

EARTH OBSERVATION CLIMATE INFORMATION SERVICE

Quick Start Guide for the University of Leicester CO total column product

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Table of Contents

Table of	Contents	3
1. Quic	ck Start: University of Leicester Total Column CO Data Product (CO_ULIRS)	4
1.1	What products are available?	5
1.2	Summary information	6
1.3	Variables summary information	6
1.4	What can these products be used for?	8
1.5	Where to find these products for download	8
1.6	Using downloaded data	8
1.7	Import Data	9
1.8	Re-Gridding/Formatting	10
1.9	Data Reduction/Subsetting	12
1.10	Interactive visualisation / data access	14
1.11	Your obligations when using these products	14
1.12	Further Information	14
1.12	.1 Summary of retrieval processing	14
History o	of modifications / Change Log	15
Related [Documents / Reference Documents	15
Acronym	as and/or Abbreviations	15
General o	definitions	15



1. Quick Start: University of Leicester Total Column CO Data Product (CO_ULIRS)

The following will provide you with sufficient information to quickly get to grips with the University of Leicester Total Column CO (CO ULIRS) dataset product and to gain some familiarity with the information available. The CO ULIRS product is derived from measurements made by the Infrared Atmospheric Sounding Interferometer (IASI) onboard the MetOp satellite series. CO ULIRS uses an optimal estimation approach to derive carbon monoxide total column amounts from IASI spectra using the University of Leicester IASI Retrieval Scheme (ULIRS). The retrieval algorithm uses an iterative retrieval scheme based on Bayesian optimal estimation to retrieve a set of atmospheric and surface parameters, referred to as the state vector, from measured spectral radiances (Illingworth et al., 2011). The ULIRS employs a line-by-line radiative transfer model, the Oxford reference forward model (https://eodg.atm.ox.ac.uk/RFM/) for radiative transfer calculations using an optimised look-up-table approach. The RFM splits any ray path calculation into equivalent homogeneous path segments for each absorber and calculates an absorption coefficient k(v,p,T) for each segment, where v is the wavenumber and p and T are the Curtis-Godson equivalent pressure and temperature for the segment (i.e., absorber-weighted averages for the path within each atmospheric layer). The line-by-line approach is computationally expensive and for the mid-infrared, where a large number of transitions are involved, it is quicker to use pre-tabulated look-up tables (LUTs) of k [m2/kmol] (1 kmol approx 6e26 molecules). To reduce the loss of accuracy dense sampling was chosen in the p, T domain. Extensive validation of our retrieved CO ULIRS has been performed against the Network for the Detection of Atmospheric Composition Change (NDACC), a global network of ground-based high-resolution Fourier Transform Spectrometers (FTS) recording mid-infrared solar transmission spectra at high spectral resolution, itself validated against balloon and aircraft measurements.





Figure 1 - Longitudinally averaged global mean carbon monoxide total column concentrations [10^18 molecules / cm2] derived from IASI for the 2013 to 2024 period. Particularly strong regional signals are observed in the data, in particular the large CO emissions over Indonesia during late 2015 and early 2016, and the CO emissions associated with exceptionally large Siberian fires during summer 2021.



Figure 2 - The number of IASI soundings per month in the final CO_ULIRS dataset, starting in June 2013 and ending in December 2024. Counts are provided for the global total. Gaps are generally caused by periods of IASI instrument calibration.

Figure 2 shows the number of successful retrievals broken down by month. This figure is particularly useful as it highlights any systematic differences in data density over time (e.g., from changes in the IASI sampling strategy) and highlights abrupt data gaps (e.g., from instrument anomalies). It also shows that during September 2014 the number of pixels increases, which may be due to a change in level 2 cloud filtering changes for IASI.

1.1 What products are available?

Product name and acronym	Filename example	Version
University of Leicester total column CO	EOCIS-FIRE-L2-CO-IASI_METOP_B-	1.0
(CO_ULIRS)	ULIRS_20230101-fv1.0.nc	

Table 1 Dataset Products covered in this document



1.2 Summary information

Product Name	University of Leicester IASI CO Data Product (CO_ULIRS)
Main observed variable(s)	Total column carbon monoxide in 10^18 molecules/ cm2
Geographical range of dataset	-90 to 90 and -180 to 180
Temporal range of dataset	06/2013 to 12/2024
Spatial resolution / gridding	IASI pixel footprint (12 km at nadir)
Temporal sampling	Global coverage in 12 hours
characteristics	
Level of processing	Level 2 Ground-Pixel Satellite Data Product.
Main auxiliary content	CO uncertainty, Averaging kernels
Dataset citation	Will be available when data are on CEDA
Dataset journal reference	Illingworth, S. M., Remedios, J. J., Boesch, H., Moore, D. P., Sembhi, H., Dudhia, A., and Walker, J. C.: ULIRS, an optimal estimation retrieval scheme for carbon monoxide using IASI spectral radiances: sensitivity analysis, error budget and simulations, Atmos. Meas. Tech., 4, 269–288, https://doi.org/10.5194/amt-4-269-2011, 2011.

Table 2 Summary Information for University of Leicester IASI Total Column CO Data Product

1.3 Variables summary information

Variable name	Description	Units
solar_zenith_angle	Angle between line of sight to the sun and local vertical	degree
sensor_zenith_angle	Angle between the line of sight to the sensor and the local vertical	degree
solar_azimuth_angle	horizontal angle between the line of sight to the sun and a reference direction (north)	degree
sensor_azimuth_angle	horizontal angle between the line of sight from the observation point to the sensor	degree
land_area_fraction	land cover within the sensor pixel in percentage	1
longitude	Centre longitude	degrees east
latitude	Centre latitude	degrees north
surface_altitude	Altitude is the (geometric) height above the geoid, which is the reference geopotential surface	m
surface_temperature	the temperature at the surface and air interface, not the bulk temperature of the surface above or below	К
air_pressure	Vertical air pressure coordinate defining the retrieval levels	hPa



altitude_levels	Altitude is the (geometric) height above the geoid, which is the reference geopotential surface. Vertical altitude coordinate defining the retrieval levels.	m
co_profile_apriori	A-priori mole fraction profile of atmospheric CO in ppb.	1e ⁻⁹
air_temperature_apriori	Air temperature is the bulk temperature of the air, not the surface (skin) temperature.	К
h2o_profile_apriori	A-priori mole fraction profile of atmospheric H ₂ O in ppm.	1e ⁻⁶
co2_profile_apriori	A-priori mole fraction profile of atmospheric CO ₂ in ppm.	1e ⁻⁶
co_profile_apriori_uncertaint y	Statistical uncertainty of a-priori mole fraction profile of atmospheric CO in ppb (1σ).	1e ⁻⁹
co_profile	Retrieved mole fraction profile of atmospheric CO in ppb.	1e ⁻⁹
co_profile_uncertainty	total uncertainty in retrieved mole fraction profile of atmospheric CO in ppb	1e ⁻⁹
co_total_column	Retrieved total column dry-air mole fraction of atmospheric carbon monoxide in molecules cm ⁻² .	1e ¹⁸
co_total_column_uncertainty	Total uncertainty on the retrieved total column dry-air mole fraction of atmospheric carbon monoxide in molecules cm ⁻² .	1e ¹⁸
co_profile_averaging_kernel	CO profile averaging kernel (a profile = vector for each single observation). Quantifies the altitude sensitivity of the CO profile retrieval.	1
chim	retrieved cost function value.	1
dofs	Degrees of freedom for signal which quantifies the vertical resolution of the retrieval profile.	1
nstep	The average number of retrieval steps.	1
cloud_flag	Percentage of cloud in the IASI pixel derived from the EUMETSAT operational level 2 product (-1 indicates that the scene is between 0 and 9 % cloudy, otherwise the number indicated is the percentage of cloud within the scene).	1
time	Measurement time.	seconds since 1970-01-01 00:00:00

Table 3 Summary information for each variable for University of Leicester CO (CO_ULIRS)dataset product



1.4 What can these products be used for?

The CO dataset can be used for the following

- 1) Study of temporal and spatial variability: assessing carbon monoxide concentration changes over time and across different regions, providing insights into emission sources and atmospheric transport patterns.
- 2) Integrating with Global Climate Models: IASI CO data can be used as input for atmospheric and climate models to improve their accuracy, better understand their contribution to climate change and inform mitigation strategies.
- 3) Trend analysis and anomalies: IASI CO measurements provide a long-term record, which is crucial for tracking changes in atmospheric carbon monoxide levels over time and assessing the effects of fire events.
- 4) Global flux inversions: One of the primary applications for the IASI CO has been as input to model global flux inversions which are essential for understanding carbon monoxide emissions, and to estimate the sources and sinks across the globe.

Known limitations and issues are following

- As data are retrieved from the mid-infrared part of the spectrum there is some limited sensitivity to direct surface emissions, unless local conditions allow. This is usually where the surface is much warmer/cooler than the adjacent atmospheric layer (generally referred to as thermal contrast).
- The retrieval uses a single a priori profile and a priori uncertainty derived from a combination of model data (troposphere) and ACE satellite data (stratosphere). This approach may under estimate total column CO values for very large fire events.
- Data gaps the retrieval struggles to reach convergence over some very cold surfaces, even though surface T is retrieved as part of the state vector. Care should be taken over these surfaces and the user should consider sampling density of the data alongside the chi-square number.

1.5 Where to find these products for download

The UoL IASI CO data will be made available from the Centre for Environmental Data Analysis data repository. For now, data are available directly from David Moore (<u>dpm9@leicester.ac.uk</u>) and are stored on the JASMIN group workspace "eo_shared_data"

(/gws/nopw/j04/eo_shared_data_vol1/satellite/iasi/ulirs_ms/eocis/metopb/)

1.6 Using downloaded data

The final total column CO data product is stored in the co_total_column variable which is derived from the co_profile data alongside the retrieval pressure levels stored in the variable pressure_levels. It is recommended that users use this variable unless explicitly interested in the retrieved profiles, which are useful for model comparisons using the included averaging kernels stored in co_profile_averaging_kernel. The ULIRS_CO data product is stored in NetCDF format with all IASI soundings on a single day stored in one file. The data product contains a number of metrics with which a user can choose to filter the data. The simplest test is via application of "chim" which can filter pixels where convergence has been reached, but the fit between the forward model and



the IASI data is poor. A value of 10 is recommended in the first instance although the user can adjust as necessary. A second filter is to look at the dofs variable where a dofs of 1.0 means that the data for the pixel contain at least one independent piece of information from the IASI spectral measurements to constrain the vertical distribution of CO. It is recommended to look at data where dofs are greater than or equal to one. A final test uses the variable nstep to filter data which converged slowly. A typical retrieval will complete where nstep is less than 6. Cloud-clearing is performed on the IASI L1C spectra prior to retrieval of CO, using a threshold of 25% (i.e. pixels are only included if the cloud percentage within the pixel is less 5 than or equal to 25%). If stricter cloudclearing is required use the cloud_flag variable.

We also include other important variables, such as averaging kernels, errors, and geolocation data in the netCDF files. All vertically resolved data is provided on pressure and altitude levels (as opposed to layers). This is especially important when for example applying the averaging kernels to model data. A dimension of n refers to the number of retrievals per file, which is 17 equidistant pressure levels. Over high terrain this means that pressure levels are closer together than over the ocean. The lowest pressure for each sounding is 50 hPa due to decreasing sensitivity of IASI at pressures lower than this. Users reading averaging kernel and pressure level information will always see 17 levels. Please see table 3 for the full data file content.

1.7 Import Data

The data are stored in NetCDF format which can be read with standard tools in the common programming languages (IDL, Matlab, Python, Fortran90, C++, etc). In python you can use the netCDF4 or xarray libraries to read the data. An example code to read a single daily file using xarray is given below.

Example Code: using xarray

```
import xarray as xr
pathname = r'/gws/nopw/j04/eo_shared_data_vol1/satellite/iasi/ulirs_ms/eocis/me
topb/2024/01' # Give the pathname to data files
file_name = 'EOCIS-FIRE-L2-CO-IASI_METOP_B-ULIRS-20240101-fv1.0.nc' # e.g., file
dataset = xr.open_dataset(pathname+'/'+file_name) # Open the ULIRS_CO IASI NetCDF
file
co_total_column_data = dataset.variables['co_total_column'][:] # Access co_total_
column variable
lat=dataset['latitude'] # Access Latitude values
lon=dataset['longitude'] # Access Longitude values
print(dataset) # Print the dataset structure
```

Illustrative Results:

<xarray.dataset> Size: 1GB</xarray.dataset>	
Dimensions:	(n: 552688, m: 17, o: 17)
Dimensions without coordinates: n, m, o	
Data variables: (12/29)	
solar_zenith_angle	(n) float32 2MB
sensor_zenith_angle	(n) float32 2MB
solar_azimuth_angle	(n) float32 2MB
sensor_azimuth_angle	(n) float32 2MB



land_area_fraction	(n) int8 553kB
longitude	(n) float32 2MB
<pre>co_profile_averaging_kernel</pre>	(n, o, m) float32 639MB
chim	(n) float32 2MB
dofs	(n) float32 2MB
nstep	(n) float32 2MB
cloud_flag	(n) float32 2MB
time	<pre>(n) datetime64[ns] 4MB</pre>
Attributes: (12/40)	
title:	IASI METOP-B infrared carbon monoxide retrievals
institution:	University of Leicester and National Centre f
source:	IASI L1B version v6.5-v12.0
history:	Product generated at the University of Leices
references:	https://doi.org/10.5194/amt-4-269-2011
tracking id:	128a8571-dec1-4e3a-9388-b6cb7b3f6e49
•••	•••
platform:	Metop-B
sensor:	IASI
spatial_resolution:	12km x 12km at nadir (typically)
geospatial lat units:	degrees north
geospatial lon units:	degrees east
key_variables:	co_profile, co_total_column

1.8 Re-Gridding/Formatting

Re-gridding/Formatting

co_total_column is a 1-dimensional variable that gives measurements across and along the orbit track. To regrid 1D co_total_column data into a 2D grid using the corresponding longitude and latitude variables, we can use interpolation or binning techniques. The example code given below generates the global map of co_total_column for June 2023 by regridding them to a regular 2D latitude-longitude grid. It loads carbon monoxide data from multiple NetCDF files, filtering to include only high-quality measurements. The carbon monoxide values are then averaged within 2-degree latitude and longitude bins using binned_statistic_2d to create a global grid of mean co_total_column concentrations. The resulting data is plotted on a global map with matplotlib and cartopy, showing spatial patterns in co_total_colum.

Example Code:

```
import xarray as xr
import numpy as np
import glob
# Combining Daily XCH4 Data into a Monthly Dataset
pathname = r'/gws/nopw/j04/eo_shared_data_vol1/satellite/iasi/ulirs_ms/eocis/me
topb/2024/01' # Give the pathname to data files
filenames = glob.glob(pathname+'/EOCIS-FIRE-L2-CO-IASI_METOP_B-ULIRS-202401*.nc
')
datasets = [xr.open_dataset(file)[['co_total_column', 'latitude', 'longitude']]
for file in filenames] # List of all individual datasets
monthly_merged_dataset = xr.concat(datasets, dim='n').set_coords(['latitude', '
longitude']) # Concatenate all datasets along the 'n' dimension
```



```
print(monthly merged dataset)
Illustrative Results:
<xarray.Dataset> Size: 197MB
Dimensions:
                    (n: 16398578)
Coordinates:
                     (n) float32 66MB -69.61 -69.74 -69.75 ... 64.82 64.97 65.11
    latitude
    longitude
                     (n) float32 66MB 12.74 11.54 13.27 ... -45.48 -43.88 -42.07
Dimensions without coordinates: n
Data variables:
    co_total_column (n) float32 66MB 1.104 0.8175 0.9939 ... 1.268 1.268 1.595
Attributes: (12/40)
                                IASI METOP-B infrared carbon monoxide retrievals
    title:
    institution:
                               University of Leicester and National Centre f...
                               IASI L1B version v6.5-v12.0
    source:
                               Product generated at the University of Leices...
    history:
    references:
                               https://doi.org/10.5194/amt-4-269-2011
                               128a8571-dec1-4e3a-9388-b6cb7b3f6e49
    tracking id:
    . . .
                                . . .
    platform:
                               Metop-B
                               IASI
    sensor:
    spatial_resolution:
                               12km x 12km at nadir (typically)
    geospatial_lat_units:
                               degrees_north
                               degrees_east
    geospatial_lon_units:
                               co_profile, co_total_column
    key_variables:
# Converting 1D co_total_column_data of to 2D to map the data onto a regular gr
id (1°x1°) based on the longitude and latitude variables
from scipy.stats import binned statistic 2d
import cartopy.crs as ccrs
import matplotlib.pyplot as plt
Lat_bins = np.arange(-90, 91, 2)# Define bin edges for Latitudes and Longitudes
lon_bins = np.arange(-180, 181, 2)
mean_co, xedges, yedges, binnumber = binned_statistic_2d (
      monthly_merged_dataset['latitude'], monthly_merged_dataset['longitude'],
      monthly_merged_dataset['co_total_column'], statistic='mean',
      bins= [lat_bins, lon_bins]
      ) # Compute the mean value in each bin
plt.figure(figsize=(13, 5))
ax = plt.axes(projection=ccrs.PlateCarree())
im=ax.imshow(mean co,origin='lower', extent=[-180, 180, -90, 90],
cmap='viridis', aspect='auto')
ax.gridLines(color='gray', linestyle='--', linewidth=0.5)
ax.set_extent([-180,180,-60,85], crs=ccrs.PlateCarree())
ax.coastlines()
plt.colorbar(im, label='Mean CO total column [molecules cm<sup>-2</sup>]',
orientation='vertical', pad=0.02)
plt.title('Global Map of CO total column for January 2024')
```



plt.xlabel('Longitude')
plt.ylabel('Latitude')
plt.show()



Figure 3 - Global map of mean CO total column for January 2024 at a grid resolution of 2° x 2°.

1.9 Data Reduction/Subsetting

The following example code shows the colour map of mean CO total column data over the UK for 2024.

```
import xarray as xr
import matplotlib.pyplot as plt
import glob
import numpy as np
from scipy.stats import binned_statistic_2d
import cartopy.crs as ccrs
pathname =
r'/gws/nopw/j04/eo_shared_data_vol1/satellite/iasi/ulirs_ms/eocis/metopb/2024/*
filenames = glob.glob(pathname+'/EOCIS-FIRE-L2-CO-IASI METOP B-ULIRS-2024*.nc')
datasets = [xr.open_dataset(file) [['co_total_column', 'latitude',
'longitude']] for file in filenames] # list of all individual datasets for the year
2024
monthly merged dataset = xr.concat(datasets, dim='n').set coords(['latitude',
'longitude']) # concatenate all datasets along the 'n' dimension
uk_data = monthly_merged_dataset.where(
    (monthly merged dataset['latitude'] >= 49) &
(monthly merged dataset['latitude'] <= 61) &</pre>
    (monthly_merged_dataset['longitude'] >= -10) &
(monthly_merged_dataset['longitude'] <= 2),</pre>
    drop=True
```



)

```
lat_bins = np.arange(49, 61, 0.5) # Adjust the boundaries and grid size for UK
lon_{bins} = np.arange(-10, 2, 0.5)
mean_co, xedges, yedges, binnumber = binned_statistic_2d (
    uk_data['latitude'], uk_data['longitude'], uk_data['co_total_column'],
    statistic='mean', bins= [lat_bins, lon_bins]
    ) # Compute the mean value in each bin
plt.figure(figsize= (7, 8)) # plotting mean total_column_co over UK
ax = plt.axes(projection=ccrs.PlateCarree())
im = ax.imshow(mean_co, origin='lower', extent= [-10, 2, 49, 61],
cmap='viridis', aspect='auto')
ax.coastLines()
ax.gridLines(color='gray', linestyle='--', linewidth=0.5)
ax.set_extent([-10, 2, 49, 61], crs=ccrs.PlateCarree())
plt.colorbar(im, label='Mean CO total column [molecules cm-2]',
orientation='vertical', pad=0.0)
plt.title('Mean CO total column over the UK for 2024')
plt.xlabel('Longitude')
plt.ylabel('Latitude')
plt.show()
```





Figure 4 - Spatial map of mean CO total column for 2024 at a grid resolution of 0.1° x 0.1°.

1.10 Interactive visualisation / data access

Not applicable

1.11 Your obligations when using these products

By accessing the University of Leicester CO Data Product from IASI (ULIRS_CO), you agree to cite the dataset digital object identifier (DOI) and corresponding journal article describing the dataset every time you publish results obtained in whole or in part by use of UK EOCIS products. These citations are given under Summary Information.

The reference to the dataset should mention "created by the UK Earth Observation Climate Information Service". The product name and acronym in Table 1 and should be used to avoid confusion and enable traceability.

Regarding usage of this data, we would just ask that you let us know if the data is presented anywhere and that you discuss co-authorship where appropriate prior to any peer-reviewed publication.

1.12 Further Information

1.12.1Summary of retrieval processing

The latest version of the operational EUMETSAT Level 1B files are acquired directly from the EUMETSAT data store (https://user.eumetsat.int/data-access/data-store) and is processed with the University of Leicester IASI Retrieval Scheme (ULIRS) pre-processing scheme to extract the measured radiances along with all required sounding-specific ancillary information such as the measurement time, location, and geometry and which have already had the relevant calibration applied. We then perform a second pre-processing step to format the spectral data for input into the ULIRS algorithm and generate a number of files containing all the ancillary data necessary to create the retrieval a priori information, once clearing of cloudy pixels is performed via the IASI L2 operational data (also obtained via the EUMETSAT data store) with a threshold of 25%. Only IASI soundings where the initial cloud screening has been successful are processed to retrieve the total column carbon monoxide. For soundings that pass the cloud screening procedure described above, retrievals with the ULIRS algorithm for CO total column profiles are carried out. The state vector for these retrievals consists of 17 equidistant-pressure level profiles from the surface to 50 hPa. Convergence is determined once the d-test criteria are met, which in practise means that two consecutive iterations of the ULIRS return a d test value of < 0.01. This value was found to be sufficient for fast retrievals but maintaining an excellent degree of accuracy for the total column values when compared to NDACC ground-station data. No post-retrieval quality filtering is carried out although the user is encouraged to consider 1) chi-square (chim) of less than 10, 2) degrees of freedom (dofs) of > 1.03) use the variable nstep to filter data which converged slowly. A typical retrieval will complete where nstep is less than 6. Data are included for the whole globe, but some caution should also be considered over ice surfaces which sometimes is difficult to distinguish low cloud from the snow-covered surface.



History of modifications / Change Log

Version	Date	Changes	Person
1.0	05/03/2025	Initial Draft	DM
1.1	20/06/2025	modified pressure co-	DM
		ordinate, added reference	
		document	

Related Documents / Reference Documents

Document	Author	Reference
ULIRS retrieval	S.	Illingworth, S. M., Remedios, J. J., Boesch, H., Moore, D. P.,
algorithm	Illingworth	Sembhi, H., Dudhia, A., and Walker, J. C.: ULIRS, an optimal
outline	, University	estimation retrieval scheme for carbon monoxide using IASI
	of	spectral radiances: sensitivity analysis, error budget and
	Leicester	simulations, Atmos. Meas. Tech., 4,
		https://amt.copernicus.org/articles/4/269/2011/

Acronyms and/or Abbreviations

Acronym / Abbreviation	Definition
EOCIS	Earth Observation Climate Information Service
EUMETSAT	European Organisation for the Exploitation of Meteorological
	Satellites
IASI	Infrared Atmospheric Sounding Interferometer
L1B	Level 1B
МЕТОР	Meteorological Operational Polar Satellite
NetCDF	Network Common Data Format
NDACC	Network for the Detection of Atmospheric Composition Change
ppb	Parts per billion
ppm	Parts per million
RFM	The University of Oxford Reference Forward Model
ULIRS	University of Leicester IASI retrieval scheme
UoL	University of Leicester, United Kingdom

General definitions

Term	Definition	
L1	Level 1 satellite data product: geolocated radiance (spectra)	
L2	Level 2 satellite-derived data product: Here: H2O, temperature information for	
	each ground-pixel	



References and Further Reading

/Bruno et al., 2023/ Bruno, A. G., Harrison, J. J., Chipperfield, M. P., Moore, D. P., Pope, R. J., Wilson, C., Mahieu, E., and Notholt, J.: Atmospheric distribution of HCN from satellite observations and 3-D model simulations, Atmos. Chem. Phys., 23, 4849–4861, https://doi.org/10.5194/acp-23-4849-2023, 2023.

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/Parker et al., 2016/ Parker, R. J., Boesch, H., Wooster, M. J., Moore, D. P., Webb, A. J., Gaveau, D., and Murdiyarso, D.: Atmospheric CH4 and CO2 enhancements and biomass burning emission ratios derived from satellite observations of the 2015 Indonesian fire plumes, Atmos. Chem. Phys., 16, 10111–10131, https://doi.org/10.5194/acp-16-10111-2016, 2016.