Synthetic XCO_2, CO and NO_2 observations for the CO2M and Sentinel-5 satellites

SMARTCARB data1 package

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Synthetic XCO_2, CO and NO_2 observations for the CO2M and Sentinel-5 satellites	**ESA Project SMARTCARB** Study on use of satellite measurements of auxiliary reactive trace gases for fossil fuel carbon dioxide emission estimation contract no 4000119599/16/NL/FF/mg	Empa Materials Science and Technology ETH zürich Max Planck Institute for Biogeochemistry

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Applicable documents

	Reference	Title
(data1)	4000119599/16/NL/FF/mg	Data1 dataset and code of ESA study contract n° 4000119599/16/NL/FF/mg
(FR)	4000119599/16/NL/FF/mg	Final report of ESA study contract n° 4000119599/16/NL/FF/mg

Acronyms

CO	Carbon monoxide
CO_2	Carbon dioxide
COSMO	Consortium for Small-Scale Modelling
GHG	Greenhouse Gases
MODIS	Moderate Resolution Imaging Spectrometer
netCDF	Network Common Data Form
NO_2	Nitrogen dioxide
NO_x	Nitrogen oxides (NO + NO_2)
SMARTCARB	Satellite Measurements of Auxiliary Reactive Trace gases for fossil fuel CARBon dioxide emission estimation
SRON	Netherlands Institute for Space Research
XCO_2	Column averaged dry air mole fraction of CO_2

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1. Introduction

The SMARTCARB project was funded by the European Space Agency (ESA) to study the use of satellite measurements of auxiliary reactive trace gases for fossil fuel carbon dioxide emission estimation. In the project, synthetic satellite observations were generated from high-resolution CO_2, CO and NO_2 fields (1×1 km^2 resolution) simulated with the COSMO-GHG model. The vertically integrated model fields, the synthetic satellite observations, and the code for generating additional satellite observations (Level-2 creator) were delivered to ESA as "data1 package".

This dataset is a subset of the SMARTCARB "data1 package" that includes vertically integrated model fields and some synthetic satellite observations. The satellite observations were generated for a CO_2, CO and NO_2 imaging satellite with 2 km x 2 km resolution and a 250-km wide swath and a CO and NO_2 imaging satellite with 7 km x 7 km resolution at nadir and a 2650 km wide swath. The instrument specifications are based on the Copernicus CO_2 monitoring (CO2M) mission and the Sentinel 5 instrument, respectively.

This version does not include the code (Level-2 creator) used for generating synthetic satellite observations for different satellite orbits. The code was written by Gerrit Kuhlmann (gerrit.kuhlmann@empa.ch) and builds on the SRON orbit simulator provided by Jochen Landgraf and Joost aan de Brugh. Please contact Gerrit Kuhlmann, if you are interested in the code.

The SMARTCARB study is described in the final report of the project:

- G. Kuhlmann, V. Clément, J. Marshall, O. Fuhrer, G. Broquet, C. Schnadt-Poberaj, A. Löscher, Y. Meijer, and D. Brunner: SMARTCARB – Use of Satellite Measurements of Auxiliary Reactive Trace Gases for Fossil Fuel Carbon Dioxide Emission Estimation, Final report of ESA study contract n°4000119599/16/NL/FF/mg, https://doi.org/10.5281/zenodo.4034266, 2018.

Furthermore, the following publications have been published in peer-reviewed journals:

- Brunner, D., Kuhlmann, G., Marshall, J., Clément, V., Fuhrer, O., Broquet, G., Löscher, A., and Meijer, Y.: Accounting for the vertical distribution of emissions in atmospheric CO_2 simulations, Atmos. Chem. Phys., 19, 4541–4559, https://doi.org/10.5194/acp-19-4541-2019, 2019.
- Kuhlmann, G., Broquet, G., Marshall, J., Clément, V., Löscher, A., Meijer, Y., and Brunner, D.: Detectability of CO_2 emission plumes of cities and power plants with the Copernicus Anthropogenic CO_2 Monitoring (CO2M) mission, Atmos. Meas. Tech., 12, 6695–6719, https://doi.org/10.5194/amt-12-6695-2019, 2019.
- Kuhlmann, G., Brunner, D., Broquet, G., and Meijer, Y.: Quantifying CO_2 emissions of a city with the Copernicus Anthropogenic CO_2 Monitoring satellite mission, Atmos. Meas. Tech. Discuss., https://doi.org/10.5194/amt-2020-162, in review, 2020.

1.1 Known issues:

Users should consider the following issues when using the dataset:

- In January and July 2015, CO_2 and NO_x emissions of Berlin are too high, because some large point sources were wrongly counted twice. The effected tracers are {XCO2,NO2}_B0, {XCO2,NO2}_BV and {XCO2,NO2}_BC. To create a consistent dataset, we recommend to compute time-varying CO_2/NO_2 fields for these two months as follows:

$$XCO2_{BV,corrected} = 0.55 \cdot XCO2_{B0} + XCO2_{B1} + XCO2_{B2}$$

- The model fields include a relaxation zone where boundary conditions are merged into COSMO-GHG model domain. We recommend not to use grid cells that are within ~50 km distance of the model boundary. Note that these data are not flagged in the Level-2 product.

2. Data product

2.1 Vertically integrated model fields

The vertically integrated (or column averaged in case of CO_2) model fields were computed from the hourly, three-dimensional model fields of two simulations with the COSMO-GHG model covering the first and second half of the year 2015, respectively. The simulations and computation of the integrated model fields are described in the final report of the SMARTCARB study.

The data are stored in netCDF4 files in two folders named "cosmo2D_2015-01" and "cosmo2D_2015-07". The first folder contains the output files for the period 1 January to 3 July 2015 and second folder for the period 1 July to 25 December 2015.

The file names are "cosmo_2d_YYYYMMDDHH.nc" where "YYYY" is the year, "MM" is the month, "DD" is the day and "HH" is the hour of the timestamp. Each file contains the variables listed in Table 1.

Table 1: Variables in vertically-integrated COSMO-GHG output files

Variable(s)	**Description**
	Geolocation
rlon, rlat	longitude and latitude in rotated pole coordinates (units: degrees)
rotatedpole	definition of rotated pole coordinates
lon, lat	geographical longitude and latitude (units: degrees)
	Meteorological variable
CLCT	total cloud cover (units: 1)
PS	surface pressure (units: Pa)
	Carbon dioxide (units: ppm)
XCO2_BG	time-varying background CO_2 column-averaged dry-air mole fraction transported from lateral boundaries
XCO2_GPP	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 surface flux from gross primary production
XCO2_RA	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 surface flux from respiration
XCO2_TOT	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 emissions for all sources in domain
XCO2_SURF	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 emissions for all sources in domain but emitted at surface
xCO2_A	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 emissions for all sources in domain excl. Berlin and power plants
XCO2_BV	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 emissions for all sources in Berlin
XCO2_BC	CO_2 column-averaged dry-air mole fraction of time-constant CO_2 emissions for all sources in Berlin
XCO2_B[0..2]	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 emissions for industry (0), heating (1) and traffic (2) in Berlin

XCO2_T0[0..7]	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 emissions in Berlin for eight 3-hourly time intervals
XCO2_JV	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 emissions for six major power plants (incl. Jänschwalde)
XCO2_JC	CO_2 column-averaged dry-air mole fraction of time-constant CO_2 emissions for six major power plants (incl. Jänschwalde)
XCO2_NPR	CO_2 column-averaged dry-air mole fraction of time-varying CO_2 emissions for six major power plants (incl. Jänschwalde) without plume rise
YCO2_BG	time-varying CO_2 column-averaged moist-air mole fraction at lateral boundary
	Carbon monoxide columns (units: molecules cm^{-2})
CO_BG	CO background vertical column density of mass fraction transported from lateral boundaries
CO_TOT	CO vertical column density of time-varying CO emissions for all sources in domain
CO_SURF	CO vertical column density of time-varying CO emissions for all sources in domain but emitted at surface
CO_A	CO vertical column density of time-varying CO emissions for all sources in domain excl. Berlin and power plants
CO_BV	CO vertical column density of time-varying CO emissions for all sources in Berlin
CO_BC	CO vertical column density of time-constant CO emissions for all sources in Berlin
CO_B[0..2]	CO vertical column density of time-varying CO emissions for industry (0), heating (1) and traffic (2) in Berlin
CO_JV	CO vertical column density of time-varying CO emissions for six major power plants (incl. Jänschwalde)
CO_JC	CO vertical column density of time-varying CO emissions for six major power plants (incl. Jänschwalde)
CO_NPR	CO vertical column density of time-varying CO emissions for six major power plants (incl. Jänschwalde) without plume rise
	Nitrogen dioxide columns (units: molecules cm^{-2})
NOX_BG	NO_2background vertical column density transported from lateral boundaries
NOX_TOT	NO_2 vertical column density of time-varying NO_x emissions for all sources in domain
NOX_SURF	NO_2 vertical column density of time-varying NO_x emissions for all sources in domain but emitted at surface
NOX_A	NO_2 vertical column density of time-varying NO_x emissions for all sources in domain excl. Berlin and power plants
NOX_BV	NO_2 vertical column density of time-varying NO_x emissions for all sources in Berlin
NOX_BC	NO_2 vertical column density of time-constant NO_x emissions for all sources in Berlin
NOX_Bx	NO_2 vertical column density of time-varying NO_x emissions for industry (0), heating (1) and traffic (2) in Berlin
NOX_R[0,2,12,24]	NO_2 vertical column density of time-varying NO_x emissions in Berlin for inert (0) and decaying NO_x (e-folding times: 2, 12, and 24 hours)
NOX_JV	NO_2 vertical column density of time-varying NO_x emissions for Jänschwalde
NOX_JC	NO_2 vertical column density of time-constant NO_x emissions for Jänschwalde
NOX_NPR	NO_2 vertical column density of time-varying NO_x emissions for six major power plants (incl. Jänschwalde) without plume rise

2.2 Level-2 data

The *level2* folder contains Level-2 data generated from the vertically integrated fields for different instrument scenarios as described in the SMARTCARB final report (FR). For each instrument scenario a subfolder was created with individual Level-2 data. The Python code used for creating the Level-2 data is described in Section 3.

The instrument scenarios are:

- *Sentinel_5* (Sentinel 5 satellite with 2650 km wide swath)
- *Sentinel_7_CO2* (Sentinel CO_2 mission with 250 km swath and 2 km resolution)
- *Sentinel_7_NO2_1km* (Sentinel CO_2 mission with 350 km swath and 1 km resolution without CO_2 fields)
- *Sentinel_7_NO2_2km* (Sentinel CO_2 mission with 350 km swath and 2 km resolution without CO_2 fields)
- *Sentinel_7_NO2_4km* (Sentinel CO_2 mission with 350 km swath and 4 km resolution without CO_2 fields)

Each subfolder has one file per orbit with the following file name:

{instrument_scenario}_{YYYYmmddHH}_o{orbit}_l{equator_starting_longitude}.nc

with:

- *instrument_scenario*: the instrument scenario above
- *YYYYmmddHH*: date string: year, month, day and hour of overpass
- *orbit*: orbit number
- *equator_starting_longitude*: starting longitude at equator of the first orbit

Each file contains the input parameter used for computing the orbit, geolocation fields, e.g. longitude and latitude for pixel centres and corners, meteorological fields, tracer fields and pre-computed uncertainties. The variables are summarized in Table 2 and Table 3.

Table 2: Variables in Level-2 data files (except uncertainties: see Table 3).

Variable(s)	**Description**
	Input
Input	Variable with attributes describing input parameters used in orbit simulator
	Geolocation
time	time of measurement since 2015-01-01 00:00:00 (units: s)
longitude	pixel center longitude (dims: nobs, nrows)
latitude	pixel center latitude (dims: nobs, nrows)
longitude_corners	pixel corner longitudes (dims: nobs, nrows, ncorners)
latitude_corners	pixel corner latitudes (dims: nobs, nrows, ncorners)
solar_zenith_angle	solar zenith angle (units: degrees)

	Meteorological fields
CLCT	total cloud cover (units: 1)
PS	surface pressure (units: Pa)
Albedo_NIR	MODIS white-sky albedo Band 2 (841-867 nm) with data gaps filled
Albedo_SWIR	MODIS white-sky albedo Band 6 (1623-1652 nm) with data gaps filled
	Tracer fields
	(for each tracer, s**ee Table 1; Sentinel-5 does not include XCO_2 fields**)
CO_XX	CO column densities at satellite pixel
XCO2_XX	XCO_2 at satellite pixel
NO2_XX	NO_2 column density at satellite pixel

Table 3: Uncertainty variables in Level-2 data files for the different instrument scenarios.

Variable(s)	**Description**
	Sentinel_5
uNO_2	NO_2 random uncertainty
uCO	CO random uncertainty
	Sentinel_7_CO2
uXCO2	XCO_2 random uncertainty computed with error parametrization formula
uNO2_low	NO_2 random uncertainty for low noise scenario
uNO2_high	NO_2 random uncertainty for high noise scenario
uCO_low	CO random uncertainty for low noise scenario
uCO_high	CO random uncertainty for high noise scenario
	Sentinel_7_NO2_1km, _2km and 4_km
	same fields as for Sentinel_7_CO2 except no CO_2 fields

2.3 MODIS surface reflectance

The MODIS folder contains two netCDF files with daily MODIS surface reflectances (BSA: black-sky albedo and WSA: white-sky albedo) in the near-infrared (Band 2) and shortwave infrared (Band 6) channel. The albedos are projected on the SMARTCARB model domain. For each channel, raw data and processed data with filled data gaps are provided. The data are used for computing XCO_2 uncertainties (see FR for details). Table 4 and Table 5 describe the variables in the two files.

Table 4: Variables in file: COSMO_2D_MCD43A3.006_BSA.nc

Variable	**Description**
time	seconds since 2015-01-01 00:00
rlon	Longitude in rotated pole coordinates
rlat	Latitude in rotated pole coordinates
rotpole	Definition of rotated pole coordinates
Albedo_BSA_Band2	raw MODIS black-sky albedo in the near infrared (Band 2)
Albedo_BSA_Band2_filled	gap-filled MODIS black-sky albedo in the near infrared (Band 2)
Albedo_BSA_Band6	raw MODIS black-sky albedo in the shortwave infrared (Band 6)
Albedo_BSA_Band6_filled	gap-filled MODIS black-sky albedo in the shortwave infrared (Band 6)

Table 5: Variables in file: COSMO_2D_MCD43A3.006_WSA.nc

Variable	**Description**
time	seconds since 2015-01-01 00:00
rlon	Longitude in rotated pole coordinates
rlat	Latitude in rotated pole coordinates
rotpole	Definition of rotated pole coordinates
Albedo_WSA_Band2	raw MODIS white-sky albedo in the near infrared (Band 2)
Albedo_WSA_Band2_filled	gap-filled MODIS white-sky albedo in the near infrared (Band 2)
Albedo_WSA_Band6	raw MODIS white-sky albedo in the shortwave infrared (Band 6)
Albedo_WSA_Band6_filled	gap-filled MODIS white-sky albedo in the shortwave infrared (Band 6)