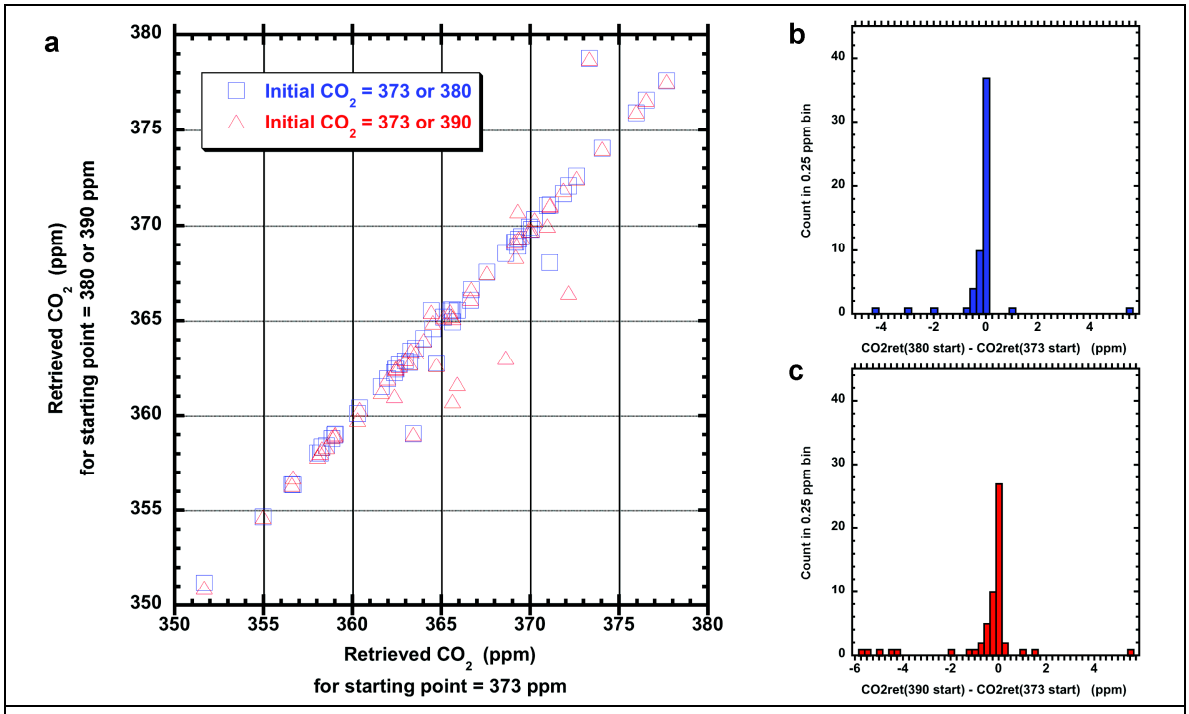

Figure 3: Independence of VPD solution from starting value for CO_2. Solution for 52 retrievals over Western Siberia and the Arctic Ocean on Jan 20, 2003. (**a**) Scatter plot showing range of CO_2 solutions for the three starting values; (**b**) Histogram of differences of solution for starting values of 373 ppm and 380 ppm; (**c**) Histogram of differences of solution for starting values of 373 ppm and 390 ppm.

We have also observed that negligible correlations among T(p), H_2O(p), O_3(p), and CO_2 are introduced by the VPD algorithm, as in the case illustrated in Figure 4. Here, R is Pearson's correlation coefficient assuming CO_2 is one variable and either T(p), H_2O(p) or O_3(p) is the other variable. However in some other cases, we do observe correlations, as would be expected when physical mechanisms such as stratospheric intrusions and stratospheric-tropospheric exchanges are present, as in the case of the sudden stratospheric warming noted in Figure 4 of Chahine et al. [2008].

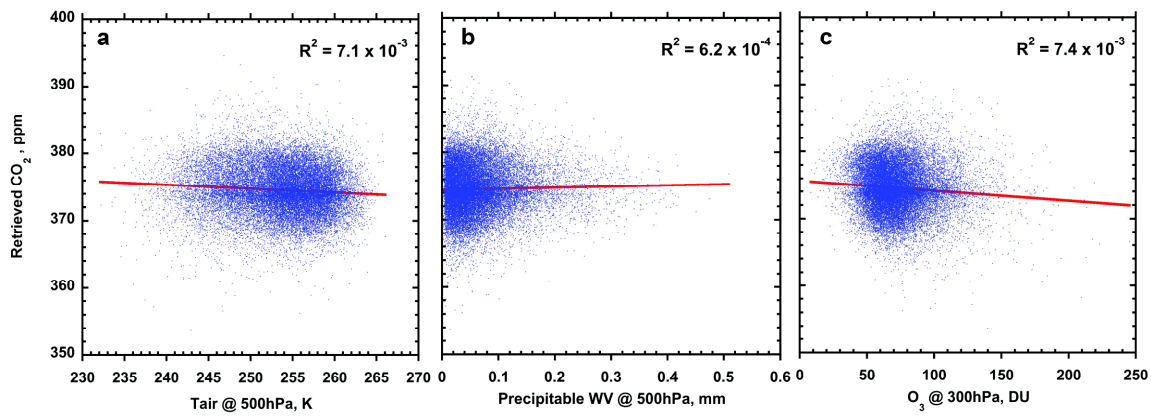

Figure 4: Lack of correlation of CO2 solution with temperature, water vapor and ozone.

Demonstration of lack of correlation among the VPD solutions for 24,635 retrievals of CO_2 and (**a**) T(500 hPa); (**b**) H_2O(500 hPa); (**c**) O_3(300 hPa) during January 2003 in the latitude band 30N to 40N. R^2 represents the portion of the variance in CO_2 that could be explained by the variance in the other parameter and is less than 0.8% in all cases. No more than 0.8% of the variance in CO_2 can be attributed to the variance of one of the other parameters.

Chahine et al. [2005] determined that the errors in the retrieved CO_2 are uncorrelated so that a reduction in the CO_2 error by averaging is possible. Averaging allowed tracking of the monthly seasonal variations of CO_2 between September 2002 and March 2004 with an agreement of 0.43 ± 1.20 ppm with respect to collocated aircraft measurements made by Matsueda [Matsueda et al., 2002], now incorporated into the Comprehensive Observation Network for Trace gases by AIrLiner (CONTRAIL).

Auxiliary AIRS CO2 Weighting Function Data File

The Level 2 CO_2 product files contain averaging kernels. The averaging kernel defines the layers in the atmosphere over which a perturbation of CO_2 at a given level is propagated in retrieval by estimation techniques and in data assimilation. On the other hand, the AIRS weighting function for CO_2 is the derivative of the atmospheric transmission function with respect the natural logarithm of the pressure, $\frac{\partial \tau(\nu, p)}{\partial \ln p}$, and quantifies the fraction of emitted radiation arising from the various layers in the atmosphere. It is an essential parameter in the physical inverse solution of the radiative transfer equation, used in the AIRS Level 2 retrievals. The VPD algorithm necessarily computes the weighting function for

each infrared channel at each iteration step during the retrieval as part of the forward calculation of radiances for the atmospheric state.

Direct validation the AIRS retrieved CO_2 is accomplished by convolving *in situ* CO_2 profiles with the AIRS weighting function to derive a value that is directly comparable to the AIRS result. As an aid to researchers, an ancillary tab-delimited file provides the AIRS CO2 weighting functions for the Thermodynamic Initial Guess Retrieval (TIGR) database [Chedin et al., 1985] tropical, mid-latitude summer, sub-polar winter atmospheres and Air Force Geophysical Laboratory (AFGL) 1976 US standard atmospheres [Anderson et al., 1986]. The unnormalized weighting functions are for constant CO_2 volume mixing ratio profiles of 330, 370 and 390 ppm and are given for each of the 101 levels of the supplementary pressure array. The file name is

AIRS_mid_trop_CO2_330_370_390_wgt_func.txt

We advise interested researchers to use these AIRS CO_2 weighting functions to derive a value from their measured profiles that may be compared to the AIRS retrieved CO_2. Care must be taken to interpolate each of the 101 levels taking into account the time growth of CO_2 over time and the latitude of their *in situ* measurement. A summary of the preferred algorithm is:

1. Interpolate the *in situ* measurement onto the 101 pressure levels
2. From the date of *in situ* measurement, calculate a global average CO_2 using the relationship for **Climatology_CO2** provided in the introduction of this document.
3. For each level of each model, linearly interpolate a new weighting function value for the calculated global average CO_2. The result is a new set of weighting functions for each model.
4. From the latitude of the *in situ* measurement, interpolate the new weighting functions for each level amongst the three TIGR models. The result is a weighting function profile for that date and location. Alternatively, choose the result in step #2 for the model that most closely matches the latitude of the *in situ* measurement.
5. Level-by-level, multiply the interpolated *in situ* measurement with the corresponding weighting function that results from step #4. Divide by the sum of the weights applied. The result is a value that can be directly compared to the AIRS CO_2 retrievals.

Figure 5 depicts representative AIRS vertical weighting functions and averaging kernels for the Thermodynamic Initial Guess Retrieval (TIGR) database [Chedin et al., 1985] tropical, mid-latitude summer and sub-polar winter atmospheres. Depending upon the atmosphere, AIRS peak sensitivity, shown by the averaging kernels, occurs at 285 hPa (tropical) and 425 hPa (polar), and the kernel width at

half-maximum varies from spanning 120 hPa to 515 hPa (tropical) to spanning 235 hPa to 640 hPa (polar).

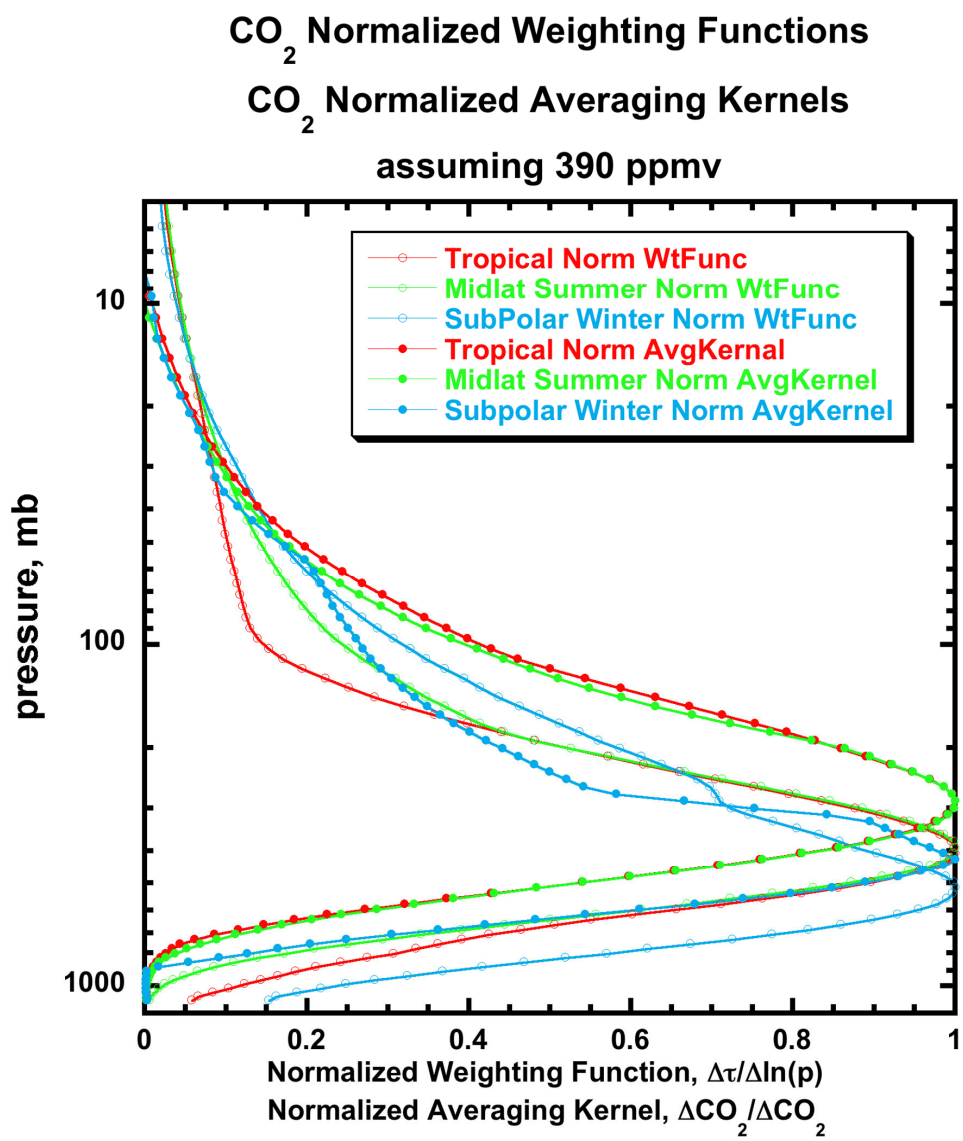

Figure 5: CO2 weighting functions and averaging kernels for three model atmospheres.

Comparison of CO_2 weighting functions and averaging kernels. All have been normalized to unity at their peaks.

ACKNOWLEDGMENT

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

Copyright 2009 California Institute of Technology, Government sponsorship acknowledged.

ACRONYMS

AFGRL	Air Force Geophysical Laboratory
AIRS	Atmospheric InfraRed Sounder
AMSU	Advanced Microwave Sounding Unit
CONTRAIL	Comprehensive Observation Network for Trace gases by AIrLiner
FOV	Field of View
GES DISC	Goddard Earth Sciences Data and Information Services Center
RMS	Root Mean Square
TCCON	Total Carbon Column Observing Network
TOA	Top of Atmosphere
TOVS	TIROS Operational Vertical Sounder
TIGR	Thermodynamic Initial Gues Retrieval
VPD	Vanishing Partial Derivative

REFERENCES

Anderson, G. P., S. A. Clough, F. X. Kneizys, J. W. Chetwynd, and E. P. Shettle (1986), AFGL atmospheric constituent profiles (0 – 120 km), *Tech. Rep. AFGL-TR-86-0110*, Phillips Lab., Hanscom Air Force Base, Mass.

Boering, K. A. (1996), Stratospheric Mean Ages and Transport Rates from Observations of Carbon Dioxide and Nitrous Oxide, *Science, 274*, 1340-1343, doi: 10.1126/science.274.5291.1340.

Chahine, M.T., C. Barnet, E. T. Olsen, L. Chen, and E. Maddy (2005), On the determination of atmospheric minor gases by the method of vanishing partial derivatives with application to CO2, *Geophys. Res. Lett., 32*, L22803, doi:10.1029/2005GL024165.

Chahine, M.T. *et al.,* (2006), AIRS: Improving Weather Forecasting and Providing New Data on Greenhouse Gases, *Bull. Am. Meteor. Soc., 87*, 911-926, doi:10.1175/BAMS-87-7-911

Chahine, M.T. et al., (2008), Satellite Remote Sounding of Mid-Tropospheric CO2, *Geophys. Res. Lett., 35*, L17807, doi:10.1029/2008GL035022.

Chedin, A., N. A. Scott, C. Wahiche and P. Moulinier, (1985), The improved initialization inversion method: a high resolution physical method for temperature retrievals from satellites of the TIROS-N series, *J. Appl. Meteorol., 24*, 128-143, doi: 10.1175/1520-0450(1985)024<0128:TIIIMA>2.0.CO;2

Engelen, R. J., and A. P. McNally (2005), Estimating atmospheric CO2 from advanced infrared satellite radiances within an operational four-dimensional variational (4D-Var) data assimilation system: Results and validation, *J. Geophys. Res., 110*, D18305, doi:10.1029/2005JD005982.

Engelen, R. J., S. Serrar, and F. Chevallier (2009), Four-dimensional data assimilation of atmospheric CO2 using AIRS observations, *J. Geophys. Res., 114*, D03303, doi:10.1029/2008JD010739.

Jiang, X. et al. (2008), Simulation of upper troposphere CO2 from chemistry and transport models, *Global Biogeochemical Cycles*, 22, doi:10.1029/2007GB003049.

Matsueda, H., H. Y. Inoue, and M. Ishii (2002), Aircraft observation of carbon dioxide at 8-13 km altitude over the western Pacific from 1993 to 1999. *Tellus*, *54B*(1), 1- 21,
doi: 10.1034/j.1600-0889.2002.00304.x; (Data are available at ftp://gaw.kishou.go.jp/pub/data/current/co2/event/eom999900.mri.am.fl.co2.nl.ev.dat).

Maddy E. S., C. D. Barnet, M. Goldberg, C. Sweeney, X. Liu (2008), CO2 retrievals from the Atmospheric Infrared Sounder: Methodology and validation, *J. Geophys. Res., 113*, D11301, doi:10.1029/2007JD009402.

Morgan, C. G., M. Allen, M. C. Liang, R. L. Shia, G. A. Blake, and Y. L. Yung (2004), Isotopic fractionation of nitrous oxide in the stratosphere: Comparison between model and observations, *J. Geophys. Res., 109*, D04305, doi:10.1029/2003JD003402.

Shia, R. L., M. C. Liang, C. E. Miller and Y. L. Yung (2006), CO2 in the Upper Troposphere: Influence of Stratophere-Troposphere Exchange, *Geophys. Res. Lett. 33*, doi:10, 1029/2006/GRL026141.

Strow, L. L., S. E. Hannon, (2008), A 4-year zonal climatology of lower tropospheric CO2 derived from ocean-only Atmospheric Infrared Sounder observations, *J. Geophys. Res., 113*, D18302, doi:10.1029/2007JD009713.

Waugh, D., and T. Hall (2002), Age of stratospheric air: Theory, observations, and models, *Rev. Geophys., 40*(4), 1010, doi:10.1029/2000RG000101.