TROPESS Ammonia
Level 2 Standard Data Product User Guide

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1 Introduction

1.1 Overview and Document Scope

This document is to be used as a “Quick Start “user guide for using the TROPESS AIRS and CrIS Level 2 Standard Product Files for ammonia (NH_3). 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 ammonia (NH_3).

Table 1: Dataset Description

Product Information	Description
Parameters	NH3 profile, NH3 total column
Data Product Provenance	MUSES Version 1.11
Approximate file size	15 MB for this collection
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	Ammonia is concentrated mainly in the boundary layer. Estimates of ammonia concentrations from thermal infrared satellite observations are most sensitive to NH3 variability between 900 and 650 mb. However, sensitivity depends on the observed scene parameters such as thermal contrast , cloud optical depth and boundary layer thickness. Users should assess individual retrieval sensitivity using the averaging kernel (AK) for NH3 profiles, and degrees of freedom for signal (DFS) or column AK for total column NH3.
Data quality	The data 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. However, AIRS NH3 retrievals over ocean use a low level background prior, and will rarely provide any information; this also applies to AIRS and CrIS retrievals over medium to thick clouds. CrIS retrievals over ocean may occasionally show unphysically high values, which should not be used.
Uncertainty	Uncertainty on the profiles and columns varies from 10 to 50%, with larger uncertainties on smaller amounts.

Validation Stage	Stage 1, according to NASA guidelines https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels
Retrieval Levels	15 levels from surface to TOA
FillValues	-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_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

The following references were 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.

Shephard, M.W. and Cady-Pereira, K.E., Cross-track Infrared Sounder (CrIS) satellite observations of tropospheric ammonia, ***Atmos. Meas. Tech****., 8(3):1323–1336, 03 2015*.

Shephard, M. W., Cady-Pereira, K. E., Luo, M., Henze, D. K., Pinder, R. W., Walker, J. T., Rinsland, C. P., Bash, J. O., Zhu, L., Payne, V. H., and Clarisse, L.: TES ammonia retrieval strategy and global observations of the spatial and seasonal variability of ammonia***, Atmos. Chem. Phys****., 11, 10743–10763*, https://doi.org/10.5194/acp-11-10743-2011, 2011.

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.

1. How to Compare TROPESS NH_3 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 NH3 profile using the model or aircraft 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 NH3 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 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 zeroth entry for x as x_{true}. If your test operation (steps 1-3) matches the variable x_test then the operation is correct.

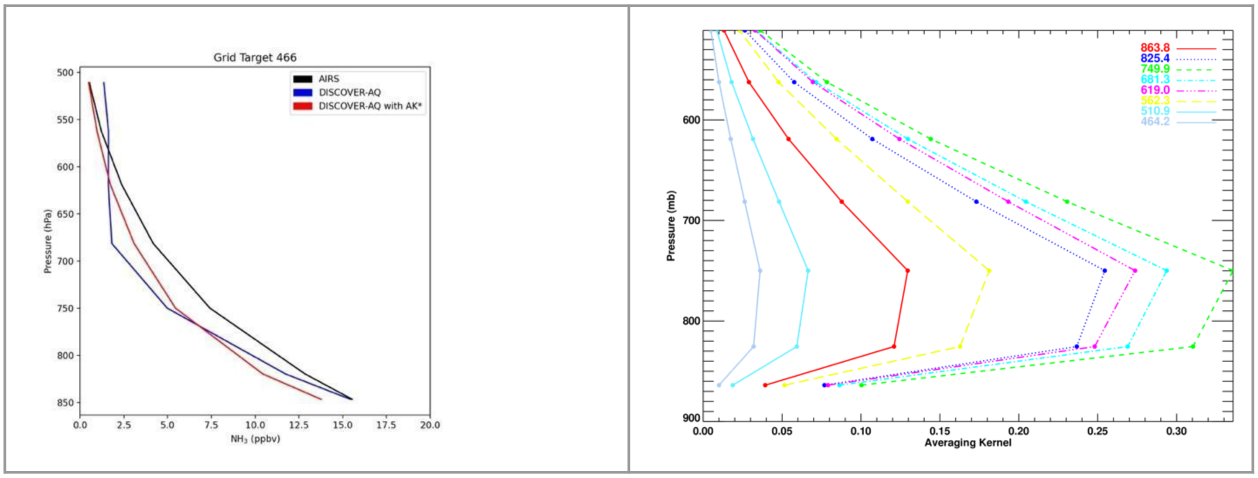

Figure 1. Co-located AIRS NH3 and aircraft profiles from DISCOVER-AQ Colorado The red curve shows the aircraft profile with the AIRS operator applied (left). Corresponding averaging kernel (right).

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

The averaging kernel matrix (see previous section) is the sensitivity of the estimate to the true state. To determine if the estimate is sensitive to a particular altitude look at the value of diagonal of the AK at that altitude. In the example (Figure 1, right panel) the peak of the sensitivity is at ~750 mbar, which is typical for a daytime retrieval in a region with no thermal inversion. To determine how much information the estimate provides over the entire profile, look at the DOFS, which is defined as the trace of the averaging kernel matrix. A value of DOFS ~1 means the estimate can quantify the full range of variability and a value >1 means there is information about the vertical distribution. A value of zero means no sensitivity to the measurement. A good rule of thumb is to trust results in which DOFS > 0.5.

The most useful metrics from the TROPESS NH3 product are the total column and the surface value, in that order. The retrieval has reduced sensitivity to surface values when there are thermal inversions in the observed profile.

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 avg_kernel) **A** in order to compare the AIRS estimates with either aircraft data or models or some other constructed profile (***see previous section***).

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

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

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

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

4.3 Error example from the DISCOVER-AQ Colorado 2014 campaign

The error analsyis from the DISCOVER-AQ Colorado campaign (Figure 2) show that the retrieval provides a useful amount of information, as the difference between the retrieved profiles and the aircraft measurements is much smaller than the difference between the a priori and the aircraft data. This analysis also suggests that the estimated error is biased high between 800 and 500 hPa.

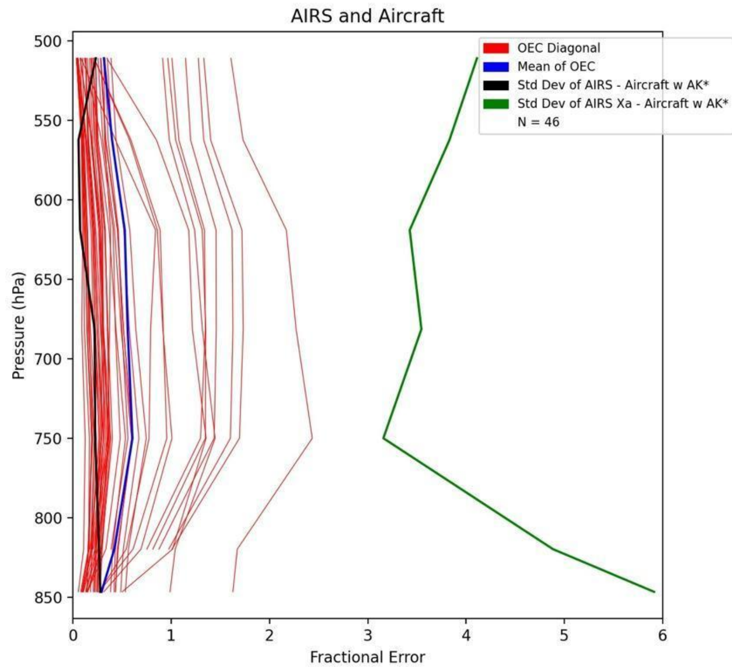

Figure 2. AIRS estimated (observational) errors for 46 (red) observations over Colorado during the DISCOVER-AQ campaign in July and August, mean estimated error (blue) and measured error (black).

5 Validation Summary

Summary Statement: Based on the NASA Validation Guidelines (see link in Table 1), we determined the validation level of the TROPESS L2 Standard NH_3 products at stage 1. AIRS NH_3 has been compared against a very limited set of profiles from aircraft measurements, while CrIS NH_3 is currently being evaluated against surface measurements from a small network in Idaho. No large scale analysis has yet been completed.

Figure 3 compares the NH_3 aircraft measurements taken during the Colorado DISCOVER-AQ campaign with co-located AIRS retrievals; both profiles (left panel) and total columns (right panel) are shown. The AIRS profiles are basically unbiased, while the total columns are biased high except for very low values. A similar analysis is under way for CrIS NH_3.

CrIS NH_3 is also being evaluated against surface data collected from a small network in the Magic Valley region of Idaho, which provides two week means of ground level NH_3 from 2018 through 2020. A first step comparison shows qualitative agreement in the seasonal cycle (Figure 4). Since the temporal (instantaneous measurements at 1:30 local time vs two week means) and spatial (profile vs point) sampling are very different between CrIS and the ground data quantitative comparisons require a more detailed analysis that is ongoing.

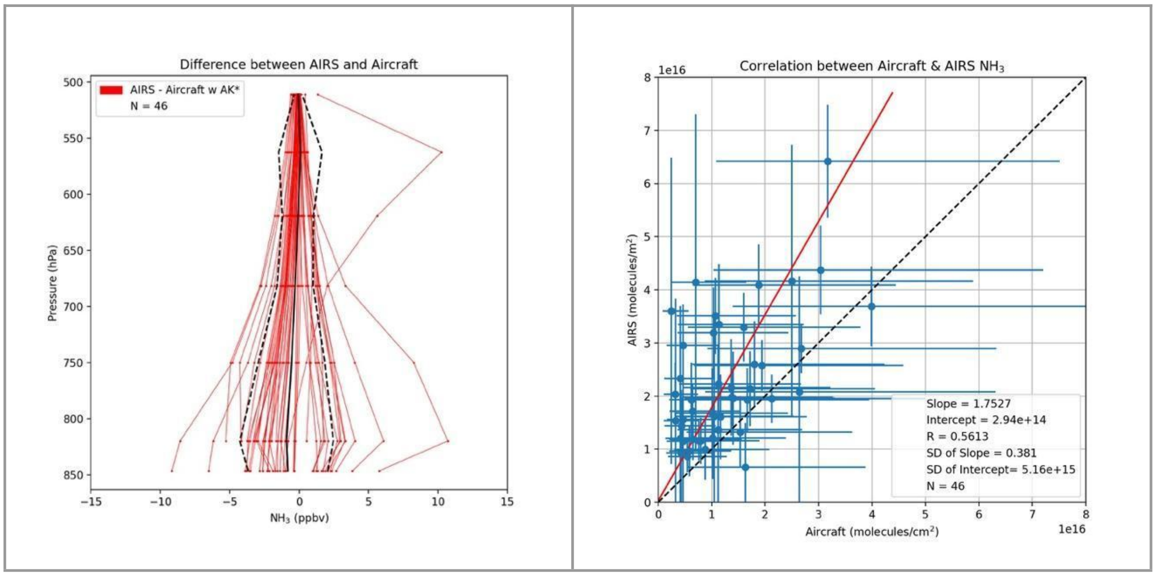

Figure 3. NH_3 from the DISCOVER-AQ campaign in Colorado (2014); AIRS-aircraft profile differences (left) and total column scatter plot (right).

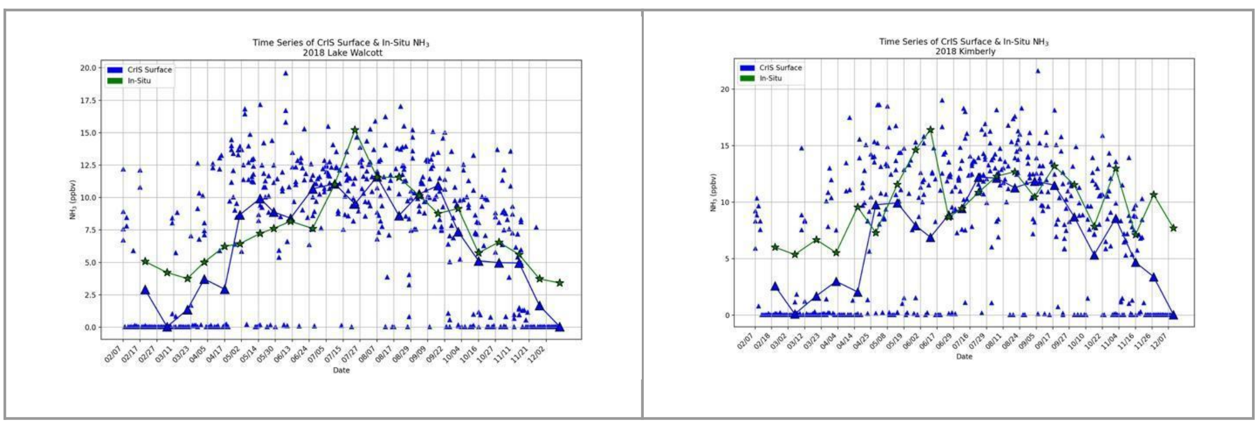

Figure 4: Time series of surface NH_3 from CrIS (daily and averaged) and two monitoring sites (two week means) in 2018.

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	562.3420
9	510.8980
10	464.1600
11	383.1170
12	316.2270
13	261.0160
14	215.4440
15	0.1000

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