ESA Project **METHANE+**	**DP description & AUM**	Version: Draft 0.9 Doc ID: TN-D4and5-CH4PLUS Date: 3 June 2020

Data Pool (DP) description / Auxiliary dataset User Manual (AUM)

ESA project METHANE+ led by SRON

Task 2, WP 2000, Deliverables 4 and 5 (D4 & 5)

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Change log

Version	Date	Status	Authors	Reason for change
Draft 0.9	03-June-2020	First complete draft	All	New document

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1. Overview

This project uses a range of auxiliary products (from other satellite, air-borne and ground-based sources) in the production and assessment of the main methane datasets. Following the SoW, this auxiliary data is collectively referred to as a data pool (DP). The DP is required to be made accessible to ESA (subject to any restrictions on proprietary external datasets). The content of the DP is to be described in the auxiliary data user manual (AUM), including an overview of the data contents and their specific use within this project.

This document describes the DP and covers the scope of the AUM.

For completeness, we include all input data sets to the project in the scope of this document, including L1 datasets which are to be processed during the study.

In this project most (all, tbc) of the auxiliary datasets are available to ESA via the relevant host organisation website. We do not plan to duplicate such data-bases on the METHANE+ project website. This document contains links to the relevant websites hosting each dataset, together with descriptions of the specific sub-sets of data (and versions) used within this project.

2. Auxiliary data set descriptions

2.1. TCCON

2.1.1. Overview

"The Total Carbon Column Observing Network (TCCON) is a network of ground-based Fourier Transform Spectrometers that record spectra of the sun in the near-infrared. From these spectra, accurate and precise column-averaged abundances of atmospheric constituents including CO_2, CH_4, N_2O, HF, CO, H_2O, and HDO, are retrieved."[1]

Within this project TCCON measurements of methane (CH_4) are used to validate the satellite retrievals.

2.1.1. References

Wunch, D., G.C. Toon, J.-F.L. Blavier, R.A. Washenfelder, J. Notholt, B.J. Connor, D.W.T. Griffith, V. Sherlock, P.O. Wennberg. The Total Carbon Column Observing Network. Phil. Trans. R. Soc. A (2011) 369, doi:10.1098/rsta.2010.0240
Xiong , Xiaozhen, Chris Barnet, Eric Maddy, Colm Sweeney, Xingpin Liu,, Lihang Zhou, and Mitch Goldberg, Characterization and validation of methane products from the Atmospheric Infrared Sounder (AIRS), JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 113, G00A01, doi:10.1029/2007JG000500, 2008

2.1.2. Data source / URL

The main TCCON data archive: https://tccondata.org/

2.1.3. Data policy / restrictions of use

See https://tccon-wiki.caltech.edu/Network_Policy/Data_Use_Policy

Note that the right to redistribute data are reserved. Also PIs of the data from each individual station need to be notified in advance of "publication or presentation" of results using TCCON data and the station specific DOI needs to be cited in any publication.

[1] Quoted from https://tccon-wiki.caltech.edu/

2.1.4. Version used

This project will use the latest version of “GGG2014” data available in time for the required work. Data from each TCCON station is available in a specific file, with specific DOI. DOIs of the datasets used will be quoted in the final version of this document.

2.1.5. Sub-set of data used

The following TCCON sites provide during the time period relevant to this project. All data from these stations will be used:

Ascension Island (SH), Anmeyondo (KR), Bialystok (PL), Bremen (DE), Burgos (PH), Caltech (US), Darwin (AU), Edwards (US), East Trout Lake (CA), Eureka (CA), Garmisch (DE), Izana (ES), Jet Propulsion Laboratory (US), Saga (JP), Karlsruhe (DE), Lauder (NZ), Lamont (US), Orléans (FR), Park Falls (US), Paris (FR), Réunion Island (RE), Rikubetsu (JP), Sodankylä (FI), Ny Ålesund (SJ), Tsukuba (JP), Wollongong (AU), Zugspitze (DE).

2.1.6. Contents of data

Data file contents are described here:
https://tccon-wiki.caltech.edu/Network_Policy/Data_Use_Policy/Data_Description

2.1.7. Tools used to read / access the data

Standard tools to read NetCDF format files.

2.2. Aircore

2.2.1. Overview

The AirCore is an atmospheric sampler flying under a meteorological balloon. It allows the measurement of the vertical profiles (from the surface up to 30 km of altitude) of atmospheric concentration of greenhouse gases (CO2, CH4 and CO).

Its concept, initially proposed by NOAA, is extremely simple: it consists of a long tube of stainless steel placed under a meteorological balloon which, in the ascending phase, empties its air by its open end, to fill with air during its downward phase. The captured air column is then interpreted in terms of the vertical gas concentration profile using a Picarro type laser diode analyser. This system makes it possible to access altitudes not attainable by aircraft flights and to obtain very good vertical resolution.

In this project, AirCore data will be available from two sources. First, vertical profiles of CH4 will be made available from the French AirCore program. The AirCore-Fr program, led by LMD and established in 2013, is now performing regular/monthly measurements at 3 stations in France: Aire-sur-l'Adour, MDH-Reims and Trainou-Orléans. For the period mid-2018 to mid-2019, about 40 profiles are available, including profiles acquired during the MAGIC2019 campaign (https://magic.aeris-data.fr) that aimed at performing validation of IASI and TROPOMI level1 and level2 data.

Aircore CH4 profiles will also be made available by prof.dr. H. Chen (RUG) for use in the Methane+ project. Namely data taken at Sodankyla on a regular basis (9 profiles in 2018, and 6 profiles in 2019 covering nearly all months from April to October), and in total taken on 4 days; 6 profiles obtained during the Ringo-project campaign at Trainou during a 2 weeks (June 10 – 22, 2019), and Aircore profiles planned during a two weeks campaign at Kiruna in Aug./Sept. 2020 that is postponed to summer 2021 due to Covid-19. Possibly more Aircore profiles will become available in 2021 but that is subject to proposals getting funded and uncertain if these will be in time to be used in Methane+.

2.2.2. References

Membrive O., Crevoisier C., Sweeney C., Danis F., Hertzog A., Engel A., Bönisch H. and Picon L., AirCore-HR: A high resolution column sampling to enhance the vertical description of CH4 and CO2, Atmos. Meas. Tech., 10, 2163-2181, 2017, https://doi.org/10.5194/amt-10-2163-2017

2.2.3. Data source / URL

Data should be made available in the coming months on the French AirCore program website at https://aircore.aeris-data.fr In the meantime, profiles for the period considered in the project will be provided by LMD.

At the moment, regular AirCore profiles in Sodankyla and RINGO RUG AirCore profiles are only available by email request. Working in progress to make the data online.

2.2.4. Data policy / restrictions of use

The right to redistribute data are reserved. Also PIs of the data from each individual station need to be notified in advance of publication or presentation of results using AirCore-Fr data. When available, specific DOI needs to be cited in any publication.

2.2.5. Version used

The latest version will be available for the project.

2.2.6. Contents of data

Data files contain atmospheric profiles of pressure, CO2, CH4, CO, temperature, relative humidity, latitude, longitude and time. Format is NASA AMES.

2.2.7. Tools used to read / access the data

Standard tools to read ascii files.

2.3. ATOM 4

2.3.1. Overview

The Atmospheric Tomography Mission (ATom) comprises dedicated flights of the NASA DC-8 aircraft, designed to provide continuous sampling of tropospheric profiles of trace-gases (including methane) over a wide range of latitudes, sampling each of the 4 seasons in 4 separate campaigns. Each campaign comprises several flights, taking place over several weeks; taken together the measurements in a single campaign typically form a near complete transect of observations spanning North America down to the Southern Pacific (and back).

The final campaign, Atom 4, took place between March and May 2018, providing measurements which can be use in this study to assess retrievals from S5P as well as IASI and CrIS. Atom data should enable the vertical profile information obtained from the TIR and joint SWIR/TIR retrievals to be quantitatively assessed.

2.3.1. References

Wofsy, S.C., S. Afshar, H.M. Allen, E.C. Apel, E.C. Asher, B. Barletta, J. Bent, H. Bian, B.C. Biggs, D.R. Blake, N. Blake, I. Bourgeois, C.A. Brock, W.H. Brune, J.W. Budney, T.P. Bui, A. Butler, P. Campuzano-Jost, C.S. Chang, M. Chin, R. Commane, G. Correa, J.D. Crounse, P. D. Cullis, B.C. Daube, D.A. Day, J.M. Dean-Day, J.E. Dibb, J.P. DiGangi, G.S. Diskin, M. Dollner, J.W. Elkins, F. Erdesz, A.M. Fiore, C.M. Flynn, K.D. Froyd, D.W. Gesler, S.R. Hall, T.F. Hanisco, R.A. Hannun, A.J. Hills, E.J. Hintsa, A. Hoffman, R.S. Hornbrook, L.G. Huey, S. Hughes, J.L. Jimenez, B.J. Johnson, J.M. Katich, R.F. Keeling, M.J. Kim, A. Kupc, L.R. Lait, J.-F. Lamarque, J. Liu, K. McKain, R.J. Mclaughlin, S. Meinardi, D.O. Miller, S.A. Montzka, F.L. Moore, E.J. Morgan, D.M. Murphy, L.T. Murray, B.A. Nault, J.A. Neuman, P.A. Newman, J.M. Nicely, X. Pan, W. Paplawsky, J. Peischl, M.J. Prather, D.J. Price, E. Ray, J.M. Reeves, M. Richardson, A.W. Rollins, K.H. Rosenlof, T.B. Ryerson, E. Scheuer, G.P. Schill, J.C. Schroder, J.P. Schwarz, J.M. St.Clair, S.D. Steenrod, B.B. Stephens, S.A. Strode, C. Sweeney, D. Tanner, A.P. Teng, A.B. Thames, C.R. Thompson, K. Ullmann, P.R. Veres, N. Vieznor, N.L. Wagner, A. Watt, R. Weber, B. Weinzierl, P.O.

Wennberg, C.J. Williamson, J.C. Wilson, G.M. Wolfe, C.T. Woods, and L.H. Zeng. 2018. ATom: Merged Atmospheric Chemistry, Trace Gases, and Aerosols. ORNL DAAC, Oak Ridge, Tennessee, USA. https://doi.org/10.3334/ORNLDAAC/1581

2.3.2. Data source / URL

Main page for the ATom project: https://espo.nasa.gov/atom/content/ATom

Data access: https://daac.ornl.gov/cgi-bin/dsviewer.pl?ds_id=1581

2.3.3. Data policy / restrictions of use

https://daac.ornl.gov/about/#citation_policy

There are no restrictions on the use of the data, though

2.3.4. Version used

This project will used v1.4 of the merged “atmospheric chemistry, trace gases, and aerosols” product, which has the following doi:

https://doi.org/10.3334/ORNLDAAC/1581

2.3.5. Sub-set of data used

Methane data from Atom 4 campaign found to be co-located with S5P/IASI/CrIS orbit tracks/ sampling time.

2.3.6. Contents of data

See doi reference above

2.3.7. Tools used to read / access the data

Standard tools to read NetCDF files.

2.4. S5P L1B data (bands 6,7,8)

2.4.1. Overview

S5P TROPOMI L1B radiance spectra from band 6 (L1B_RA_BD6), band 7 (L1B_RA_BD7) and band 8 (L1_RA_BD8) are used.

TROPOMI performs a solar irradiance measurement approximately every 15 orbits (i.e. once a day). L1B irradiance spectra from bands 1-6 (L1B_IR_UVN) and bands 7-8 (L1B_IR_SIR) are used.

2.4.1. References

[ATBD] Algorithm theoretical basis document for the TROPOMI L01b data processor
source: KNMI; ref: S5P-KNMI-L01B-0009-SD; issue: 8.0.0; date: 2017-06-01;
url: https://sentinels.copernicus.eu/documents/247904/2476257/Sentinel-5P-TROPOMILevel-1B-ATBD

[IODS] Input/output data specification for the TROPOMI L01b data processor
source: KNMI; ref: S5P-KNMI-L01B-0012-SD; issue: 9.0.0; date: 2018-04-01;
url: https://sentinels.copernicus.eu/documents/247904/3119978/Sentinel-5P-Level-01Binput-output-data-specification

[MDS] Metadata specification for the TROPOMI L1b products
source: KNMI; ref: S5P-KNMI-L01B-0014-SD; issue: 5.0.0; date: 2018-04-01;
url: https://sentinels.copernicus.eu/documents/247904/3119978/Sentinel-5P-L01Bmetadata-specifications

[PRF] S5P Mission Performance Centre Level 1b Readme
source: KNMI; ref: S5P-MPC-KNMI-PRF-L1B; issue: 2.2.0; date: 2019-10-31;
url: http://www.tropomi.eu/sites/default/files/files/publicS5P-MPC-KNMI-PRF-L1B_v01.00.00_2.2.0_20191031.pdf

2.4.2. Data source / URL

All L1B data are available on the Copernicus Open Data Hub
https://s5phub.copernicus.eu/dhus/#/home

2.4.3. Data policy / restrictions of use

Data are publicly available free and open access to the user community.

2.4.4. Version used

L1B data produced with the processor version 01.00.00 (current available version as of April 2020) will be used in off-line timeliness (OFFL)(PRF)

2.4.5. Sub-set of data used

Two years of data will be used, corresponding to the operational phase of S5P-TROPOMI starting April 2018.

2.4.6. Contents of data

Details of the data format are provided in the Input/Output Data Specification document (IODS).

2.4.7. Tools used to read / access the data

To access the data batch scripting with wget or similar tools for data query can be used (see (https://scihub.copernicus.eu/twiki/do/view/SciHubUserGuide/BatchScripting?redirectedfrom=SciHubUserGuide.8BatchScripting#odata_demo_script). Data is in NetCDF4 format, so standard netCDF libraries and tools are used to read the data.

2.5. TM5 CO and CH4 prior information

2.5.1. Overview

The operational and offline TROPOMI XCO and XCH4 retrieval algorithms make use of model simulated vertical profiles of CO and CH4 mixing ratios as a priori. These mixing ratio profiles are derived from the TM5-4DVAR inverse modelling system applied to CO, making use of the setup developed by Hooghiemstra et al (2012), and to CH4, using the Copernicus Atmosphere Monitoring Surface (CAMS) reanalysis as documented in Segers et al (2020). Because of the near real-time operational processing of S5p data this information needs to be available ahead of time, and is therefore a prediction of future CO and CH4 mixing ratios based on the long-term trend and the climatological global variation in space and time (Landgraf et al, 2016). Section 2.5.2 provides description of the approach that is followed to derive these data.

2.5.2. Method description

CO a priori

Inverse modelling calculations in TM5-4DVAR have been performed for the period 2010-2015 using surface measurements from background sites of the NOAA-ESRL flask sampling network. The setup of the inversion followed the methodology of

Hooghiemstra et al (2012), using ECMWF ERA interim meteorology at 6ºx4º and 25 vertical hybrid sigma pressure levels. The optimized concentration output is used to compute a single climatological year, by collecting and averaging the available output per month.
To extrapolate the monthly CO climatology to the future time window for which the data will applied, output is sampled at four background sites of the NOAA ESRL network: SUM (38.42ºW; 72.60ºN; 3215masl), MLO (155.58ºW; 19.53ºN; 3402masl), ASK (5.63ºE; 23.26ºN; 2715masl), and SPO (24.80ºW; -89.98ºS; 2815masl). These stations have been selected because they represent background conditions, have a multi-year gap free data record and span the full north-south gradient.

For each measurement site a trend is determined by linear regression to the available measurements since 2010. From this trend line the mean CO level is determined for the future time window for which a priori data are needed. The TM5-4DVAR derived climatology is sampled at the same location and the difference between climatological CO level and the extrapolated station concentration is calculated to determine the offset to the climatology that is required to bring it to the extrapolated CO level. This procedure is repeated for the 4 stations. The offsets are averaged to obtain a single offset that the turns the climatology into an a priori CO dataset that is valid for the time window of its application.
The resulting dataset is evaluated against NOAA ESRL measurement sites to evaluate its validity. Optionally the uniform offset can be extended with a trend correction. However, so far this was not needed as the global trend in CO during the past decade has been quite small (~1% reduction per year). The seasonal amplitude (30-50%) is large compared to the trend. Because of this, there is also no need to correct for jumps between subsequent a priori data submissions.

CH4 a priori

The CH4 a priori is derived from the CAMS CH4 multi-year reanalysis that is delivered to ECMWF by TNO on an annual basis. Optimised CH4 mixing ratio are taken from the most recent multi-year inversion production chain using surface measurements that is available from the CAMS server (currently v18r1, spanning the period 1990 – 2018). Mixing ratios are available at 6 hourly time interval at 3ºx2º degree and 34 vertical pressure-sigma levels. From these data a monthly climatology is computed for the most recent 6 years. The vertical resolution is degraded to the default 25 layers by linear interpolation.

To extrapolate the monthly CH4 climatology to the future time window for which the data will applied, output is sampled at four background sites of the NOAA ESRL network: SUM (38.42ºW; 72.60ºN; 3215masl), MLO (155.58ºW; 19.53ºN; 3402masl), ASK (5.63ºE; 23.26ºN; 2715masl), and SPO (24.80ºW; -89.98ºS; 2815masl). These stations have been selected because they represent background conditions, have a multi-year gap free data record and span the full north-south gradient.

For each measurement site a trend is determined by linear regression to the available measurements since 2012. From this trend line the mean CH4 level is determined for the future time window for which a priori data are needed. The TM5-4DVAR derived climatology is sampled at the same location and the difference between climatological CH4 level and the extrapolated station concentration is calculated to determine the offset to the climatology that is required to bring it to the extrapolated CH4 level. This procedure is repeated for the 4 stations. The offsets are averaged to obtain a single offset that the turns the climatology into an a priori CH4 dataset that is valid for the time window of its application. The a priori dataset consists of daily CH4 data, which are derived from the monthly means by linear interpolation.
The resulting dataset is evaluated against NOAA ESRL measurement sites to evaluate its validity. Optionally the uniform offset can be extended with a trend correction. So far this was not needed, but the trend has been corrected for an offset due to the 2015-2016 El Nino. Jumps between two subsequent a priori data submissions are smoothened by linear interpolation applied to the first month of every new submission.

2.5.3. References

Hooghiemstra, P. B., M. C. Krol, P. Bergamaschi, A.T.J. de Laat, G.R. van der Werf, P.C. Novelli, M.N. Deeter, I. Aben, T. Röckmann, 2012, Comparing optimized CO emission estimates using MOPITT or NOAA surface network observations, J. Geophys. Res., 117, D06309, doi:10.1029/2011JD017043.

Segers, A. and S. Houweling, 2020, Description of the CH4 Inversion Production Chain, Copernicus Atmosphere Monitoring Service, https://atmosphere.copernicus.eu/sites/default/files/2020-01/CAMS73_2018SC1_D73.5.2.2-2019_202001_production_chain_v1.pdf

Landgraf, J., Brugh, J. De, Scheepmaker, R., Borsdorff, T., Hu, H., Houweling, S., … Hasekamp, O. (2016). Carbon monoxide total column retrievals from TROPOMI shortwave infrared measurements, 4955–4975. Atmos. Meas. Tech., https://doi.org/10.5194/amt-9-4955-2016.

2.5.4. Data source / URL

Contained in TROPOMI L2 files: https://s5phub.copernicus.eu/dhus/#/home

2.5.5. Data policy / restrictions of use

Public data.

2.5.6. Version used

The a priori data are made available in overlapping 12 monthly batches, submitted twice per year. The version that is used varies with the timestamp of the retrieved data.

2.5.7. Sub-set of data used

n.a.

2.5.8. Contents of data

Vertical profiles of the CO and CH4 mixing ratio at 25 levels from the surface to top of atmosphere for each TROPOMI retrieval.

2.5.9. Tools used to read / access the data

Standard tools for processing netcdf data.

2.6. GMTED2010 and GLCC

2.6.1. Overview

A digital elevation model is required for the selection and interpolation of suitable precalculated reference spectra. For this purpose, the Global Multi-resolution Terrain Elevation Data 2010 (GMTED2010) and the Global Land Cover Characterization (GLCC) of the United States Geological Survey (USGS) (United States Geological Survey) are used to compute surface elevation and land fraction for every sounding of the satellite.

2.6.2. References

Danielson, J. J., and Gesch, D. B., 2011, Global multi-resolution terrain elevation data 2010 (GMTED2010): U.S. Geological Survey Open-File Report 2011–1073, https://doi.org/10.3133/ofr20111073

2.6.3. Data source / URL

Global Multi-resolution Terrain Elevation Data 2010 (GMTED2010):
https://doi.org/10.5066/F7J38R2N

Global Land Cover Characterization (GLCC):
https://doi.org/10.5066/F7GB230D

2.6.4. Data policy / restrictions of use

Public access:
https://www.usgs.gov/atom/72352

2.6.5. Version used

There is only a single version of data

2.6.6. Sub-set of data used

Global data

2.6.7. Contents of data

See technical documentation on webpage

2.6.8. Tools used to read / access the data

The provided raster data is converted to netCDF using IDL routines.

2.7. GOSAT SRON CH4 data products

2.7.1. Overview

SRON generates GOSAT CH4 products using the RemoTeC retrieval algorithm as a part of C3S, CAMS and CCI+ GGH. In this project we will use the GOSAT RemoTec CH4 Proxy product generated as part of C3S.

2.7.2. References

Butz, A., et al.: Toward accurate CO2 and CH4 observations from GOSAT Geophys. Res. Lett., 38(L14812), doi:10.1029/2011GL047888, 2011.

Guerlet, S., et al., Impact of aerosol and thin cirrus on retrieving and validating XCO2 from GOSAT shortwave infrared measurements, J. Geophys. Res. Atmos., 118, 4887–4905, doi:10.1002/jgrd.50332, 2013.

Schepers, D., et al., Methane retrievals from Greenhouse Gases Observing Satellite (GOSAT) shortwave infrared measurements: Performance comparison of proxy and physics retrieval algorithms, J. Geophys. Res., 117, D10307, doi:10.1029/2012JD017549, 2012

2.7.3. Data source / URL

Data can be accessed via SRON ftp
ftp://ftp.sron.nl/pub/pub/RemoTeC/C3S/CH4_GOS_SRPR/2.3.9/

2.7.4. Data policy / restrictions of use

The data can be freely downloaded via the ftp site (see 2.7.3). There are no restrictions in the use of the data, but SRON team should be contacted upon scientific findings.

2.7.5. Version used

Version 2.3.9 of the data set will be used.

2.7.6. Sub-set of data used

Two years of data will be used, corresponding to the operational phase of S5P-TROPOMI starting April 2018. GOSAT has a thin spatial sampling, therefore the data has to be collocated in time and space with TROPOMI observations.

2.7.7. Contents of data

The GOSAT proxy product contains the retrieved column averaged dry air mixing ratio, both corrected (xch4) and non-corrected (xch4_raw) variables. It is recommended to use the corrected xch4.

2.7.8. Tools used to read / access the data

Standard netCDF libraries/tools can be used to access and read the data.

2.8. L1 data from Metop B (IASI, AMSU, MHS)

2.8.1. Overview

Data from the Metop sounders used in this project is provided by Eumetsat.

Two years of Metop-B data, acquired during the operational phase of S5P will be analysed in this project. This is currently assumed to be April 2018-20.

Offline data in native format, acquired from the Eumetsat archive will be used by RAL.
LMF will use Metop-B data provided through EUMETCast and made available by the French data center AERIS.

2.8.1. References

2.8.2. Data source / URL

Eumetsat archive:
https://www.eumetsat.int/website/home/Data/DataDelivery/EUMETSATDataCentre/index.html

2.8.3. Data policy / restrictions of use

See
https://www.eumetsat.int/website/wcm/idc/idcplg?IdcService=GET_FILE&dDocName=PDF_LEG_DATA_POLICY&RevisionSelectionMethod=LatestReleased&Rendition=Web

Note that re-distribution of IASI data acquired from the archive is not permitted.

2.8.4. Version used

Only a single version of data from the 3 sounders is available for any given date. However the L1 data version used in the ground-segment evolves with time. The following versions are relevant to the period considered in this project:

- IASI L1C: v8.0 (13 Sept 2017 to 24 Sept 2019), v8.2 (24 Sept 2019 onwards)
- AMSU and MHS L1B: Version 1.0

2.8.5. Sub-set of data used

All L1 data within the 2 year METHANE+ study period will be used.

2.8.6. Contents of data

Refer to the EUMETSAT product specification documents:

ATOVS Level 1b Product Guide, EUMETSAT, Doc.No. : EUM/OPS-EPS/MAN/04/0030, Issue : v3:
http://www.eumetsat.int/website/wcm/idc/idcplg?IdcService=GET_FILE&dDocName=pdf_v2a_atovs_level_1b&RevisionSelectionMethod=LatestReleased&Rendition=Web

IASI Level 1: Product Guide
EUMETSAT; Doc.No. EUM/OPS-EPS/MAN/04/0032. Issue: v5 e-signed; Date: 6 September 2019:
http://www.eumetsat.int/website/wcm/idc/idcplg?IdcService=GET_FILE&dDocName=PDF_IASI_LEVEL_1_PFS&RevisionSelectionMethod=LatestReleased&Rendition=Web

2.8.7. Tools used to read / access the data

RAL use IDL routines ("READ_FIXED_EPS") provided by Eumetsat to read the native format data from IASI, AMSU and MHS.

2.9. L1 data from Suomi NPP (CrIS, ATMS)

2.9.1. Overview

Within the METHANE+ product the RAL IASI IMS and methane schemes will also be applied to the CrIS TIR spectrometer and ATMS microwave sounder on Suomi NPP.

CrIS full spectral resolution (FSR) data files are used, available after the operation of the instrument was changed to allow this on November 2, 2015. The FSR files have 2,223 channels: 637 shortwave channels from 3.9 to 4.7 microns (2555 to 2150 cm-1), 869 midwave channels from 5.7 to 8.05 microns (1752.5 to 1242.5 cm-1), and 717 longwave channels from 9.1 to 15.41 microns (1096.25 to 648.75 cm-1). Each CrIS field-of-regard (FOR, ~50x50km at nadir) contains 9 (~12km diameter) field-of-views (FOVs) arranged in a 3X3 array. (I.e. the FOR are similar to IASI, but CrIS obtains 9 observations within each compared to 4 for IASI.)

The ATMS instrument is a cross-track scanner with 22 microwave channels in the range 23.8-183.31 Gigahertz (GHz). The beam width is 1.1 degrees for the channels in the 160-183 GHz range, 2.2 degrees for the 80 GHz and 50-60 GHz channels, and 5.2 degrees for the 23.8 and 31.4 GHz channels. Since the SNPP satellite is orbiting at an altitude of about 830 km, the instantaneous spatial resolution on the ground at nadir is about 16 km, 32 km, or 75 km depending upon the channel. There are 96 samples in the cross-track direction.

Within this project we will use all data available in the selected 2 year time period for joint analysis with S5P.

2.9.1. References

Han, Y. et al. Suomi NPP CrIS measurements, sensor data record algorithm, calibration and validation activities, and record data quality. *J. Geophys. Res.* **118**, 12734–12748 (2013).

Kim, E., Lyu, C.-H. J., Anderson, K., Leslie, R. V., and Blackwell, W. J. (2014), S-NPP ATMS instrument prelaunch and on-orbit performance evaluation, *J. Geophys. Res. Atmos.*, 119, 5653– 5670, doi:10.1002/2013JD020483.

2.9.2. Data source / URL

ATMS: https://snpp-sounder.gesdisc.eosdis.nasa.gov/data/SNPP_Sounder_Level1/SNPPATMSL1B.2/

CrIS L1B (full spectral resolution):
https://snpp-sounder.gesdisc.eosdis.nasa.gov/data/SNPP_Sounder_Level1/SNPPCrISL1B.2/

2.9.3. Data policy / restrictions of use

Data are available free to the user community. See NASA Earth Science Data and Information Policy: https://science.nasa.gov/earth-science/earth-science-data/data-information-policy/

2.9.4. Version used

CrIS Version 2.11 FSR

ATMS Version 2.11

2.9.5. Sub-set of data used

All L1 data within the 2 year METHANE+ study period will be used

2.9.6. Contents of data

See product user guides:

NASA Cross Track Infrared Sounder (CrIS) Level 1B Product Users' Guide Version 2.11. Product Version: 2.11.1, Software Version: 2.1.3, December 2018: https://docserver.gesdisc.eosdis.nasa.gov/public/project/JPSS-1/NASA_CrIS_L1B_Product_Users_Guide_V2.11.pdf

NASA Advanced Technology Microwave Sounder (ATMS), Level 1B Data Product User Guide, August 2019, Product Version 2.11, Software Version 2.11.2: https://docserver.gesdisc.eosdis.nasa.gov/public/project/JPSS-1/SNDRJ1ATMSL1B.2.Readme.12AUG2019.pdf

2.9.7. Tools used to read / access the data

Standard netCDF reading tools are used.

2.10. ECMWF ERA-5 analysis

2.10.1. Overview

ERA-5 is the latest ECMWF re-analysis product spanning. Currently data from 1979 to present is available (it is planned to extend back to 1950).

RAL use the following variables from the hourly analysis fields stored at 0.125 degree resolution at the UK Centre for Environmental Data Analysis (CEDA):

- Surface temperature
- Surface pressure
- Temperature profile
- Humidity profile
- Vorticity profile
- 2m temperature and humidity

Data is produced by ECMWF in grib2 format, though it can be acquired from the C3S datastore in netCDF format. The data used by RAL at CEDA is netCDF format.

2.10.2. References

Hersbach, H, Bell, W, Berrisford, P, Horányi, A, J., M-S, Nicolas, J, Radu, R, Schepers, D, Simmons, A, Soci, C, Dee, D, Global reanalysis: goodbye ERA-Interim, hello ERA5,ECMWF Newsletter 159, Apr 2019, https://www.ecmwf.int/node/19027

Dataset citable as: Copernicus Climate Change Service (C3S) (2017): ERA5: Fifth generation of ECMWF atmospheric reanalyses of the global climate . Copernicus Climate Change Service Climate Data Store (CDS), 2019.
https://cds.climate.copernicus.eu/cdsapp#!/home

2.10.3. Data source / URL

Main page at ECMWF:
https://www.ecmwf.int/en/forecasts/datasets/reanalysis-datasets/era5

Documentation:
https://confluence.ecmwf.int/display/CKB/ERA5%3A+data+documentation

Data access via Copernicus C3S data store:
https://cds.climate.copernicus.eu/#!/search?text=ERA5&type=dataset

Data access from CEDA:
http://data.ceda.ac.uk/badc/ecmwf-era5/

2.10.4. Data policy / restrictions of use

See Copernicus C3S/CAMS License agreement:
http://apps.ecmwf.int/datasets/licences/copernicus/

2.10.5. Version used

Data available in 2019/20

2.10.6. Sub-set of data used

All data hourly analysis data for variables listed above, duing period analysed in study.

2.10.7. Contents of data

Each model field, at a given time step is stored in a separate file. See links to documentation and C3S datastore above for more details.

2.10.8. Tools used to read / access the data

Standard netCDF tools.

2.11. ECMWF Operational Analysis

2.11.1. Overview

In SRON retrievals, the atmospheric conditions are derived from the ECMWF (European Centre for Medium-Range Weather Forecasts) first analysis after the forecast, provided 6-hourly.

2.11.2. References

2.11.3. Data source / URL

Data is obtained from ECMWF archive catalogue from the MARS archiving system.

2.11.4. Data policy / restrictions of use

Data access is granted to SRON in the framework of the TROPOM project.

2.11.5. Version used

2.11.6. Sub-set of data used

Two years of data will be used, corresponding to the operational phase of S5P-TROPOMI starting April 2018.

2.11.7. Contents of data

Temperature profile, H_2O column, surface pressure and surface elevation data are obtained on a reduced Gaussian grid, N640.

2.11.8. Tools used to read / access the data

The ECMWF data are downloaded in GRIB files, and ingested by a pre-processing system used at SRON for spatial and temporal collocation of input data with TROPOMI data.

2.12. CAMS CH4 global CH4 flux-inversion re-analysis

2.12.1. Overview

The CAMS greenhouse-gas (GHG) flux inversions provide global methane analyses based on the assimilation of ground-based measurements to infer methane surface fluxes. Depending on the dataset version, satellite observations may also be assimilated. The dataset provides methane profiles which are useful for assessment of height resolved methane retrievals, allowing the effects of vertical sensitivity to be properly accounted for by applying of averaging kernels to the model profiles.

To date, RAL have used the dataset (“v10-S1NOAA_ra”) which spans 2000-2012, based on the assimilation of NOAA surface level flask measurements. As well as direct comparisons of IASI and CAMS, RAL also use the CAMS data to account for the impact of averaging kernels on comparisons between TCCON and IASI. The most recent v18r1 data covers the period from 1990 up to the end of 2018. This will enable comparisons to be made during the period of the S5P mission.

2.12.2. References

Segers, A. and S. Houweling, 2020, Description of the CH4 Inversion Production Chain, Copernicus Atmosphere Monitoring Service, https://atmosphere.copernicus.eu/sites/default/files/2020-01/CAMS73_2018SC1_D73.5.2.2-2019_202001_production_chain_v1.pdf

Houweling, S., Bergamaschi, P., Chevallier, F., Heimann, M., Kaminski, T., Krol, M., Michalak, A. M., and Patra, P.: Global inverse modeling of CH_4 sources and sinks: an overview of methods, Atmos. Chem. Phys., 17, 235–256, https://doi.org/10.5194/acp-17-235-2017, 2017.

2.12.3. Data source / URL

CAMS flux inversion data store at ECMWF:
https://apps.ecmwf.int/datasets/data/cams-ghg-inversions/

2.12.4. Data policy / restrictions of use

The data is publically available.

2.12.5. Version used

v18r1

2.12.6. Sub-set of data used

During the METHANE+ analysis period.

2.12.7. Contents of data

Global 3D CH4 dry air mixing ratios at 2^ox3^o horizontal resolution, 34 vertical levels, and 6 hourly time interval.

2.12.8. Tools used to read / access the data

Standard netcdf tools.

2.13. HITRAN spectroscopic data

2.13.1. Overview

HITRAN is a compilation of spectroscopic parameters, which is used in the forward model to compute the lookup table for the radiances and their derivatives.

2.13.2. References

Gordon, I. E., Rothman, L. S., Hill, C., Kochanov, R. V., Tan, Y., Bernath, P. F., Birk, M., Boudon, V., Campargue, A., Chance, K. V., Drouin, B. J., Flaud, J.-M., Gamache, R. R., Hodges, J. T., Jacquemart, D., Perevalov, V. I., Perrin, A., Shine, K. P., Smith, M.-A., Tennyson, J., Toon, G. C., Tran, H., Tyuterev, V. G., Barbe, A., Császár, A. G., Devi, V. M., Furtenbacher, T., Harrison, J. J., Hartmann, J.-M., Jolly, A., Johnson, T., Karman, T., Kleiner, I., Kyuberis, A., Loos, J., Lyulin, O. M., Massie, S. T., Mikhailenko, S. N., Moazzen-Ahmadi, N., Müller, H. S. P., Naumenko, O. V., Nikitin, A. V., Polyansky, O. L., Rey, M., Rotger, M., Sharpe, S., Sung, K., Starikova, E., Tashkun, S. A., Vander Auwera, J., Wagner, G., Wilzewski, J., Wcisło, P., Yu, S., and Zak, E. J.: The HITRAN2016 molecular spectroscopic database, J. Quant. Spectrosc. Ra., 203, 3–69, https://doi.org/10.1016/j.jqsrt.2017.06.038, 2017.

2.13.3. Data source / URL

https://hitran.org/

2.13.4. Data policy / restrictions of use

Public access

2.13.5. Version used

HITRAN 2016

2.13.6. Sub-set of data used

Line-by-line data for H_2O, CO_2, N_2O, CO, CH_4, O_2

2.13.7. Contents of data

See technical documentation on the webpage:
https://hitran.org/docs/

2.13.8. Tools used to read / access the data

Standard FORTRAN tools are used.

2.14. GEISA spectroscopic data

2.14.1. Overview

GEISA is a compilation of spectroscopic parameters, which is used in the 4A forward radiative transfer code to compute spectral radiances and associated Jacobians, which are then used in the retrieval procedure of LMD.

2.14.2. References

N. Jacquinet-Husson, R. Armante, N.A. Scott, A. Chedin, L. Crépeau, C. Boutammine, A. Bouhdaoui, C. Crevoisier, V. Capelle, C. Boonne, N. Poulet-Crovisier, A. Barbe, D. Chris Benner, V. Boudon, L.R. Brown, J. Buldyreva, A. Campargue, L.H. Coudert, V.M. Devi, M.J. Down, B.J. Drouin, et al., The 2015 edition of the GEISA spectroscopic database, *J. Mol. Spectrosc.*, 327, 31-72, http://dx.doi.org/10.1016/j.jms.2016.06.007 (2016)

2.14.3. Data source / URL

https://geisa.aeris-data.fr

2.14.4. Data policy / restrictions of use

Public access

2.14.5. Version used

GEISA2015

2.14.6. Contents of data

See technical documentation on the webpage:
https://geisa.aeris-data.fr

2.14.7. Tools used to read / access the data

Standard FORTRAN tools are used.

2.15. SEOM-IAS spectroscopic data

2.15.1. Overview

The SEOM-Improved Atmospheric Spectroscopy Databases (IAS) Project produced a new specptroscopic database for improving retrievals from Remote Sensing missions.

2.15.2. References

Birk, M.,Wagner, G., Loos, J.,Wilzewski, 5 J., Mondelain, D., Campargue, A., Hase, F., Orphal, J., Perrin, A., Tran, H., Daumont, L., Rotger-Languereau, M., Bigazzi, A., and Zehner, C.: Methane and water spectroscopic database for TROPOMI Sentinel 5 Precursor in the 2.3um region, vol. 19, p. 4652, EGU General Assembly, 2017.

2.15.3. Data source /URL

All Databases are available from the website (https://www.wdc.dlr.de/seom-ias/) and from the Open Access platform zenodo.org.

2.15.4. Data policy / restrictions of use

Data is open access and is free to the user community.

2.15.5. Version used

The 2017 version is used.

2.15.6. Sub-set of data used

See 2.14.7

2.15.7. Contents of data

The database contains measurements for retrieval of absorption line parameters of H2O, CO and CH4 in the spectral range 4190-4340 cm^{-1}. These cross-section lookup-tables are calculated from the databases assuming Voigt line shapes

2.15.8. Tools used to read / access the data

Standard programming tools are used to read and manipulate the data.

3. Acronyms and abbreviations

Acronym	Meaning
ACOS	Atmospheric CO2 Observations from Space (algorithm)
ATBD	Algorithm Theoretical Basis Document
AU	Country code: Australia
AUM	Auxiliary Data User Manual
BESD	Bremen optimal estimation DOAS
C3C	Copernicus Climate Change Service
CCI	Climate Change Initiative (of ESA)
CA	Country code: Canada
CAMS	Copernicus Atmosphere Monitoring Service
CEDA	Centre for Environmental Data Analysis (UK data centre)
CrIS	Cross-track Infrared Sounder
DE	Country code: Germany
DOI	Data Object Identifier
DP	Data Pool
ECMWF	European Centre for Medium Range Weather Forecasting
ENVISAT	Environmental Satellite
EUMETSAT	European Organisation for the Exploitation of Meteorological Satellites
ESA	European Space Agency
FI	Country code: Finland
FR	Country code: France
FSR	Full Spectral Resolution (wrt CriS L1B)
GEISA	Gestion et Etude des Informations Spectroscopiques Atmosphériques: Management and Study of Atmospheric Spectroscopic Information
GOSAT	Greenhouse Gases Observing Satellite
IASI	Infrared Atmospheric Sounding Interferometer
IDL	Interactive Data Language
IUP-UB	Institute of Environmental Physics (Institut für Umweltphysik), University of Bremen, Germany
JP	Country code: Japan
KR	Country code: South Korea
L1	Level 1
L2	Level 2
LMD	Laboratoire de Météorologie Dynamique/Institut Pierre-Simon Laplace

NIR	Near Infra Red (band)
NRT	Near Real Time
NZ	Country code: New Zealand
NPOES	National Polar-orbiting Operational Environmental Satellite System
NPP	NPOESS Preparatory Project
PH	Country code: Philippines
PL	Country code: Poland
RAL	Rutherford Appleton Laboratory
RE	Country code: Réunion
RemoTeC	SRON retrieval algorithm
SCIAMACHY	Scanning Imaging Absorption Spectrometers for Atmospheric Chartography
SH	Country code: Saint Helena, Ascension and Tristan da Cunha
SJ	Country code: Svalbard and Jan Mayen
SRON	SRON netherlands institute for space research
SWIR	Short Wave Infrared
TCCON	Total Carbon Column Observing Network
US	Country code:United States of America

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