

TROPES Methane Level 2 Standard Data Product User Guide

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1 Introduction

1.1 Overview and Document Scope

This document is to be used as a Quick start user guide for using the TROPES AIRS and CrIS methane (CH₄) Level 2 Standard Product Files.

1.2 Dataset Description

This user guide describes the TROPES AIRS and CRIS Level 2 Standard (Product Files

TROPES CH4 Level 2 Standard Product User Guide

| Product Information | Description |
|-------------------------|--|
| Parameters | CH4 |
| Data Product Provenance | MUSES Program Version 1.11 |
| Approximate file size | ~15 MB per file |
| Spatial coverage | Nominally 50S to 70N coverage on a subset of observations. |
| Temporal coverage | Each L2 nominal Standard file contains 1 day of data |
| File format | netcdf |
| Vertical sensitivity | CH4 has sensitivity between approximately 800 hPa and the tropopause with approximately 1 degree of freedom. |
| Data quality | The data have undergone a pre-quality check, which involves checks for retrieval convergence and vertical sensitivity. |
| Uncertainty | Kulawik et al. (2020): 30 ppb single, 17 ppb daily, 10 ppb seasonal errors |
| Validation Stage | AIRS CH4 is at validation level 3 based on NASA guidelines (see below). CRIS CH4 is at validation stage 1 https://science.nasa.gov/earth-science/earth-science-data/data-maturity-levels |
| Retrieval Levels | 26 levels: from surface to top-of-atmosphere |
| FillValues | -999 |

1.3 Filename

The Standard Products adhere to the following filename convention:

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

Example:

```
TROPESS_AIRS-Aqua_L2_Standard_CH4_20200912_MUSES_R1p11_FS_F0p1.nc
```

2 Product File Contents and Parameter Description

Please see the README for a list of variables included in the L2 Standard product Files

3 References

3.1 Citing these data

Please cite the following references if you intend to use these data:

1. Kulawik, S. S., Worden, J. R., Payne, V. H., Fu, D., Wofsy, S. C., McKain, K., Sweeney, C., Daube Jr., B. C., Lipton, A., Polonsky, I., He, Y., Cady-Pereira, K. E., Dlugokencky, E. J., Jacob, D. J., and Yin, Y.: Evaluation of single-footprint AIRS CH4 profile retrieval uncertainties using aircraft profile measurements, *Atmos. Meas. Tech.*, 14, 335–354, <https://doi.org/10.5194/amt-14-335-2021>, 2021..

4 Extended User Guide: L2 Standard Product

This extended user guide shows how to compare these fields to aircraft or model fields, calculate uncertainties.

4.1 How to compare to aircraft or model fields

All comparisons between remotely sensed data and *in situ* measurements or high resolution model fields must account for the sensitivity of the remotely sensed measurement and any regularization used with the remotely sensed measurements. Otherwise *large* errors will be incurred with the comparisons.

We first construct an observation operator that is used for comparison of the TROPESS CH4 data to models or vertical profile measurements such as from aircraft:

- 1) Calculate the CH4 profile using the model or aircraft fields (for the purpose of this demonstration we will call this x_{true}).
- 2) Construct the observation operator as the following :

$$H(\cdot) = \ln(x_a) + A(\ln(\cdot) - \ln(x_a))$$

- 3) Apply observation operator to the CO profile:

$$\hat{x} = \exp[H(x_{true})]$$

In the netcdf product file and in the equation, x_a is the constraint vector used to regularize the retrieval. $H(\cdot)$ is the observation operator, where the (\cdot) represents a model or *in situ* profile. A is the averaging kernel matrix and must be matrix multiplied by $\ln(x_{true}) - \ln(x_a)$. After this operation one can compare the modified CH4 profile (\hat{x}) to the retrieved “x” variable in the netcdf product file. Note that the averaging kernel matrix (A) is not symmetric, so getting the row/column order of A correct is critical.

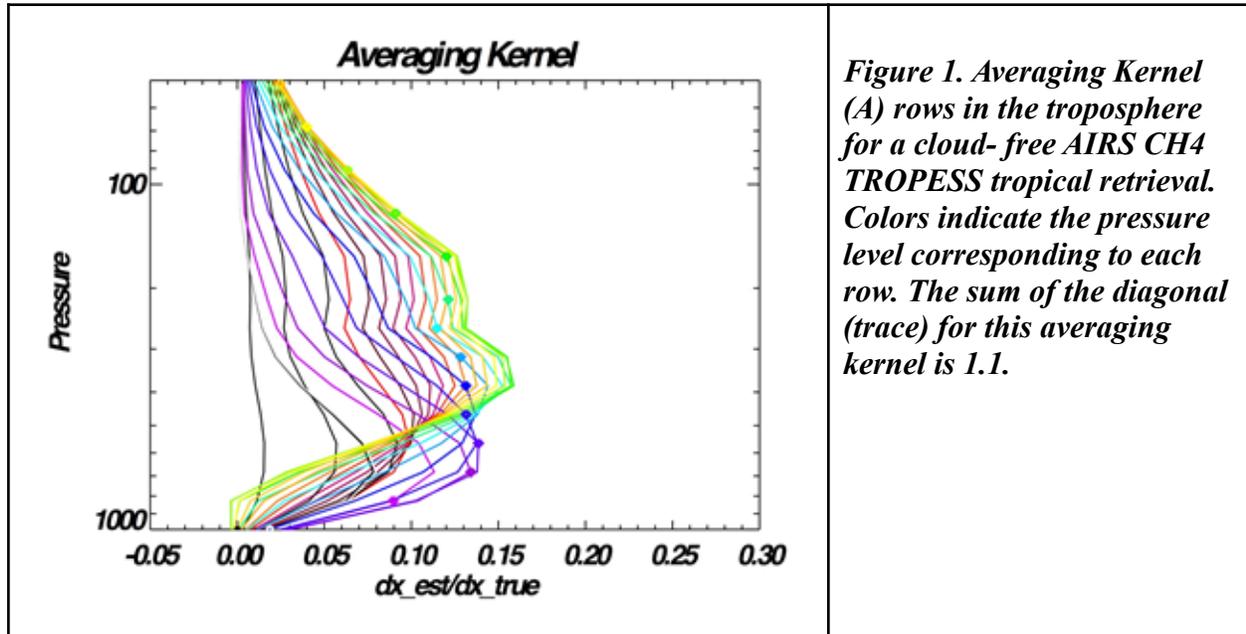
4.2 Verifying your equations

You can check your work by using the above equation with the zeroth entries for the averaging kernel, x_a and using the zeroth entry for x as x_{true} . If your test operation (steps 1-3) matches the variable x_{test} then the operation is correct.

4.3 Sensitivity of methane to the true state

Figure 1 shows an example of the averaging kernel rows for a AIRS CH4 retrieval over a tropical ocean scene. Figure 2 shows an example of applying the averaging kernels from

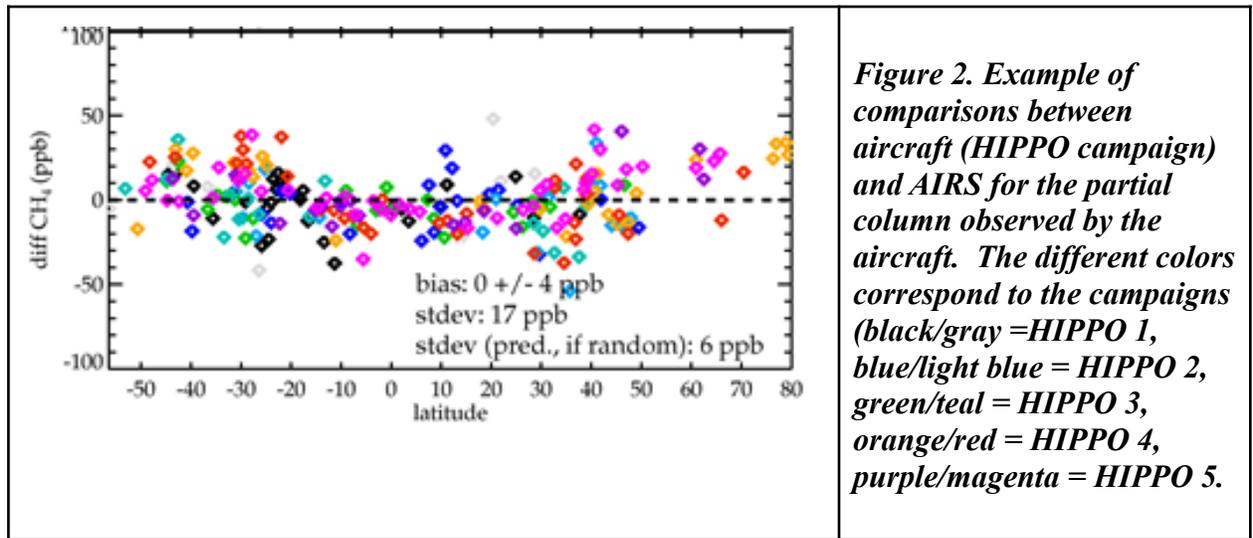
TROPESS AIRS CH4 retrievals to in situ profiles from the HIPPO campaign over a wide range of latitudes.



5 Validation Summary

Summary Statement for AIRS CH4: Based on the NASA Validation criteria listed subsequently, we determined that the validation level of the TROPESS AIRS L2 Standard CH4 products as Level 2. The CH4 error has been quantified for single observations, daily averages, weekly averages, monthly averages, 3-month averages, and seasonal averages are shown in Kulawik et al., 2021. AIRS CH4 was validated versus ATom and GML aircraft profiles. AIRS CH4 has a variable bias for land, ocean, and pressure, as seen in Table 1, which varies from 0 to 25 ppb. AIRS CH4 standard deviation versus validation data reduces with increasing averaging, 22 ppb for single observations, 16 ppb for daily averages, and 9 ppb for monthly averages, as seen in Kulawik et al (2021).

Summary Statement for CrIS CH4: Based on the NASA Validation criteria listed subsequently, we determined that the validation level of the TROPESS AIRS L2 Standard CH4 products as Level 1. The CrIS CH4 has not had bias correction applied and has not had formal validation.



Appendix A. Bias correction and quality flags

Bias correction

The CH4 estimates in these files have a bias correction to correct a high bias, possibly due to spectroscopy. This is corrected with the following formula:

pressure > 400 hPa:

$$\delta bias[ind] = -6.1e-5 * pressure[ind]$$

pressure < 400 hPa:

$$\delta bias[ind] = -0.09 + 0.00018 * pressure[ind]$$

The bias correction formula is:

$$\ln(x_corrected) = \ln(x_original) + \text{averaging_kernel}(\delta bias)$$

Note that the bias correction must be done on the full state pressure grid rather than the retrieval pressure grid, so that if you are applying the bias correction yourself, you need to use the archival product.

Quality Flags

Here are the quality flags recommended by Kulawik et al. (2021):

Radiance residual rms < 1.5.

|Radiance residual mean| < 0.15.

TSUR < near-surface atmospheric temperature value + 30K.

Cloudtop pressure > 90 hPa.

Cloud OD < 0.3.

Cloud variability versus wavenumber < 1.5 * cloud OD.

dofs > 1.1

ch4_doftrop > 0.7

ch4_dofstrat < 0.5

column750_error < 53 ppb

Note that the value in the L2 and Summary products are bias corrected. The value in the CH4 archive is not bias corrected.

Next release:

Change column lowest pressure value from 750 to 825.4 hPa to match retrieval pressure grid.

Appendix B. Retrieval levels

The table below contains the nominal retrieval levels. For each sounding, the surface pressure level is inserted into the retrieval levels set. Any retrieval levels below the surface pressure level are omitted.

| Index | Pressure [hPa] |
|--------------|-----------------------|
| 1 | 1040.0000 |
| 2 | 1000.0000 |
| 3 | 825.4020 |
| 4 | 681.2910 |
| 5 | 562.3420 |
| 6 | 464.1600 |
| 7 | 383.1170 |
| 8 | 316.2270 |
| 9 | 261.0160 |
| 10 | 215.4440 |
| 11 | 161.5610 |
| 12 | 121.1520 |
| 13 | 90.8518 |
| 14 | 68.1295 |
| 15 | 51.0896 |
| 16 | 38.3119 |
| 17 | 28.7299 |
| 18 | 21.5443 |
| 19 | 16.1560 |
| 20 | 12.1153 |
| 21 | 9.0851 |

| | |
|----|--------|
| 22 | 6.8129 |
| 23 | 4.6416 |
| 24 | 1.6156 |
| 25 | 0.6813 |
| 26 | 0.1000 |

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