CON CERTO

Deliverable D4.3 – New top-down isoprene flux datasets based on TROPOMI HCHO

Lead Beneficiary: BIRA-IASB

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Contents

Preface

We present the top-down isoprene emission dataset submitted as part of the CONCERTO project (deliverable 4.3). This dataset has been developed with the aim of improving our understanding of ecosystem responses to environmental factors, such as heatwaves, droughts, etc. We make use of remote sensing tools to observationally constrain biogenic volatile organic compound emissions from space based on formaldehyde (HCHO) measurements acquired from the TROPOMI satellite instrument. This emission dataset serves as a tool to evaluate isoprene fluxes calculated by land surface models, and to reduce uncertainties in the carbon cycle. In this document, we provide a short description of the methodology in deriving the emissions from satellite data, a description of the file structure, and sample python code for data reading and visualization.

Summary

The dataset consists of global top-down biogenic isoprene emission fluxes at daily temporal resolution and 0.5°×0.5° spatial resolution for the 2019 to 2024 period. The emissions are provided in NetCDF format, with one file of 300 MB per year containing daily emission estimates. The dataset is published at Zenodo under DOI (https://doi.org/10.5281/zenodo.20540268).

List of Abbreviations

MAGRITTE – Model of Atmospheric composition at Global and Regional scales using Inversion Techniques for Trace gas Emissions

CTM – Chemistry Transport Model

CCI – Climate Change Initiative

FTIR – Fourier Transform InfraRed

VOC – Volatile Organic Compound

1. Methodology

The dataset has been derived from an emission inversion using the MAGRITTEv1.2 chemistry-transport model (Müller et al. 2019). It features a detailed isoprene oxidation mechanism based on the Leuven Isoprene Model (LIM, Peeters et al., 2009, 2014) and the Caltech oxidation mechanism (Wennberg et al., 2018). The mechanism comprises 243 reactions involving 93 chemical species. The global model is run with a horizontal resolution of 2.0° × 2.5° and a vertical resolution of 40 levels from the surface up to 44 hPa. Meteorological fields used in the model are taken from ERA5 reanalysis data (Hersbach et al., 2020). The forward model simulations use a daily time step with diurnal correction factors calculated using a simulation with 20-min time step.

The adjoint-based inversion setup is described in Oomen et al. (2026) and is constrained by TROPOMI HCHO columns from the CCI+precursors project (De Smedt et al., 2025). We use the L3 data product with a bias correction derived from FTIR validation data ($y = 1.315x - 0.934$, Compernolle et al., 2025). The MAGRITTE model uses a priori emission data from bottom-up inventories: biogenic VOC emissions from MEGAN-MOHYCAN (Stavrakou et al., 2018), pyrogenic emissions from QFEDv2.4 (Darmenov and da Silva, 2015) with emission factors from Andreae (2019), and anthropogenic emissions from CAMS-GLOB-ANTv5.3 (Soulie et al., 2024). The three emission categories are optimized simultaneously by minimizing the cost function between the modelled and TROPOMI HCHO columns using a large-scale quasi-Newton algorithm (Gilbert & Lemaréchal, 1989). The emission factors are optimised at monthly resolution and 2.0° × 2.5°, and then upscaled to the native spatiotemporal resolution of the a priori emission inventories (0.5° × 0.5°, daily). Finally, note that the present dataset will be extended to 2025, as soon as the TROPOMI CCI data become available.

2. File structure

Each yearly NetCDF file follows the naming convention:

```
CONCERTO_top-down_isoprene_bira-iasb_YYYY0101-YYYY1231.nc
```

2.1. Dimensions

- Time: daily index (1—365/366)
- Latitude: 360 grid cells
- Longitude: 720 grid cells

2.2. Coordinates

- Latitude: 89.75° N to 89.75° S

- Longitude: 0.25° E to 359.75° E

2.3. Main variable

Variable	Units	Dimensions	Description
isoprene_flux	molec. cm^{-2} s^{-1}	(time, latitude, longitude)	Top-down isoprene emission flux

3. User manual

3.1. Reading in the Python data

The dataset can be read using xarray.

```
import xarray as xr

ds = xr.open_dataset(
    "CONCERTO_top-down_isoprene_bira-iasb_20190101-20191231.nc"
)

print(ds)
```

Access the main variable:

```
flux = ds["isoprene_flux"]
print(flux.shape)
```

Extract emissions for a specific day:

```
day1 = flux.sel(time=1)
```

3.2. Example map

Daily global emissions can be visualized using:

```
import matplotlib.pyplot as plt
import cartopy.crs as ccrs

day = ds["isoprene_flux"].sel(time=180)

fig, ax = plt.subplots(1, 1, figsize=(12,5),
```

```
                        subplot_kw={'projection':
ccrs.PlateCarree()})

borders = [-180, 180, -60, 80] # [lower lon, upper lon, lower lat,
upper lat]
ax.set_extent(borders, crs=ccrs.PlateCarree())

gl = ax.gridlines(draw_labels=True, color = "None")
gl.top_labels = False
gl.right_labels = False

day.plot(ax=ax, transform=ccrs.PlateCarree(),
    cmap="viridis",
    robust=True
)

plt.title("Top-down isoprene emissions (Day 180)")

plt.tight_layout()
plt.savefig("example_map.png", dpi=300)
plt.show()
```

Figure 1 shows an example emission map on a day during Northern Hemisphere summer.

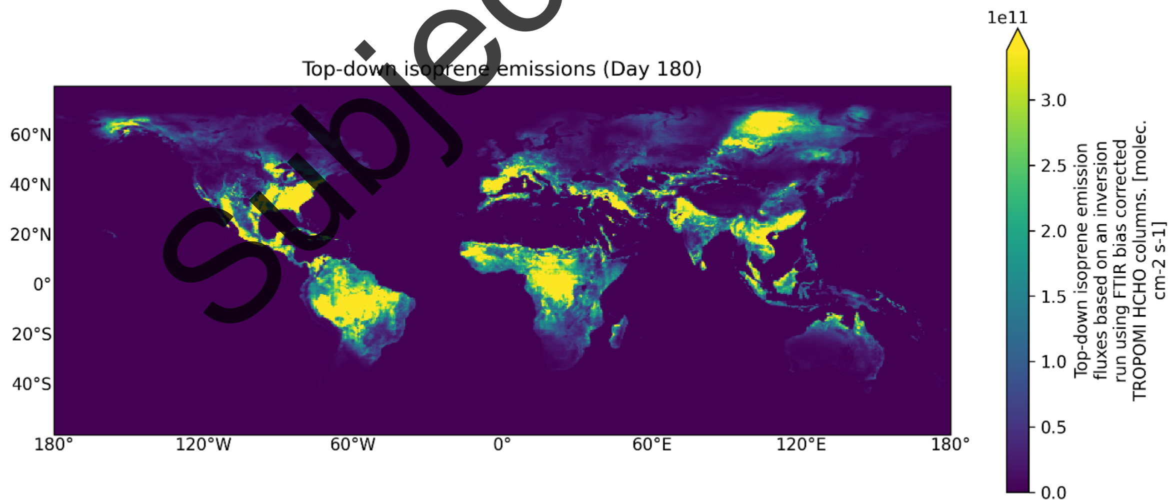

Figure 1: Example of daily top-down isoprene emission fluxes on day 180 in 2019.

3.3. Example time series

To use data over specific regions, we can use extract chunks from the xarray data structure.

```
import numpy as np
import matplotlib.dates as mdates

fig,ax=plt.subplots(figsize=(10,4))

time = ds["time"].values

# Select Amazon region (70 W to 60 W, 0 N to 10 S)
amazon = ds["isoprene_flux"].sel(
    longitude=slice(290, 300),
    latitude=slice(0, -10)
)

# Spatial average
amazon_mean = amazon.mean(dim=["latitude", "longitude"])

# plot time series
plt.plot(time, amazon_mean, 'b-', linewidth=1)

ax.xaxis.set_major_locator(mdates.MonthLocator())
ax.xaxis.set_major_formatter(mdates.DateFormatter('%b'))
ax.set_xlabel('2019', fontsize=9)
ax.set_ylabel('Isoprene  emissions\n[molec  cm$^{-2}$  s$^{-1}$]', fontsize=9)
ax.tick_params(labelsize=9)
ax.yaxis.get_offset_text().set_fontsize(9)



plt.savefig("example_time_series.png", dpi=300)
plt.show()
```

Figure 2 displays a time series of isoprene fluxes In the Amazon for 2019. Dry season in the Amazon runs from August to November and is characterised by higher temperatures and reduced cloudiness, which lead to higher isoprene emissions and larger HCHO columns.

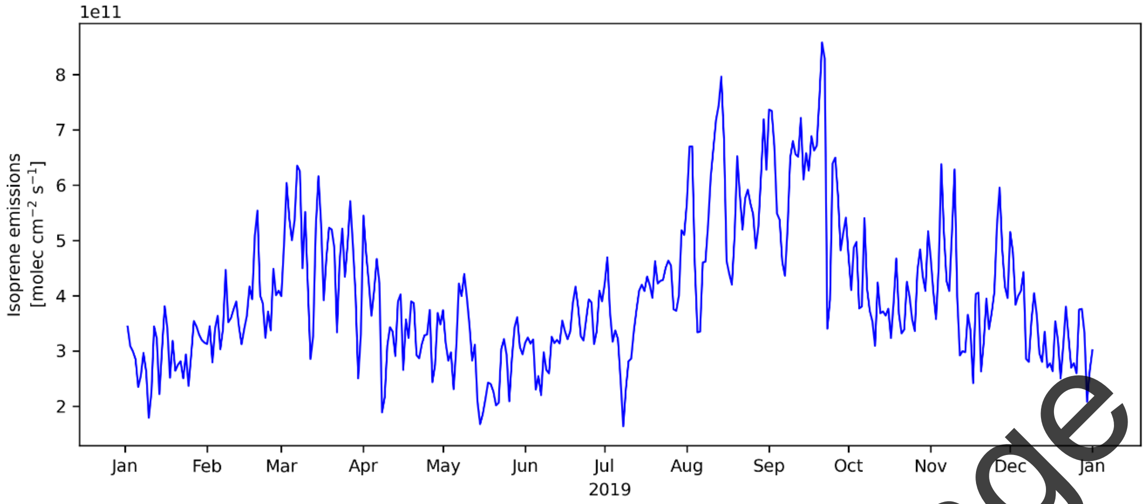

Figure 2: Time series of isoprene emissions over the Amazon (0°-10°S, 60°-70°W) for 2019.

4. Conclusions and future developments

The top-down isoprene emission fluxes presented in this deliverable provides an observationally-constrained benchmark for evaluating and improving land surface and Earth system models. The emissions are inferred from the latest version of TROPOMI HCHO data developed as part of the ESA CCI+ precursors project (De Smedt et al. 2025). The global emission dataset has been made available at high resolution (daily, $0.5° \times 0.5°$) for the years 2019 to 2024. Extension of this dataset to 2025 will be performed upon availability of the TROPOMI CCI+ HCHO dataset (foreseen in late 2026).

Within the CONCERTO project, the dataset will support the assessment of model representations of BVOC emissions and their responses to environmental drivers such as temperature, radiation, drought, and ecosystem stress. The daily temporal resolution and global coverage facilitate comparisons with model simulations (ICL's P model of isoprene, CMCC's CLM model) and allow investigating regional and seasonal variations in isoprene emissions. We will also use the dataset to evaluate existing bottom-up emission inventories, to analyse the interannual variability in biogenic fluxes, and to study the role of emissions from vegetation in the carbon cycle and air quality.

In the coming years of CONCERTO, additional top-down emission products will be developed using the inversion framework designed for and coupled with the MAGRITTE CTM. These include updated isoprene fluxes for 2025, following the release of the corresponding TROPOMI HCHO product, but also isoprene fluxes constrained by the latest version of CrIS isoprene columns. These new top-down datasets will be carefully evaluated against independent ground-based and aircraft observations.

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