EmissV: an R package to create vehicular and other emissions for air quality models

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Summary

Air quality models need input data containing information about atmosphere (such as temperature, wind, humidity), terrestrial data (such as terrain, land use, soil types) and emissions. Therefore, the emission inventories are easily seen as the scapegoat if a mismatch is found between modelled and observed concentrations of air pollutants (Pulles & Heslinga, 2010). The anthropogenic emissions, especially vehicular emissions, are highly dependent on human activity and constantly changing due to various factors ranging from economic (such as the state of conservation of the fleet, renewal of the fleet and the price of fuel) to legal aspects (such as the vehicle routing).

The EmissV is an R package that estimates vehicular emissions by a top-down approach, the emissions are calculated using the statistical description of the fleet at available level (National, State, City, etc). The following steps show an example of the workflow for calculating vehicular emissions, this emissions are initially temporally and spatially disaggregated, and then distributed spatially and temporally to be used as input in numeric air quality models such WRF-Chem (Grell et al., 2005).

I. Total: emission of pollutants is estimated from the fleet (number, type and year of vehicles), vehicular activity (km/day) and emission factors (g/km) by pollutant for each interest area (cities, states, countries, etc) or alternatively the totals of some inventory can be used.

II. Spatial distribution: the package has functions to read information from tables, georeferenced images (tiff), shapefiles (sh), openstreetmap data (osm), global inventories in NetCDF format (nc) to calculate point, line and area sources.

III. Emission calculation: calculates the final emission from all different sources and converts to model units and resolution.

IV. Temporal distribution: a set of hourly profiles that represents the mean activity (by hour and day of the week) calculated from traffic counts of toll stations located at São Paulo city available for apply in the emissions.

The package has additional functions for creating emissions from individual sources (including plume rise parameterizations) and to estimate the vehicular emissions of volatile organic compounds from exhaust (through the exhaust pipe), liquid (carter and evaporative) and vapor (fuel transfer operations).

Functions and data

EmissV counts with the folllwing functions:

Function	Description
areaSource	Distribution of emissions by area
emission	Emissions in the format for atmospheric models
emissionFactors	Tool to set-up vehicle emission factors
gridInfo	Read grid information from a NetCDF file
lineSource	Distribution of emissions by streets
perfil	Dataset with temporal profile for vehicular emissions
plumeRise	Calculate plume rise height
pointSource	Emissions from point sources
rasterSource	Distribution of emissions by a georeferenced image
read	Read NetCDF data from global inventories
streedDist	Distribution by OpenStreetMap street
totalEmission	Calculate total emissions
totalVOC	Calculate total VOCs emissions
vehicles	Tool to set-up vehicle data frame

Examples

The following example creates an area source for São Paulo State (Brasil). The `vehicles` function creates a `data.frame` with information about the São Paulo Fleet using data from (DETRAN, 2015), the `emissionFactors` creates a `data.frame` with emission factors for CO and PM (CETESB, 2015). The `totalEmission` calculates the total emissions of CO for these vehicles and this emission factors. The next 3 lines opens different data: wrf file, a raster and the area shapefiles. These data are the input for `areaSouce` that creates an area source based on an image of persistent lights of the Defense Meteorological Satellite Program (DMSP) for São Paulo and Minas Gerais (Brasil) states and finally the function `emission` calculates the CO emissions.

```r
library(EmissV)

fleet <- vehicles(example = T)
# using a example of vehicles (DETRAN 2016 data and SP vahicle distribution):
#                                 Category     Type  Fuel       Use       SP ...
# Light Duty Vehicles Gasohol     LDV_E25      LDV   E25    41 km/d 11624342 ...
# Light Duty Vehicles Ethanol     LDV_E100     LDV   E100   41 km/d   874627 ...
# Light Duty Vehicles Flex          LDV_F      LDV   FLEX   41 km/d  9845022 ...
# Diesel Trucks                  TRUCKS_B5  TRUCKS   B5    110 km/d   710634 ...
# Diesel Urban Busses              CBUS_B5     BUS    B5    165 km/d   792630 ...
# Diesel Intercity Busses          MBUS_B5     BUS    B5    165 km/d    21865 ...
# Gasohol Motorcycles             MOTO_E25    MOTO   E25   140 km/d  3227921 ...
# Flex Motorcycles                  MOTO_F    MOTO   FLEX  140 km/d   235056 ...

# dropping the fleet from Rio de Janeiro (RJ), Parana (PR) and Santa Catarina (SC)
fleet <- fleet[,c(-6,-8,-9)]

EF      <- emissionFactor(example = T)
# using a example emission factor (values calculated from CETESB 2015):
#                                   CO          PM
# Light Duty Vehicles Gasohol   1.75 g/km 0.0013 g/km
# Light Duty Vehicles Ethanol  10.04 g/km 0.0000 g/km
# Light Duty Vehicles Flex      0.39 g/km 0.0010 g/km
# Diesel Trucks                 0.45 g/km 0.0612 g/km
# Diesel Urban Busses           0.77 g/km 0.1052 g/km
```
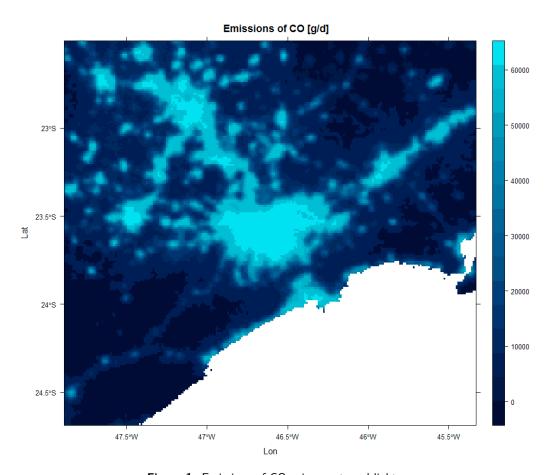
```r
# Diesel Intercity Busses        1.48 g/km 0.1693 g/km
# Gasohol Motorcycles            1.61 g/km 0.0000 g/km
# Flex Motorcycles               0.75 g/km 0.0000 g/km

TOTAL  <- totalEmission(fleet,EF,pol = c("CO"),verbose = T)
# Total of CO : 1128297.0993334 t year-1

grid   <- gridInfo(paste(system.file("extdata", package = "EmissV"),
                   "/wrfinput_d02",sep=""))
# Grid information from: .../EmissV/extdata/wrfinput_d02

raster <- raster::raster(paste(system.file("extdata", package = "EmissV"),
                         "/dmsp_hi-res.tiff",sep=""))

shape  <- raster::shapefile(paste(system.file("extdata", package = "EmissV"),
                           "/BR.shp",sep=""),verbose = F)[12,1]

Minas_Gerais <- areaSource(shape,raster,grid,name = "Minas Gerais")
# processing Minas Gerais area ...
# fraction of Minas Gerais area inside the domain = 0.0147607845622591

shape  <- raster::shapefile(paste(system.file("extdata", package = "EmissV"),
                           "/BR.shp",sep=""),verbose = F)[22,1]

Sao_Paulo <- areaSource(shape,raster,grid,name = "Sao Paulo")
# processing Sao Paulo area ...
# fraction of Sao Paulo area inside the domain = 0.473260323300595

sp::spplot(raster::merge(drop_units(TOTAL$CO[[1]]) * Sao_Paulo,
                         drop_units(TOTAL$CO[[2]]) * Minas_Gerais),
           scales = list(draw=TRUE),ylab="Lat",xlab="Lon",
           # main=list(label="Emissions of CO [g/d]"),
           col.regions = c("#031638","#001E48","#002756","#003062",
                           "#003A6E","#004579","#005084","#005C8E",
                           "#006897","#0074A1","#0081AA","#008FB3",
                           "#009EBD","#00AFC8","#00C2D6","#00E3F0"))

CO_emissions <- emission(TOTAL,"CO",list(SP = Sao_Paulo, MG = Minas_Gerais),
                         grid,mm=28, plot = T)
# calculating emissions for CO using molar mass = 28 ...
```

The emissions of CO calculated in this example can be seen in Figure 1 in `g/d` (by pixel) and the final emissions on Figure 2 in MOL `h-1 km-1` (by model grid cell). This emissions can be written to WRF-Chem emission files using some package that makes the interface with NetCDF format such as **ncdf4** (Pierce, 2017), **RNetCDF** (Michna & Milton Woods, 2017), **ncdf.tools** (Buttlar, 2015) or with the **eixport** (Ibarra-Espinosa & Schuch, 2018). Some output values (also figures generated by EmissV) might differ slightly depending on the EmissV package-version (as well as different versios of ncdf4, units, raster, sf, lwgeom, etc) and changes to the sample files.

The R package EmissV is available at the repository https://github.com/atmoschem/EmissV. And this installation is tested automatically on Linux via TravisCI and Windows via Appveyor continuous integration systems. Also, EmissV is already on CRAN https://CRAN.R-project.org/package=EmissV.

Figure 1: Emissions of CO using nocturnal lights.

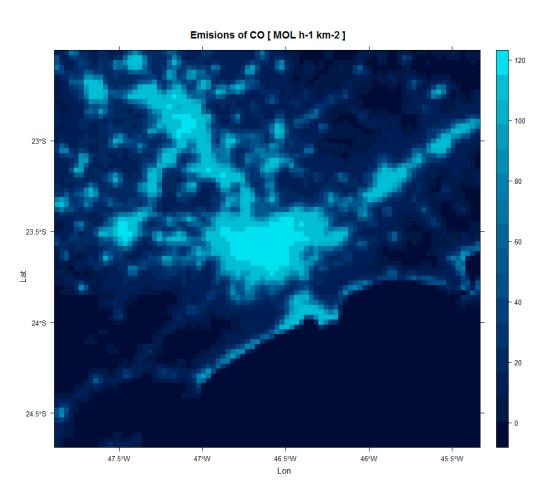**Figure 2:** CO emissions ready for use in air quality model.

Schuch et al., (2018). EmissV: an R package to create vehicular and other emissions for air quality models. *Journal of Open Source Software*, 5
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Acknowledgements

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