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EmissV: A Preprocessor for WRF-Chem Model

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ABSTRACT

Air quality models are tools capable to predict the physical and chemical processes that affect air pollutants as they disperse and reacts in the atmosphere. These models need input containing meteorological data, terrestrial data and emissions. Meteorological and terrestrial data comes from different sources such as meteorological stations and satellite images which are important to represent the current state of the atmosphere and are available at least on a daily frequency. On the other hand, the emission data comes from pollution inventories generated mainly from governmental reports, this data needs to be processed by various reasons such as the correction of outdated emissions, for combining inventories or to speciate the emitted pollutants to different chemical mechanisms. EmissV is a code written into a high-level programming language to create emissions input for these atmospheric models. The emissions from EmissV are coherent with the total and the spatial distribution of emissions obtained from other preprocessors.

1. Introdution

EmissV is an abbreviation for vehicular emission, it was written in R-programming language [1] and available in the form of a package distributed on Github [2] and CRAN [3] repositories. The goal of this code is to create the input for numerical air quality, including booth vehicular emissions and non-vehicular from other sources such as agriculture, agricultural waste burning, aircraft, fuel production and distribution, industry processes, residential, ships, solvents and waste [4]. Once for real world application, the emission comes from different sources and purely vehicular emission has little practical utility for most cities around the world.

Emission inventories have been compiled for a broad range of applications by an increasing number of institutions and scientists as they contains the basic information that is needed for studies on the environmental issues from air pollution to climate change [5]. In special some of these inventories are in form of a gridded database for use in global and regional modelling which covers different time periods, such as the Emission Database for Global Atmospheric Research, EDGAR [6], and MACCITY [7].

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2. Methodology

Figure 1 shows a simple diagram of the workflow for using EmissV as a preprocessor, the rectangle represents external files for input and output and the circles represents functions available on the package. The process needs NetCDF grided inventory file(s) (EDGAR and MACCITY are supported) and an input file (for example, wrfinput_d01 for domain 1) or an emission file (for example, wrfchem_d02_<date><time> for domain 2) contains information about the model grid.
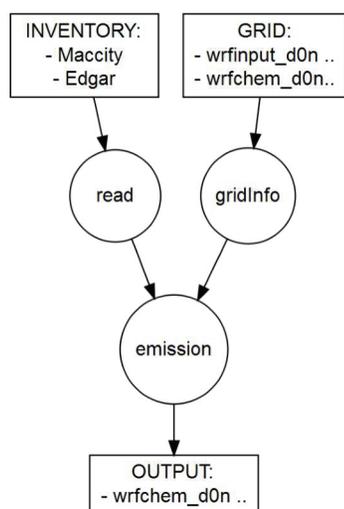

Figure 1. Diagram of the workflow.

The process of using a gridded inventory starts with a high-level function (read) that reads the emission in NetCDF format and return a Raster object that represents a georeferenced pixel image from the pollutant. This function is capable to read several source files and merge the emissions assigning weights to different files and variables. This approach, along with a set of messages that can detail what the function is performing, gives to the user the power to easily control the input data that comes from inventories and use this information to make projections, create scenarios, or simply combine the desired variables to this own application. An additional feature is the ability to speciate the emission into several species for different chemical mechanisms with data from the package (nitrogen oxide (NOX) [8,9], particulate matter (PM) [10], volatile organic compounds (VOC) from total emissions [11] and from mobile sources [12] and for EDGAR-4.3.2 [13] for different chemical mechanisms) or data provided by the user.

A function (emission) has the role to convert the emissions into data for the model. The processes converts the emission from the inventory units (kg s-1 m-2) to model units for gases (MOL h-1 km-2) and aerosol (μg s-1 m-2),

and uses a bilinear spatial interpolation for the model grid. The model domain information accessed by a function (gridInfo) that reads the information needed to convert the emission for a specific domain. Additionally, the function shows a graph of the emissions, as is showed in Figure 2, since the output of this function is unitless and without spatial reference.
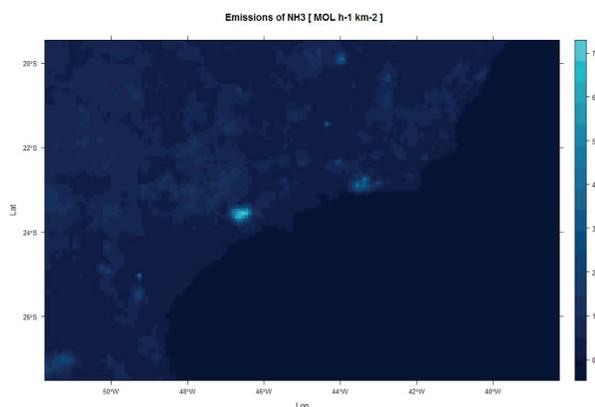

Figure 2. Output from the emission function.

The output from emission function can be written to model files at the time WRF-Chem [14], is the only model full implemented. Several R-packages has the ability to interact with NetCDF files such as ncdf4 [15], RNetCDF [16] and ncdf.tools [17]. The package eixport [18] has high-level functions to create a WRF-Chem emission file for WRF-Chem (version v3.6.1 or higher) and to write the emission function output.

3. Results

As a test case, we choose two nested domains, one outer domain (d01) on the southeast region of Brazil with 150x100 horizontal grid points and 9 km of spacing, and an inner domain (d02) the Metropolitan area of São Paulo with 64x52 horizontal grid points with 3 km of spacing, the boundaries are shown in Figure 3.
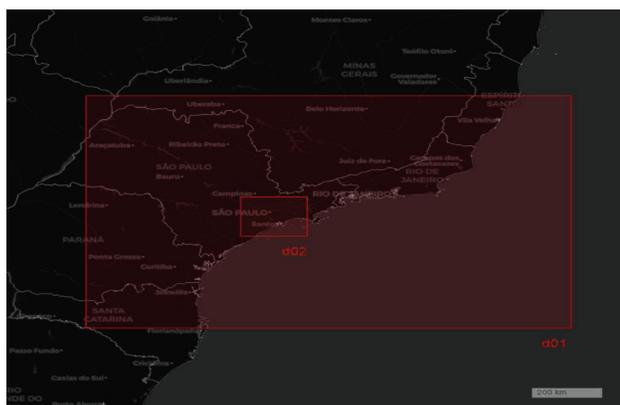

Figure 3. WRF nested domains.

In this example the chosen ammonia (NH3) for visualization purposes. Figure 4 shown the global emission of EDGAR for NH3 from the industry, energy, residential and agriculture sectors from for 2010 over the globe (combined with the read function). The transport sector will not be used for not double count the vehicular emissions allowing the use of emission from another models or sources.
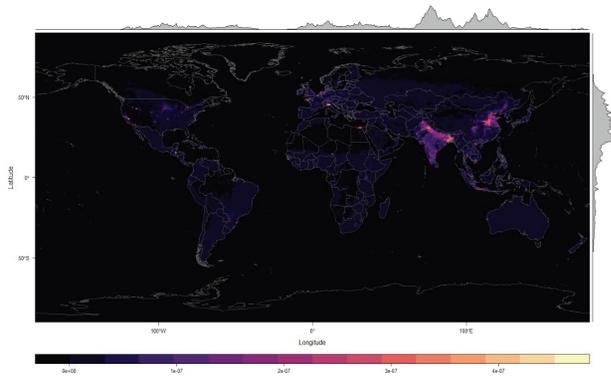

Figure 4. EDGAR global emission for NH_3 (kg m-2 s-1).

Using the gridInfo function for both domains and the EDGAR the emission function generates the emission and saves on file ready to be used on a simulation. Figure 5 and 6 shows the emission in domain d01 and d02 respectively.
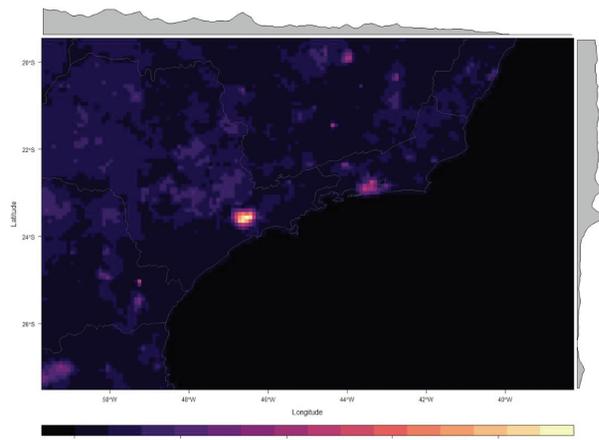

Figure 5. NH3 Emissions for domain d01 (MOL km-2 h-1).

In Figure 5 and 6 seven Brazilian states are (partially) inside the domain d01 in the same way of Figure 3. Figure 6 shows domain d02, which is a region inside the São Paulo State with a high urbanized area that concentrates a big amount of emissions.

4. Discussion

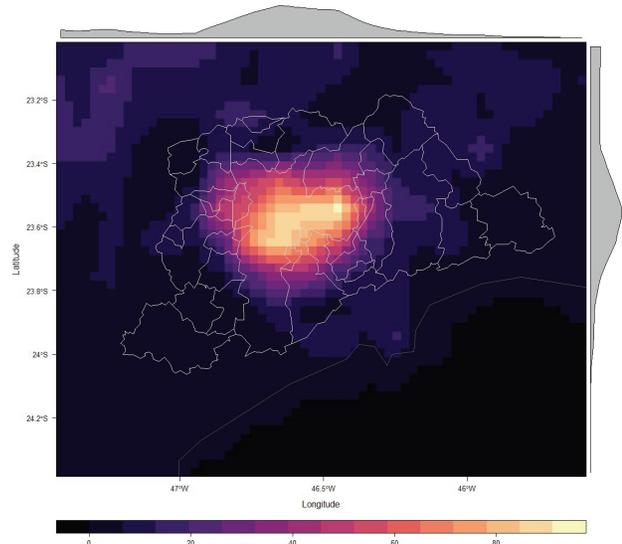For the purpose of comparison, two set of emissions was calculated using the EmissV and the Antro emiss prepro-

Figure 6. NH3 Emissions for domain d02 (MOL km-2 h-1).

cessor [19] using the same input from the EDGAR inventory. Figure 7 shows the contour lines of EmissV emissions for domain d01 (b) and d02 (b) and for Anthro emiss d01 (c) and domain d02 (d). Both emissions exhibit the same patterns with almost no difference regard the spatial distribution of the emission species.

Statistically, both emissions are very compatible. The average values of the EmissV emissions are 97.8% for domain d01 and 101.2 % for domain d02. The EmissV maximum values are 102.5 % and 100.3 % of the calculated by the Anthro emiss.

5. Conclusions

The output emissions from EmissV are coherent with the emissions obtained from Anthro emiss using the same input and the spatial distribution of the emissions of both preprocessors are very coherent with the distribution of the sources on the Metropolitan Area of São Paulo which is a highly urbanized area.

The EmissV is a tool available for the creation of emission files for use in numerical air quality models, regarding the use of the top-down vehicular estimation which can combine inventories into a high-level programming language. The support for another models and inventories is the next development steps in case of interest of the package users.

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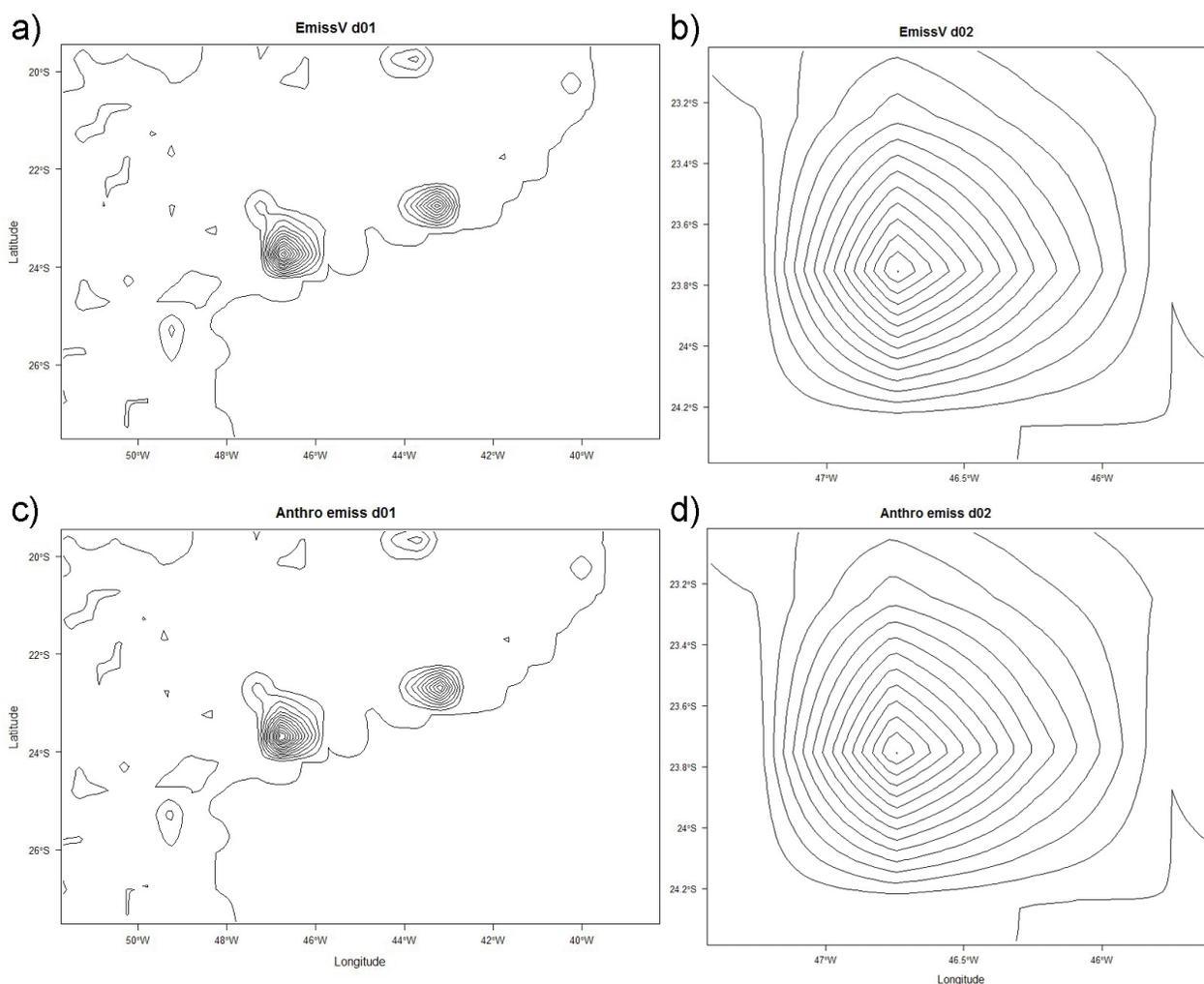
Figure 7. Contour of the emissions: a) EmissV for domain d01, b) EmissV for domain d02, c) Anthro emiss for domain d01 and d) Anthro emiss for domain d02.

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