EDGAR v5.0 Global Air Pollutant Emissions for MOZART chemical mechanism

Technical documentation

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Contents

1 Introduction **1**

2 Inventory processing **2**
2.1 Pollutant species and sectors 2
2.2 NMVOCs speciation to MOZART 2

3 Adapting for WRF-Chem use **4**

4 Code information **4**

5 License **6**

6 How to cite **6**

References **6**

1 Introduction

Emissions inventories need to be prepared to be ready to be used in chemical transport models (CTMs). They usually need ad-hoc preprocessing based on the chemical mechanism used in the CTM, including speciation of non-methane volatile organic compounds (VOCs). Here we report monthly EDGAR v5.0 global air pollutant emissions for the year 2015, speciated for the MOZART chemical mechanism. The dataset is also ready to be used in the WRF-Chem anthro_emiss preprocessing tool with the MOZART-MOSAIC options. The folder contains:

1. edgar_v5_MOZART_data.tar.gz: EDGAR v5.0 monthly emissions for the year 2015 (NetCDF format), speciated for MOZART chemical mechanism. Both total and individual sector emissions are included in each file.
2. edgarv5_MOZART_MOSAIC.inp: Input file for anthro_emiss preprocessing tool for MOZART-MOSAIC options in WRF-Chem.
3. code folder: scripts used to prepare 1).
4. technical_note_EDGARv5_MOZART.pdf: this technical documentation.

This technical documentation supports the dataset provided, and describes how the EDGAR v5.0 emission inventory was speciated for the MOZART chemical mechanism and prepared for use by the WRF-Chem model.

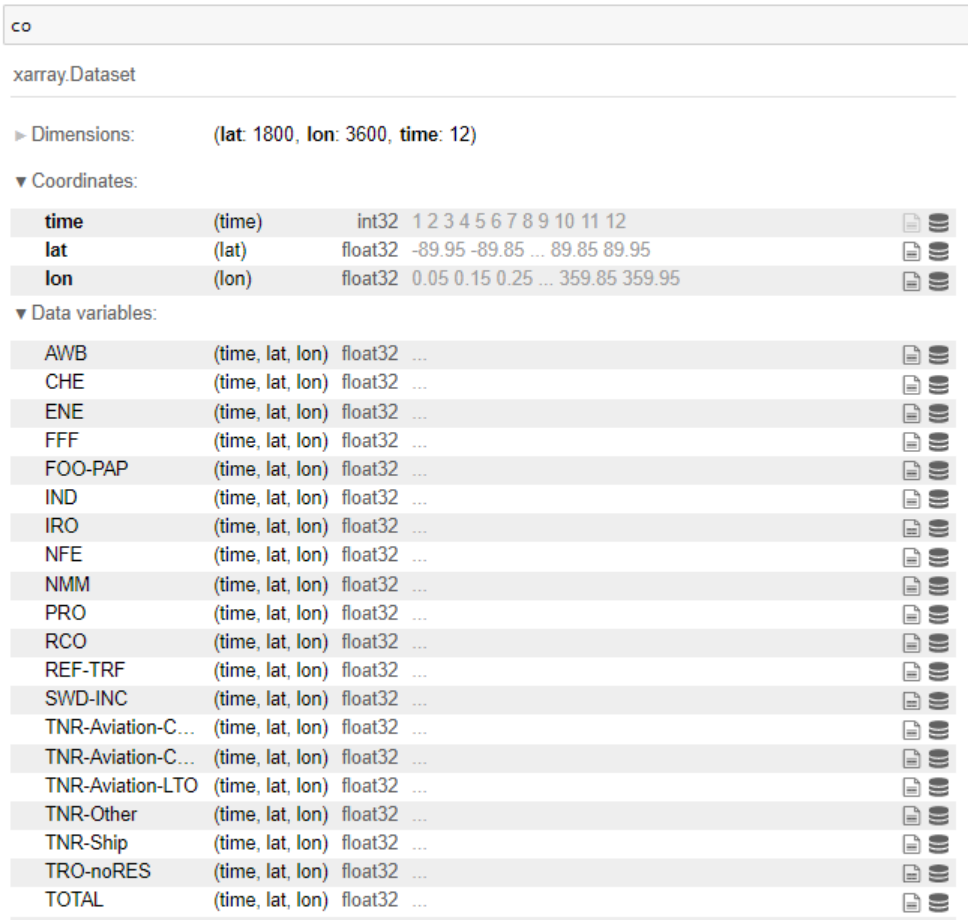

Figure 1: Dataset structure for each emission file. Example for the CO species. Data variables are explained in Table 1.

2 Inventory processing

2.1 Pollutant species and sectors

EDGAR v.5.0 monthly global gridded air pollutant emissions at 0.1°x0.1° resolution for the year 2015 (Crippa et al., 2019b,a,c, 2020) have been downloaded from the repository at https://data.jrc.ec.europa.eu/dataset/377801af-b094-4943-8fdc-f79a7c0c2d19#contact. EDGAR v.5.0 considers the following air pollutant species: BC, CO, NH_3, NO_x, OC, $PM_{2.5}$, PM_{10}, SO_2 and total NMVOCs for 27 anthropogenic sectors. We consider here all sectors except for supersonic aviation (for which no monthly emissions are available). Table 1 list the sectors and their identification code. We also provide total emissions for each species, calculated from summing all the individual sector emissions for the given species. The original files downloaded have been aggregated by pollutant species in the form shown in Figure 1.

2.2 NMVOCs speciation to MOZART

Total NMVOCs in EDGAR v.5.0 are speciated to the MOZART chemical mechanism using the fractional mass contribution obtained from the EDGAR v4.3.2 NMVOCs as follows.

We first obtain sector specific monthly EDGAR v4.3.2 NMVOCs for year 2010 at 0.1°x0.1° resolution Huang et al. (2017a,b) from the repository https://data.jrc.ec.europa.eu/dataset/jrc-edgar-edgar_v432_voc_spec_gridmaps, and we reorganise them by pollutant species as in we did for original EDGAR v5.0 files in Figure 1. EDGAR v4.3.2 NMVOCs are speciated using the GEIA 25 NMVOCs groups. We relate these NMVOC groups to the MOZART chemistry using the mapping provided in Emmons et al. (2020) and reproduced in Table 2. Since EDGAR v4.3.2 NMVOCs emissions are

sector name	sector id
Power industry	ENE
Oil refineries and Transformation industry	REF_TRF
Combustion for manufacturing	IND
Aviation landing&takeoff	TNR_Aviation_LTO
Aviation cruise	TNR_Aviation_CRS
Aviation climbing&descent	TNR_Aviation_CDS
Road transportation no resuspension	TRO_noRES
Road transportation resuspension	TRO_RES
Railways, pipelines, off-road transport	TNR_Other
Shipping	TNR_Ship
Energy for buildings	RCO
Fuel exploitation	PRO
Non-metallic minerals production	NMM
Chemical processes	CHE
Iron and steel production	IRO
Non-ferrous metals production	NFE
Non energy use of fuels	NEU
Solvents and products use	PRU_SOL
Food and Paper	FOO_PAP
Manure Management	MNM
Agricultural waste burning	AWB
Agricultural Soils	AGS
Solid waste landfills	SWD_LDF
Solid waste incineration	SWD_INC
Waste water handling	WWT
Fossil Fuel Fires	FFF

Table 1: Anthropogenic emissions sectors for EDGAR v5.0 air pollutant emissions. The sector_id column is used as sector identifier in the dataset we provide. More information on sectors definition are available at EDGAR v5.0 air pollutant emissions official website (Crippa et al., 2019b).

provided in mass and not in molar units, we obtain a mass mapping of Table 2 by applying the molecular weights for the GEIA NMVOC groups. Molecular weights for the GEIA VOC species are taken from http://www.globalchange.umd.edu/data/ceds/README-CEDS-VOC-speciation_2017-05-18.txt. Figure 1 shows the resulting monthly MOZART VOC distributions described on a uniform 0.1°x0.1° grid. We then calculate the gridded map of total NMVOCs mass by adding up the contribution of the individual MOZART species. For each MOZART VOCs species, we obtain a gridded map of its mass fractional contribution to total NMVOCs by dividing it by the gridded map of total NMVOC mass. We then apply these fractional gridded maps to the total EDGAR v5.0 NMVOCs file to obtain disaggregated NMVOCs emissions for the MOZART mechanism. The resulting EDGAR v5.0 MOZART VOCs are monthly gridded maps at 0.1°x0.1° in the form of Figure 1. All the original EDGAR v5.0 NMVOC sectors are included in the MOZART NMVOCs dataset, except for manure management (MNM, ipcc1996:4B), which is not included in the EDGAR v4.3.2 NMVOCs dataset. In addition, since the definition of sectors is slightly different between EDGARv4.3.2 and EDGAR v5.0 sectors, we needed to remap some of the NMVOCs sectors:

- Process emissions during production and application:
  PPA (EDGAR v.4.3.2) = CHE+FOO_PAP+IRO+PRU-SOL+NMM (EDGAR v5.0)
- Waste solid and wastewater:
  SWD (EDGAR v.4.3.2) = SWD_INC+SWD_LDF+WWT (EDGAR v5.0)
- Oil refineries and Transformation industry:
  REF+TRF (EDGAR v.4.3.2) = REF_TRF (EDGAR v.5.0)

The final speciated NMVOCs files that we report contain the mapped sectors (PPA,SWD,REF+TRF) and not the original EDGARv5.0 ones.

MOZART	GEIA/CEDS
C2H6	VOC02-ethane
C3H8	VOC03-propane
BIGALK	VOC04-butanes + VOC05-pentanes + VOC06-hexanes-pl + VOC18-esters + VOC19-ethers
C2H4	VOC07-ethene
C3H6	VOC08-propene
C2H2	VOC09-ethyne
BIGENE	VOC12-other-alke
BENZENE	VOC13-benzene
TOLUENE	VOC14-toluene
XYLENES	VOC15-xylene+VOC16-trimethylb+ VOC17-other-arom
CH2O	VOC21-methanal
CH3CHO	VOC22-other-alka
CH3OH	0.15*VOC01-alcohols
C2H5OH	0.85*VOC01-alcohols
CH3COCH3	0.2*VOC23-ketones
MEK	0.8*VOC23-ketones
HCOOH	0.5*VOC24-acids
CH3COOH	0.5*VOC24-acids

Table 2: Molar Mapping of NMVOCs species from GEIA/CEDS to MOZART chemistry. Adaptation of Table S3 from Emmons et al. (2020)

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3 Adapting for WRF-Chem use

We made the EDGAR v5.0 inventory speciated to MOZART obtained from Sec. 2 ready to be used in WRF-Chem with the anthro-emiss utility (MOZART-MOSAIC options). We added to the data files monthly *date* and *datesec* variables, the attribute units: $[kg\ m^{-2}\ s^{-1}]$ to each variable, and create the anthro-emiss input file (edgarv5-MOZART-MOSAIC.inp).

4 Code information

All the data processing described in Sec. 2 and Sec. 3 has been performed using scripts in Python 3.6, summarised by the flowchart in Figure 2. For each step of the process the corresponding code is found in the following scripts. For more details, see the individual Python scripts in the "code" folder.

- 1) download_edgarv5.sh
- 2)edgarv5_format.ipynb
- 3)download_nmvoc_edgarv432.sh
- 4) nmvoc4.3.2_format.ipynb
- 5) CEDS_MOZART_VOCmap.xlsx
- 6) nmvoc4.3.2_map_mozart_mass.ipynb
- 7), 8) nmvoc4.3.2_map_mozart_fractions.ipynb
- 9): edgarv5_NMVOC_map_sectors.xlsx; map_v5_to_v4.3.2_nmvoc_sectors.ipynb
- 10) edgarv5_nmvoc_speciate_to_mozart.ipynb
- 11) add_total_emissions.ipynb
- 12) edgarv5_to_WRFChem_anthroemiss.ipynb

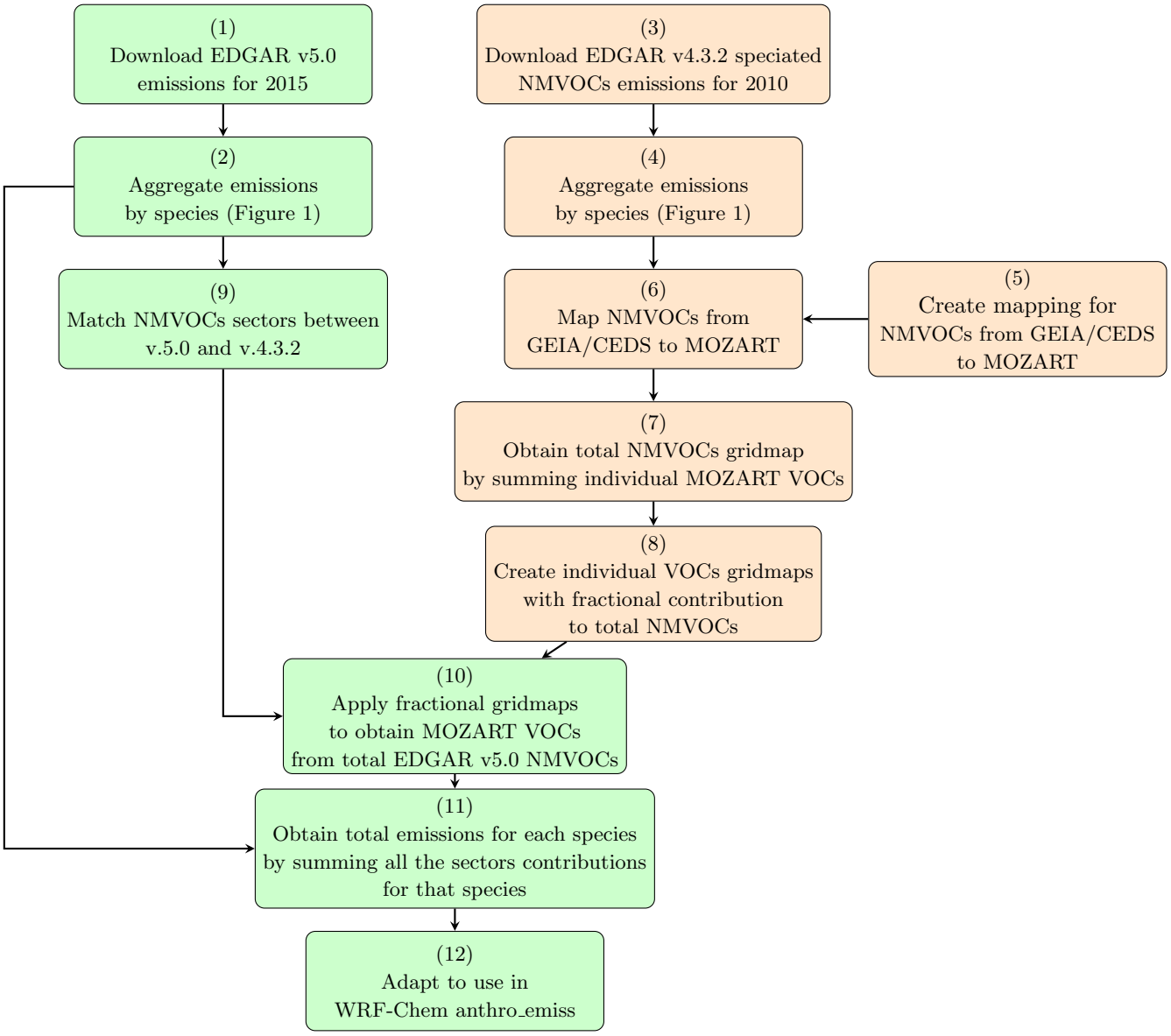

Figure 2: Flowchart of the data processing for preparing EDGAR v5.0 air pollutant emissions for MOZART chemistry. Green rectangles represent EDGAR v5.0 data processing, orange rectangle EDGAR v.4.3.2 NMVOCs data processing.

5 License

All the material provided (the dataset, the input file for anthro_emiss, the code and the present technical documentation) is distributed under MIT License.

6 How to cite

If you use this ready-to-use EDGAR v5.0 inventory and/or part of the code for an academic publication or any other work, we ask you to include the following acknowledgment:
"We acknowledge the use of the EDGAR v5.0 emissions inventory as prepared by Mogno and Marvin (2022)"
or directly cite the zenodo repository:
TO DO: ADD FINAL ZENODO REP

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