

# *TROPESS Ammonia*

## *Level 2 Summary Data Product User Guide*

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### **Table of Contents**

<b>1</b>	<b><i>Introduction.....</i></b>	<b><i>2</i></b>
1.1	<b><i>Overview and Document Scope.....</i></b>	<b><i>2</i></b>
1.2	<b><i>Dataset Description.....</i></b>	<b><i>2</i></b>
1.3	<b><i>Filename.....</i></b>	<b><i>3</i></b>
<b>2</b>	<b><i>Product File Contents and Parameter Description.....</i></b>	<b><i>3</i></b>
2.1	<b><i>Variables included in the L2 Summary Product.....</i></b>	<b><i>3</i></b>
<b>3</b>	<b><i>How to Compare TROPESS NH3 columns to aircraft or model fields.....</i></b>	<b><i>5</i></b>
3.1	<b><i>Evaluating the TROPESS NH3 sensitivity.....</i></b>	<b><i>6</i></b>
<b>4</b>	<b><i>References.....</i></b>	<b><i>6</i></b>
<b>4</b>	<b><i>Validation Summary.....</i></b>	<b><i>7</i></b>
<b>2</b>	<b><i>Appendix A. Bias correction and quality flags.....</i></b>	<b><i>7</i></b>
<b>3</b>	<b><i>Appendix B. Retrieval levels.....</i></b>	<b><i>7</i></b>
<b>4</b>	<b><i>Acknowledgement.....</i></b>	<b><i>8</i></b>

# 1 Introduction

## 1.1 Overview and Document Scope

This document is to be used as a “Quick Start “user guide for using the TROPESS Level 2 Summary Product Files for ammonia (NH<sub>3</sub>).

## 1.2 Dataset Description

This user guide describes the TROPESS Level 2 Summary Product Files for ammonia (NH<sub>3</sub>).

Table 1: Dataset Description

Product Information	Description
Parameters	See Table 2, in section 2.1
Data Product Provenance	Refer to ReadMe document, section 1.3.4 Algorithm Version
Approximate file size	11MB CrIS, 7MB AIRS
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 Summary 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 NH <sub>3</sub> 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 column AK for total column NH <sub>3</sub> .
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 NH <sub>3</sub> 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.
Observational uncertainty	Observational uncertainty on the columns varies from 10 to 50%, with larger uncertainties on smaller amounts.
Validation Stage	Stage 1, according to NASA guidelines <a href="https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels">https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels</a>
Retrieval Levels	15 levels from surface to TOA
FillValues	-999
Retrieval terminology	Retrieval terminology is defined in TES ATBD <a href="#">TROPESS ATBDv1.1.pdf (nasa.gov)</a>

### 1.3 Filename

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

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

**Example:**

```
TROPESS_CrIS-SNPP_L2_Summary_CO_20200912_MUSES_R1p10_FS_F01.nc
```

## 2 Product File Contents and Parameter Description

### 2.1 Variables included in the L2 Summary Product

All data fields in NH3 summary products are shown in Table 2.

Table 2. Data Fields

Data Field Name	Long_Name/Description	Type	Dimensions	Undefined Value	Units
longitude	longitude of earth view target center	float	target	-999.0	degrees_east
latitude	latitude of earth view target center	float	target	-999.0	degrees_north
time	Earth view target mid time as International Atomic Time (TAI) seconds since 1993-01-01 00:00:00	double	target	-999.0	seconds since 1993-01-01 00:00:00
datetime_utc	UTC expressed as an array of integers year, month, day, hour, minute,	int	target, datetime_utc_dim	-999	1

Data Field Name	Long_Name/Description	Type	Dimensions	Undefined Value	Units
	second				
year_fraction	Year plus fraction of the year	double	target	-999.0	year
altitude	Altitude at each target	float	target, level	-999.0	m
pressure	Atmospheric pressure used for retrieval at each target.	float	target, level	-999.0	hPa
target_id	Unique id that identifies observations across all product files.	long	target	-999	1
x	Volume mixing ratio (VMR) of Ammonia relative to dry air	double	target, level	-999.0	1
xa	A priori profile, as volume mixing ratio (VMR) relative to dry air	float	target, level	-999.0	1
col	Vertically integrated ammonia total column	double	target	-999	mol m-2
col_error	Observational uncertainty of the vertically integrated ammonia total column	double	target	-999	mol m-2
col_dry_air	Vertically integrated dry air total column	double	target	-999	mol m-2
ak_col	Linearized column averaging kernel for the column; from the surface	double	target, level	-999	mol m-2

Data Field Name	Long_Name/Description	Type	Dimensions	Undefined Value	Units
	to Top of Atmosphere (TOA); Applies to `col`				
pwf_col	Full pressure weighting function. Set of coefficients used for calculating the column volume mixing ratio average; from the surface to Top of Atmosphere (TOA).	double	target, level	-999	1
land_flag	If target is over land == 1, otherwise == 0	Int	target	-999	N/A
day_night_flag	If target is during the day == 1, otherwise == 0	Int	target	-999	N/A

### 3 How to Compare TROPESS NH3 columns to aircraft or model fields

Comparisons between remotely sensed data and *in situ* measurements or vertically-resolved model fields should account for the vertical sensitivity of the remotely sensed measurement and its uncertainty. Otherwise, the error will be larger than the observation error that is provided with this product, since the smoothing error, the error due to relatively limited vertical resolution of the retrieval, is not included in the observation error

An observation operator, which explicitly accounts for this sensitivity and facilitates comparisons with models and independent data, is applied in the following manner:

- 1) Select the NH<sub>3</sub> profile using the model or aircraft fields (for the purpose of this demonstration called  $\mathbf{x}_{true}$ ).

- 2) Construct the operation operator as the following:

$$H(\cdot) = h^T x_a + a^T (\cdot - x_a)$$

where: **h** is the pressure weighting function, denoted as `pwf_col` in the product file;  $x_a$ , the a priori profile; **a**, the column averaging kernel, denoted as `ak_col` in the product file.

- 3) Apply observation operator to the NH<sub>3</sub> "true" profile:

$$\hat{x}_{true} = H(x_{true})$$

This will provide the column in mol/m<sup>2</sup>. Should the user wish to use units of molecules/cm<sup>2</sup> **h** should be multiplied by `col_dry_air` and **a** by 6.022141e19, as presented in the product file.

- 4) Compare:  $\hat{x}_{true}$  to the satellite result,  $\hat{x}$ , denoted as `x_col` in the product file. The difference

$$\epsilon = \hat{x}_{true} - \hat{x}$$

Now accounts for the prior information and limited sensitivity in the retrieval. Differences larger than the predicted error, denoted as `x_col_error` in the file, are statistically significant.

### 3.1 Evaluating the TROPESS NH3 sensitivity

The column averaging kernel, called `ak_col`, incorporates both the pressure weighting function and the sensitivity of the retrieval to the distribution of the state. To investigate the sensitivity alone, calculate

$$a\_norm = ak\_col / pwf\_col$$

The term `a_norm` is the sensitivity versus pressure. A value of 1 for `a_norm` means perfect sensitivity, whereas a value of 0 means no sensitivity.

## 4 References

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

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## 4 Validation Summary

See L2 Standard Products User's Guide for Validation Summary.

## 2 Appendix A. Bias correction and quality flags

The data in the L2 Summary Products have been pre-filtered for quality and bias corrected. See L2 Standard Product Use's guides for definitions.

## 3 Appendix B. 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

## 4 Acknowledgement

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