*National Aeronautics and Space Administration*
*Goddard Earth Science Data Information and Services Center (GES DISC)*

# NASA S-NPP ESSPA-Ammonia Level-2 Products User Guide: File Format and Definition

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Product Version 1.0

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# Revision History

| ***Software Version*** | ***Revision Date*** | ***Changes*** | ***Author*** |
|---|---|---|---|
| v01_37_02 | 2020-07-21 | Initial Release | Evan Manning |

# 1.0 Introduction

This document provides basic information for using the Version 1 Level-2 ESSPA-NH3 product from the Cross-track Infrared and Microwave Sounding Suite (CrIMSS) instruments on the Suomi-NPP spacecraft. The CrIMSS instrument suite consists of the Cross-track Infrared Sounder (CrIS) infrared sounder and the Advanced Technology Microwave Sounder (ATMS) microwave sounder.

The products result from the Earth System Science Profiling Algorithm (ESSPA) ammonia retrieval algorithm (ESSPA-NH3). The approach of this algorithm is briefly described in Section 2.2.

The main Level-2 retrieval product contains ammonia vertical profiles arranged according to CrIS horizontal observation geometry for six minutes of observations. Only infrared observations are used directly in the ESSPA algorithm to derive ammonia concentrations, but ATMS is also used in the Community Long-term Infrared Microwave Combined Atmospheric Processing System (CLIMCAPS) algorithm, which provides the background atmospheric state. The products have been annotated with both file and variable level attributes to fully describe their contents.

## 1.1 Overview of Sounder SIPS

The Suomi-National Polar-Orbiting Partnership (S-NPP) Sounder SIPS, is one of six SIPSs formed by NASA to provide the processing of level 0 data through level 1, level 2 and level 3 from the Suomi NPP (previously known as NPP) satellite. The Suomi-NPP satellite is managed by the National Polar-orbiting Partnership (NPP) which includes elements from NASA, NOAA and DoD. Details about the S-NPP Mission can be found at: https://www.jpss.noaa.gov/

The S-NPP Sounder SIPS is a team made up of the Jet Propulsion Laboratory (JPL) and the Goddard Earth Sciences Data and Information Services Center (GES DISC). JPL provides the overall project management, science algorithm software integration, test and validation support. The GES DISC performs level 0 data acquisition and routine data processing operations. The GES DISC / Distributed Active Archive Center and distribution of the data products and associated documentation.

## 1.2 Mission Description

The S-NPP satellite was launched on October 28, 2011 from Vandenburg Air Force Base in California into an orbit with an altitude of 824 km above the Earth surface, an inclination angle of 98.7 deg and a 13:30 local time ascending node [Reference 1]. SNPP is the first in a series of next generation U.S. weather satellites of the Joint Polar Satellite System (JPSS). CrIMSS (CrIS and ATMS) are two of the five instruments onboard the S-NPP satellite. The

other instruments are: Clouds and the Earth's Radiant Energy System (CERES), Ozone Mapping and Profiler Suite (OMPS) and Visible Infrared Imaging Radiometer Suite (VIIRS).

Table 1.2.1 contains a summary of platform parameters.

**Table 1.2.1 Approximate S-NPP orbital parameters.**

| Platform | Alt | Orbit Incl. (°) | Equator X Time | Period | Repeat Orbits | Repeat Days | Launch |
|---|---|---|---|---|---|---|---|
| **S-NPP** | 824 | 98.7 | 13:30* | 101 | 228 | 16 | 28 Oct 2011 |

# 1.3 CrIS Instrument Description

The Cross-track Infrared Sounder (CrIS) is a Fourier Transform Spectrometer (FTS) which measures interferograms in three Infrared (IR) bands simultaneously. The CrIS interferometer includes a beamsplitter, a stationary and moving mirror, and a laser sampling system. The scene radiance entering the interferometer is split by the beamsplitter into two beams along two separate paths. One beam travels towards the moving mirror; the other to a stationary mirror. The two beams are reflected from the corresponding mirrors and recombine before converging on the detector. The optical path difference (OPD) traveled by the two beams is twice the physical path difference between the two mirrors. As the moving mirror sweeps from one side of the zero path difference (ZPD) to the other, a time-varying interference pattern known as the interferogram is recorded. A convolution of the interferogram with a Finite Impulse Response (FIR) numerical filter is applied in real-time on the spacecraft to reduce the internal data rate to meet telemetry requirements. This results in a complex-valued interferogram of a fixed number of sample points which is included in the downlinked data packets.

During a single scene scan mirror dwell period, one interferogram is recorded for each of 27 detectors simultaneously (3 focal planes (LW, MW, SW) each containing 9 bore-sighted detectors in a 3x3 pattern). The CrIS uses a 45-degree scene scan mirror to provide sequential views of an internal blackbody (ICT), a deep space view (DS), and 30 Earth views in the cross-track direction in a repeating pattern as the spacecraft moves along-track. The interferograms associated with the ICT and DS views and a measurement of ICT temperature are used in the ground processing software to calibrate the Earth views to produce radiance spectra. Prior to calibration, a correction is applied to account for measured signal nonlinearity of selected detectors. Corrections are also applied in the ground processing software to remove FTS self-apodization effects and to resample the spectra to a predefined user spectral grid.

For the first part of the SNPP mission, the effective spectral resolution of CrIS data received from the satellite was lower in the short-wave and mid-wave infrared bands than in the longwave infrared band. Level 0 data received during this initial period is referred to as Normal Spectral Resolution (NSR). The products from this period were produced using version 1 of the CrIS Level-1B product in Normal Spectral Resolution (NSR).

## 1.4 Data Disclaimer

Version 1.0 CrIMSS Level-2 data are released to the public as is. Every effort has been made to properly represent the data which this document describes.

All users are encouraged to read the appropriate documentation listed in the references related to these data products to further understand the contents.

## 1.5 Where to find the Product

The S-NPP Level-2 ESSPA-Ammonia products can be found at and downloaded from the NASA GES DISC. First time users are asked to register and create an EARTHDATA login account to access the GES DISC collections. There you will find additional information and documentation about this product and other products of interest. The preferred method to locate a data collection is via the unique Digital Object Identifier (DOI) link [see Table 1.5].

Alternatively, users can enter the ShortName directly into the EARTHDATA search string to quickly find CLIMCAPS level 2 products. The data at the GES DISC is organized by unique versioned ShortNames. Some just doing a general search can enter the string "Suomi-NPP CrIS NH3" (with quotes) under Data Collections.

NASA EARTHDATA login: https://disc.gsfc.nasa.gov

**Table 1.5 ECS ShortName and DOI**

| ShortName.version | DOI | Description |
|---|---|---|
| SNDRSNIL2ESPNH3_1 | 10.5067/EHW76N16L83M | Suomi NPP CrIS Level 2 ESSPA-Ammonia Normal Spectral Resolution V1 |
| ***Related data sets at GDAAC*** | | |
| | | |
| SNDRSNIML2CCPRETN.1 | 10.5067/6U9XTLE2XOTA | CLIMCAPS Level-2 retrieved product |
| TBD | | SNPP global, geolocated, granule maps |

## 1.6 Contact Information

For information, questions or concerns with this S-NPP CrIS Level-2 data set, please contact:
Ruth Monarrez at Ruth.Monarrez@jpl.nasa.gov or send your questions or comments to: sounder.sips@jpl.nasa.gov.

# 1.7 References

1. S-NPP Crosstrack Infra-red Sounder (CrIS) ESSPA-Ammonia (NH3) Retrieval Algorithm Theoretical Basis Document (ATBD)

2. NASA SNPP Cross Track Infrared Sounder (CrIS) Level 1B Product Users' Guide

3. Data Product User Guide for S-NPP Sounder SIPS CHART and CLIMCAPS CrIS and ATMS Level-2 Products

4. Shephard, M. W. and K.E. Cady-Pereira: Cross-track Infrared Sounder (CrIS) satellite observations of tropospheric ammonia, Atmos. Meas. Tech., 8, 1323-1336, doi:10.5194/amt-8-1323-2015, 2015.

5. Moncet, J.-L, Uymin G., Lipton A. E., and Snell H. E.: Infrared radiance modeling by optimal spectral sampling. J. Atmos. Sci., 65, 3917-3934, 2008.

6. NetCDF Climate and Forecast (CF) Metadata Conventions, Version 1.7, http://cfconventions.org/Data/cf-conventions/cf-conventions-1.7/cf-conventions.html

# 2.0 ESSPA-NH3 Level-2 Product Overview

## 2.1 Product Granulation and Identification

The Level-2 products are divided into a series of 6-minute segments or granules with each granule making up one file and 240 granules per day. Each file contains all observations for a given type made during a period of exactly 6 minutes. For each day, each 240 files are identified by granule number in the filename. For example, **g156** for granule 156 out of 240.

The nominal start time of granule 1 is defined to be 00:00:00. Because both CrIS and ATMS instruments are synced to TAI93, the start time of the first 8-second scanset of a day can be anywhere up to 8 seconds later. It moves 1 second with each leap second. If the first scanset starts 8 seconds after the nominal start time, then the data can extend up to 8 seconds past the nominal end time.

The ability to uniquely identify a granule is built in to the Level-1B and Level-2 products. This is extremely useful when publishing analysis results. The nominal time coverage, represented as a string: yyyymmddThhmm, is used to construct a unique granule identifier called "gran_id". gran_id is stored as a global attribute that is also used in the filename, see section 2.6 File Naming Convention.

In addition, there is an observation identifier variable called "obs_id" that can further uniquely identify an observation within the granule. The obs_id is formatted as the gran_id with observation information appended to it. Because of the different viewing geometry, ATMS and CrIS obs_ids differ. Level-2 ESSPA ammonia obs_ids follow the CrIS pattern because their retrieved information corresponds to CrIS geometry.

CrIS/Level-2 obs_id: Each field of regard (FOR), defined as a set of 9 simultaneously observed fields of view, has a globally unique ID stored in the variable "obs_id". The observation ID is created from the granule ID, with information appended to identify the FOR observation within the granule.

The dimensions of this variable (atrack=45, xtrack=30) correspond to the first two dimensions of the science data variables, such as radiances. An observation ID can be associated with data by applying the same indices into these common dimensions.

The format of the CrIS/Level-2 observation ID string is "yyyymmddThhmm.aaExx", where "aa" is the 2- digit along-track index (01-45), and "xx" is the 2-digit cross-track index (01-30). The "E" indicates that it is an earth view.

For example:

20160125T1300.01E18

FOV Observation ID: At the finest level of granularity, each field of view (FOV) within a FOR observation has a globally unique ID that is stored in a variable called "fov_obs_id". The FOV observation ID is created from the observation ID, with extra information appended to identify the FOV within the FOR observation.

The dimensions of this variable (atrack=45, xtrack=30, fov=9) correspond to the first three dimensions of the science data variables, such as radiances. A FOV observation ID can be associated with data by applying the same indices into these common dimensions.

The format of the FOV observation ID string is "yyyymmddThhmm.aaExx.f" where "f" is the 1-digit FOV number (1-9).

For example:

20160125T1300.01E18.6

## 2.2 Algorithm Background

ESSPA is a retrieval framework developed by AER; it uses an optimal estimation (OE) approach with the AER Optimal Spectral Sampling (OSS) (Moncet et al., 2008) code as a forward model.

ESSPA-NH3 obtains the background atmospheric state from the CLIMCAPS L2 product, then uses a specific configuration of input files to derive surface temperature and emissivity and ammonia from CrIS radiances. The algorithm is indifferent to the resolution of the CrIS L1b data (NSR or FSR), as the spectral range required is always at FSR resolution.

The ESSPA-NH3 retrieval reads an estimation of the atmospheric state from the CLIMCAPS Level-2 retrieval at each FOR, and the observed cloudy radiances from CrIS Level-1B. It then populates each FOV within the FOR with the L2 data. Next a surface temperature and emissivity retrieval is carried out for each FOV: this step seeks to reduce any offset in the residuals around the ammonia spectral feature; it is not designed to produce accurate surface temperature estimates. This adjusted surface temperature replaces the surface temperature from CLIMCAPS. The code then determines the strength of the ammonia signal using an on/off BT difference test, selects the ammonia a priori profile from a set of three possible profiles, and performs an optimal estimation retrieval of ammonia using data from the Q branch of ammonia $\nu_2$ band (between 960 and 970 $cm^{-1}$).

## 2.3 Data Organization

The Level-2 products are divided into a series of 6-minute segments with one segment per file. Each file contains all observations of a given type made during a period of exactly 6

minutes. For each day there are 240 files (also known as granules), identified by granule number in the filename. For granule start time details, refer to section 2.1.

## 2.4 File Format and Structure

The files are in Network Common Data Form, version 4 (netCDF4/HDF5) format.

The product format takes advantage of the netCDF4 data model and makes use of groups, dimensions, variables and attributes to fully describe the science data. See section 3.0 Data Content for a listing of key dimensions and attributes.

## 2.5 Metadata

Every effort has been made to ensure that metadata conforms to the Climate and Forecasting (CF), Version 1.6, and Attribute Conventions for Data Discovery (ACDD), Version 1.3, guidelines.

See the full product specifications in Appendix B.

For more information on CF, refer to: http://cfconventions.org/

For more information on ACDD, refer to:
http://wiki.esipfed.org/index.php?title=Category:Attribute_Conventions_Dataset_Discovery

## 2.6 File Naming Convention

File naming for Sounder SIPS products will be unique and include the following tokens separated by the delimiter '.' For each token that makes up the filename, there will be an attribute in the data product that it maps to indicated in [ ].

<Sounder_SIPS_ID>.<platform>.<inst_ID>.<granuleID>.<product_granularity>.<granule_number>.<product_type>.<variant>.<version>.<production_location>.<prod_timestamp>.<extension>

Where:

- **Sounder_SIPS_ID** is the project identifier [product_name_project] = SNDR
- **platform** [product_name_platform] = SNPP
- **inst_ID** [product_name_instr] = CRIS
- **granuleID** (yyyymmddThhmm) [gran_id] nominal start time where:
  - yyyy = year
  - mm = month of year (01-12)
  - dd = day of month (01-31)
  - hh = hour (00-24)
  - mm = minute (00-59)

- **product_granularity** [product_name_duration]= m06 (6 minute)
- **granule_number** [granule_number]= g###
- **product_type** with an optional identifier for testing [product_type_name_id]
  - L2_ESSPA_NH3_RET
- **variant** [product_name_variant] = std
- **version** vmm_mm [product_name_version] - eg. v01_34
  - Versioning will be synchronized across Sounder SIPS products
  - Version 1 Level-2 products are derived from version 1 Level-1B products
- **production_location** [product_name_producer]- J=SIPS at JPL, G=Operations, T=Test, W = CrIS Team at Univ of Wisc
- **prod_timestamp** so each product has a unique name (yymmddhhmmss) [product_name_timestamp]- 150407123456
- **Extension** (.nc)

Example Filename: 6-minute SNPP CrIS ESSPA ammonia Level-2 granule

SNDR.SNPP.CRIS.20160114T1248.m06.g129.L2_ESSPA_NH3_RET.std.v01_34_00.J.190523213454.nc

## 2.7 Time Representation

Times in the Level-2 products are generally represented as UTC. However, observation times are provided in both UTC and TAI93 representations as a convenience to users.

Coordinated Universal Time (UTC) is the international standard for representation of time. UTC times are expressed in human-readable form, as a set of values indicating year, month, day, hour and so on. In the data stream received from the satellite, observation times are represented as UTC.

Timestamps in product filenames and attributes are represented as UTC and formatted according to the "ISO 8601:2004" standard. For example, the time January 25, 2016 at 13:00 may be represented as either of the following:

2016-01-25T13:00Z
20160125T1300

The longer form is used in attributes, and the more compact form is used in filenames. The character "Z" indicates "Zulu time", or UTC.

**International Atomic Time (TAI)** is expressed as number of seconds elapsed on the surface of the Earth since some reference UTC time. The term "TAI93" indicates that the reference time is the beginning of the year 1993, or 1993-01-01T00:00:00Z. This reference time was chosen to be consistent with data products from other instruments, and to allow for precise representation of times spanning the expected mission length.

## 2.8 Data Holdings

For the initial release of v1 ESSPA-NH3, a test data set of 8 months of data is provided. This data covers the months of {January, April, July, October} of the years 2013 & 2015. This set is designed to allow research and comparisons over a full seasonal cycle and comparisons of different phases of the ENSO cycle.

# 3.0 Data Content

The Level-2 data products are written in netCDF4 format and therefore make use of groups, dimensions, variables and attributes (global & variable). Every netCDF4 file contains, at a minimum, one root group which is unnamed.

Attention should be given to quality flags and checked for fill values before being used for any analysis or higher processing of the product.

A full profile of the contents of the files is included in Appendix B.

Selected fields are highlighted in this section.

## 3.1 Dimensions

Key dimensions for ESSPA-NH3 products.

**Table 3.1 Key Dimensions**

| Name | Size | Description |
|---|---|---|
| **atrack** | 45 | along-track spatial dimension |
| **xtrack** | 30 | cross-track spatial dimension |
| **fov** | 9 | Field-of-view dimension |
| **air_pres_nh3** | 21 | Reporting atmospheric pressure levels for ammonia |

## 3.2 Global Attributes (metadata)

There are two types of attributes: global & variable. In this section we will talk about global attributes. Global attributes, sometimes referred to as 'file-level attributes', provide information about the entire file or 6-minute granule. This includes observation times, publisher and creator information, data provenance, and location information. Many attributes are required to conform to the CF & ACDD standards while other attributes are written for consistency with legacy products.

A full definition of the global attributes can be found in Appendix B.

**Table 3.2.2 Key Global Attributes**

| Name | Description |
|---|---|
| **date_created** | The date on which this version of the data was created |
| **geospatial_lat_min** | The southernmost latitude covered by the dataset |
| **geospatial_lat_max** | The northernmost latitude covered by the dataset |
| **geospatial_lon_min** | The westernmost longitude covered by the dataset. See also geospatial_lon_max. |

| | |
|---|---|
| **geospatial_lon_max** | The easternmost longitude covered by the dataset. Cases where geospatial_lon_min is greater than geospatial_lon_max indicate the bounding box extends from geospatial_lon_max, through the longitude range discontinuity at the antimeridian, to geospatial_lon_min; for example, geospatial_lon_min=170 and geospatial_lon_max=-175 incorporates 15 degrees of longitude (ranges 170 to 180 and -180 to -175). |
| **geospatial_lat_mid** | granule center latitude |
| **geospatial_lon_mid** | granule center longitude |
| **geospatial_bounds** | Describes the data's 2D or 3D geospatial extent in OGC's Well-Known Text (WKT) Geometry format. Longitude values are limited to the (-180, 180) range. Example: 'POLYGON ((40.26 -111.29, 41.26 -111.29, 41.26 -110.29, 40.26 -110.29, 40.26 -111.29))'. |
| **product_name_granule_number** | zero-padded string for granule number of day (g001-g240) |
| **gran_id** | Unique granule identifier yyyymmddThhmm of granule start, including year, month, day, hour, and minute of granule start time |
| **identifier_product_doi** | digital signature (DOI) |
| **AutomaticQualityFlag** | "Passed": the granule contains a non-degraded retrieved value in a geolocated FOV; "Suspect": the granule does not qualify as "Passed" but contains a (possibly degraded) retrieved value (possibly without associated geolocation); "Failed": the granule contains no retrieved values. “Missing” is a default value in the template that you should never see in the product unless something went seriously wrong. |
| **qa_no_data** | A simple indicator of whether this is an "empty" granule with no data from the instrument. "TRUE" or "FALSE". |

## 3.3 Variable Attributes

Each variable has its own associated attributes. Variable attributes are a CF standard and are used to describe the variable in more detail to properly interpret its value.

**Table 3.3: Variable Attributes**

| Attribute | Description |
|---|---|
| **units** | units, for variables that represent physical quantities |
| **_FillValue** | a single sentinel value indicating the data point contains fill instead of valid data |
| **standard_name** | standard name from the CF standard name table, if one exists for the quantity being represented |
| **long_name** | a longer name describing the quantity being represented, suitable for a plot title |
| **description** | a longer description of the quantity being represented |
| **valid_range** | a pair of values indicating the minimum and maximum values to be considered valid |
| **coordinates** | a space-separated list of the names of other variables that are coordinates for this variable |
| **coverage_content_type** | ACDD/ISO field categorizing types of data:<br>• image<br>• thematicClassification<br>• physicalMeasurement<br>• auxillaryInformation<br>• coordinate<br>• modelResult<br>• qualityInformation<br>• referenceInformation<br>https://geo-ide.noaa.gov/wiki/index.php?title=ISO_19115_and_19115-2_CodeList_Dictionaries#MD_CoverageContentTypeCode |
| **ancillary_variables** | a space-separated list of the names of other variables that contain information about this variable |
| **bounds** | defines the extent, for cell variables |
| **cell_methods** | describes statistical methods used to derive data, for cell variables |
| **flag_values** | These attributes collectively tell how to interpret flag variables. See the CF standard for details. In these Level-2 products, these attributes are mostly used in association with the *_qc QC ancillary variables. |
| **flag_meanings** | |
| **flag_masks** | |

## 3.4 Group Structure

One feature which was added to netCDF4 is the ability to structure files with "groups", which are similar to a directory hierarchy. SounderCDF files are designed so that all of the most commonly needed information is contained in "/", the root group. Subgroups contain more specialized information.

These are the groups for ESSPA-NH3 files:

| Group | Purpose |
|---|---|
| **/ (root)** | Main group, with ammonia profiles, along with supporting location and quality information |
| **/aux** | Supporting information primarily for the algorithm developers |

## 3.5 Geolocation

Geolocation parameters are used for determining location of each observation on Earth and associated information about that location.

Geolocation variables are located in the file at the root level. These include latitudes and longitudes associated with each observation, as well as satellite and solar geometry information, spacecraft position and orbital characteristics, surface information and related metadata.

**Table 3.5.1 Geolocation Dimensions**

| Dimension name | Size | Meaning |
|---|---|---|
| atrack | 45 | Along-track FOR horizontal dimension |
| xtrack | 30 | Cross-track FOR horizontal dimension |
| fov | 9 | CrIS FOV dimension within FOR |
| fov_poly | 8 | latitude/longitude points defining the polygon bounding an fov (anticlockwise as viewed from above) |

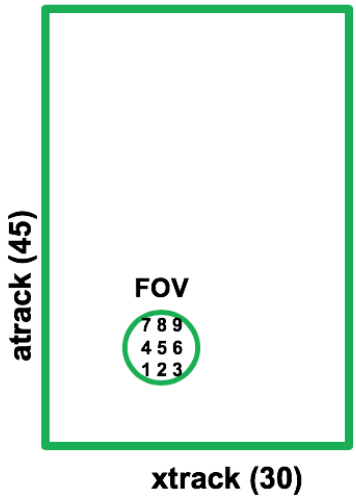


**Figure 1. geolocation horizontal dimensions**

The key geolocation variables are:

**Table 3.5.2 Key FOV Geolocation Variables**

| Geolocation Variable | Dimensions | Meaning |
|---|---|---|
| lat | atrack, xtrack, fov | latitude of FOV center |
| lon | atrack, xtrack, fov | longitude of FOV center |
| lat_bnds | atrack, xtrack, fov, fov_poly | latitude of FOV bounding polygon |
| lon_bnds | atrack, xtrack, fov, fov_poly | longitude of FOV bounding polygon |
| land_frac | atrack, xtrack, fov | Land fraction over the FOV |
| surf_alt | atrack, xtrack, fov | mean surface altitude WRT Earth model over FOV |
| obs_time_tai93 | atrack, xtrack | earth view observation midtime for each fov in units of seconds since 1993-01-01T00:00:00 |
| obs_time_utc | atrack, xtrack, utc_tuple | UTC earth view observation time as an array of integers: year, month, day, hour, minute, second, millisecond, microsecond |

Full geolocation includes information about solar geometry (sol_zen, sol_azi, sun_glint_dist), viewing geometry (sat_zen, sat_azi, view_ang, sat_range, subsat_lat, …) and orbital parameters. See Appendix B for full specification.

One key feature is boundaries. Each FOV has a bounding 8-point polygon in variables {lat_bnds, lon_bnds}. This makes it easy to place values in appropriate regions on a map, including the distorted shapes of FOVs at the edges of the swath.

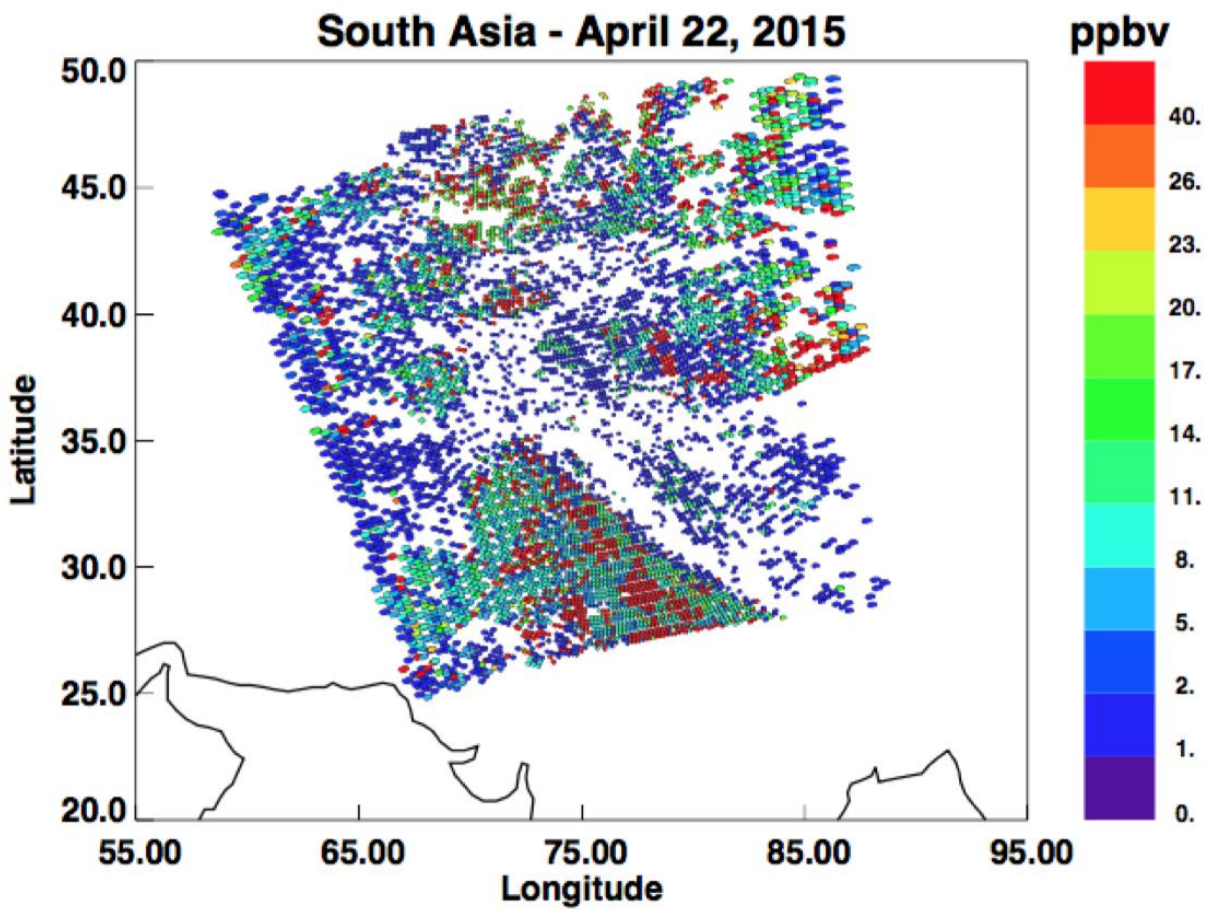


**Figure 2. Sample plot of retrieved CrIS $NH_3$ using bounding polygons**

## 3.6 Science Data Variables

The key retrieved quantities are all related to ammonia: nh3_tot, nh3_mmr, surf_nh3_mmr.

Many variables have associated quality control and error estimate information. These are contained in variables with the same name but with "_qc" and "_err" appended. For example the ammonia profile is contained in a variable named "nh3_mmr"; its error estimate is in "nh3_mmr_err" and its quality control is "nh3_mmr_qc". The "ancillary_variables" variable attribute of nh3_mmr lists "nh3_mmr_qc, nh3_mmr_err". In the tables below the ancillary variables are not listed explicitly. They are indicated in the "ancillary variables" column.

Key science data fields are defined below. See the appendixes for a full listing.

**Table 3.6.1 Key RET Science Data Variables**

| Name | Type | Dimensions | Description | Units | Ancillary Variables |
|---|---|---|---|---|---|
| nh3_tot | float32 | atrack, xtrack, fov | Total column ammonia | kg m-2 | err, qc |
| nh3_mmr | float32 | atrack, xtrack, fov, air_pres_nh3 | ammonia mass mixing ratio to dry air | unitless | err, qc |
| surf_nh3_mmr | float32 | atrack, xtrack, fov | near-surface ammonia mass mixing ratio to dry air (~2 meters above surface) | unitless | err, qc |
| nh3_dof | float32 | atrack, xtrack, fov | The trace of the averaging kernel matrix as a measure of the number of pieces of information about the ammonia profile provided by the physical retrieval step. | unitless | |

## 3.7 Quality Information

For most retrieved geophysical variables, a numerical error estimate in the same physical units is provided in a corresponding ancillary_variable with a name ending in "_err". There are also Quality Control (QC) scores of {0, 1, 2} in corresponding ancillary_variables with a name ending in "_qc".

**Table: 3.7.1 *_qc Values**

| Value | Meaning |
|---|---|
| **0** | Highest quality – use without reservation |
| **1** | Good quality – suitable for most purposes |

| | |
|---|---|
| **2** | Do not use. In some cases a physical value is present but is not considered reliable. In other cases only fill values are present. |

For ESSPA ammonia, quality flags are determined internally using thresholds on degrees of freedom (nh3_dof) and nh3_signal_strength. The same value is used for ammonia column total and for ammonia mixing ratio for all levels above the surface.

Q0 data should be used when low uncertainty is important, e.g., when validating against in situ data.

Q0 and Q1 data should be used when having a larger dataset is more important than having data with low uncertainty. More data allows the user to reduce the "noise" in the data. Thus a user looking for means over seasons or large regions should use Q0 and Q1 data.

In addition to the _qc and _err variables, there are other indicators of quality. nh3_dof are degrees-of-freedom for retrievals of ammonia. In the /aux subgroup there are more detailed internal quality indicators including chi-squared, RMS residual, ammonia signal strength, and the diagonal of the error covariance matrix.

## 3.8 Missing Data / Fill Values

Fill values are used where there is no valid data, including profiles level with pressures greater than the surface pressure. The fill value is indicated by the attribute '_FillValue'. It is advised to check the data for fill values before it is used. The fill values per variable datatype are listed in the table below.

**Table: 3.8.1 Fill Values**

| Variable Type | Fill Value |
|---|---|
| **unsigned 8-bit integer** | 255UB |
| **unsigned 16-bit integer** | 65535US |
| **unsigned 32-bit integer** | 4294967295U |
| **floating point** | 9.96921e+36 |

## 3.9 Key supporting information variables for profiles

These variables provide supporting information to interpret the science variables.

| Name | Dimensions | Description | Units |
|---|---|---|---|
| **air_pres_nh3** | air_pres | 21 Fixed pressure levels for reporting ammonia | Pa |

| | | | |
|---|---|---|---|
| **air_pres_nh3_nsurf** | atrack, xtrack, fov | Index in air_pres_nh3 of the level at the surface. Values at levels beyond this are invalid, representing data below the Earth's surface. | unitless |
| **aux/sig_lev_pres** | atrack, xtrack, fov, sig_lev | 101 pressures of hybrid signal levels per FOV. | Pa |

## 3.10 Known issues

Over ocean retrievals may be problematic.

# 4.0 Options for Reading the Data

The product files are written in netCDF4/HDF5. Because netCDF4 builds upon the classic netCDF data model using HDF5 as the storage layer, a user of the data product can take full advantage of tools and libraries readily available to access the data.

Every netCDF4 file is considered an HDF5 file, however, not every HDF5 file is necessarily a netCDF4 file. A limited subset of the HDF5 data model and file format features are used in netCDF4 files. Conformance to the earlier mentioned CF & ACDD standards allows for users to take advantage of most netCDF interfaces.

Tools and libraries for reading netCDF4 as well as a netCDF Users' Guide are written and maintained by Unidata and can be found online at:
http://www.unidata.ucar.edu/software/netcdf/

Panoply is a good tool for visualizing this type of files, but it doesn't handle ESSPA-NH3 very well because of the presence of 3 horizontal dimensions (atrack, xtrack, fov). You can plot one of 9 fovs at a time or preprocess the data down to 2 dims. https://www.giss.nasa.gov/tools/panoply/

There are a number of interfaces available for reading netCDF for different programming languages including: C/C++, Fortran, Matlab, IDL, Python and Perl.

The files can also be accessed with HDF5 tools and libraries available at:
https://www.hdfgroup.org/products/hdf5_tools/

There is a prototype tool that uses collocated VIIRS cloud fraction and brightness temperature to flag and reject pixels with low NH3 values. Users interested in this tool should contact the PI (kcadyper@aer.com).

# 5.0 Data Services

The products are available to the user community via the Goddard Earth Sceinces Data and Information Services Center (GES DISC). https://disc.gsfc.nasa.gov/

In addition to the netCDF data files, there you can also get daily granule maps, showing the location of each granule of each day.

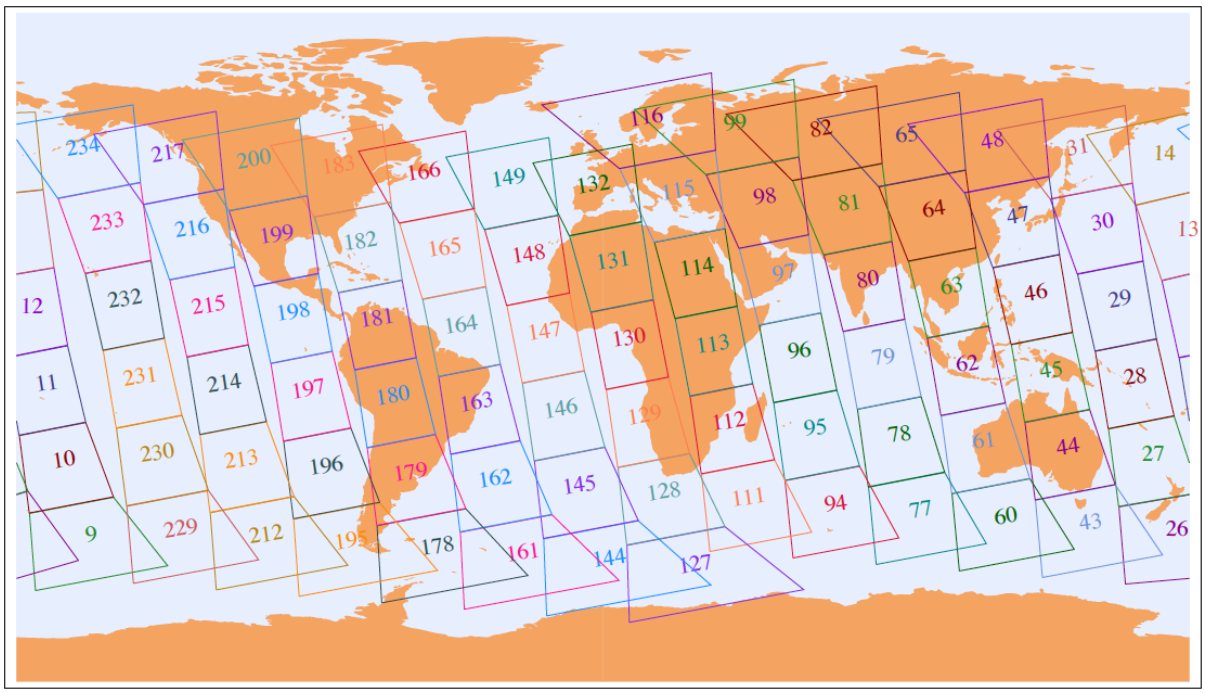


**Figure 3. Granule map for daytime data 2015-04-22, used in figures A1-1 and A1-2a.**

# Appendix A: Sample images

These images show the spatial variability in surface NH3 captured by CrIS. The figure on the left is a composite of six granules (46,47,63,64,80,81) from April 22, 2015. Note the elevated values over the Indian subcontinent, the Taklimakan desert, and the Sea of Bohai. The expected source for all of these high values is agricultural activity. The figure on the right is a composite of five granules ([110,111,126,127,144) from January 16, 2013. The elevated NH3 amounts between the Equator and 20 N are likely a product of biomass burning, which is very intense in this season. All pixels are plotted with their true shapes.

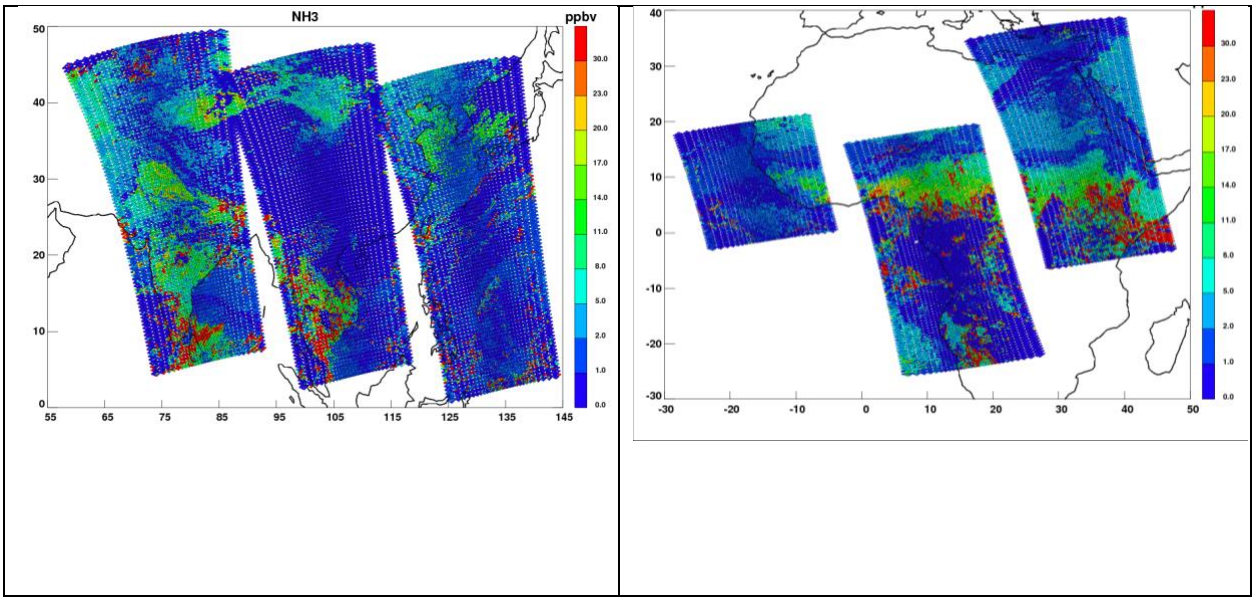


**Figure A1: Surface NH3 from CrIS: south Asia, April 22, 2015 (left); Africa, January 13, 2016 (right).**

Both figures present significant regions with very low NH3 (in dark blue). These low values may reflect low NH3 amounts; however, since NH3 is nearly always concentrated in the boundary layer, they could be due to blocking of the NH3 signals by clouds; these pixels should be rejected when the data are temporally or spatially averaged, since they may bias the results, especially over regions with frequent cloudy periods. We have developed a prototype tool that uses collocated VIIRS cloud fraction and brightness temperature to flag these pixels. The figures below illustrate the impact of rejecting these low NH3 values. Note that this algorithm does not use the VIIRS cloud mask, as this product was found to reject many pixels with reasonable NH3 values. Users interested in this tool should contact the PI (kcadyper@aer.com).

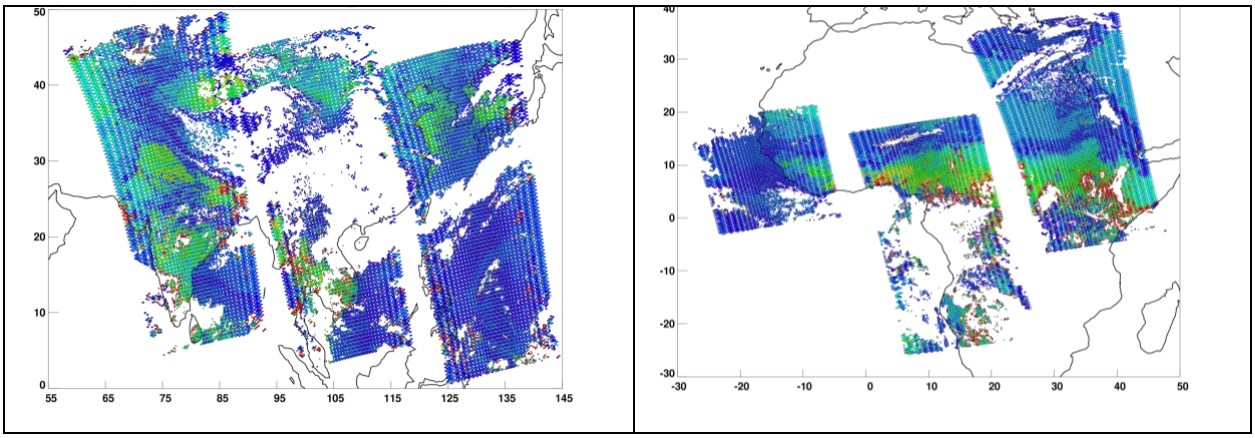


**Figure A2: Surface NH3 from CrIS with rejection of cloudy pixels: south Asia, April 22, 2015 (left); Africa, January 13, 2016 (right).**

# Appendix B: Detailed file format

These tables show all of the dimensions, global attributes, and variables in the ESSPA-NH3 product files.

For clarity, some variable attributes are omitted, including long_name, standard_name, coverage_content_type, axis, valid_range, coordinates, and _FillValue.

Ancillary variables are also omitted. The presence of “bnds” in the ancillary_variables column for “lat” means that there is also a variable named “lat_bnds”.

To get a complete listing including all variable attributes, apply “ncdump -h” to any netCDF4 product file.

# SNPP L2 ESSPA NH3 Interface Specification

Interface Specification Version 02.00.36
01-07-2020

## Global Groups

| Path | Description |
|---|---|
| / | Main science data |
| /aux | Internal product team data |

## Global Dimensions

| Name | Size | Description |
|---|---|---|
| atrack | 45 | along-track horizontal dimension |
| xtrack | 30 | cross-track horizontal dimension |
| fov | 9 | Field-of-view dimension |
| air_pres_nh3 | 21 | Coarse/fine atmospheric pressure levels for NH3 starting from the top |
| fov_poly | 8 | lat_bnds, lon_bnds points defining the polygon bounding an FOV (anticlockwise as viewed from above) |
| utc_tuple | 8 | parts of UTC time: year, month, day, hour, minute, second, millisec, microsec |
| spatial | 3 | directions: x, y, z for satellite position and velocity |
| attitude | 3 | roll, pitch, yaw |

## Global Attributes

| Name | Type | Size | Value | Description |
|---|---|---|---|---|
| keywords | string | 1 | EARTH SCIENCE > ATMOSPHERE > ATMOSPHERIC CHEMISTRY > NITROGEN COMPOUNDS > AMMONIA | A comma-separated list of key words and/or phrases. Keywords may be common words or phrases, terms from a controlled vocabulary (GCMD is often used), or URIs for terms from a controlled vocabulary (see also "keywords_vocabulary" attribute). |
| Conventions | string | 1 | CF-1.6\, ACDD-1.3 | A comma-separated list of the conventions that are followed by the dataset. |
| history | string | 1 | | Provides an audit trail for modifications to the original data. This attribute is also in the NetCDF Users Guide: 'This is a character array with a line for each invocation of a program that has modified the dataset. Well-behaved generic netCDF applications should append a line containing: date, time of day, user name, program name and command arguments.' To include a more complete description you can append a reference to an |

| Name | Type | Size | Value | Description |
|---|---|---|---|---|
| | | | | ISO Lineage entity; see NOAA EDM ISO Lineage guidance. |
| source | string | 1 | CrIS instrument telemetry | The method of production of the original data. If it was model-generated, source should name the model and its version. If it is observational, source should characterize it. This attribute is defined in the CF Conventions. Examples: 'temperature from CTD #1234'; 'world model v.0.1'. |
| processing_level | string | 1 | 2 | A textual description of the processing (or quality control) level of the data. |
| comment | string | 1 | | Miscellaneous information about the data or methods used to produce it. Can be empty. |
| acknowledgment | string | 1 | Support for this research was provided by NASA. | A place to acknowledge various types of support for the project that produced this data. |
| license | string | 1 | Limited to Sounder SIPS affiliates | Provide the URL to a standard or specific license, enter "Freely Distributed" or "None", or describe any restrictions to data access and distribution in free text. |
| standard_name_vocabulary | string | 1 | CF Standard Name Table v28 | The name and version of the controlled vocabulary from which variable standard names are taken. (Values for any standard_name attribute must come from the CF Standard Names vocabulary for the data file or product to comply with CF.) Example: 'CF Standard Name Table v27'. |
| date_created | string | 1 | Unassigned | The date on which this version of the data was created. (Modification of values implies a new version, hence this would be assigned the date of the most recent values modification.) Metadata changes are not considered when assigning the date_created. The ISO 8601:2004 extended date format is recommended, as described in the Attribute Content Guidance section. |
| creator_name | string | 1 | Unassigned | The name of the person (or other creator type specified by the creator_type attribute) principally responsible for creating this data. |
| creator_email | string | 1 | Unassigned | The email address of the person (or other creator type specified by the creator_type attribute) principally responsible for creating this data. |
| creator_url | string | 1 | Unassigned | The URL of the person (or other creator type specified by the creator_type attribute) principally responsible for creating this data. |
| institution | string | 1 | Unassigned | Processing facility that produced this file |
| project | string | 1 | Sounder SIPS | The name of the project(s) principally responsible for originating this data. Multiple projects can be separated by commas, as described under Attribute Content Guidelines. Examples: 'PATMOS-X', 'Extended Continental Shelf Project'. |

| Name | Type | Size | Value | Description |
|---|---|---|---|---|
| product_name_project | string | 1 | SNDR | The name of the project as it appears in the file name. 'SNDR' for all Sounder SIPS products, even AIRS products. |
| publisher_name | string | 1 | Unassigned | The name of the person (or other entity specified by the publisher_type attribute) responsible for publishing the data file or product to users, with its current metadata and format. |
| publisher_email | string | 1 | Unassigned | The email address of the person (or other entity specified by the publisher_type attribute) responsible for publishing the data file or product to users, with its current metadata and format. |
| publisher_url | string | 1 | Unassigned | The URL of the person (or other entity specified by the publisher_type attribute) responsible for publishing the data file or product to users, with its current metadata and format. |
| geospatial_bounds | string | 1 | | Describes the data's 2D or 3D geospatial extent in OGC's Well-Known Text (WKT) Geometry format (reference the OGC Simple Feature Access (SFA) specification). The meaning and order of values for each point's coordinates depends on the coordinate reference system (CRS). The ACDD default is 2D geometry in the EPSG:4326 coordinate reference system. The default may be overridden with geospatial_bounds_crs and geospatial_bounds_vertical_crs (see those attributes). EPSG:4326 coordinate values are latitude (decimal degrees_north) and longitude (decimal degrees_east), in that order. Longitude values in the default case are limited to the (-180, 180) range. Example: 'POLYGON ((40.26 -111.29, 41.26 -111.29, 41.26 -110.29, 40.26 -110.29, 40.26 -111.29))'. |
| geospatial_bounds_crs | string | 1 | EPSG:4326 | The coordinate reference system (CRS) of the point coordinates in the geospatial_bounds attribute. This CRS may be 2-dimensional or 3-dimensional, but together with geospatial_bounds_vertical_crs, if that attribute is supplied, must match the dimensionality, order, and meaning of point coordinate values in the geospatial_bounds attribute. If geospatial_bounds_vertical_crs is also present then this attribute must only specify a 2D CRS. EPSG CRSs are strongly recommended. If this attribute is not specified, the CRS is assumed to be EPSG:4326. Examples: 'EPSG:4979' (the 3D WGS84 CRS), 'EPSG:4047'. |
| geospatial_lat_min | float | 1 | 9.9692099683868690e+36f | Describes a simple lower latitude limit; may be part of a 2- or 3-dimensional bounding region. Geospatial_lat_min specifies the southernmost latitude covered by the dataset. |
| geospatial_lat_max | float | 1 | 9.9692099683868690e+36f | Describes a simple upper latitude limit; may be part of a 2- or 3-dimensional bounding region. Geospatial_lat_max specifies the |

| Name | Type | Size | Value | Description |
|---|---|---|---|---|
| | | | | northernmost latitude covered by the dataset. |
| geospatial_lon_min | float | 1 | 9.9692099683868690e+36f | Describes a simple longitude limit; may be part of a 2- or 3-dimensional bounding region. geospatial_lon_min specifies the westernmost longitude covered by the dataset. See also geospatial_lon_max. |
| geospatial_lon_max | float | 1 | 9.9692099683868690e+36f | Describes a simple longitude limit; may be part of a 2- or 3-dimensional bounding region. geospatial_lon_max specifies the easternmost longitude covered by the dataset. Cases where geospatial_lon_min is greater than geospatial_lon_max indicate the bounding box extends from geospatial_lon_max, through the longitude range discontinuity meridian (either the antimeridian for -180:180 values, or Prime Meridian for 0:360 values), to geospatial_lon_min; for example, geospatial_lon_min=170 and geospatial_lon_max=-175 incorporates 15 degrees of longitude (ranges 170 to 180 and -180 to -175). |
| time_coverage_start | string | 1 | | Nominal start time. Describes the time of the first data point in the data set. Use the ISO 8601:2004 date format, preferably the extended format as recommended in the Attribute Content Guidance section. |
| time_of_first_valid_obs | string | 1 | | Describes the time of the first valid data point in the data set. Use the ISO 8601:2004 date extended format. |
| time_coverage_mid | string | 1 | | Describes the midpoint between the nominal start and end times. Use the ISO 8601:2004 date format, preferably the extended format as recommended in the Attribute Content Guidance section. |
| time_coverage_end | string | 1 | | Nominal end time. Describes the time of the last data point in the data set. Use ISO 8601:2004 date format, preferably the extended format as recommended in the Attribute Content Guidance section. |
| time_of_last_valid_obs | string | 1 | | Describes the time of the last valid data point in the data set. Use the ISO 8601:2004 date extended format. |
| time_coverage_duration | string | 1 | P0000-00-00T00:06:00 | Describes the duration of the data set. Use ISO 8601:2004 duration format, preferably the extended format as recommended in the Attribute Content Guidance section. |
| product_name_duration | string | 1 | m06 | Product duration as it appears in product_name (m06 means six minutes) |
| creator_type | string | 1 | institution | Specifies type of creator with one of the following: 'person', 'group', 'institution', or 'position'. If this attribute is not specified, the creator is assumed to be a person. |

| Name | Type | Size | Value | Description |
|---|---|---|---|---|
| creator_institution | string | 1 | Jet Propulsion Laboratory -- California Institute of Technology | The institution of the creator; should uniquely identify the creator's institution. This attribute's value should be specified even if it matches the value of publisher_institution, or if creator_type is institution. |
| product_version | string | 1 | v01.37.02 | Version identifier of the data file or product as assigned by the data creator. For example, a new algorithm or methodology could result in a new product_version. |
| keywords_vocabulary | string | 1 | GCMD:GCMD Keywords | If you are using a controlled vocabulary for the words/phrases in your "keywords" attribute, this is the unique name or identifier of the vocabulary from which keywords are taken. If more than one keyword vocabulary is used, each may be presented with a prefix and a following comma, so that keywords may optionally be prefixed with the controlled vocabulary key. Example: 'GCMD:GCMD Keywords, CF:NetCDF COARDS Climate and Forecast Standard Names'. |
| platform | string | 1 | SUOMI-NPP > Suomi National Polar-orbiting Partnership | Name of the platform(s) that supported the sensor data used to create this data set or product. Platforms can be of any type, including satellite, ship, station, aircraft or other. Indicate controlled vocabulary used in platform_vocabulary. |
| platform_vocabulary | string | 1 | GCMD:GCMD Keywords | Controlled vocabulary for the names used in the "platform" attribute. |
| product_name_platform | string | 1 | SNPP | Platform name as it appears in product_name |
| instrument | string | 1 | CrIS > Cross-track Infrared Sounder | Name of the contributing instrument(s) or sensor(s) used to create this data set or product. Indicate controlled vocabulary used in instrument_vocabulary. |
| instrument_vocabulary | string | 1 | GCMD:GCMD Keywords | Controlled vocabulary for the names used in the "instrument" attribute. |
| product_name_instr | string | 1 | CRIS | Instrument name as it appears in product_name |
| product_name | string | 1 | SNDR.SNPP.CRIS.<gran_id >.m06.g<granule_number>.L2_ESSPA_NH3_RET_NSR.std.v01_37_02.J.< product_name_timestamp >.nc | Canonical fully qualified product name (official file name) |
| product_name_variant | string | 1 | std | Processing variant identifier as it appears in product_name. 'std' (shorthand for 'standard') is to be the default and should be what is seen in all public products. |
| product_name_version | string | 1 | v01_37_02 | Version number as it appears in product_name (v01_37_02) |
| product_name_producer | string | 1 | J | Production facility as it appears in product_name (single character) 'T' is the default, for unofficial local test products |
| product_name_timestamp | string | 1 | yymmddhhmmss | Processing timestamp as it appears in product_name (yymmddhhmmss) |

| Name | Type | Size | Value | Description |
|---|---|---|---|---|
| product_name_extension | string | 1 | nc | File extension as it appears in product_name (typically nc) |
| granule_number | ushort | 1 | | granule number of day (1-240) |
| product_name_granule_number | string | 1 | g000 | zero-padded string for granule number of day (g001-g240) |
| gran_id | string | 1 | yyyymmddThhmm | Unique granule identifier yyyymmddThhmm of granule start, including year, month, day, hour, and minute of granule start time |
| geospatial_lat_mid | float | 1 | 9.9692099683868690e+36f | granule center latitude |
| geospatial_lon_mid | float | 1 | 9.9692099683868690e+36f | granule center longitude |
| featureType | string | 1 | point | structure of data in file |
| data_structure | string | 1 | swath | a character string indicating the internal organization of the data with currently allowed values of 'grid', 'station', 'trajectory', or 'swath'. The 'structure' here generally describes the horizontal structure and in all cases data may also be functions, for example, of a vertical coordinate and/or time. (If using CMOR pass this in a call to cmor_set_cur_dataset_attribute.) |
| cdm_data_type | string | 1 | Swath | The data type, as derived from Unidata's Common Data Model Scientific Data types and understood by THREDDS. (This is a THREDDS "dataType", and is different from the CF NetCDF attribute 'featureType', which indicates a Discrete Sampling Geometry file in CF.) |
| id | string | 1 | Unassigned | An identifier for the data set, provided by and unique within its naming authority. The combination of the "naming authority" and the "id" should be globally unique, but the id can be globally unique by itself also. IDs can be URLs, URNs, DOIs, meaningful text strings, a local key, or any other unique string of characters. The id should not include white space characters. |
| naming_authority | string | 1 | Unassigned | The organization that provides the initial id (see above) for the dataset. The naming authority should be uniquely specified by this attribute. We recommend using reverse-DNS naming for the naming authority; URIs are also acceptable. Example: 'edu.ucar.unidata'. |
| identifier_product_doi | string | 1 | Unassigned | digital signature |
| identifier_product_doi_authority | string | 1 | Unassigned | digital signature source |
| algorithm_version | string | 1 | ESSPA_NH3 v17; OSS v1.2 | The version of the algorithm in whatever format is selected by the developers. After the main algorithm name and version, versions from multiple sub-algorithms may be concatenated with semicolon separators. (ex: 'CCAST 4.2; BB emis from MIT 2016-04-01') Must be updated with every delivery that changes numerical results. |

| Name | Type | Size | Value | Description |
|---|---|---|---|---|
| production_host | string | 1 | squall | Identifying information about the host computer for this run. (Output of linux "uname -a" command.) |
| format_version | string | 1 | v02.00.36 | Format version. |
| input_file_names | string | 1 | | Semicolon-separated list of names or unique identifiers of files that were used to make this product. There will always be one space after each semicolon. There is no final semicolon. |
| input_file_types | string | 1 | | Semicolon-separated list of tags giving the role of each input file in input_file_names. There will always be one space after each semicolon. There is no final semicolon. |
| input_file_dates | string | 1 | | Semicolon-separated list of creation dates for each input file in input_file_names. There will always be one space after each semicolon. There is no final semicolon. |
| orbitDirection | string | 1 | | Orbit is ascending and/or descending. Values are "Ascending" or "Descending" if the entire granule fits that description. "NorthPole" and "SouthPole" are used for polar-crossing granules. "NA" is used when a determination cannot be made. |
| day_night_flag | string | 1 | | Data is day or night. "Day" means subsatellite point for all valid scans has solar zenith angle less than 90 degrees. "Night" means subsatellite point for all valid scans has solar zenith angle greater than 90 degrees. "Both" means the dataset contains valid observations with solar zenith angle above and below 90 degrees. "NA" means a value could not be determined. |
| AutomaticQualityFlag | string | 1 | Missing | "Passed": the granule contains a non-degraded calibrated brightness temperature, radiance, or retrieved value for at least one value in a geolocated FOV; "Suspect": the granule does not qualify as "Passed" but contains a (possibly degraded) calibrated or retrieved value (possibly without associated geolocation); "Failed": the granule contains no calibrated or retrieved values. “Missing” is a default value in the template that you should never see in the product unless something went seriously wrong. |
| qa_pct_data_missing | float | 1 | | Percentage of expected observations that are missing. |
| qa_pct_data_geo | float | 1 | | Percentage of expected observations that are successfully geolocated. |
| qa_pct_data_sci_mode | float | 1 | | Percentage of expected observations that were taken while the instrument was in science mode and are successfully geolocated. |
| qa_no_data | string | 1 | TRUE | A simple indicator of whether this is an "empty" granule with no data from the instrument. "TRUE" or "FALSE". |

| Name | Type | Size | Value | Description |
|---|---|---|---|---|
| title | string | 1 | Level-2 ESSPA-NH3 SNPP CrIS | a succinct description of what is in the dataset. (= ECS long name) |
| summary | string | 1 | The Level-2 ESSPA-NH3 product includes ammonia retrieval products from the ESSPA-NH3 algorithm for one six-minute interval. | A paragraph describing the dataset, analogous to an abstract for a paper. |
| shortname | string | 1 | SNDRSNIL2ESPNH3 | ECS Short Name |
| product_group | string | 1 | l2_esspa_nh3 | The group name to be used for this product when it is collected in a multi-group file type, like SNO or calsub |
| metadata_link | string | 1 | Unassigned | A URL that gives the location of more complete metadata. A persistent URL is recommended for this attribute. |
| references | string | 1 | Shephard\, M. W. and K.E. Cady-Pereira: Cross-track Infrared Sounder (CrIS) satellite observations of tropospheric ammonia\, Atmos. Meas. Tech.\, 8\, 1323-1336\, doi:10.5194/amt-8-1323-2015\, 2015. | ATDB and design documents describing processing algorithms. Can be empty. |
| contributor_name | string | 1 | Karen Cady-Pereira; Mark Shephard; Alan Lipton; Jean-Luc Moncet; Igor Polonski | The names of any individuals or institutions that contributed to the creation of this data. |
| contributor_role | string | 1 | NH3 Retrieval PI; Retrieval developer; Retrieval PI; Retrieval PI; Forward Model | The roles of any individuals or institutions that contributed to the creation of this data. |

## Global Variables

| Name | Type | Dimensions | Description | Units | Ancillary Variables |
|---|---|---|---|---|---|
| obs_id | string | atrack, xtrack | unique observation identifier: yyyymmddThhmm.aaSxx. Includes gran_id plus 2-digit along-track index (01-45), scene identifier (E=earth, H=hot, C=cold) and 2-digit cross-track index (01-30). | | |
| fov_obs_id | string | atrack, xtrack, fov | unique observation identifier for FOV: yyyymmddThhmm.aaSxx.f . Includes gran_id plus 2-digit along-track index (01-45), scene identifier (E=earth, H=hot, C=cold) , 2-digit cross-track index (01-30), and 1-digit FOV number (1-9). | | |
| obs_time_tai93 | double | atrack, xtrack | earth view observation midtime for each FOV | seconds since 1993-01-01 00:00 | bnds |
| obs_time_utc | uint16 | atrack, xtrack, utc_tuple | UTC earth view observation time as an array of integers: year, month, day, hour, minute, second, millisec, microsec | | |
| lat | float | atrack, xtrack, fov | latitude of FOV center | degrees_north | bnds |

| Name | Type | Dimensions | Description | Units | Ancillary Variables |
|---|---|---|---|---|---|
| lat_geoid | float | atrack, xtrack, fov | latitude of FOV center on the geoid (without terrain correction) | degrees_north | |
| lon | float | atrack, xtrack, fov | longitude of FOV center | degrees_east | bnds |
| lon_geoid | float | atrack, xtrack, fov | longitude of FOV center on the geoid (without terrain correction) | degrees_east | |
| land_frac | float | atrack, xtrack, fov | land fraction over the FOV | unitless | |
| surf_alt | float | atrack, xtrack, fov | mean surface altitude wrt earth model over the FOV | m | |
| surf_alt_sdev | float | atrack, xtrack, fov | standard deviation of surface altitude within the FOV | m | |
| sun_glint_lat | float | atrack | sun glint spot latitude at scan_mid_time. Fill for night observations. | degrees_north | |
| sun_glint_lon | float | atrack | sun glint spot longitude at scan_mid_time. Fill for night observations. | degrees_east | |
| sol_zen | float | atrack, xtrack, fov | solar zenith angle at the center of the FOV | degree | |
| sol_azi | float | atrack, xtrack, fov | solar azimuth angle at the center of the FOV (clockwise from North) | degree | |
| sun_glint_dist | float | atrack, xtrack, fov | distance of sun glint spot to the center of the FOV | m | |
| view_ang | float | atrack, xtrack, fov | off nadir pointing angle | degree | |
| sat_zen | float | atrack, xtrack, fov | satellite zenith angle at the center of the FOV | degree | |
| sat_azi | float | atrack, xtrack, fov | satellite azimuth angle at the center of the FOV (clockwise from North) | degree | |
| sat_range | float | atrack, xtrack, fov | line of sight distance between satellite and FOV center | m | |
| asc_flag | ubyte | atrack | ascending orbit flag: 1 if ascending, 0 descending | | |
| subsat_lat | float | atrack | sub-satellite latitude at scan_mid_time | degrees_north | |
| subsat_lon | float | atrack | sub-satellite longitude at scan_mid_time | degrees_east | |
| scan_mid_time | double | atrack | TAI93 at middle of earth scene scans | seconds since 1993-01-01 00:00 | |
| sat_alt | float | atrack | satellite altitude with respect to earth model at scan_mid_time | m | |
| sat_pos | float | atrack, spatial | satellite ECR position at scan_mid_time | m | |
| sat_vel | float | atrack, spatial | satellite ECR velocity at scan_mid_time | m s-1 | |
| sat_att | float | atrack, attitude | satellite attitude at scan_mid_time. An orthogonal triad. First element is angle about the +x (roll) ORB axis. +x axis is positively oriented in the direction of orbital flight. Second element is angle about +y (pitch) ORB axis. +y axis is oriented normal to the orbit plane with the positive sense | degree | |

| Name | Type | Dimensions | Description | Units | Ancillary Variables |
|---|---|---|---|---|---|
| | | | opposite to that of the orbit's angular momentum vector H. Third element is angle about +z (yaw) axis. +z axis is positively oriented Earthward parallel to the satellite radius vector R from the spacecraft center of mass to the center of the Earth. | | |
| local_solar_time | float | atrack, xtrack, fov | local apparent solar time in hours from midnight | hours | |
| mean_anom_wrt_equat | float | atrack | spacecraft mean anomaly measured with respect to the ascending node | degree | |
| sat_sol_zen | float | atrack | solar zenith angle at the satellite | degree | |
| sat_sol_azi | float | atrack | solar azimuth angle at the satellite (clockwise from North) | degree | |
| asc_node_lon | float | | Longitude of the last ascending node of spacecraft orbit before time_coverage_end. | degrees_east | |
| asc_node_tai93 | double | | TAI93 time of the last ascending node of spacecraft orbit before time_coverage_end. | seconds since 1993-01-01 00:00 | |
| asc_node_local_solar_time | float | | local apparent solar time at the last ascending node before time_coverage_end in hours from midnight | hours | |
| solar_beta_angle | float | | Beta angle for the spacecraft orbit, determining the percentage of the orbit that the spacecraft is in direct sunlight. | degree | |
| attitude_lbl | string | attitude | list of rotational directions (roll, pitch, yaw) | | |
| spatial_lbl | string | spatial | list of spatial directions (X, Y, Z) | | |
| utc_tuple_lbl | string | utc_tuple | names of the elements of UTC when it is expressed as an array of integers year,month,day,hour,minute,second,millisecond, microsecond | | |
| nh3_tot | float32 | atrack, xtrack, fov | Total column ammonia | kg m-2 | err, qc |
| nh3_mmr | float32 | atrack, xtrack, fov, air_pres_nh3 | ammonia mass mixing ratio to dry air | unitless | err, qc |
| surf_nh3_mmr | float32 | atrack, xtrack, fov | near-surface ammonia mass mixing ratio to dry air (~2 meters above surface) | unitless | err, qc |
| nh3_dof | float32 | atrack, xtrack, fov | The trace of the averaging kernel matrix as a measure of the number of pieces of information about the ammonia profile provided by the physical retrieval step. | unitless | |
| air_pres_nh3_nsurf | int16 | atrack, xtrack, fov | Index in air_pres_nh3 of the level at the surface. Values at levels beyond this are invalid, representing data below the Earth's surface. | unitless | |
| air_pres_nh3 | float32 | air_pres_nh3 | NH3 pressure levels | Pa | |

aux Dimensions

| Name | Size | Description |
|---|---|---|
| surf_wnum_ir | 12 | IR surface emissivity hinge points |
| sig_lev | 101 | Hybrid sigma levels |

## aux Variables

| Name | Type | Dimensions | Description | Units | Ancillary Variables |
|---|---|---|---|---|---|
| nh3_mmr_sig_lev | float32 | atrack, xtrack, fov, sig_lev | ammonia mass mixing ratio to dry air | unitless | |
| nh3_rms_resid | float32 | atrack, xtrack, fov | Ammonia root-mean-square residual | Kelvin | |
| chi2_nh3 | float32 | atrack, xtrack, fov | Ammonia Chi^2 | unitless | |
| prior_surf_ir_emis | float32 | atrack, xtrack, fov, surf_wnum_ir | prior infrared surface emissivity | unitless | |
| surf_temp | float32 | atrack, xtrack, fov | radiative temperature of the surface | Kelvin | err, qc |
| prior_surf_pres | float32 | atrack, xtrack, fov | surface pressure from forecast | Pa | |
| sig_lev_pres | float32 | atrack, xtrack, fov, sig_lev | sigma level pressure | Pa | |
| num_iter | ushort | atrack, xtrack, fov | Number of iterations | unitless | |
| nh3_signal_strength | ushort | atrack, xtrack, fov | Ammonia signal strength - prior profile classification | | |
| nh3_err_covar_diagonal | float32 | atrack, xtrack, fov, sig_lev | Ammonia error covariance matrix diagonal | unitless | |
| surf_wnum_ir | float32 | surf_wnum_ir | Infrared surface emissivity frequencies (hinge points) | cm-1 | |