TROPESS Carbon Monoxide Level 2 Standard Data Product User Guide

Authors: Kevin Bowman[1], John Worden[1], Helen Worden[2], Karen Cady-Pereira[3], Gene Francis[2], Jennifer Hegarty[3], Ming Luo[1], Vivienne Payne[1], Susan Kulawik[4], Sirvard Akopyan[1], Valentin Kantchev[1], and Kristen Fahy[1]

[1] Jet Propulsion Laboratory, California Institute of Technology
[2] National Center for Atmospheric Research
[3] Atmospheric and Environmental Research, Inc.
[4] NASA Ames Research Center

Table of Contents

1. Introduction

1.1 Overview and Document Scope

This document is the User Guide for the TROPESS AIRS and CrIS carbon monoxide (CO) Level 2 Standard Product Files. This document is intended to be used with the README, which describes the variables included in the data products.

1.2 Dataset Description

This user guide describes the TROPESS AIRS and CrIS Level 2 Standard Product Files for CO.

Table 1. Dataset Description

Product Information	Description
Parameters	CO profile
Data Product Provenance	Refer to ReadMe document, section 1.3.4 Algorithm Version
Approximate file size	15 MB
Spatial coverage	Regular collections have global coverage: Nominal latitude range: 70 N to 50 S Nominal longitude range: -180 to 180 Special collections: Spatial coverage varies by collection
Temporal coverage	Each L2 Standard file contains 1 day of data.
File format	netcdf
Vertical sensitivity	Estimates of carbon monoxide concentrations from thermal infrared satellite observations are most sensitive to CO variability between 850 and 200 mb. However, sensitivity depends on observed scene parameters such as thermal contrast and can be variable. Users should assess individual retrieval sensitivity using the averaging kernel (AK) for CO profiles and degrees of freedom for signal (DFS) or column AK for total column CO.
Data quality	The L2 Standard data products have undergone a pre-quality check, which involves checks for retrieval convergence and measurement sensitivity. There are no checks for clouds or land versus ocean as we do not find these to substantively affect the quality of the retrieval as long as the retrieval has converged. Note that retrievals over thick clouds will not be sensitive to CO below the clouds.
Uncertainty	Profiles levels have approximately 7% observational error (does not include vertical smoothing error).
Validation Stage	Stage 3 according to NASA guidelines https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels
Retrieval Levels	14 levels: from surface to top-of-atmosphere
_FillValues	-999

1.3   Filename

The Level 2 Standard Products adhere to the following filename convention:

```
[TROPESS]_ [Instrument-
Platform]_[ProductLevel]_[ProductType]_[ProductName]_[DateStamp]_[Algor
ithmName]_[AlgorithmVersion]_[ProcessingStrategy]_[FormatVersion].nc
```

Example:

```
TROPESS_CrIS-SNPP_L2_Standard_CO_20200912_MUSES_R1p10_FS_F01.nc
```

2. Product File Contents and Parameter Description

2.1   Variables included in the L2 Standard Product

Please see the README for a list of variables included in the L2 Standata product Files

3. References

Citing these data
Please cite the following references if you intend to use these data:

Hegarty et al., Validation and Error Estimation of AIRS MUSES CO Profiles with HIPPO, ATom and NOAA ESRL Aircraft Observations, AMTD 2021.

The following references were also used in the development of this documentation and can be cited for model/data comparisons.

Bowman, K.W.; Rodgers, C.D.; Kulawik, S.S.; Worden, J.; Sarkissian, E.; Osterman, G.; Steck, T.; Lou, M.; Eldering, A.; Shephard, M.; Worden, H.; Lampel, M.; Clough, S.; Brown, P.; Rinsland, C.; Gunson, M.; Beer, R., Tropospheric Emission Spectrometer: Retrieval Method and Error Analysis, *IEEE Trans. Geosci. Remote Sensing*, *44, 1297- 1307*, May 2006.

Buchholz, R. R., Worden, H. M., Park, M., et al., Air pollution trends measured from Terra: CO and AOD over industrial, fire-prone, and background regions, **Remote Sensing of Environment**, 256, 112275, doi: 10.1016/j.rse.2020.112275, 2021.

Deeter, M. N., D. P. Edwards, G. L. Francis, J. C. Gille, D. Mao, S. Martinez-Alonso, H. M. Worden, D. Ziskin, and M. O. Andreae (2019), Radiance-based retrieval bias mitigation for the MOPITT instrument: the version 8 product, *Atmos. Meas. Tech.*, *12*(8), 4561–4580, doi:10.5194/amt-12-4561-2019.

D. Fu, K. W. Bowman, H. M. Worden, V. Natraj, J. R. Worden, S. Yu, P. Veefkind, I. Aben, J. Landgraf, L. Strow, and Y. Han. High-resolution tropospheric carbon monoxide profiles retrieved from CrIS and TROPOMI. Atmos. Meas. Tech., 9(6):2567–2579, 06 2016.

D. B. A. Jones, K. W. Bowman, P. I. Palmer, J. R. Worden, D. J. Jacob, R. N. Hoffman, I. Bey, and R. M. Yantosca. Potential of observations from the Tropospheric Emission Spectrometer to constrain continental sources of carbon monoxide. J. Geophys. Res.-Atmospheres, 108(D24):4789, 2003.

Luo, M., C. P. Rinsland, C. D. Rodgers, J. A. Logan, H. Worden, S. Kulawik, A. Eldering, A. Goldman, M. W. Shephard, M. Gunson, and M. Lampel, Comparison of carbon monoxide measurements by TES and MOPITT: the influence of a priori data and instrument characteristics on nadir atmospheric species retrievals, *J. Geophys. Res.*, *112, D09303*, doi: 10.1029/2006JD007663 , May 3, 2007.

Rodgers, C. D., and B. J. Connor (2003), Intercomparisons of remote sounding instruments, *J. Geophys. Res.*, **108**(D3), 4116, doi:10.1029/2002JD002299

Worden, H. M., M. N. Deeter, C. Frankenberg, M. George, F. Nichitiu, J. Worden, I. Aben, K. W. Bowman, C. Clerbaux, P. F. Coheur, A. T. J. de Laat, R. Detweiler, J. R. Drummond, D. P. Edwards, J. C. Gille, D. Hurtmans, M. Luo, S. Martínez-Alonso, S. Massie, G. Pfister, and J. X. Warner (2013), Decadal record of satellite carbon monoxide observations, *Atmos. Chem. Phys.*, *13*(2), 837–850, doi:10.5194/acp-13-837-2013.

4. Extended User Guide: L2 Standard Product

This extended user guide shows how to compare these fields to aircraft or model fields and calculate uncertainties.

How to Compare TROPESS CO profiles to aircraft or model fields
All comparisons between remotely sensed data an *in situ* measurements or high resolution model fields must account for the sensitivity of the remotely sensed measurement and any regularization used with the remotely sensed measurements. Otherwise *large* errors will be incurred with the comparisons.
We first construct an observation operator that is used for comparison of the TROPESS CO data to models or vertical profile measurements such as from aircraft:
1) Calculate the CO profile using the model or aircraft fields (for the purpose of this demonstration we will call this $x_{\_true}$).
2) Construct the operation operator as the following :
$$H(\cdot) = ln(x_a) + A(ln(\cdot) - ln(x_a))$$
3) Apply observation operator to the CO profile:
$$\hat{x} = exp[H(x_{true})]$$

In the netcdf product file and in the equation, x_a is the constraint vector used to regularize the retrieval. $H(\cdot)$ is the observation operator, where the $(\cdot)$ represents a model or *in situ* profile. A is the averaging kernel matrix and must be matrix multiplied by $ln(x_{true}) - ln(xa)$. After this operation one can compare the modified CO profile ($\hat{x}$) to the retrieved "x" variable in the netcdf product file. Note that the averaging kernel matrix (**A**) is not symmetric, so getting the row/column order of A correct is critical. You can check your work by using the above equation with the zeroth entries for the averaging kernel, **xa** and using the zero[th] entry for **x** as x_{true}. If your test operation (steps 1-3) matches the variable x_test then the operation is correct.

Figure 1 shows an example of the averaging kernel rows for a CrIS CO retrieval over a tropical ocean scene. Figure 2 shows an example of applying the averaging kernels from TROPESS AIRS CO retrievals to in situ profiles from the HIPPO campaign in plume and background conditions.
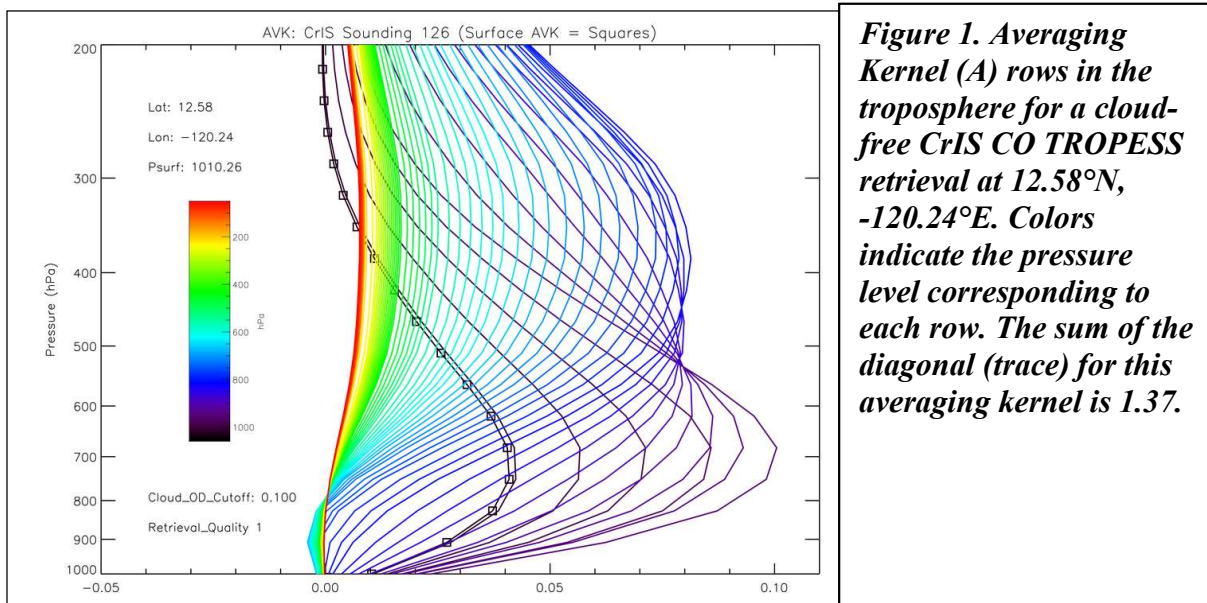

Figure 1. Averaging Kernel (A) rows in the troposphere for a cloud-free CrIS CO TROPESS retrieval at 12.58°N, -120.24°E. Colors indicate the pressure level corresponding to each row. The sum of the diagonal (trace) for this averaging kernel is 1.37.
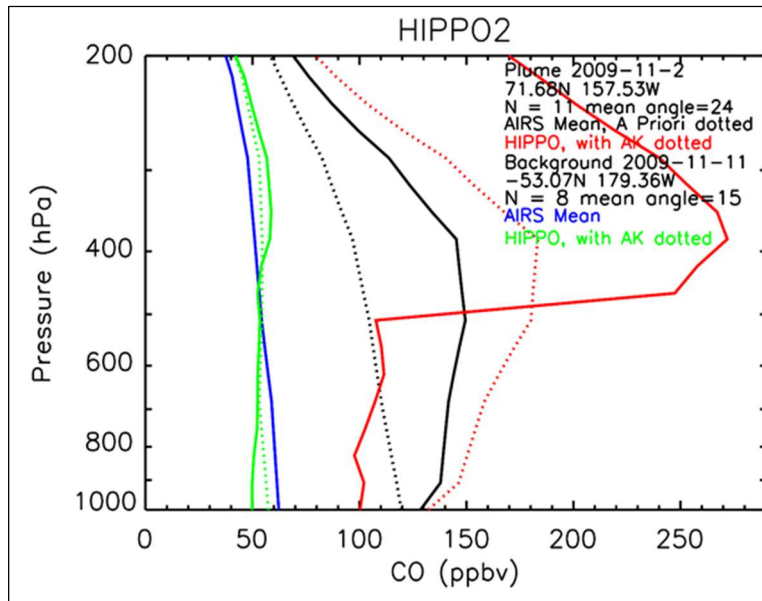
5

Figure 2. Example of comparisons between aircraft (HIPPO-2 campaign) and AIRS CO profiles (taken from Hegarty et al., 2021). The solid red and green lines show the HIPPO in-situ profiles for plume (red) and background (green) cases. Dashed red and green lines show the HIPPO profiles after applying the AIRS AK and apriori and represent the profiles as they would be observed by AIRS and retrieved with TROPESS.

4.1 Calculation of the Degrees of Freedom for Signal (DOFS)

The DOFS is the number of independent pieces of information that can be resolved and is therefore a useful diagnostic of the retrieval. The Averaging kernel matrix (see previous section) is the sensitivity of the estimate to the true state. The DOFS is defined as the trace of the averaging kernel matrix. To determine if the estimate is sensitive to a particular altitude a good place to check is the DOFS. The expected range of DOFS varies by species. A good rule of thumb for CO is to use data where DOFS > 0.7. A value of zero means no sensitivity to the retrieved profile. For the averaging kernel rows plotted in Fig. 1, the DOFS is 1.37, which is in the typical range (~1 to 1.5) for thermal infrared (TIR) spectral CO observations over cloud free ocean, (except in polar regions). For cloud-free land observations, DOFS can be > 1.5 in cases of high thermal contrast.

4.2 Error Derivation Used for Process Studies and Model or Aircraft Comparisons

Errors are calculated based on the derivation in Bowman *et al*. (2006). The TROPESS AIRS product files provide the averaging kernel (or AK) **A** in order to compare the CO estimates with either aircraft data or models or some other constructed profile.

The uncertainties can be calculated by taking the expectation of the difference between the estimate and the true state.

$$E(\hat{x} - \underline{x})((\hat{x} - \underline{x})^T = (I - A)S_a(I - A)^T + S^{meas} + S^{int}$$

The first term represents the smoothing error and covariances, $S^{obs} = S^{meas} + S^{int}$ are provided with the TROPESS product files. The smoothing error terms are not needed for comparisons since aircraft or model profiles are smoothed by the averaging kernel before comparing. The product files provide the following error diagnostic terms:

A = AVG_KERNEL
S^{obs} = OBS_ERROR

5 Validation Summary

Summary Statement: Based on the NASA Validation Guidelines (see link in Table 1), we determined that the TROPESS L2 Standard CO products are at Validation Stage 3. Both TROPESS AIRS CO (Fig. 3) and TROPESS CrIS CO (Fig. 4) retrievals have similar biases with respect to in situ data, around +5% in the lower troposphere and -5% in the upper troposphere. Calculated observational error is ~7% (Fig. 5) and varies with altitude.

Our rationale for this validation stage and these uncertainties is that retrieved profiles and calculated errors have been evaluated by comparing against independent satellite and aircraft data sets in the tropics, mid-latitudes, and high-latitudes (Hegarty et al., 2021). Figure 3 shows a representative plot from Hegarty et al. (2021) with AIRS CO comparisons to HIPPO and ATom aircraft profiles. Figure 4 shows CrIS CO comparisons with ATom (Note that CrIS data were not available during the HIPPO campaigns). Here we only report data where the species retrieval quality is sufficient for science analysis. The CO data are **not** bias corrected.
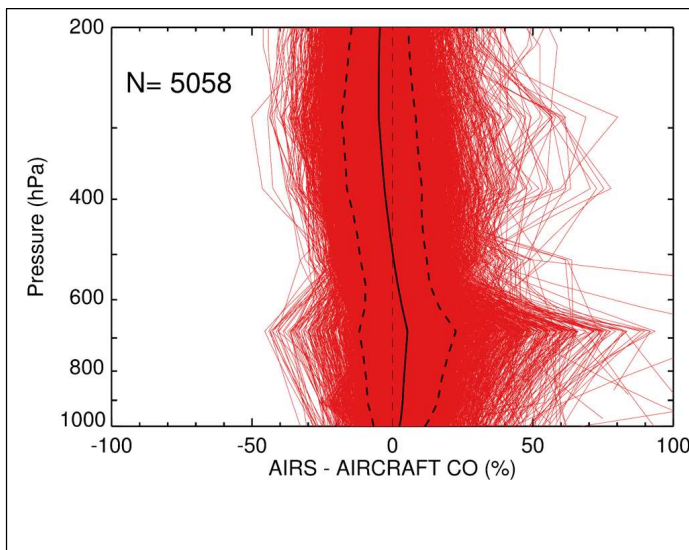

Figure 3. Differences (%) between AIRS TROPESS CO profiles and smoothed aircraft profiles (taken from Hegarty et al., 2021). Aircraft data are from all 5 HIPPO missions and ATom campaigns 1-3. The number of matched profiles was 5058, with 50 km, 9 hour coincidence criteria for 563 unique aircraft profiles. The red lines are individual comparisons, the black solid line indicates the mean bias, and the dashed black lines are one standard deviations from the mean. Grey dashed line is the 0% bias reference.

Figure 4. Differences (%) between CrIS TROPESS CO profiles and smoothed ATom (50km, 9 hr coincidence). Colors indicate latitude ranges for individual comparisons. Black line with error bars shows mean bias, standard deviation. Grey dashed line is the 0% bias reference.
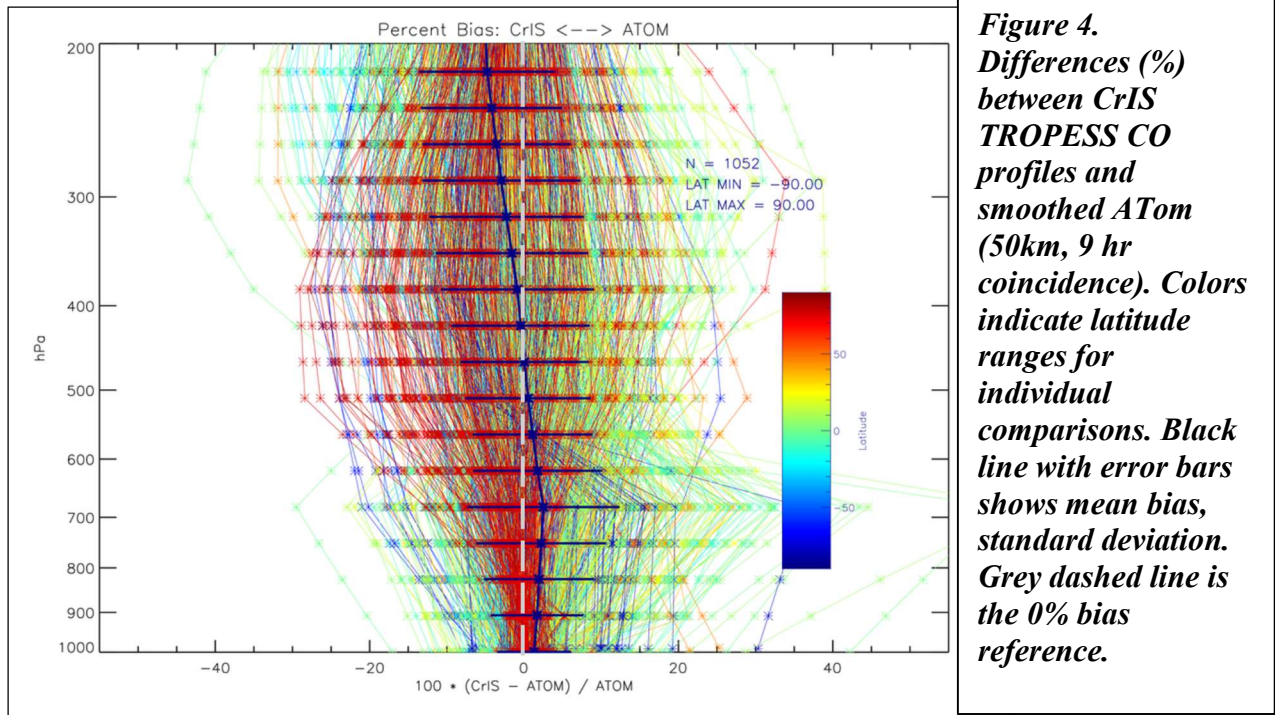
We made comparisons of CrIS-SNPP and CrIS-JPSS1 CO data processed with the Release Version 1.8 for the same months of Jan 2019 to May 2020. For the global monthly data sets, we calculated the percent differences of their volume mixing ratios at 681 hPa and derived the comparison statistics in latitude bands. At 681 hPa, the percent differences of the two CO fields show slightly larger numbers in the tropics compared to higher latitude. They are 0-4% with rms of 2-5%. The retrieval precisions are 4-8%. Compared to the retrieval precision and considering the atmospheric variability of CO, the CO retrievals of CrIS-SNPP and CrIS-JPSS1 are in good agreement.

5.1 Example of error validation

Figure 5 shows how the average calculated or theoretical error, S^{obs} in Sec. 4.3 compares with the empirical error calculation using the standard deviation of multiple comparisons for CrIS and ATom profiles. The average calculated error is reasonably close, but smaller than the empirical error, as can be expected for the somewhat broad coincidence criteria used for comparisons (see Fig. 4). Figure 5 also shows how both calculated and empirical errors are reduced from the prior

8

fractional error, and also improved from the standard deviation for comparisons of prior-ATom CO profiles in the free troposphere.
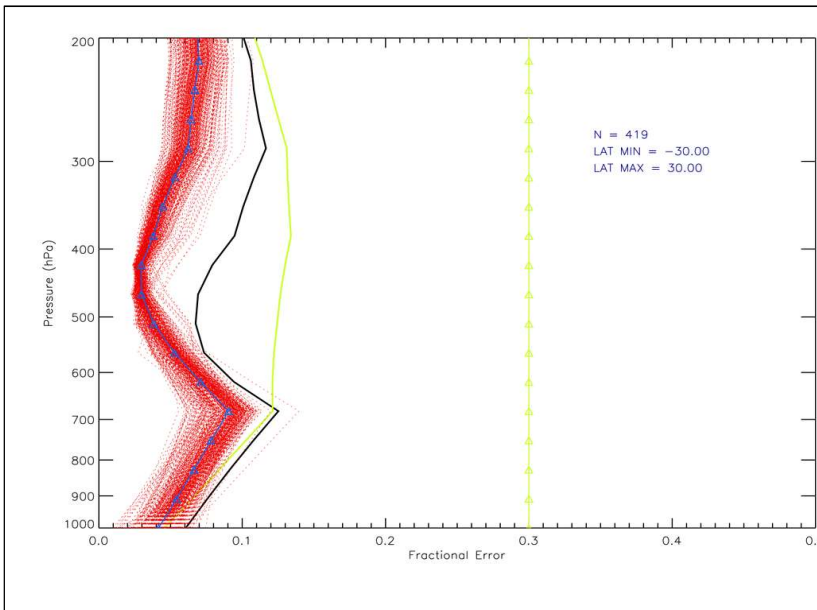

Figure 5. CrIS CO calculated vs. empirical errors for CrIS-ATom comparisons between 30°S and 30°N. Prior fractional error (0.3) is shown in yellow with triangles. Solid yellow is the standard deviation of Prior-ATom. Red lines are the calculated errors for each TROPESS retrieval with average in blue triangles. Black line is the empirical error (standard deviation of CrIS-ATom).

5.2 Intercomparisons of TROPESS AIRS and CrIS CO with MOPITT CO retrievals

The MOPITT instrument on NASA/Terra was launched in 1999 and its global observations of CO profiles have been widely used in air quality and climate studies. MOPITT CO data products have also been validated against in-situ measurements (Deeter et al., 2019) and together with other satellite retrievals in time trend analyses (Worden et al., 2013; Buchholz et al., 2021). Same as comparisons of satellite retrievals and in-situ or model species profiles, the comparisons of the profile retrievals derived from different satellite remote sensing observations also need to consider the influences of the a Priori assumptions (Rodgers and Connor, 2003; Luo et al, 2007). We used two step adjustment to make comparisons between the MUSES retrieved CO from the CrIS measurements and the MOPITT version 8 TIR-only (V8T) CO products making use of the a Priori info and the retrieval characteristic data provided by the two instrument teams. Table 3, below, lists the comparisons of TROPESS AIRS and CrIS with MOPITT CO retrievals at the lower and upper troposphere pressures and the total column. For selected four days in four seasons of 2019, the closest in distance profiles are identified within 500 km of the two instruments. The global averaged percent differences and the rms of all the paired data are examined. Table 4 gives the average and rms of reported errors along with CO variability within the 500km coincidence criteria.

Table 3. Comparisons of TROPESS CrIS and MOPITT V8T CO for lower/upper troposphere and total column.

		681 hPa		215 hPa		Total Column	
		Percent Differences (MUSES-MOPITT)/Mean	Percent rms	Percent Differences (MUSES-MOPITT)/Mean	Percent rms	Percent Differences (MUSES-MOPITT)/Mean	Percent rms
Direct Compare	CrIS	5.8%	20.4%	-7.5%	31%	1.9%	15%
	AIRS	8.3%	30%	-6.6%	30%	3.4%	16%
Adjust Xa to MOPITT Xa	CrIS	3.6%	20%	-5.2%	30%		
	AIRS	6.1%	30%	-4.5%	29%		
Adjust Xa to MOPITT Xa + Apply TROPESS operator to MOPITT profile	CrIS	3%	17%	-2.8%	19%		
	AIRS	5.7%	28%	-2.5%	19%		

Table 4. Mean and variability of observation errors, total retrieval errors for TROPESS CrIS and MOPITT V8T CO retrievals and CO variability for 500km coincidence criteria.

		681 hPa		215 hPa		Total Column	
		Percent Mean	Percent rms	Percent Mean	Percent rms	Percent Mean	Percent rms
Measurement Error	CrIS	4.4%	2.8%	6.5%	1.8%		
	AIRS	4.1%	2.6%	6.4%	1.9%		
	MOPITT	2.1%	0.8%	3%	0.8%		
Total Retrieval Error	CrIS	26.5%	3.7%	24.5%	2.8%	12%	4.3%
	AIRS	28%	3.2%	25%	2.9%	12.6%	3.6%
	MOPITT	12.3%	0.6%	11.5%	1.1%	9.3%	3.4%
MOPITT CO Variability Within 500km of CrIS-MOPITT matches		(700 hPa) 3%	(700 hPa) 1.3%	(200 hPa) 4.4%	(200 hPa) 2.8%		

To summarize these intercomparisons with MOPITT CO: (1) The comparisons agreed better after we adjusted the a Priori to a common one and applied MUSES-CrIS retrieval operator to MOPITT retrievals. (2) In the lower troposphere, CrIS CO is about 3% higher and in the upper troposphere, CrIS CO is about 3% lower than MOPITT CO. (3) The comparison differences are

within the measurement errors of the two instruments (2-7%). The CO atmospheric variability within the matched pairs of the two instrument is 3-5%.

5.3 Known Issues

A set of data quality screening criteria have been used to remove the problematic CO retrievals in L2 standard product, such as the radiance residual rms (radResRMS) indicating the degree of agreement between the measured spectral radiance and the modeled one. For the CrIS CO retrievals, the max limit for radResRMS is set larger than AIRS CO in keeping some realistically high CO retrievals over fire plumes. However, in some non-fire or non-heavily polluted regions we also see a few anomalously high CO VMRs in the mid-troposphere in a given month's CrIS CO data. Users are encouraged to use their judgment to identify the anomalous CO profiles in their applications; or if possible, to use a more strict radResRMS criterion in addition to the current quality screening set when accessing the archived data.

Appendix A. Retrieval levels

The table below contains the nominal retrieval levels. For each sounding, the surface pressure level is inserted into the retrieval levels set. Any retrieval levels below the surface pressure level are omitted.

Index	Pressure [hPa]
1	1040.0000
2	908.5139
3	681.2910
4	510.8980
5	383.1170
6	287.2980
7	215.4440
8	161.5610
9	121.1520
10	90.8518
11	51.0896
12	28.7299
13	4.6416
14	0.1000

Acknowledgement