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Goddard Earth Science Data Information and
Services Center (GES DISC)*

README Document for TROPESS CrIS-SNPP L2 Carbon Monoxide, Ozone, Ammonia, and Peroxyacetyl Nitrate West Coast Fires, Standard Product

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1.0 Introduction

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

These data products include atmospheric composition measurements of ozone (O₃), carbon monoxide (CO), ammonia (NH₃), and peroxyacetyl nitrate (PAN) derived from radiances measured by the NASA CrIS-SNPP sounder and focused over North America during the time of the California and Colorado fires from August through October 2020. The lat/lon range region in this dataset is 20N - 60N latitude, and 40W - 150W longitude. The data is subsampled using a grid sampling approach where the region is divided into 0.7 degree lat x 0.7 degree lon grid boxes. 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.

Table 1. Datasets / collections described in this document.

Long Name	Short Name	DOI
TROPESSE CrIS-SNPP L2 Ozone for West Coast Fires, Standard Product	TRPSDL2O3CRSWCF	10.5067/N4CJ9HTW7WJL
TROPESSE CrIS-SNPP L2 Carbon Monoxide for West Coast Fires, Standard Product	TRPSDL2COCRSWCF	10.5067/HXARUSIEQ4KM
TROPESSE CrIS-SNPP L2 Ammonia for West Coast Fires, Standard Product	TRPSDL2NH3CRSWCF	10.5067/U54WBM8OXJO7
TROPESSE CrIS-SNPP L2 Peroxyacetyl Nitrate for West Coast Fires, Standard Product	TRPSDL2PANCRSWCF	10.5067/EAZVCIS0JH00

1.1 Description of the Datasets

These data are processed by the NASA Tropospheric Ozone and Precursors from Earth System Sounding (TROPESSE) 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 vertical distribution of retrieved atmospheric states, formal uncertainties, and diagnostic information. These ancillary data are used to construct observation operators, which facilitate data assimilation and intercomparison, and 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.jpl.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-Spectral, 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. These ESDRs have accuracies superior to composition measurements derived from any single instrument, and these data are based on optimal estimation retrievals, which include critical diagnostics such as observation operators and uncertainty metrics sufficient for assimilation into Earth system models.

1.3 Data Disclaimer

While an atmospheric profile of these species is 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 TROPES 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: Shepard 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.

1.4 Quality Flags

Species retrievals of CrIS data have been compared with other IR instruments (e.g., AIRS), and have been processed through the same algorithm. 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 has 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, and PAN) derived from the CrIS-SNPP 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.

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/>.

2.2 File Naming Convention

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

Below is an example of the general TROPES 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., TROPES).
- **[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 TROPESSE collections are Level 2 (L2) products, following the [NASA Data Processing Levels](#).
 - **[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:
 - O3 = Ozone
 - CO = Carbon monoxide
 - NH3 = Ammonia
 - PAN = Peroxyacetyl nitrate
 - **[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: "Rxx"
 - **[ProcessingStrategy]**: a two-letter code for the processing strategy used in generating the L2 science data products. Allowable values are:
 - FS: Forward Stream. 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: "Fxx".

Table 2. TROPES file naming conventions

Short Name	Filename Pattern
TRPSDL2O3CRSWCF	TROPES_CrIS-SNPP_L2_Standard_O3_20200912_MUSES_R1p10_FS_F01.nc
TRPSDL2COCRSWCF	TROPES_CrIS-SNPP_L2_Standard_CO_20200912_MUSES_R1p10_FS_F01.nc
TRPSDL2NH3CRSWCF	TROPES_CrIS-SNPP_L2_Standard_NH3_20200912_MUSES_R1p10_FS_F01.nc
TRPSDL2PANCRSWCF	TROPES_CrIS-SNPP_L2_Standard_PAN_20200912_MUSES_R1p10_FS_F01.nc

2.3 Key Science Data Fields

The TROPES 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	Type	Dimensions	Undefined Value	Units
x	Retrieved state, as volume mixing ratio (VMR) relative to dry air.	float	target, level	-999.0	1
xa	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 ln(VMR). For PAN, retrieved states are linear.	float	target, level, level	-999.0	1
observation_error	Measurement + systematic + cross-state error. Use for	float	target, level, level	-999.0	1

	comparisons with other measurements and for assimilations				
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3.0 Data Contents

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	Type
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

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	Type
_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 TROPES team to trace back to source.	string

3.3 Geolocation Fields

Geolocation fields appear for every data observation and are shown in Table 6.

Table 6. Geolocation fields.

Global Attribute	Description	Type
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

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*).

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
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.

4.1 Data Fields

The science data fields are shown in Table 8.

Table 8. Data fields.

Data Field Name	Long_Name/Description	Type	Dimensions	Undefined Value	Units
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x	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 ln(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
xa	A priori state, as volume mixing ratio relative to dry air	float	target, level	-999.0	1

4.2 Fill Values

Fill values are indicated in Table 9.

Table 9. Fill values.

Variable Type	Fill Value
float	-999.0

5.0 Options for Reading the Data

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.

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>

- [ncap](#) and [ncap2](#): netCDF Arithmetic Processors ([examples](#)) -- algebraic manipulation of data

- [ncatted](#): netCDF Attribute Editor ([examples](#)) -- modify metadata
- [ncbo](#): netCDF Binary Operator (includes ncadd, ncsubtract, ncmultiply, ncdivide) -- ([examples](#)) -- 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
- [ncflint](#): netCDF File Interpolator ([examples](#)) -- 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
- [ncra](#): netCDF Record Averager ([examples](#)) -- average across time (record dimension)
- [ncrcat](#): netCDF Record Concatenator ([examples](#)) -- combine sequential files
- [ncrename](#): netCDF Renamer ([examples](#)) -- rename dimensions, variables, or attributes
- [ncwa](#): netCDF Weighted Averager ([examples](#)) -- weighted average over one file

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

6.1 How to Articles

The GESDISC web site contains many informative articles under the “[How To Section](#)”, “[FAQ](#)” (frequently asked questions), “[News](#)”, “[Glossary](#)”, and “[Help](#)”. 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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