

Emiproc: A Python package for emission inventory processing

Constantin Lionel ¹, Brunner Dominik ¹, Thanwerdas Joel ¹, Keller Corina ¹, Steiner Michael ¹, and Koene Erik ¹

 ${f 1}$ Empa, Laboratory for Air Pollution / Environmental Technology, Switzerland * These authors contributed equally.

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@einaraz @mikapfl

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Summary

Emission inventories are created by countries and regions to assess and address air quality and climate change targets. An emission inventory is a spatial dataset that reports the yearly amount of pollutants released into the atmosphere, often broken down by specific source sectors or individual sources. Atmospheric modellers use such inventories to simulate the transport of emitted species in order to compute their distribution and assess their potential impact on the environment. The simulations are often compared with measurements to verify if the declared emissions and their trends are consistent with the observed changes in the atmosphere, thereby enhancing confidence in the inventories.

Figure 1 presents an example of a gridded inventory.

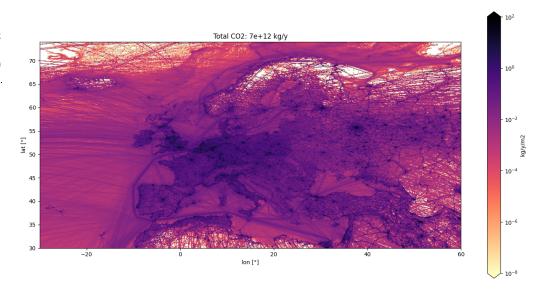


Figure 1: Anthropogenic CO2 emissions of the year 2022 from the EDGARv6 inventory .

Inventories are created in multiple different formats and resolutions, which makes it difficult to compare and use them in atmospheric transport models. For example, TNO (Dutch Organization for Applied Scientific Research) provides inventories which contains both, area emissions on a regular grid and point sources at their exact locations. Other inventories, such as one from the city of Zurich, are provided as vector data with various shapes (points, lines, polygons) depending on the category of the source. Atmospheric models require emission



inventories to be in a specific file format. For example ICON-ART (Schröter et al., 2018) requires emissions on a semi-structured triangular grid and temporal profiles to scale the emissions with hourly, daily and monthly variability.

Statement of need

emiproc is a Python package that provides tools for processing emission inventories, harmonizing datasets, and preparing such data as inputs for atmospheric transport models. Designed to be flexible and extendable, emiproc allows users to easily add custom functionality, read new inventories or export data to other formats.

When modellers design their simulations, they are often interested in modifying the inventories. For example, they could do the following: scale emissions based on future scenarios, aggregate emissions by sector or pollutant to simplify their simulations or combine multiple inventories to represent different sources such as anthropogenic and natural emissions. emiproc provides this functionality and has already been successfully applied for different use cases:

- Steiner et al. (2024) produced emission files for ICON-ART-OEM based on the EDGARv6 inventory (Monforti Ferrario et al., 2021) (Emissions Database for Global Atmospheric Research).
- Dönmez et al. (2024) conducted urban climate simulation using emissions produced with emiproc for cities of Zurich and Basel.
- Ponomarev et al. (2024) used emiproc to nest the Zurich city inventory inside the Swiss national inventory and to further nest the Swiss inventory inside the European TNO inventory.

emiproc shares some of its functionality with another Python tool, HERMESv3 (Guevara et al., 2019), which is also designed to process emission data and generate input files for atmospheric transport models.

Compared to HERMESv3, which relies on specific configuration files, emiproc is more flexible, extensible and practical as it can be integrated in existing Python-based workflows.

History

An earlier version of emiproc was already published by Jähn et al. (2020), but it was limited to specific models and inventories. Starting in 2022 emiproc has been refactored to satisfy the requirements of high flexibility and modularity. This included major changes to code structure, the addition of new capabilities, a major performance increase for the task of spatial regridding, a comprehensive documentation and the addition of test examples.

Since then the package is regularly updated with new features and bug fixes.



Design

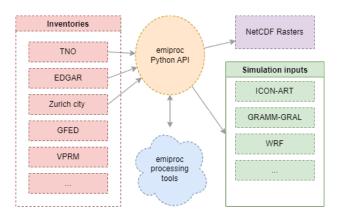


Figure 2: Design of emiproc.

The API of emiproc leverages the advantages of object-oriented programming. The main class is Inventory. It provides a common data structure to represent and harmonize all the different emission inventories. The Grid object represent the spatial distribution of the emission. It is flexible enough to implement all kinds of grids, from regular latitude-longitude grids to the icosahedral grid from the ICON Model (ICON partnership (DWD; MPI-M; DKRZ; KIT; C2SM), 2024). Finally TemporalProfile and VerticalProfile are used for the distribution of emissions in time and height.

Thanks to the harmonization of the data, functions for additional data processing can easily be applied to the different inventories once loaded into emiproc. These functions are listed in the API documentation. Examples of operations on inventory data are among others:

- remapping to different model grids
- aggregating emissions by sector or pollutant
- crop an inventory over a specific area

emiproc also allows for generation of additional emission sectors not always present in the inventories. For example, the vegetation emissions can be modelled through VPRM (Vegetation Photosynthesis and Respiration Model) (Mahadevan et al., 2008).

The export of inventories for various atmospheric models is done through custom functions that produce all emission input files required by the model.

For data vizualisation emiproc provides custom functions based on matplotlib (Hunter, 2007). Figure 1 was created using such a function.

emiproc is built on top of geopandas (Jordahl et al., 2020), which allows storing the geometries of the emission maps and offers many functionalities related to geometric operations. Within emiproc, the emission data of the inventory is stored as a geopandas.GeoDataFrame.

Availability

The package is available on GitHub and the documentation is available on readthedocs.

Tutorials are available to guide new users. A good first start is the EDGAR processing tutorial which shows how emiproc can be used to load, process and export a freely available inventory.



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References

- Dönmez, K., Emmenegger, L., & Brunner, D. (2024). Urban climate and CO2 simulations with the new atmospheric model ICON-ART accounting for spatially varying urban morphology and material properties. *EGU General Assembly 2024*. https://doi.org/10.5194/egusphere-egu24-3375
- Guevara, M., Tena, C., Porquet, M., Jorba, O., & Pérez García-Pando, C. (2019). HERMESv3, a stand-alone multi-scale atmospheric emission modelling framework part 1: Global and regional module. *Geoscientific Model Development*, 12(5), 1885–1907. https://doi.org/10.5194/gmd-12-1885-2019
- Hunter, J. D. (2007). Matplotlib: A 2D graphics environment. *Computing in Science & Engineering*, 9(3), 90–95. https://doi.org/10.1109/MCSE.2007.55
- ICON partnership (DWD; MPI-M; DKRZ; KIT; C2SM). (2024). *ICON release 2024.01*. World Data Center for Climate (WDCC) at DKRZ. https://doi.org/10.35089/WDCC/lconRelease01
- Jähn, M., Kuhlmann, G., Mu, Q., Haussaire, J.-M., Ochsner, D., Osterried, K., Clément, V., & Brunner, D. (2020). An online emission module for atmospheric chemistry transport models: Implementation in COSMO-GHG v5.6a and COSMO-ART v5.1-3.1. *Geoscientific Model Development*, 13(5), 2379–2392. https://doi.org/10.5194/gmd-13-2379-2020
- Jordahl, K., Bossche, J. V. den, Fleischmann, M., Wasserman, J., McBride, J., Gerard, J., Tratner, J., Perry, M., Badaracco, A. G., Farmer, C., Hjelle, G. A., Snow, A. D., Cochran, M., Gillies, S., Culbertson, L., Bartos, M., Eubank, N., maxalbert, Bilogur, A., ... Leblanc, F. (2020). *Geopandas/geopandas: v0.8.1* (Version v0.8.1). Zenodo. https://doi.org/10.5281/zenodo.3946761
- Mahadevan, P., Wofsy, S. C., Matross, D. M., Xiao, X., Dunn, A. L., Lin, J. C., Gerbig, C., Munger, J. W., Chow, V. Y., & Gottlieb, E. W. (2008). A satellite-based biosphere parameterization for net ecosystem CO2 exchange: Vegetation photosynthesis and respiration model (VPRM). Global Biogeochemical Cycles, 22(2). https://doi.org/10.1029/2006GB002735
- Monforti Ferrario, F., Crippa, M., Guizzardi, D., Muntean, M., Schaaf, E., Lo Vullo, E., Solazzo, E., Olivier, J., & Vignati, E. (2021). EDGAR (Emissions Database for Global Atmospheric Research) v6.0 Greenhouse Gas Emissions. European Commission, Joint Research Centre (JRC) [Dataset]. http://data.europa.eu/89h/97a67d67-c62e-4826-b873-9d972c4f670b
- Ponomarev, N., Steiner, M., Koene, E., Constantin, L., Rubli, P., Grange, S., Emmenegger, L., & Brunner, D. (2024). Estimation of CO2 fluxes in the city of zurich using the mesoscale atmospheric transport and inversion model ICON-ART-CTDAS. *EGU General Assembly*



2024. https://doi.org/10.5194/egusphere-egu24-7420

- Schröter, J., Rieger, D., Stassen, C., Vogel, H., Weimer, M., Werchner, S., Förstner, J., Prill, F., Reinert, D., Zängl, G., Giorgetta, M., Ruhnke, R., Vogel, B., & Braesicke, P. (2018). ICON-ART 2.1: A flexible tracer framework and its application for composition studies in numerical weather forecasting and climate simulations. *Geoscientific Model Development*, 11(10), 4043–4068. https://doi.org/10.5194/gmd-11-4043-2018
- Steiner, M., Peters, W., Luijkx, I., Henne, S., Chen, H., Hammer, S., & Brunner, D. (2024). European CH₄ inversions with ICON-ART coupled to the CarbonTracker data assimilation shell. *Atmospheric Chemistry and Physics*, *24*(4), 2759–2782. https://doi.org/10.5194/acp-24-2759-2024