TROPESS Water Vapor
Level 2 Standard Data Product User Guide

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Table of Contents

1 Introduction

1.1 Overview and Document Scope

This document is the User Guide for the TROPESS AIRS and CrIS water vapor (H_2O) 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 H_2O.

Table 1. Dataset Description

Product Information	Description
Parameters	H2O profile
Data Product Provenance	MUSES Version 1.11
Approximate file size	13MB
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 water vapor concentrations from thermal infrared satellite observations are most sensitive to H2O variability between 825 and 300 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 H2O profiles and degrees of freedom for signal (DOFS) or column AK for total column H2O.
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 H2O below the clouds.
Uncertainty	Profiles levels have approximately 20% observational error (does not include vertical smoothing error).
Validation Stage	Stage 4 according to NASA guidelines https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels
Retrieval Levels	17 levels: from surface to top-of-atmosphere
Fill Values	-999

1.3 Filename

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

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

Example:

```
TROPESS_CrIS-SNPP_L2_Standard_H2O_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 Standard Product Files

3 References

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

Herman, R. L., Worden, J., Noone, D., Henze, D., Bowman, K., Cady-Pereira, K., Payne, V. H., Kulawik, S., and Fu, D.: Comparison of optimal estimation HDO/H2O Retrievals from AIRS with ORACLES measurements, Supplement of ***Atmos. Meas. Tech.***, ***13***, 1825–1834, 2020, https://doi.org/10.5194/amt-13-1825-2020-supplement

The following references were also used in the development of this documentation and should 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.

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

Worden, J., Kulawik, S., Frankenberg, C., Payne, V., Bowman, K., Cady-Pereira, K., Wecht, K., Lee, J.-E., and Noone, D.: Profiles of CH_4 , HDO, H_2O, and N_2O with improved lower tropospheric vertical resolution from Aura TES radiances, **Atmos. Meas. Tech.**, **5**, 397–411, https://doi.org/10.5194/amt-5- 397-2012, 2012.

Worden, J. R., Kulawik, S. S., Fu, D., Payne, V. H. , Lipton, A. E., Polonsky, I., He, Y., Cady-Pereira, K., Moncet, J.-L., Herman, R. L., Irion, F. W., and Bowman, K. W., "Characterization and Evaluation of AIRS-Based Estimates of the Deuterium Content of Water Vapor", ***Atmos. Meas. Tech.,*** **12**, 2331-2339, 2019, https://doi.org/10.5194/amt-12-2331-2019.

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 H_2O 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 H_2O data to models or vertical profile measurements such as from aircraft:

1) Calculate the H_2O profile using the model or radiosonde fields (for the purpose of this demonstration we will call this $\boldsymbol{x}_{true}$).
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 H_2O profile:
$$\hat{x} = exp[H(x_{true})]$$

In the netcdf product file and in the equation *xa* is the constraint vector used to regularize the retrieval. The $H(\cdot)$ is the observation operator, where the $(\cdot)$ represents the 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 H_2O 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 zeroth 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 an AIRS H_2O retrieval over a tropical ocean scene.

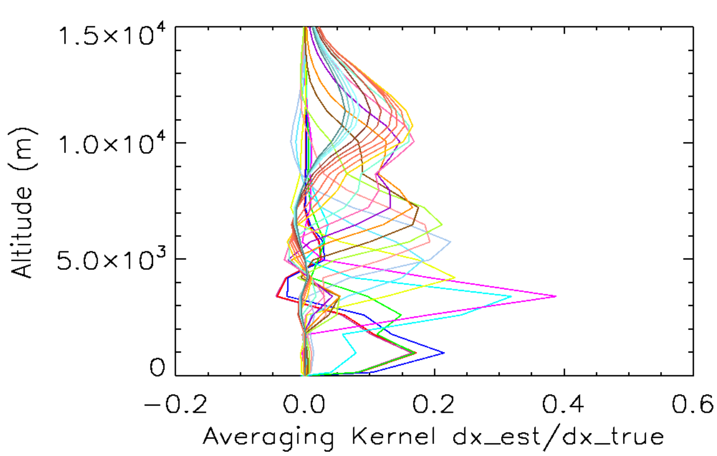

Figure 1. Averaging Kernel (A) rows in the troposphere for a cloud-free AIRS H_2O TROPESS retrieval. Colors indicate the pressure level corresponding to each row.

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 H_2O is to use data where DOFS > 2.
A value of zero means no sensitivity to the retrieved profile. The typical range of DOFS for thermal infrared (TIR) spectral H_2O observations over cloud free ocean is 2 to 4, (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 H_2O 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.

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

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:

$\boldsymbol{A}$ = AVG_KERNEL
S^{obs} = OBS_ERROR

5 Validation Summary

Based on the NASA Validation criteria listed subsequently, we list the validation level of the TROPESS L2 H_2O product as Level 4. One year of global radiosonde measurements from the NOAA Global Systems Laboratory database have been compared to AIRS H_2O, as shown in the

figure below [https://ruc.noaa.gov/raobs/General_Information.html, M. Govett, pers. comm.]. The mean difference (AIRS minus radiosonde with averaging kernel applied) is between +10% and -10% for the troposphere, 825 hPa to 200 hPa.
H_2O validation has also been carried out with in situ aircraft measurements during the ORACLES Earth Venture mission [see supplement of Herman et al., 2020]. Both TROPESS AIRS H_2O and TROPESS CrIS H_2O have similar biases.

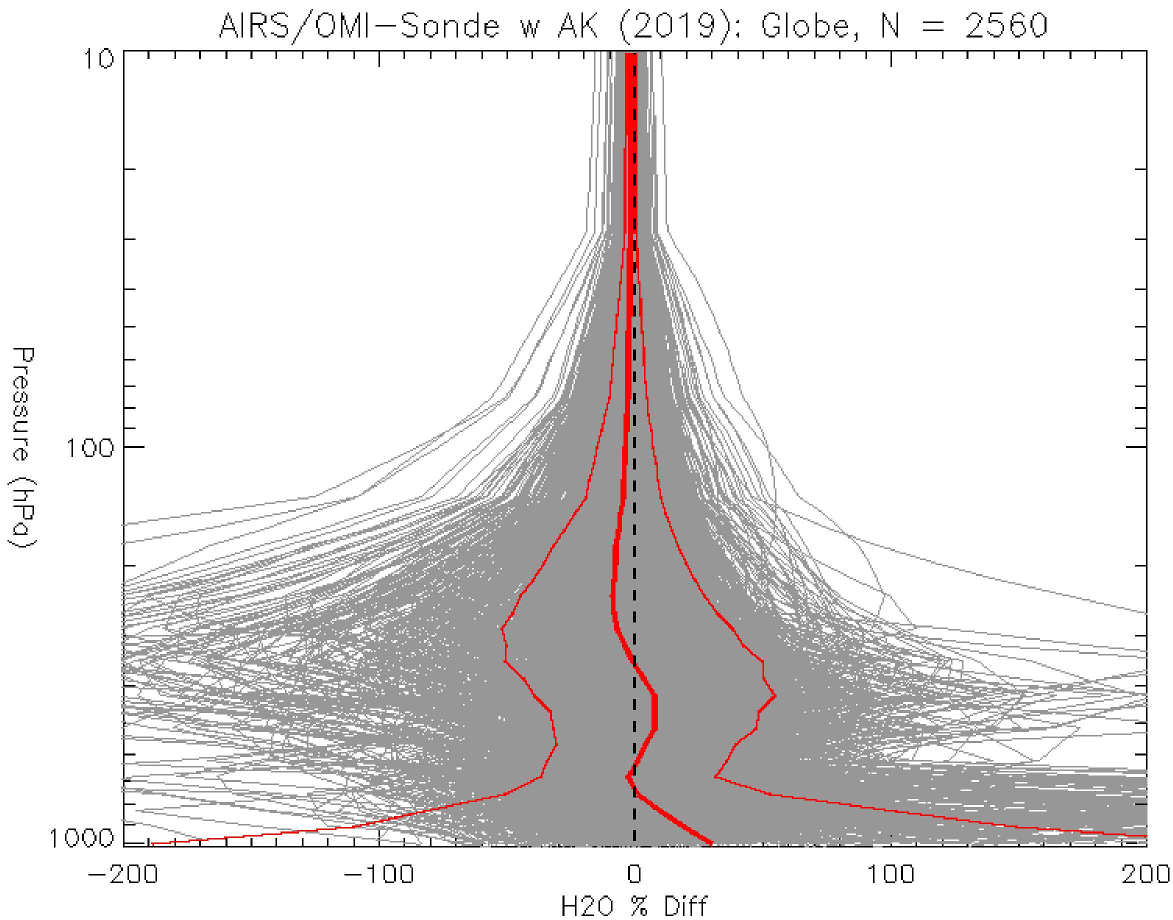

Figure 2. Validation of TROPESS AIRS H_2O with radiosondes. There are 2560 matches during calendar year 2019 within 50 km and +1.5/-0.5 hours coincidence. For AIRS minus radiosonde (with averaging kernel), both the mean (solid red line) and rms (dashed red line) are shown.

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	1000.0000
3	908.5140
4	825.4020
5	749.8930
6	681.2910
7	618.9660
8	510.8980
9	421.6980
10	348.0690
11	287.2980
12	237.1370
13	177.8290
14	133.3520
15	74.9896
16	28.7299
17	0.1000

Acknowledgement

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