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

Technical Document

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October 22, 2021

Introduction

Emissions inventories needs to be prepared to be ready to be used in chemical transport model (CTMs). They usually need ad-hoc preprocessing based on the chemical mechanism used in the CTM. In particular, speciation of non-methane volatile organic compounds (VOCs) is chemical-mechanism dependent. Here the EDGAR v5.0 global air pollutant emission for year 2015 s provided as monthly emissions 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 v5.0 monthly emissions for year 2015 (NetCDF format), speciated for MOZART chemical mechanism. Both total and individual sectors emissions are included.
2. Input file (*.inp) for anthro_emiss preprocessing tool for MOZART-MOSAIC options in WRF-Chem.
3. Code used to prepare 1).

This document supports the dataset provided, and describes how EDGAR v5.0 was speciated for MOZART chemical mechanism.

Inventory processing

EDGAR v.5.0 (Crippa et al., 2019b,a,c, 2020) monthly global gridded air polluant emissions at 0.1x0.1 for year 2015 have been downloaded from the repository at https://cidportal.jrc.ec.europa.eu/ftp/jrc-opendata/EDGAR/datasets/v50_AP. For speciating NMVOCs we make also use of EDGAR v4.3.2 global speciated NMVOCs monthly emissions for year 2010 Huang et al. (2017a,b) that have been downloaded from the repository https://jeodpp.jrc.ec.europa.eu/ftp/jrc-opendata/EDGAR/datasets/v432_VOC_spec.

Pollutant species and sectors

EDGAR v.5.0 considers the following air pollutant species: BC, CO, NH_3, NO_x, OC, $PM_{2.5}$, PM_{1O}, SO_2 and total NMVOCs for 27 anthropogenic sectors. All sectors are here considered except for supersonic aviation (no monthly emissions are available). Table 1 list the sectors, their identification code, and their IPCC identifier. Data provided have also total emissions for each species, calculated from summing all the individual sector emissions for the given species.

NMVOCs speciation to MOZART

Total NMVOCs in EDGAR v.50 are speciated to MOZART chemical mechanism using the fractional mass contribution obtained from the EDGAR v4.3.2 NMVOCs as follow.

We first map monthly EDGAR v4.3.2 NMVOCs for year 2010 for each sector to MOZART chemical mechanism: EDGAR.v4.3.2 NMVOCs are available speciated in the GEIA 25 NMVOCs groups, and

sector name	sector id	ipcc_2006	ipcc_1996
Power industry	ENE	1A1a	1A1a
Oil refineries and Transformation industry	REF_TRF	1A1b+1A1ci+1A1cii+1A5biii+ 1B1b+1B2aiii6+1B2biii3+1B1c	1A1b+1A1c+1A5b1+1B1b+ 1B2a5+1B2a6+1B2b5+2C1b
Combustion for manufacturing	IND	1A2	1A2
Aviation landing&takeoff	TNR_Aviation_LTO	1A3a_LTO	1A3a_LTO
Aviation cruise	TNR_Aviation_CRS	1A3a_CRS	1A3a_CRS
Aviation climbing&descent	TNR_Aviation_CDS	1A3a_CDS	1A3a_CDS
Road transportation no resuspension	TRO_noRES	1A3b_noRES	1A3b_noRES
Road transportation resuspension	TRO_RES	1A3b_RES	1A3b_RES
Railways, pipelines, off-road transport	TNR_Other	1A3c+1A3e	1A3c+1A3e
Shipping	TNR_Ship	1A3d	1A3d+1C2
Energy for buildings	RCO	1A4+1A5	1A4
Fuel exploitation	PRO	1B1a+1B2aiii2+1B2aiii3+ 1B2bi+1B2bii	1B1a+1B2a1+1B2a2+ 1B2a3+1B2a4+1B2c
Non-metallic minerals production	NMM	2A	2A
Chemical processes	CHE	2B	2B
Iron and steel production	IRO	2C1+2C2	2C1a+2C1c+2C1d+ 2C1e+2C1f+2C2
Non-ferrous metals production	NFE	2C3+2C4+2C5+2C6+2C7	2C3+2C4+2C5
Non energy use of fuels	NEU	2D1+2D2+2D4	2G
Solvents and products use	PRU_SOL	2D3+2E+2F+2G	3
Food and Paper	FOO_PAP	2H	2D
Manure Management	MNM	3A2	4B
Agricultural waste burning	AWB	3C1b	4F
Agricultural Soils	AGS	3C2+3C3+3C4+3C7	4C+4D
Solid waste landfills	SWD_LDF	4A+4B	6A+6D
Solid waste incineration	SWD_INC	4C	6C
Waste water handling	WWT	4D	6B
Fossil Fuel Fires	FFF	5B	7A

Table 1: Anthropogenic emissions sectors for EDGAR v5.0 air pollutant emissions. Table adapted from EDGAR v5.0 air pollutant emissions official website (Crippa et al., 2019b). The sector_id column is used as sector identifier in the dataset provided.

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/CESM2 to MOZART chemistry. Adaptation of Table S3 from (Emmons et al., 2020). Molar weights for the GEIA/CEDS VOCs groups are taken from the CEDS documentation at http://www.globalchange.umd.edu/data/ceds/README-CEDS-VOC-speciation_2017-05-18.txt

we map them to the MOZART chemistry using the mapping provided in (Emmons et al., 2020). and reproduced in Table 2. This molar mapping has been then converted to mass mapping, since EDGAR

EDGAR v4.3.2 NMVOCs sector name	v4.3.2 sector id	v5 sector id
Agricultural waste burning	AWB	AWB
Power generation	ENE	ENE
Combustion for manufacturing industry	IND	IND
Process emissions during production and application	PPA	CHE+FOO_PAP+IRO+PRU-SOL+NMM
Fuel exploitation	PRO	PRO
Energy for buildings	RCO	RCO
Waste solid and wastewater	SWD	SWD_INC+SWD_LDF+WWT
Aviation climbing&descent	TNR_Aviation_CDS	TNR_Aviation_CDS
Aviation cruise	TNR_Aviation_CRS	TNR_Aviation_CRS
Aviation landing&takeoff	TNR_Aviation_LTO	TNR_Aviation_LTO
Railways, pipelines, off-road transport	TNR_Other	TNR_Other
Shipping	TNR_Ship	TNR-Ship
Oil refineries + Transformation industry	REF+TRF	REF_TRF
Road transportation	TRO	TRO_noRES
Fossil Fuel Fires	FFF	FFF

Table 3: Mapping of EDGAR v5.0 sectors to match EDGAR v4.3.2 NMVOCs sectors.

v4.3.2 NMVOCs emissions are provided in mass and not in molar units. Then for each MOZART VOC species we obtain gridded maps with their mass fractional contribution to total NMVOCs by dividing each VOC by the total NMVOC mass. Finally we apply these fractional gridded maps to the total EDGAR v5.0 NMVOCs to obtain disaggregated NMVOCs emissions for MOZART. Since there is no biunivocal correspondence between EDGARv4.3.2 NMVOCs sectors and EDGARv5 NMVOC sectors, we map EDGAR v5.0 NMVOCs sectors to be compliant with EDGAR v3.4.2 ones, as indicated in Table 3. All the original EDGAR v5.0 NMVOCs sectors are included in the dataset, except for manure management (MNM, ipcc1996:4B), which is not included in the original EDGAR v4.3.2 NMVOCs dataset.

Adapting emissions files for WRF-Chem use

To make the inventory ready to be used in WRF-Chem anthro-emiss utility with MOZART-MOSAIC options, we add to the data files monthly *date* and *datesec* variables, the attribute units: $[kgm-2s-1$ to each variable, and create the anthro-emiss input file (edgarv5-MOZART-MOSAIC.inp).

Code information

All the data processing described above has been performed using scripts in Python 3.6, ad it is summarised in the flowchart in Figure 1. For each step of the process the corresponding code is found in the following scripts:

- Get EDGAR v5.0 monthly emissions: download_edgarv5.sh
- Get EDGAR v4.3.2 NMVOCs monthly emissions: download_nmvoc_edgarv432.sh
- Format: edgarv5_format.ipynb
- Format NMVOCs: nmvoc4.3.2_format.ipynb
- Map NMVOCs GEIA/CEDS to MOZART: CEDS_MOZART_VOCmap.xlsx
- Speciate NMVOCs to MOZART (mass): nmvoc4.3.2_map_mozart_mass.ipynb
- Create VOCs gridmaps with fractional contribution to total NMVOCs: nmvoc4.3.2_map_mozart_fractions.ipynb
- Match NMVOCs sectors v.5.0to v.4.3.2: edgarv5_NMVOC_map_sectors.xlsx; map_v5_to_v4.3.2_nmvoc_sectors.ipynb
- Speciate EDGAR v.5.0 NMVOCs to MOZART: edgarv5_nmvoc_speciate_to_mozart.ipynb
- Add total emissions: add_total_emissions.ipynb

- Adapt to use in WRF-Chem anthro_emiss: edgarv5_to_WRFChem_anthroemiss.ipynb

For more details, see the individual Python scripts in the 'code' folder.

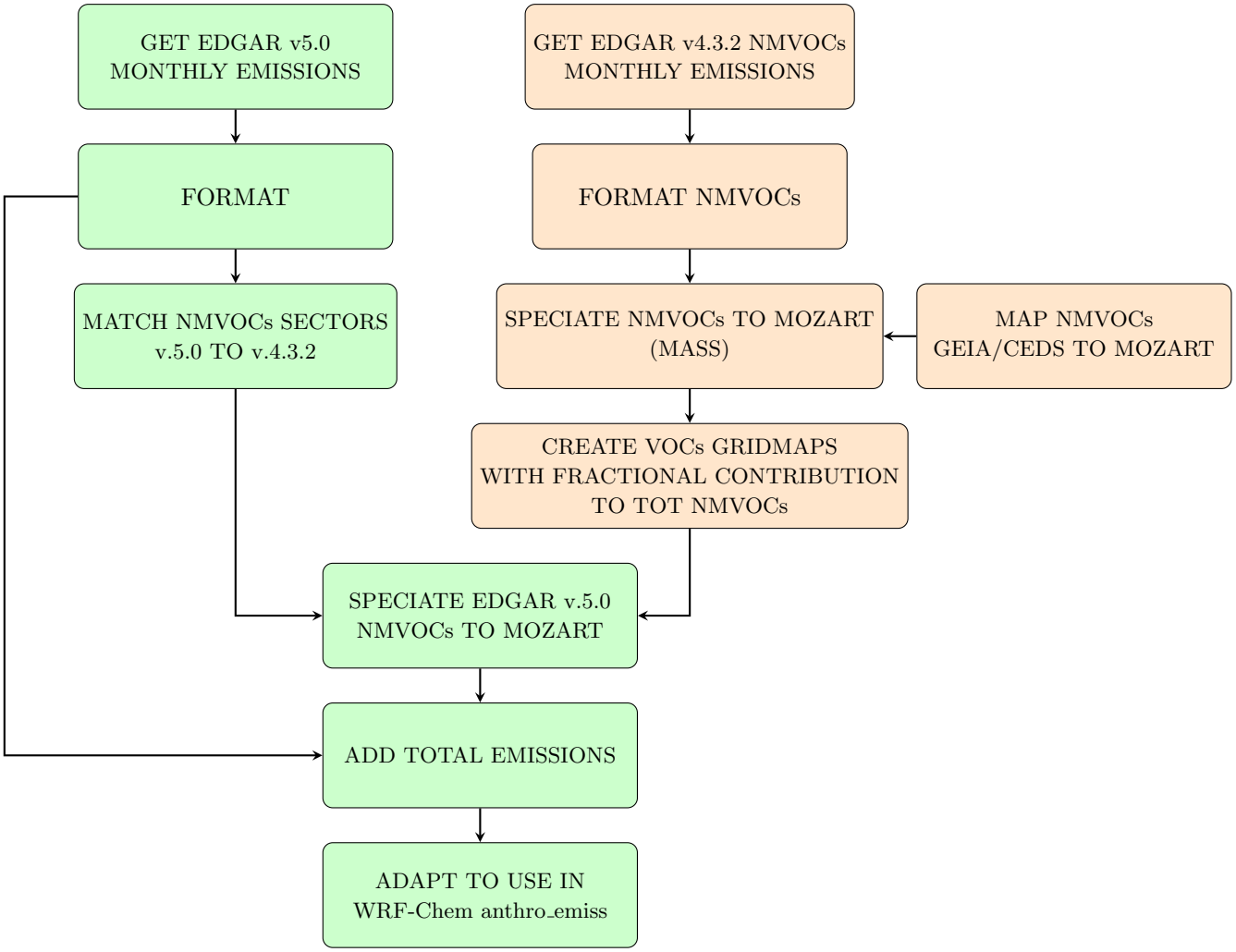

Figure 1: Flowchart of the data processing for preparing EDGAR v5.0 air pollutant emissions for MOZART chemistry. Green rectangles represent EDGAR v5.0 data processing, orange rectangle EDGAR v.4.3.2 NMVOCs data processing.

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