

README Document for TROPESS Forward Stream, Standard and Summary Products

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• 1.0 Introduction

This document provides basic information for using the TROPESS datasets listed in Table 1.

The TROPESS forward processing stream generates products that include atmospheric composition measurements of ozone (O_3), carbon monoxide (CO), ammonia (NH_3), peroxyacetyl nitrate (PAN), methane (CH_4), and deuterated water vapor (HDO) derived from radiances measured by the NASA CrIS, Aqua AIRS, and Aura OMI sounders. These products provide global coverage. The data are subsampled using a grid sampling approach where the region is divided into 0.7 degree latitude (lat) x 0.7 degree longitude (lon) grid boxes for AIRS-OMI products, and 0.8 degree lat x 0.8 degree lon grid boxes for the CrIS products. The single, center most target within each box is selected to be included in the dataset. The dataset provides both day and night time coverage.

The CrIS products described in this document are generated from 2 input sources. TROPESS CrIS products from February 1, 2021 through May 21, 2021 were generated from L1B input files from the Suomi-NPP CrIS instrument. Due to the loss of the Longwave Band on the side A electronics on Suomi-NPP CrIS instrument first encountered on May 21, 2021, subsequent CrIS processing has switched to using the L1B input files from the JPSS1/NOAA20 CrIS instrument in order to mitigate impact on TROPESS retrieval product accuracy.

Table 1. Datasets / collections described in this document.

Long Name	Short Name	DOI
	Standard Products	
TROPESS AIRS-OMI L2 Ozone for Forward Stream, Standard Product	TRPSDL2O3AIRSOMIFS	10.5067/V9HA0ZB6Y3UZ
TROPESS OMI L2 Ozone for Forward Stream, Standard Product	TRPSDL2O3OMIFS	10.5067/HL2UFH62ELJO
TROPESS AIRS L2 Ozone for Forward Stream, Standard Product	TRPSDL2O3AIRSFS	10.5067/1OOD0AX232CJ
TROPESS AIRS L2 Carbon Monoxide for Forward Stream, Standard Product	TRPSDL2COAIRSFS	10.5067/I1NONOEPXLHS
TROPESS AIRS L2 Atmospheric Temperature for Forward Stream, Standard	TRPSDL2TATMAIRSFS	10.5067/XGCPC0JSDJCN

Long Name	Short Name	DOI
Product		
TROPESS AIRS L2 Deuterated Water Vapor for Forward Stream, Standard Product	TRPSDL2HDOAIRSFS	10.5067/K3OGAJGRUAB8
TROPESS AIRS L2 Water Vapor for Forward Stream, Standard Product	TRPSDL2H2OAIRSFS	10.5067/GAAB1GIBBQKU
TROPESS AIRS L2 Methane for Forward Stream, Standard Product	TRPSDL2CH4AIRSFS	10.5067/LP1B3RFV5WK7
TROPESS AIRS L2 Ammonia for Forward Stream, Standard Product	TRPSDL2NH3AIRSFS	10.5067/EYXLPVGTSWFF
TROPESS CrIS L2 Ozone for Forward Stream, Standard Product	TRPSDL2O3CRSFS	10.5067/8LMUGJ8X1ZXB
TROPESS CrIS L2 Carbon Monoxide for Forward Stream, Standard Product	TRPSDL2COCRSFS	10.5067/EA7G2TTV84RV
TROPESS CrIS L2 Atmospheric Temperature for Forward Stream, Standard Product	TRPSDL2TATMCRSFS	10.5067/XL382B4YZJP5
TROPESS CrIS L2 Deuterated Water Vapor for Forward Stream, Standard Product	TRPSDL2HDOCRSFS	10.5067/XTPEDYJ62GGN
TROPESS CrIS L2 Water Vapor for Forward Stream, Standard Product	TRPSDL2H2OCRSFS	10.5067/YUE7KKLKA1RS
TROPESS CrIS L2 Methane for Forward Stream, Standard Product	TRPSDL2CH4CRSFS	10.5067/MRTPR45H95EC
TROPESS CrIS L2 Ammonia for Forward Stream, Standard Product	TRPSDL2NH3CRSFS	10.5067/B4TF7ND8A3O7

Long Name	Short Name	DOI
TROPESS CrIS L2 Peroxyacetyl for Forward Stream, Standard Product	TRPSDL2PANCRSFS	10.5067/MQITF51HVPNW
TROPESS CrIS-JPSS1 L2 Ozone for Forward Stream, Standard Product	TRPSDL2O3CRS1FS	10.5067/WUKWENW76N5P
TROPESS CrIS-JPSS1 L2 Carbon Monoxide for Forward Stream, Standard Product	TRPSDL2COCRS1FS	10.5067/BYIIUV3PR9L6
TROPESS CrIS-JPSS1 L2 Atmospheric Temperature for Forward Stream, Standard Product	TRPSDL2TATMCRS1FS	10.5067/DBWOVPBIHL90
TROPESS CrIS-JPSS1 L2 Deuterated Water Vapor for Forward Stream, Standard Product	TRPSDL2HDOCRS1FS	10.5067/WS2EO2ZDOM75
TROPESS CrIS-JPSS1 L2 Water Vapor for Forward Stream, Standard Product	TRPSDL2H2OCRS1FS	10.5067/MRHSM2PY0DZZ
TROPESS CrIS-JPSS1 L2 Methane for Forward Stream, Standard Product	TRPSDL2CH4CRS1FS	10.5067/QOFZLQYMGA72
TROPESS CrIS-JPSS1 L2 Ammonia for Forward Stream, Standard Product	TRPSDL2NH3CRS1FS	10.5067/7I3KMUCCJNEN
TROPESS CrIS-JPSS1 L2 Peroxyacetyl for Forward Stream, Standard Product	TRPSDL2PANCRS1FS	10.5067/W0W6L8M6J85X
Summary Products		

TROPESS AIRS-OMI L2 Ozone for Forward Stream, Summary Product	TRPSYL2O3AIRSOMIFS	10.5067/YOQS41ON99CE
TROPESS OMI L2 Ozone for	TRPSYL2O3OMIFS	10.5067/ZFQQYOR9H4OX

Forward Stream, Summary Product		
TROPESS AIRS L2 Ozone for Forward Stream, Summary Product	TRPSYL2O3AIRSFS	10.5067/C1MS8SM5FBDO
TROPESS AIRS L2 Carbon Monoxide for Forward Stream, Summary Product	TRPSYL2COAIRSFS	10.5067/GRQCDD4L9P18
TROPESS AIRS L2 Atmospheric Temperature for Forward Stream, Summary Product	Not Provided	N/A
TROPESS AIRS L2 Deuterated Water Vapor for Forward Stream, Summary Product	TRPSYL2HDOAIRSFS	10.5067/2UILXXXCZLQN
TROPESS AIRS L2 Water Vapor for Forward Stream, Summary Product	Not Provided	N/A
TROPESS AIRS L2 Methane for Forward Stream, Summary Product	TRPSYL2CH4AIRSFS	10.5067/2N3XGOWWH69U
TROPESS AIRS L2 Ammonia for Forward Stream, Summary Product	TRPSYL2NH3AIRSFS	10.5067/NJU5C9752RD4
TROPESS CrIS L2 Ozone for Forward Stream, Summary Product	TRPSYL2O3CRSFS	10.5067/LT66296ATQD7
TROPESS CrIS L2 Carbon Monoxide for Forward Stream, Summary Product	TRPSYL2COCRSFS	10.5067/VJPF383IL5E1
TROPESS CrIS L2 Deuterated Water Vapor for Forward Stream, Summary Product	TRPSYL2HDOCRSFS	10.5067/5X25TK595WAF
TROPESS CrIS L2 Methane for Forward Stream, Summary Product	TRPSYL2CH4CRSFS	10.5067/DBLUVSN1KWX2

TROPESS CrIS L2 Ammonia for Forward Stream, Summary Product	TRPSYL2NH3CRSFS	10.5067/87GYER1R69D2
TROPESS CrIS L2 Peroxyacetyl for Forward Stream, Summary Product	TRPSYL2PANCRSFS	10.5067/ITM51B0FIBDV
Mega City Products		
See Appendix: Mega Cities		

0 1.1 Description of the Datasets

TROPESS L2 Standard Products are for users that are doing full analysis with avenging kernel and covariance corresponding to retrieved vertical profiles. L2 Summary products have a smaller files size and are more convenient for first-look and rapid analysis. Summary products are total and partial column product and include column averaging kernel.

These data are processed by the NASA TRopospheric Ozone and Precursors from Earth System Sounding (TROPESS) project, which uses an optimal estimation algorithm whose heritage comes from the NASA Tropospheric Emission Spectrometer (TES) satellite project (Beer et al, 2006, Bowman et al, 2006).

Consequently, the data sets include the retrieved atmospheric states (vertical profiles), and diagnostic information including observation operators, (averaging kernels), to facilitate data assimilation and intercomparison, and error covariances that characterize the accuracy and precision. The organization of the data structures and variables described in this document are similar to the TES data. More information about these data can be found at https://tes.ipl.nasa.gov/ and User Guides.

1.2 TRopospheric Ozone and Precursors from Earth System Sounding (TROPESS) Description

Tropospheric sounding from satellite observations provides critical information about atmospheric composition and its impact on human health and climate. The TRopospheric Ozone and Precursors from Earth System Sounding (TROPESS) project generates Earth System Data Records (ESDRs) of ozone and other atmospheric constituents by processing data from multiple satellites through a common retrieval algorithm and ground data system. These products are rigorously validated using uncertainty analysis in conjunction with independent measurements. These steps quantify the accuracies needed to make long-term trends through multi-satellite records and chemical data assimilation.

The TROPESS activity leverages innovations pioneered by the Tropospheric Emission Spectrometer (TES) team in combining data from multiple satellites to form a common retrieval framework, which is known as the MUlti-SpEctra, MUlti-SpEcies, Multi-SEnsors (MUSES) science data processing system (MUSES-SDPS). This framework has been applied to a combined suite of hyper-spectral thermal infrared, near-infrared, and ultraviolet instruments to generate ESDRs of Earth's tropospheric composition, including ozone, carbon monoxide, and water vapor deuterium. The ESDRs resulting from combinations of instruments/wavelength regions have increased sensitivity to the lower troposphere relative to composition measurements derived from any single instrument.

0 1.3 Data Disclaimer

While atmospheric profiles of these species are provided from the surface to the top-of-atmosphere, the user should primarily focus their analyses on the vertical range where the sensitivity of the measurements is greatest. That sensitivity can vary, and should be diagnosed from the averaging kernel (Bowman *et al.*, 2002). For most species, peak sensitivity is in the free troposphere. However, for some species, such as NH₃, the sensitivity is in the lower troposphere.

The TROPESS / MUSES retrievals of atmospheric composition in this collection have not yet been formally validated by aircraft or ground measurements. However, the following evaluations have been done:

- O₃: Informal comparison of CrIS O₃ retrievals have been made with AIRS and TES data, which in turn have been validated (Nassar *et al.*, 2008; Boxe *et al.*, 2010; Verstraten *et al.*, 2013; Fu et al., 2018) and show that CrIS retrievals are consistent with the AIRS and TES retrievals.
- CO: CrIS CO retrievals have been compared to MOPITT CO, which agree on average between 3-10% (Fu *et al.*, 2016).
- PAN: CrIS PAN retrievals have been informally compared with TES PAN (Payne *et al.*, 2014) and have shown to be broadly consistent. CrIS PAN data have also been provisionally validated using in situ aircraft profiles from the Atmospheric Tomography Mission (ATom).
- NH₃: The CrIS NH₃ retrievals have been compared to CrIS retrievals processed with the algorithms described in Shepard *et al.*, (2011) and Shepard and Cady-Pereira (2015). Both algorithms are derived from the TES algorithm. The retrievals compare within expected uncertainties.

■ 1.3.1 Data Citation and Acknowledgment

The datasets may be acknowledged in publications using the Digital Object Identifiers (DOIs) listed in Table 1.

If you plan on using any of these data please cite the following for a general description of the TROPESS retrieval algorithm: (Bowman *et al.*, 2006; Worden *et al.*, 2012; Fu *et al.*, 2018).

In addition, there are several specific algorithm papers related to the retrieval and validation of each species, please cite depending on which data product is used:

- For validation methods and indirect comparisons with TES ozone retrievals, please reference the following: H. Worden *et al.* (2007), Boxe *et al.* (2010), Verstraeten *et al.*, (2013).
- For validation of CO retrievals please reference the following: Luo *et al.* (2007a; 2007b), Fu *et al.*, (2016), Buchholz et al., (2021).
- For validation of NH₃ retrievals please cite the following: Shephard and Cady-Pereira (2015).
- For discussion of the PAN retrieval please cite: Payne *et al.*, (2014).

■ 1.3.2 Contact Information

Please contact John Worden (john.r.worden@jpl.nasa.gov) for any additional information needed about these data.

■ 1.3.3 Version 1

This is the first version of this product.

■ 1.3.4 Algorithm Version

Algorithm Version	Change Description
1.20.0	Fixed the retrieval strategy for Methanol for CrIS. Other products are not affected by this change.
1.19.0	 Modified radiative transfer approach Switched from using VLIDORT 2.5 to an approach using scalar LIDORT 3.8¹ Utilizing a Principal Component Analysis based approach to speed up multiple scattering computations² Incorporated the use of the ReFRACtor reusable software framework for atmospheric composition

Algorithm Version	Change Description
	 Spurr, R., Christi, M. (2019). The LIDORT and VLIDORT Linearized Scalar and Vector Discrete Ordinate Radiative Transfer Models: Updates in the Last 10 Years. In: Kokhanovsky, A. (eds) Springer Series in Light Scattering. Springer Series in Light Scattering. Springer, Cham. https://doi.org/10.1007/978-3-030-03445-0_1 Natraj, V., Shia, R. L., & Yung, Y. L. (2010). On the use of principal component analysis to speed up radiative transfer calculations. Journal of Quantitative Spectroscopy and Radiative Transfer, 111(5), 810-816.
1.18.0	Add `xa` prior variable to PAN summary products First public release for all summary products Use `desert_emis_qa quality > 0.925` filter for PAN
1.17.0	Implement strategy for CrIS to move the methanol step processing AFTER the ammonia step. Correcting AveragingKernelDiagonal calculation.
1.16.0	Using CAMELv2 emissivity dataset instead of UWIS for AIRS and CrIS Incorporated a new strategy in CrIS processing without the mid-wave channel. This will not produce HDO and CH4 products. Fixed a bug in prior column calculations Adding H2O columns to CO and PAN summary products
1.15.0	Processing pipeline is fully implemented in Python. This introduced statistically insignificant differences in the products compared to previous version 1.14.0.
1.14.0	PAN updates: Fixed the code for handling negative PAN values.

Algorithm Version	Change Description
1.13.0	Incorporated a fix to improve NLLS Solver output.
1.12.0	Fixed HDO error calculation. Updated standard product files and official summary products.
1.11.0	New NH3 microwindows for AIRS.
1.10.0	Fixed to use correct observation time in CrIS products.
1.9.0	New NH3 microwindows for CrIS data processing, improved NH3 algorithm.
1.8.0	Implemented the use of a new CO covariance matrix. For AIRS data processing, better handling of solar irradiance coefficients.
1.7.0	OMI Retrieval algorithm updates.
1.6.0	AIRS retrieval algorithm updates.
1.5.0	First Release.

0 1.4 Quality Flags

There are a number of internal metrics of retrieval performance, e.g., statistics of spectral residuals, that are evaluated and used to calculate quality flags. For the standard products, these quality flags have already been applied such that only data that satisfies these flags are provided. Since quality flags vary by species, not all species are available at the same geolocation. Users will need to use the geolocation fields (see § 3.3) to match the targets for comparing species. Code for matching targets can be found in links in § 5.1.1 Code examples: Python, Matlab, IDL. Quality flags are subject to change in light of new sources of validation. The approaches used are described in detail in algorithm documentation.

2.0 Data Organization

These data represent a compilation of observations of different species (O₃, CO, NH₃, CH₄, PAN, HDO, H₂O, and TATM) derived from the CrIS-SNPP, and AIRS-Aqua, OMI-Aura L1B retrievals.

There is 1 file per species, and the data are divided into a series of daily segments with one segment per file.

Each file contains all observations of a given species made during a period of exactly 1 day, identified by the date in the filename.

0 2.1 File Format and Structure

The files in these collections are in NetCDF-4 format. NetCDF is a set of software libraries and self-describing, machine-independent data formats that support the creation, access, and sharing of array-oriented scientific data that was developed by UCAR/Unidata: https://www.unidata.ucar.edu/software/netcdf/.

0 2.2 File Naming Convention

The filenames for these data products are described in Table 2, where YYYYMMDDD should be replaced by the observation date.

Below is an example of the general TROPESS file naming convention used to identify each granule:

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

where:

- **[ProjectID]**: corresponds to the project identifier for the collection (i.e., TROPESS).
- **[Instrument-Platform]**: corresponds to the instrument/sensor and corresponding platform used as L1B input dataset(s) used in the generation of the L2 data products. For Collections where more than one [INSTRUMENT-PLATFORM] combination is used as throughout the

record, the original heritage of the L1B input datasets will be traceable in the filename. For sensor-platform sets we use a `-` (dash) for the platform specification. For multi-sensor and platform combinations, we use an `_` (underscore) to delineate the different instruments.

Examples:

- Single sensor: [INSTRUMENT-PLATFORM]
 - [AIRS-Aqua]
 - [OMI-Aura]
 - [CrIS-SNPP]
 - [CrIS-JPSS1]
 - [CrIS-JPSS2]
 - [TROPOMI-S5P]
- Multi-sensor: [INSTRUMENT-PLATFORM_INSTRUMENT-PLATFORM]
 - [AIRS-Aqua_OMI-Aura]
 - [CrIS-SNPP_TROPOMI-S5P]
 - [CrIS-JPSS1_TROPOMI-S5P]
 - [CrIS-JPSS2_TROPOMI-S5P]
- **[ProductLevel]**: The data processing level of the file. All TROPESS collections are Level 2 (L2) products, following the <u>NASA Data Processing Levels</u>.
- [ProductName]: Short name to describe the data product name. Allowable values: Full, Standard and Summary. Standard products contain a subset of the parameters in the Full archival product.
- **[ProductType]**: A short name to describe the primary atmospheric species or parameter included in the data file. Gas phase species names follow the chemical compound name and contain the symbols of the atoms of the elements present in the compound, as well as how many there are for each element in the form of subscripts. Acceptable values are:
 - \circ O3 = Ozone
 - CO = Carbon monoxide
 - NH3 = Ammonia
 - PAN = Peroxyacetyl nitrate
 - CH4 = Methane
 - HDO = Deuterated water vapor
 - H2O = Water vapor
 - TATM = Atmospheric temperature
- **[DateStamp]**: Date stamp is the observation period of the data contained in the product. Products are aggregated daily and will use the [DateStamp] notation *YYYYMMDD*, where:
 - YYYY: is the full calendar year.
 - MM: is the 2-digit month of the year. Single-digit months employ a leading zero.
 - *DD*: is the 2-digit day of the month. Single-digit days employ a leading zero.
- **[AlgorithmName]**: The algorithm used to produce the data products (MUSES). Information indicating where the data were processed is covered in the global attributes.
- **[AlgorithmVersion]**: 2-digit (zero-padded) version number following capital "R". The initial version will be R0.0, with the first release being R1.0. This will reset only with Major version updates. Example: "Rxpx"
- **[ProcessingStrategy]**: a two-letter code for the processing strategy used in generating the L2 science data products. Allowable values are:

- FS: Forward Steam. Low-latency data products generated from the MUSES-SDPS forward processing streams.
- RS: Reanalysis Stream. Products are generated from the MUSES-SDPS reanalysis processing streams.
- SC: Special Collections. Provided on an as-needed and as-available basis to support NASA field missions and individual-investigator requests over specific regions.
- **FormatVersion**: 2-digit number, prefixed by a capital F. A change in the format version signals a change in the netcdf file layout, which would likely require a change in the users' data readers. Example: "Fxpx".

Table 2. TROPESS file naming conventions

Short Name	Filename Pattern
TRPSDL2O3AIRSOMIFS	TROPESS_AIRS-Aqua_OMI- Aura_L2_Standard_O3_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2O3OMIFS	TROPESS_OMI-Aura_L2_Standard_O3_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2O3AIRSFS	TROPESS_AIRS-Aqua_L2_Standard_03_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2COAIRSFS	TROPESS_AIRS-Aqua_L2_Standard_CO_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2TATMAIRSFS	TROPESS_AIRS-Aqua_L2_Standard_TATM_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2HDOAIRSFS	TROPESS_AIRS-Aqua_L2_Standard_HDO_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2H2OAIRSFS	TROPESS_AIRS-Aqua_L2_Standard_H2O_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2CH4AIRSFS	TROPESS_AIRS-Aqua_L2_Standard_CH4_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2NH3AIRSFS	TROPESS_AIRS-Aqua_L2_Standard_NH3_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2O3CRSFS	TROPESS_Cris-SNPP_L2_Standard_03_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2COCRSFS	TROPESS_CrIS-SNPP_L2_Standard_CO_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2TATMCRSFS	TROPESS_Cris-SNPP_L2_Standard_TATM_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2HDOCRSFS	TROPESS_Cris-SNPP_L2_Standard_HDO_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2H2OCRSFS	TROPESS_CrIS-SNPP_L2_Standard_H20_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2NH3CRSFS	TROPESS_CrIS-SNPP_L2_Standard_NH3_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSDL2PANCRSFS	TROPESS_Cris-SNPP_L2_Standard_PAN_20200912_MUSES_R1p11_FS_F0p1.nc

TRPSYL2O3AIRSOMIES	TROPESS_AIRS-Aqua_OMI-
	Aura_L2_Summary_03_20200912_MUSES_R1p11_FS_F0p1.nc

TRPSYL2O3OMIFS	TROPESS_OMI-Aura_L2_Summary_O3_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2O3AIRSFS	TROPESS_AIRS-Aqua_L2_Summary_03_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2COAIRSFS	TROPESS_AIRS-Aqua_L2_Summary_CO_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2HDOAIRSFS	TROPESS_AIRS-Aqua_L2_Summary_HDO_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2CH4AIRSFS	TROPESS_AIRS-Aqua_L2_Summary_CH4_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2NH3AIRSFS	TROPESS_AIRS-Aqua_L2_Summary_NH3_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2O3CRSFS	TROPESS_CrIS-SNPP_L2_Summary_03_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2COCRSFS	TROPESS_CrIS-SNPP_L2_Summary_CO_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2HDOCRSFS	TROPESS_CrIS-SNPP_L2_Summary_HDO_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2NH3CRSFS	TROPESS_CrIS-SNPP_L2_Summary_NH3_20200912_MUSES_R1p11_FS_F0p1.nc
TRPSYL2PANCRSFS	TROPESS_CrIS-SNPP_L2_Summary_PAN_20200912_MUSES_R1p11_FS_F0p1.nc

o 2.3 Key Science Data Fields

The TROPESS L2 Standard Products have been designed with users in mind. The Key Science Data Fields expected to be of interest for most users are:

Table 3. Key science data fields.

Data Field Name	Long_Name/Description	Туре	Dimensions	Undefined Value	Units
Х	Retrieved state, as volume mixing ratio (VMR) relative to dry air.	float	target, level	-999.0	1
ха	A priori state, as volume mixing ratio relative to dry air	float	target, level	-999.0	1
averaging_kernel	Sensitivity of the retrieved state to the true state. For CO, O3, and NH3 retrieved states are in In(VMR). For PAN,	float	target, level, level	-999.0	1

	retrieved states are linear.				
observation_error	Measurement + systematic + cross-state error. Use for comparisons with other measurements and for assimilations	float	target, level, level	-999.0	1

• 3.0 Data Contents

o 3.1 Data Set Attributes (File Metadata)

A summary of global attributes present in all files is shown in Table 4 below.

Table 4. Global data attributes.

Global Attribute	Description	Туре
ShortName	ESDT short product name	string
LongName	Full product name	string
VersionID	Version ID for this product	int
IdentifierProductDOIAuthority	Organization providing DOI information	string
IdentifierProductDOI	DOI value	string
Format	Data file format	string
ProcessingLevel	Level of data product	string
SouthBoundingCoordinate	South bounding latitude	double
NorthBoundingCoordinate	North bounding latitude	double
WestBoundingCoordinate	West bounding longitude	double
EastBoundingCoordinate	East bounding longitude	double
Conventions	Name of convention(s) for metadata	string
MeasuredParameter	Species measured for this product	string

Platform	Platform for measuring instrument	string
Instrument	The measuring instrument	string

o 3.2 Variable Data 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 (see Table 5).

Table 5. Per variable data attributes.

Variable Attribute	Description	Туре
_FillValue	single value indicating the data point contains fill instead of valid data	float
long_name	longer name describing the quantity being represented; typically used for plot titles	string
standard_name	standard name from CF standard name table, if one exists for the quantity being represented	string
comment	description or comment for the quantity being represented	string
units	units for variables that represent physical quantities	string
coordinates	space-separated list of the names of other variables that are coordinates for this variable	string
missing_value	same as _FillValue	float
source	identifies variable from the input product from which this quantity is derived from; used internally by TROPESS team to trace back to source.	string

o 3.3 Geolocation Fields

Geolocation fields appear for every data observation and are shown in Table 6. Note that the geolocation for AIRS and CrIS is specified differently in the TROPESS products, following the

geolocation information in the respective L1B files. CrIS geolocation is specified by along-track and cross-track field of regard (FOR) indices within a granule, and by field of view (FOV) within each FOR. AIRS geolocation is specified according to individual FOVs along-track and cross-track within each granule.

Table 6. Geolocation fields.

Global Attribute	Туре			
CrlS Geolocation Fields				
cris_atrack	CrIS Suomi-NPP along-track index (1-45)	int		
cris_xtrack	CrIS Suomi-NPP cross-track index (1-30)	int		
cris_fov	CrIS Suomi-NPP field-of-view index (1-9)	int		
cris_view_ang	CrIS Suomi-NPP view angle	float		
cris_granule	CrIS Suomi-NPP granule number (1-240)	int		
	AIRS Geolocation Fields			
airs_atrack	AIRS along-track index (1-135)	int		
airs_xtrack	AIRS cross-track index (1-90)	int		
airs_view_ang	AIRS scan angle	float		
airs_granule	AIRS granule number (1-240)			
	OMI Geolocation Fields			
omi_atrack_index	OMI along-track index (1-1643)	int		
omi_xtrack_uv1	OMI cross-track UV1 index (1-30)	int		
omi_xtrack_uv2	OMI cross-track UV2 index (1-60)	int		
omi_view_ang	OMI UV2 solar zenith angle	float		

Since quality flags vary by species, some species may not be available at the same geolocation. Consequently, users are recommended to employ these geolocation fields to match the targets for comparing species (for more information, see §5.1.1 Code examples: Python, Matlab, IDL).

o 3.4 Dimensions

The variable dimensions associated with the data products are shown in Table 7.

Table 7. Data dimensions.

Global Attribute	Description	Dimension Size
target	target/observation identifier	Varies*
level	atmospheric pressure in hPa	CO: 14 NH ₃ : 15 PAN: 16 O ₃ : 26 CH ₄ : 26 HDO: 17 H ₂ O: 17 TATM: 31
datetime_utc_dim	UTC expressed as an array of integers year, month, day, hour, minute, second	6

^{*}Note: Dimensions of "target" vary by file and date. Number of targets range from (7000-10000).

• 4.0 Products/Parameters

The science data variables are described in the table below

0 4.1 L2 Standard Product Data Fields

The science data fields are shown in Table 8.

Table 8. Data fields.

Data Field Name	Long_Name/Description	Туре	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_nort
time	Earth view target mid time as International	double	target	-999.0	seconds since 1993-01-01

	Atomic Time (TAI) seconds since 1993-01-01 00:00:00				00:00:00
datetime_utc	UTC expressed as an array of integers year, month, day, hour, minute, second	int	target, datetime_utc _dim	-999	1
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
х	Retrieved state, as volume mixing ratio (VMR) relative to dry air.	float	target, level	-999.0	1
averaging_kernel	Sensitivity of the retrieved state to the true state. For CO, O3, and NH3 retrieved states are in In(VMR). For PAN, retrieved states are linear.	float	target, level, level	-999.0	1
observation_error	Measurement + systematic + cross-state error. Use for comparisons with other measurements and for assimilations	float	target, level, level	-999.0	1
signal_dof	Degrees of Freedom for Signal; trace of averaging kernel	float	target	-999.0	1

x_test	The estimated state for target 0 based on x[0], xa[0], and avg_kernel[0], as volume mixing ratio (VMR) relative to dry air.	float	level	-999.0	1
ха	A priori state, as volume mixing ratio relative to dry air	float	target, level	-999.0	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

0 4.2 L2 Summary Product Data Fields

See L2 Summary Product User's Guide.

• 5.0 Options for Reading the Data

O 5.1 Tools/Programming Languages

Support for reading NetCDF is offered in many programming languages, including Python, Matlab, IDL, C/C++ and Fortran. NetCDF4 files are legal HDF5 files with additional bookkeeping information managed by the NetCDF4 library.

The following link provides a list of software and tools for manipulating and displaying NetCDF (*.nc) data files: https://www.unidata.ucar.edu/software/netcdf/software.html.

■ 5.1.1 Code examples: Python, Matlab, IDL

Code examples for product usage from different programming languages are available at: https://github.com/NASA-TROPESS. In addition, code for matching targets is included at the link above.

0 5.2 Command Line Utilities

■ 5.2.1 ncdump

Outputs contents of a netCDF file as ascii. From Unidata, part of the NetCDF libraries. ncdump documentation:

https://www.unidata.ucar.edu/software/netcdf/docs/netcdf utilities guide.html#ncdump guide

The ncdump tool can be used as a simple browser for HDF data files, to display the dimension names and sizes; variable names, types, and shapes; attribute names and values; and optionally, the values of data for all variables or selected variables in a netCDF file. The most common use of ncdump is with the —h option, in which only the header information is displayed.

■ 5.2.2 NCO

NCO is a package of command-line utilities for manipulating netCDF files. Each NCO command does one very specific kind of manipulation, but you can combine them to powerful effect.

NCO Documentation: http://nco.sourceforge.net/nco.html

- <u>ncap</u> and <u>ncap2</u>: netCDF Arithmetic Processors (<u>examples</u>) -- algebraic manipulation of data
- <u>ncatted</u>: netCDF Attribute Editor (<u>examples</u>) -- modify metadata
- <u>ncbo</u>: netCDF Binary Operator (includes ncadd, ncsubtract, ncmultiply, ncdivide) -- (<u>examples</u>) -- math involving two files
- ncea: netCDF Ensemble Averager (examples) -- average across multiple input files
- ncecat: netCDF Ensemble Concatenator (examples) -- combine files into a single record
- <u>ncflint</u>: netCDF File Interpolator (<u>examples</u>) -- combine inputs via weighted interpolation
- ncks: netCDF Kitchen Sink (examples) -- copies data to ascii or output file
- ncpdq: netCDF Permute Dimensions Quickly, Pack Data Quietly (examples) -- rearrange dimensions or pack data
- <u>ncra</u>: netCDF Record Averager (<u>examples</u>) -- average across time (record dimension)
- ncrcat: netCDF Record Concatenator (examples) -- combine sequential files
- <u>ncrename</u>: netCDF Renamer (<u>examples</u>) -- rename dimensions, variables, or attributes
- ncwa: netCDF Weighted Averager (examples) -- weighted average over one file

o 5.3 GUI Tools

■ 5.3.1 Panoply

Panoply is a good generic and free visualization tool for any netCDF file. A strength

of the tool is that data can be previewed "remotely" over the network - i.e., a user can preview file content of HDF files stored on a remote site, without downloading them.

Panoply is available from Goddard Institute for Space Studies (GISS) here: https://www.giss.nasa.gov/tools/panoply/

5.3.2 HDFView

HDFView is a visual tool for browsing and editing HDF (HDF5 and HDF4) and NetCDF files. It can be downloaded from here: https://www.hdfgroup.org/downloads/hdfview/.

• 6.0 GES DISC Data Services Help Desk

If you need assistance or wish to report a problem:

Email: gsfc-dl-help-disc@mail.nasa.gov

Voice: 301-614-5224 **Fax:** 301-614-5268

Address:

Goddard Earth Sciences Data and Information Services Center NASA Goddard Space Flight Center Code 610.2 Greenbelt, MD 20771 USA

O 6.1 How to Articles

The GESDISC web site contains many informative articles under the "<u>How To Section</u>", "<u>FAQ</u>" (frequently asked questions), "<u>News</u>", "<u>Glossary</u>", and "<u>Help</u>". A sample of these articles includes:

Earthdata Login for Data Access

How to Obtain Data in NetCDF Format via SSW

How to Download Data Files from HTTPS Service with wget

How to Obtain Data in NetCDF Format via OpeNDAP

Quick View Data with Panoply

How to Read Data in NetCDF Format with R

How to Read Data in HDF-5 or netCDF Format with GrADS

How to read and plot NetCDF MERRA-2 data in Python

How to Subset Level-2 Data

How to use the Level 3 and 4 Subsetter and Regridder

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Appendix: Mega Cities

The table below describes the Mega City collection with a Latitude and Longitude boundary.

Long Name	Short Name	DOI	Lat	Lon				
Mega City Standard Products								
Tokyo, Japan	TRPSDL2ALLCRSMGTOK	10.5067/65ZEOTLVV7EZ	35.68N	139.77E				
Mexico City	TRPSDL2ALLCRSMGMEX	10.5067/PECEC1AZ5R1J	19.13N	99.40W				
Delhi, India	TRPSDL2ALLCRSMGDEL	10.5067/NILL9KD1K78G	29.02N	77.38E				
São Paulo, Brazil	TRPSDL2ALLCRSMGSAO	10.5067/SQVOPBQTHU10	23.50S	46.62W				
Lagos, Nigeria	TRPSDL2ALLCRSMGLAG	10.5067/4UH0WF2HOHHB	6.60N	3.30E				
Los Angeles, USA	TRPSDL2ALLCRSMGLOS	10.5067/0QPQFIXDET1X	34.05N	118.24W				
Beijing, China	TRPSDL2ALLCRSMGBEI	10.5067/IUJHNI1MM1QA	39.91N	116.40E				
Mega City Summary Products								
Tokyo, Japan	TRPSYL2ALLCRSMGTOK	10.5067/RAD13QSZ61JY	35.68N	139.77E				
Mexico City	TRPSYL2ALLCRSMGMEX	10.5067/YTO4AV07QQOW	19.13N	99.40W				
Delhi, India	TRPSYL2ALLCRSMGDEL	10.5067/IHXG5JVO98VC	29.02N	77.38E				
São Paulo, Brazil	TRPSYL2ALLCRSMGSAO	10.5067/AA26EWZUNMDK	23.50S	46.62W				
Lagos, Nigeria	TRPSYL2ALLCRSMGLAG	10.5067/G2FKY92PRSF5	6.60N	3.30E				
Los Angeles, USA	TRPSYL2ALLCRSMGLOS	10.5067/H66DGC3ICJMQ	34.05N	118.24W				
Beijing, China	TRPSYL2ALLCRSMGBEI	10.5067/GBMBES47TUOI	39.91N	116.40E				