Sergio Ibarra-Espinosa

Vehicular emissions inventory with VEIN


VEIN

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Preface

This book is about the process for estimating vehicular emissions. This process is complex and *can* be dificult. It is required a big amount of information related to traffic, emissions factors and then process the outpus for the desired purpose. In this book this process is addressed with the **VEIN** (Ibarra-Espinosa et al., 2018c) model, which is an R package available at `https://CRAN.R-project.org/package=vein`}.

Purpose

I wrote this book to provide instructions to all possible users who want to estimate vehicular emissions using VEIN. VEIN provides several function which are related to each other reading different traffic sources and emission factors for different pollutants. However, incorporating all the functions with input/output (I/O) process can be difficult. Moreover, communicating the recommended practices and instructions to a increasingly broader audience can be more difficult. Therefore, the purpose of this book is to reach the maximum amount of interested people in a simple way. The language chosen is engligh because it is the global language.

Structure

Chapter 1 covers the introduction to this book including the installation of R packages and dependent libraries to several operative systems. Chapter 2 covers basics commands using R. Chapter 3 presents the function

inventory to produce an structure of directories and scripts for runnin vein. Chapter 4 covers the required traffic data for inputting into VEIN including differenttypes and sources of information. Chapter 5 includes the emission factors that are included into the package and also, examples for inputing and creating new emission factors. Chapter 6 presents the estimations functions and tips. Chapter 7 includes the functions to do post-estimations to generate emission data-bases and also emissions at each street. Chapter 8 and 9 provides applications into air quality modeling, some studies with to investigte health effects and lastly, the use of VEIN as a tool for environmental planning.

About the author

Sergio Ibarra Espinosa is a chilean Environmental and Loss Prevention Engineer from the Technologycal Metropolitan University (UTEM) where study the health effects of air pollution using R in year 2007. Then started working at the National Center for Environment (CENMA) in Chile focused on emissions from vehicles, airports, biomass burning and minning industry. Then obtained a MSc. in Environmental Planning and Managment from the University of Chile, with a scholarship form CENMA. Then obtained a PhD. in Meteorology at the Institute of Astronomy, Geophysics and Atmospheric Sciences (IAG) from the University of São Paulo (USP) with scholarship from CAPEs during the first year and Becas Chile for the last three years. During his PhD. he learned programming with R and developed the R package VEIN.

1

Introduction

1.1 Definitions and sources of information

Developing emissions inventories is a complex task. Therefore, before entering into the details of the functions, it is good to provide some initial definitions.

A good starting point is the book *"The Art of Emissions Inventorying"* (Pulles and Heslinga, 2010). This book provides general description of what is an emissions inventory. One of the early sources of information about emissions inventories and emissions factors is the Environmental Protection Agency (U.S.EPA) and its compilation of emission factors AP42 (`https://www.epa.gov/air-emissions-factors-and-quantification`). A third source of information are the European EMEP/EEA air pollutant emission inventory guidebook (`https://www.eea.europa.eu/themes/air/emep-eea-air-pollutant-emission-inventory-guidebook/`).

An emissions inventory is the compilation of all mass emitted into the atmosphere by activities in a defined area during a lapse of time. The Eq. ((1.1) shows the general form (McGlade and Vidic, 2009):

$$Emission_{pollutant} = \sum_{activities} Activityreate \cdot Emissionfactor_{activity,pollutant} \tag{1.1}$$

There are two main types of inventories based on the application, one type is for policy application and the other for scientific application (Pulles and Heslinga, 2010).

- Inventories for policy application include the National Greenhouse

Gas Inventory for the parties under the United Nations Framework on Climate Change (UNFCCC, 2017).
- Emissions inventories with scientific applications include the Emission Database for Global Atmospheric Research EDGAR (EJ-JRC/PBL, 2016).

Emissions inventories can be also multimedia inventories, such as the Pollutant Release and Transfer Registers (PRTR) which include pollutants released to air, water and soil and transferred off-site for treatment or disposal (`http://www.oecd.org/chemicalsafety/pollutant-release-transfer-register/`). However, the type of inventory covered in this book cover only the emissions released into the atmosphere.

1.1.1 Approaches

It is necessary show some definitions of vehicular emissions inventories approaches, which in this case comes from the European Emissions Guidelines (Ntziachristos and Samaras, 2016):

- **Top-down** inventories are using input activity traffic data as fleet statistics, fuel consumption, representative speeds and country balances. The emissions factors are based on representative speeds. These inventories are also know as *static*.
- **Bottom-up** invetories are using input activity traffic data from traffic counts, traffic simulations, vehicle composition, speed recordings and length of roads. The emission factors are speed or/and acceleration functions. These inventories are also know as *dynamic*.
- **Reconciliation** Both approaches can be reconciliated in urban emissions inventories with comparison of total mileage, cold start mileage or emission factors to ensure that the comparison with the total fuel consumption in the study area is satisfactory. This means that bottom-up and top-down vehicular emissions must match the fuel sales over a region of study.

1.2 Installation

The VEIN r-package can be installed from Comprehensive R Archive Network CRAN[1] directly:

```
# CRAN
install.packages("vein")
```

VEIN can be also installed from github:

```
library(devtools)
install_github("ibarraespinosa/vein")
```

The github installation requires that the *devtools* package (Wickham and Chang, 2017) must be installed, including its dependencies.

1.3 Required R packages and dependencies

VEIN improts functions from other R packages. HEnce, these packages are necessary::

sf is a package that provides simple features access for R (Pebesma, 2017). It depends on the library GEOS (`http://trac.osgeo.org/geos`), 'Geospatial' Data Abstraction Library ('GDAL') (`http://www.gdal.org/`) and PROJ (`http://proj4.org/`). **data.table** is a package that provides simple features access for R (Pebesma, 2017). It can be installed. - **sp**. This is a package that provides classes and methods for spatial data (Pebesma and Bivand, 2005) considering points, lines, polygons and grids. few function of sp are imported, most of them comes from sf. **eixport** is a package (Ibarra-Espinosa et al., 2017b) that creates inputs for atmospheric models (Ibarra-Espinosa et al., 2018b). - **units**. It is a package for measurement units in

[1] `https://cran.r-project.org/`

R (Pebesma et al., 2016). This package depends on the library udunits2 (`http://www.unidata.ucar.edu/software/udunits/`). I

```
install.packages(c("sf", "data.table", "sp", "eixport", "units"))
```

In order to install **sf** package it is necessary to install the dependencies into each operational system.

Ubuntu

```
sudo add-apt-repository ppa:ubuntugis/ubuntugis-unstable
sudo apt-get update
sudo apt-get install libudunits2-dev libgdal-dev libgeos-dev libproj-dev
```

Fedora

```
sudo dnf install gdal-devel proj-devel proj-epsg proj-nad
geos-devel udunits2-devel
```

Debian and other

Dockerfiles from rocker geospatial[2].

Windows Via Rtools[3].

MAC OS

```
brew unlink gdal
brew tap osgeo/osgeo4mac && brew tap --repair
brew install proj
brew install geos
brew install udunits
brew install gdal2 --with-armadillo --with-complete
--with-libkml --with-unsupported
brew link --force gdal2
```

[2] `https://github.com/rocker-org/geospatial`
[3] `https://cran.r-project.org/bin/windows/Rtools/`

TABLE 1.1: Emission factors from CETESB in VEIN model

Age	Year	Pollutant	PC_G	LT
1	2015	CO	0.171	0.027
2	2014	CO	0.216	0.012
3	2013	CO	0.237	0.012
4	2012	CO	0.273	0.005
5	2011	CO	0.275	0.379
6	2010	CO	0.204	0.416

The R package eixport imports function from **ncdf4** (Pierce, 2017), therefore the library NetCDF must be installed. For Ubuntu, do:

```
sudo apt install libnetcdf-dev  netcdf-bin
```

1.4 Data inside the VEIN model

There are several datasets available inside the model:

1.4.1 Emission factors from CETESB

- **fe2015**: Emission factors from the Environmental Agency of Sao Paulo (CETESB). Pollutants included: "CH4", "CO", "CO2", "HC", "N2O", "NMHC", "NOx" and "PM". The type of vehicles included are Passenger Cars (PC).

usage:

```
library(vein, quietly = T)
data(fe2015)
```

1.4.2 Mileage functions of Brazilian Fleet

- **fkm**: A list of functions of mileage in km for the Brazilian fleet. It includes mileage functions based on more than 2 million recordings of vehicles (Bruni and Bales, 2013). It consists a list of age functions. The type of vehicles are Passneger Cars (PC), Light Commercial Vehicles (LCV), Small Busses (SBUS), Trucks, Articulated Trucks (ATRUCKS), Motorcycles (MOTO) and Light vehicles (LDV). The fuels are Gasoline using 25% of ethanol (E25), Ethanol 100% (E100) and Diesel with 5% of biodiesel (B5). There are also vehicles with flex engines which can run either with E25, E100 or any mixture in between (Giroldo et al., 2005). The Fig. (1.1 shows the mileage of PC using fuel E25.

usage:

```
library(vein, quietly = T)
data(fkm)
names(fkm)
```

```
##  [1] "KM_PC_E25"     "KM_PC_E100"    "KM_PC_FLEX"    "KM_LCV_E25"
##  [5] "KM_LCV_FLEX"   "KM_PC_B5"      "KM_TRUCKS_B5"  "KM_BUS_B5"
##  [9] "KM_LCV_B5"     "KM_SBUS_B5"    "KM_ATRUCKS_B5" "KM_MOTO_E25"
## [13] "KM_LDV_GNV"
```

```
age <- 1:50
mileage <- fkm[["KM_PC_E25"]](1:50)
par(mar = c(4, 4, .1, .1))
plot(y = mileage, x = age, pch = 19, type = "b")
```

- **net**: Road network of the west part of Sao Paulo city. It consistes in a SpatialLinesDataFrame (class of sp) with the attributes ldv (light duty vehicles, $1 \cdot h^{-1}$), hdv (heavy duty vehicles, $1 \cdot h^{-1}$), ps (peak speed, $km \cdot h^{-1}$), ffs (free flow speed, $km \cdot h^{-1}$), tstreet (type of street), lanes (number of lanes), capacity (capacity fo vehicles at each link, 1/h) and tmin (time for travelling each link, min). The Fig. (4 shows more details.

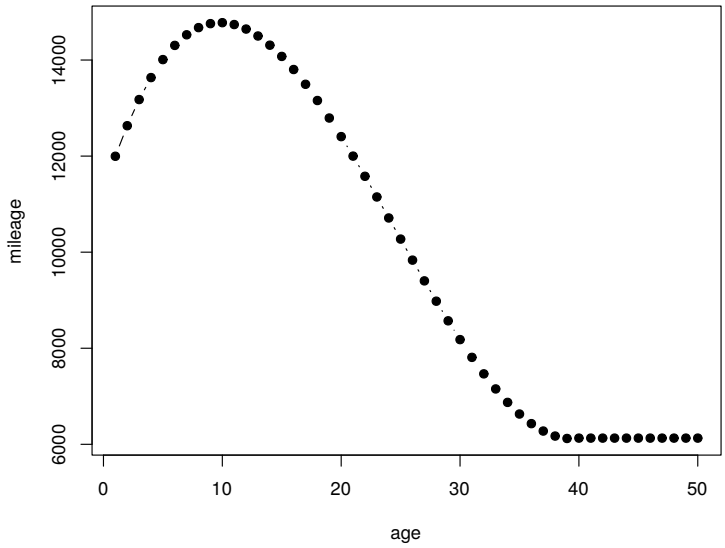

FIGURE 1.1: Mileage of PC using E25

1.4.3 Temporal factors for Passenger Cars

Temporal factors (TF) are marix of jourly traffic data normalized for the hour of interest, normally the morning rush hour 08:00-09:00 in local time (LT) (Ibarra-Espinosa et al., 2018c). This dataset cover 168 hours of one week and it is based on traffic counts of toll stations near the center of the city of SãoPaulo, Brazil. The Fig. (1.2 shows the temporal factors for PC.

usage:

```
library(vein, quietly = T)
data(pc_profile)
tf <- unlist(pc_profile)
hours <- 1:168
par(mar = c(4, 4, .1, .1))
plot(y = tf, x = hours, pch = 16, type = "b")
```

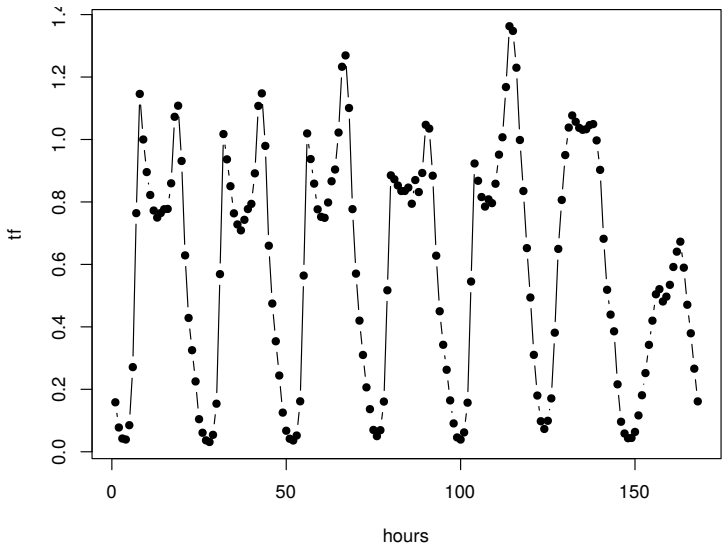

FIGURE 1.2: Temporal Factors for PC

1.4.4 Profile for cold starts of Passenger Cars

This is a profile with the hourly percentage of cold starts of Passenger Cars. This data covers 24 hours of a working day and it is based cold start recordings during the implementation of the International Vehicle Emissions (IVE) model (Davis et al., 2005) in São Paulo (Lents et al., 2004). The Fig. (1.3 shows the cold-start profile.

usage:

```
library(vein, quietly = T)
data(pc_cold)
cold <- unlist(pc_cold)
hours <- 1:24
par(mar = c(4, 4, .1, .1))
plot(y = cold, x = hours, pch = 16, type = "b")
```

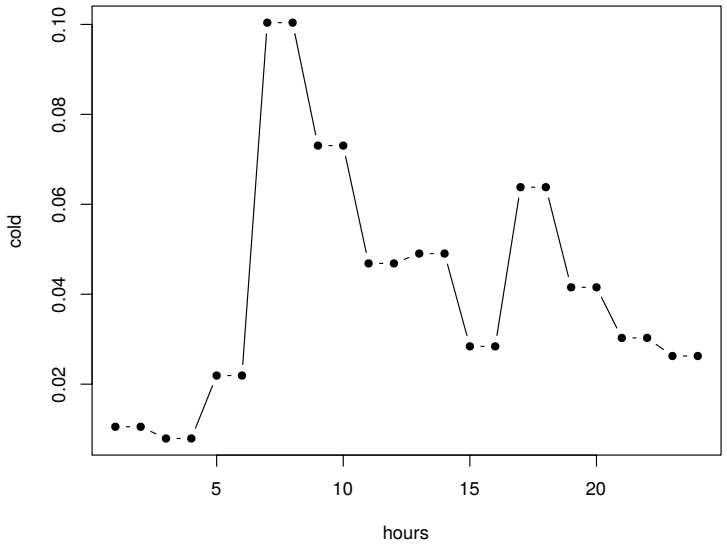

FIGURE 1.3: Cold-starts profile for PC

1.5 Acknowledgements

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2

Basics of R

2.1 Brief history

R is a programming language developed by Ross Ihaka and Robert Gentleman in 1993 (Ihaka and Gentleman, 1996). A good resource about R is the book "Programming for data science" (Peng, 2015). R can be explained as a free version of S-PLUS programming language (`http://www.solutionmetrics.com.au/products/splus/default.html`). It is free and recognized as GNU software (`https://www.gnu.org/software/software.html`) with GNU General Public License (GPLV2-GPLV3) license. This feature allowed that many developers started improving and adding code over the years.

R includes several statistical functions, therefore, users who just want to use the base capabilities of R are not forced to learn R-programming. However, the evolution from user to developer in R has been facilitated with numerous publications such as the book "R packages: organize, test, document, and share your code" (Wickham, 2015), or "The art of R programming: A tour of statistical software design" (Matloff, 2011).

2.1.1 Installation

R can be installed in different OS including Linux, Windows, Mac and Solaris. The webpage `https://cran.r-project.org/` shows how to install R in any platform. A popular Integrated development environment (IDE) is **RStudio** `https://www.rstudio.com/`, which contains many useful integrated options. However, R can be run on the terminal and any any text editor can be used to write scripts in R.

2.2 Using R

If we type at the R promt

```
x <- 1   # Not printing  results
x        # Print results
```

```
## [1] 1
```

```
print(x) # Explicit print x
```

```
## [1] 1
```

The integer 1 was *assigned* (<-) to x, then writing x or print(x) will show the value of x. Instead of numbers, other expressions such as strings, dates or other objects can be assigned. R includes several statistical functions. For instance, if we type 'pi' at the terminal, it will print the pi number.

```
pi
```

```
## [1] 3.141593
```

2.2.1 R objects

There are five basic classes (or atomic classes).

- character.
- numeric.
- integer.
- complex.
- logical (TRUE/FALSE or just T or F).

Objects of the same class can be grouped in **vectors**. Vectors are created with writing **c()** with the elements of the vector inside the parenthesis, separated by colon. In fact, **c** is a built-in function to create vectors. In this

case, the vector v1 contains a sequence of three integers, from 1 to 3. The resulting class is numeric.

```
v1 <- 1:3
v2 <- c(1, 2, 3)
identical(v1, v2)
```

```
## [1] FALSE
```

```
v1
```

```
## [1] 1 2 3
```

```
class(v1)
```

```
## [1] "integer"
```

With the operator `[` we can get specific elements of your vectors. In the following code the function `length` is used additionally, which simply returns the length of an object.

```
v1[1]          # first element of v1
```

```
## [1] 1
```

```
v1[length(v1)] # last element element of v1
```

```
## [1] 3
```

If we create a vector with numbers and letter, the resulting vector will be "character", automatically converting the numbers into characters.

```
v2 <- c(1:3,"a")
v2
```

```
## [1] "1" "2" "3" "a"
```

```
class(v2)
```

```
## [1] "character"
```

Objects can be converted to other classes with the as.* functions. For instance, if we convert the vector v2 to numeric, it will recognize the numbers adding an NA into the position of the character.

```
as.numeric(v2)
```

```
## Warning: NAs introduzidos por coerção
```

```
## [1]  1  2  3 NA
```

2.2.2 Factors

Factors represents categorical data. A typical example is a character vector of days of the week. The function `factor` creates factors. To see the help section, type `?factor`. The following example will use this function with the arguments `x` and `levels`.

```
dow <- factor(x = c("Wednesday", "Monday", "Thursday", "Friday"),
              levels =  c("Monday", "Tuesday", "Wednesday", "Thursday",
                          "Friday"))
dow
```

```
## [1] Wednesday Monday    Thursday  Friday
## Levels: Monday Tuesday Wednesday Thursday Friday
```

2.2.3 Missing Values

Missing values in data-sets are a typical source of headache for R users. Fortunatly, R counts with several tools to avoid these headaches. These tools are fhe functions `is.na` to check for NA (not available) and `is.nan` (not a number). This functions returns logical values.

```
n <- c(1, NA)
is.na(n)
```

```
## [1] FALSE  TRUE
```

```
n <- c(1, NaN)
is.na(n)
```

```
## [1] FALSE  TRUE
```

```
is.nan(n)
```

```
## [1] FALSE  TRUE
```

2.2.4 Matrices

Matrices are structure with rows and columns. They can be created using the `matrix` function and also, using vectors. Remember, if you want to know more about any function you just have to type **?** and the function (e.g. `?matrix`) and the help documentation for the function `matrix` will be opened.

Let's create a matrix using vectors:

```
a <- 1:12  #numeric vector
(m <- matrix(data = a, nrow = 3, ncol = 4))
```

```
##      [,1] [,2] [,3] [,4]
## [1,]    1    4    7   10
## [2,]    2    5    8   11
## [3,]    3    6    9   12
```

We can check the dimensions of our matrix `m` with `dim`, which are 3 and 4.

```
dim(m)
```

```
## [1] 3 4
```

In order to get the elements of matrix `m` we can use the `[` operator:

```
m[1, 1] # first element
```

```
## [1] 1
```

```
m[, 1]  # firs column
```

```
## [1] 1 2 3
```

```
m[1, ]  # firs row
```

```
## [1]  1  4  7 10
```

```
m[3,4]  # last element
```

```
## [1] 12
```

2.2.5 Arrays

Arrays are like matrices inside other matrices. In fact, a matrix is a 2-dimensional array. Let's create an array create an array using the same vector `a` and same dimensiones of `m`, 3 and 4. `array` has three arguments, `data`, `dim` and `dimnames`. In the argument `dim` let's add the number 2, resulting in an array of two matrices identical to `m`.

```
(a <- array(data = a, dim = c(3,4,2)))
```

```
## , , 1
##
##      [,1] [,2] [,3] [,4]
## [1,]    1    4    7   10
## [2,]    2    5    8   11
## [3,]    3    6    9   12
```

```
##
## , , 2
##
##      [,1] [,2] [,3] [,4]
## [1,]    1    4    7   10
## [2,]    2    5    8   11
## [3,]    3    6    9   12
```

We can subset elements from array also with the `[` operator.

```
a[1, 1, 1] # first element
```

```
## [1] 1
```

```
dim(a)     # dimensions
```

```
## [1] 3 4 2
```

```
a[3, 4, 2] # last element
```

```
## [1] 12
```

2.2.6 Lists

List are objects that can contain elements of different classes. I like to call lists as bags. In a bag you can put almost anything. Also, inside the bag, you can put other bags with different things. This means that you can have a list of lists of any R object. Lists can be created with the `list` function. Let's create an empty list. Then we will use the vecctor `a` to create another list.

```
a <- 1:3          # vector of three elements
l1 <- list()      # empty list
l1 <- list(a)     # vector of three elements
length(l1)        # length 1
```

```
## [1] 1
```

```
l1 <- as.list(a)  # vector a as list
length(l1)        # three elements
```

```
## [1] 3
```

As mentioned, the list can have lists inside.

```
l1 <- list(list(a),                    # three numeric elements
           list(TRUE, TRUE, FALSE))    # three logical elements
length(l1)                             # length 2
```

```
## [1] 2
```

2.2.7 Data-Frames

"Data-frames are used to store tabular data in R" (Peng, 2015). You can think of data-frames as spreadsheet-like objects. They are similar to matrices and you can have a matrix and a data-frame with the same dimensions. Basically, you have rows and columns, columns can have different classes, and the columns usually have a one-word name.

As this type of object is very used by scientists, there are R packages created to work with this type of ojects. Below some of them:

- `data.frame`: This is not a package. It is a class and function from the `base` library in R. With this function you can create data-frames.
- `data-table` (Dowle and Srinivasan, 2017): `data.tables` objects has the class `data.table` which inherits from the class `data-frame`, which means that they share common characteristics. However, the big difference with `data-table` is the efficiency with memory. It includes functions such as `fread` for reading millions of observations in seconds.
- `tidyr`(Wickham and Henry, 2018): Sometimes your data is in long format and you need it in wide format, and viceversa. This package does the job.
- `readxl` (Wickham and Bryan, 2017): Good package for importing Excel and LibreOffice files. I recommend this packages for newbies.

- `sf` (Pebesma, 2017): This package presents the class `sf` and introduces the list-column of spatial geometry.

Let's create a data-frame.

```
a <- 1:3
b <- 3:5
(ab <- data.frame(a, b))
```

```
##   a b
## 1 1 3
## 2 2 4
## 3 3 5
```

```
class(ab)
```

```
## [1] "data.frame"
```

2.2.8 Names

In R you can put names in almost everything. Below examples for `vectors`, `matrix` and `data.frames`.

```
names(ab)                # original names
```

```
## [1] "a" "b"
```

```
names(ab) <- c("c", "d")
names(ab)                # new names
```

```
## [1] "c" "d"
```

2.3 Inputting data into R

Your data can be in different formats. In this section I will show you how you can input text and comma separated value files, which is a very common task. Let's say that you are using a spreadsheet program such as Microsoft Excel or LibreOffice. Then you might want to import your data into R.

- Your first check is, if the first row of your data has a name or not. If they do have names, this means that they have a header.
- Then click on 'Save as' and search text file with extension .txt or .csv.
- Then you edit your file with a notepad (e.g. bloc, gedit, vi or other tool) to check if the decimal character is point '.' and the separator character is comma ',' or semicolon ';' or another character. This depends on the regional configuration of your spreadsheet software.
- If your file has the extension '.txt', use `read.table` and if it is '.csv', use `read.csv`.

Once you checked the format, you can import your '.txt' or '.csv' files in R:

```
a <- read.csv("path/to/file.csv", sep = ",", header = T)
a <- read.tablesv("path/to/file.txt", sep = ",", header = T)
```

3

Structuring an Emissions Inventory

The elaboration of vehicular emissions inventories in vein, consists of four stages:

1. pre-processing activity data,
2. preparing emissions factors,
3. estimating the emissions and
4. post-processing of emissions in maps and databases.

This means that vein provides functions to be used in each of the stages. However, in order to follow these stages, a structure of directories with scripts including vein functions is necessary. Therefore, the vein function `inventory` was created to create this structure of directories.

3.1 Overview of emissions inventorying using VEIN

3.2 The `inventory` function

The inventory function creates creates a structure of directories and scripts to run vein. This structure is a suggestion and the user can use any other. The following code shows the arguments of the function. This is done using the base function `args` with `inventory`.

```
args(inventory)
```

```
## function (name, vehcomp = c(PC = 1, LCV = 1, HGV = 1, BUS = 1,
```

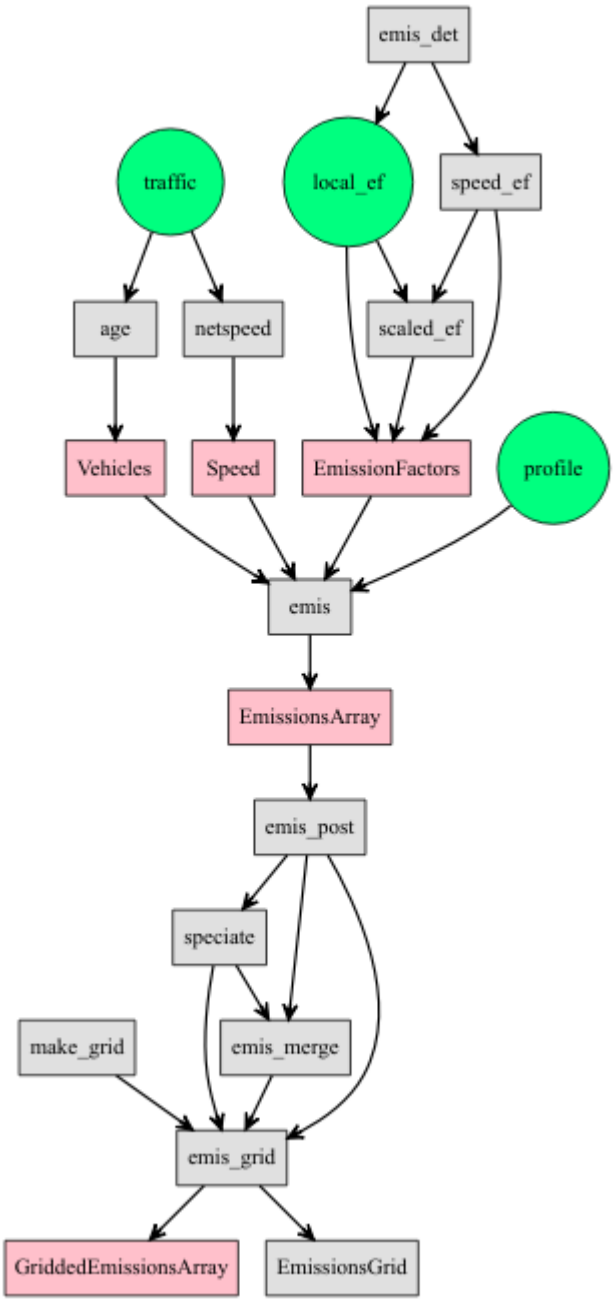


FIGURE 3.1: Structuring an emissions inventories with VEIN

```
##     MC = 1), scripts = TRUE, show.dir = TRUE, show.scripts = FALSE,
##     clear = TRUE, rush.hour = FALSE)
## NULL
```

The arguments are `name`, `vehcomp`, `scripts`, `show.dir`, `show.scripts` and `clear`.

- The argument `name`

The argument name is a word to be used as main directory where directories and scripts are stored in. It consists in *one* word with ascii characters. It is also recommended to be used without any special character or accents, for instance:

```
name = file.path(tempdir(), "YourCity")
inventory(name = name, show.dir = TRUE, show.scripts = TRUE)
```

- The argument `vehcomp` This argument is very important and comes from *Vehicular Composition*, which is the classification of the fleet by type of use, type of fuel, size of engine and gross weight, based on definitions of Corvalán et al. (2002). There is also the *technological composition* of the fleet which relates the technological modifications of the car in order to accomplish the emissions standards. However, vein uses a distribution by age of use as 4 shows.

The vehicular composition `vehcomp` has 5 types of vehicles:

1. Passenger Carss (PC).
2. Light Commercial Vehicles (LCV).
3. Heavy Good Vehicles or trucks (HGV).
4. Buses (BUS).
5. Motorcycles (MC).

The default value of this argument is: `c(PC = 1, LCV = 1, HGV = 1, BUS = 1, MC = 1)`, which means that there are 1 types of PC, 1 of LCV, 1 of trucks, 1 of buses and 1 types of motorcycles. This vehicular composition is only for ilutrasting that the user can change these values according to its own data. Appendix B shows the vehicular composition from the vehicular emissions inventory of the Environmental Agency of São Paulo,

Brazil (CETESB, 2015). In Brazil, the fuel used in vehicles is blended with ethanol with and biodiesel. The user can use **any** vehicular composition that representes its fleet with up-to 99 types of vehicles per category. For instance, if there are 4 types of PC in a fleet, `PC = 4`, and each one has aa age of use distribution.

- The argument `show.dir`

This is a logical argument to decide if the output of the function will return print the new directories or not. The use is:

```
name = file.path(tempdir(), "YourCity")
inventory(name = name, show.dir = TRUE, show.scripts = FALSE)
```

```
## files at /tmp/RtmpJQp9lK/YourCity

## Directories:
##  [1] "/tmp/RtmpJQp9lK/YourCity"
##  [2] "/tmp/RtmpJQp9lK/YourCity/ef"
##  [3] "/tmp/RtmpJQp9lK/YourCity/emi"
##  [4] "/tmp/RtmpJQp9lK/YourCity/emi/BUS_01"
##  [5] "/tmp/RtmpJQp9lK/YourCity/emi/HGV_01"
##  [6] "/tmp/RtmpJQp9lK/YourCity/emi/LCV_01"
##  [7] "/tmp/RtmpJQp9lK/YourCity/emi/MC_01"
##  [8] "/tmp/RtmpJQp9lK/YourCity/emi/PC_01"
##  [9] "/tmp/RtmpJQp9lK/YourCity/est"
## [10] "/tmp/RtmpJQp9lK/YourCity/images"
## [11] "/tmp/RtmpJQp9lK/YourCity/network"
## [12] "/tmp/RtmpJQp9lK/YourCity/post"
## [13] "/tmp/RtmpJQp9lK/YourCity/post/df"
## [14] "/tmp/RtmpJQp9lK/YourCity/post/grids"
## [15] "/tmp/RtmpJQp9lK/YourCity/post/streets"
## [16] "/tmp/RtmpJQp9lK/YourCity/profiles"
## [17] "/tmp/RtmpJQp9lK/YourCity/veh"
```

`inventory` creates the direcrory "YourCity" and the sub directories: daily, ef, emi, est, images, network and veh.

- **daily**: Directory for storing the profiles saved as .csv files. For instance, `data(pc_profile)` is a matrix that could be saved as .csv.
- **ef**: Directory for storing the emission factors data-frame, similar to `data(fe2015)` but including one column for each of the categories of the vehicular composition. For instance, if PC = 5, there should be 5 columns with emission factors in this file. If LCV = 5, another 5 columns should be present, and so on.
- **emi**: Directory with subdirectories matching the vehicular composition for saving the estimates. It is suggested to use .rds extension instead of .rda.
- **est**: Directory with subdirectories matching the vehicular composition for storing the scripts named `input.R`.
- **images**: Directory for saving images.
- **network**: Directory for saving the road network with the required attributes. This file will include the vehicular flow per street to be used by functions `age_ldv`, `age_hdv`, `age_moto` or `my_ldv`.
- **post**: Directory for storing the processed emissions. It includes the directories **df** for emissions by age of use, hour and other parameters, **streets** for storing the total emissions by streets and **grids** for storing total gridded emissions by pollutant.
- **veh**: Directory for storing the distribution by age of use of each category of the vehicular composition. Those are data-frames with number of columns with the age distribution and the number of rows as the number of streets. The class of these objects is "Vehicles".
- The argument `scripts`

This argument adds scripts into the directories. The default is TRUE. The type of scrits create are:

- main.R: Adds the `setwd("YourCity")`, `library(vein)`, `source(traffic.R)`, some comments and a loop to source all inputs. It is recommended not using the loop till it is certain that all scripts are correct.
- traffic.R: Includes two lines with exampmles of how to use the `age_ldv` function and saving the output in the directory veh.

- input.R: Each file has the scripts for reading the network, vehicles, emission factors and estimating emissions.
- The argument `show.scripts`

This argument prints the scripts created:

```
name = file.path(tempdir(), "YourCity")
inventory(name = name, show.dir = FALSE, show.scripts = TRUE)
```

```
## files at /tmp/RtmpJQp9lK/YourCity

## Scripts:
## [1] "est/BUS_01_input.R" "est/HGV_01_input.R" "est/LCV_01_input.R"
## [4] "est/MC_01_input.R"  "est/PC_01_input.R"  "main.R"
## [7] "post.R"             "traffic.R"
```

- The argument `clear`

This is a logical argument that deletes recursively when TRUE, or not when FALSE, the directory and creates another one. Default is TRUE.

The following chapters show the use of other vein functions inside an structure of directories and scripts with the name `inventory("YourCity")`.

4

Traffic data

Traffic data is read in VEIN as spatial information. In other words, traffic data must be in any vectorial line spatial format with the drivers provided by the library **GDAL** (`http://www.gdal.org/ogr_formats.html`), which is called by the packages **rgdal** or **sf**. This means that traffic data must be in in any GDAL spatial format. The Eq. (4.1) shows how traffic data is treated in VEIN.

$$F^*_{i,j,k} = Q_i \cdot VC_{i,j} \cdot Age_{j,k} \tag{4.1}$$

where $F^*_{i,j,k}$ is the vehicular flow at street link i for vehicle type j by age of use k. j defines the vehicular composition according to its type of use, type of fuel, size of engine and gross weight, based on definitions of (Corvalán et al., 2002). Q_i is the traffic flow at street link i. $VC_{i,j}$ is the fraction of vehicles varying according to the type of vehicles j in the vehicle fleet at street link i. $Age_{j,k}$ is the age distribution by vehicular composition j and age of use k.

This Equation shows that VC splits the total vehicular flow Q to identify the vehicular fraction, which varies according to the type of fuel, size of motor and gross weight. For example, if Q is light duty vehicles (LDV) and it is known that 5% of the Q are passenger cars (PC), with engines lesser than 1400 cc, VC is 0.05. This characterization of the fleet depends on the amount and quality of the available information. VEIN then multiplies the traffic with Age to obtain the amount of each type of vehicle by age of use.

4.1 Sources of traffic data

4.1.1 Travel demand outputs

VEIN was developepd according to the available traffic data in São Pauo, Brazil. In this case, the available data was a 4-stage macroscopic travel model for morning rush hours and hourly traffic counts for morning and evening rush hours. The travel model is based on data from an Origin-Destination-Survey (ODS) (Metro, 2017) which started in the decade of 1950 in São Paulo. A classic reference of a 4-stage modeling transport is (Ortuzar and Willumsen, 2002). The 4 stages of the traffic modeling include characterization of trip attractions and productions by zone in some regions, distribution of these trips, the preferred mode of transport for traveling and finally the allocation of the trips at each mode; in this case into the road network. The ODS is made every 10 years by Metro (`http://www.metro.sp.gov.br/`), which is the underground company, and they perform a smaller update of ODS after 5 years. The information gathered in the ODS is massive due to participation of thousands of commuters. It helps to identify characteristics of the trips inside MASP. CET uses the information from ODS and performs the traffic simulation. In this case, it is a macro or strategic traffic simulation which represents the equilibrium between offer and supply of transportation at maximum load of the road network, that is, at the rush hour, which is from 08:00 to 09:00 Local Time (LT).

VEIN incorporates an extract of a traffic model simulation for the west part of São Paulo named *net*. The Fig. (4.1 shows the traffic of Light Duty Vehicles (LDV). This data covers the surrounding area of the University of São Paulo. The information obtained from CET consists in:

- *ldv*: Light Duty Vehicles (1/h).
- *hdv*: Heavy Duty Vehicles (1/h).
- *lkm*: Length of the link (km).
- *ps*: Peak Speed (km/h).
- *ffs*: Free Flow Speed (km/h).
- *tstreet*: Type of street.

- *lanes*: Number of lanes per link.
- *capacity*: Capacity of vehicles in each link (1/h).
- *tmin*: Time for travelling each link (min).

The following scripts show how to load this data in R. This data has the class "SpatialLinesDataFrame" from the package (Pebesma and Bivand, 2005). This data was converted into an spatial feature "sf" object (Pebesma, 2017) because it consists of a data-frame with a list-column of geometry with the spatial attributes and it is easier to handle than an sp object class. As mentioned, future versions of VEIN will migrate to sf.

The user must call the library VEIN first, then load the data net. The object net has the class "SpatialLinesDataFrame". This data can be loaded and shown in R like this:

```
library(vein)
library(sp)
data(net)
class(net)
```

```
## [1] "SpatialLinesDataFrame"
## attr(,"package")
## [1] "sp"
```

The Fig. (4.1) shows that traffic is concentrated in main streets such as the motorway Marginal Pinheiros, located in the north east part of the area.

```
library(vein)
data(net)
net$ldv <- as.numeric(net$ldv)
spplot(net, "ldv", scales = list(draw = T),
       col.regions = rev(bpy.colors(16)))
```

4.1.2 Inteprolation of traffic counts

Travel model simulations are not always available and the user interested in estimating vehicular emisisons with a bottom-up approach would have

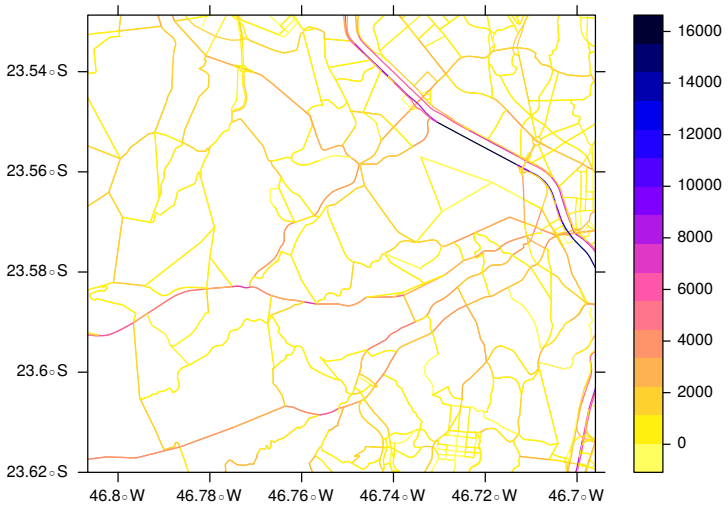


FIGURE 4.1: LDV at 08:00-09:00 (LT) in west São Paulo

to look for alternatives to obtain traffic data at street level. These alternatives cover interpolating traffic data for different temporal resolutions. For instance, Réquia Jr et al. (2015) developed a vehicular bottom-up inventory using traffic counts and a geostatistic method called Global Moran's I test (Anselin, 1995). It measures the spatial autocorrelation. However, this technique requires that the observed values are normal, which is not the case for count data.

Other authors were instested in predicting Anual Average Daily Traffic (AADT) or only ADT. Lowry (2014) presented a new method for predicting AADT based on the concept of origin-destination centrality. The idea is to obtain predictor variables directly from the road network. He identified origin and destination zones and added multiplication factors based on the land-use characteristics.

Zhao and Chung (2001) tested several multiple stepwise regressions incorporating land-use characteristics. They considered several variables: number of lanes, classificatiion of road type, employment numbers and access to expressway with correlations between 0.66 and 0.82. Lam and Xu (2000) compared neural networks and regressions for a dataset of 13 locations. Kriging methods were used in AADT interpolation by Eom et al. (2006), who predicted AADT for non-motorway streets. Also, Selby

and Kockelman (2013) compared Kriging and geographically weighted regressions in the prediction of AADT.

Another approach is to perform a spatial regression based on the distributio on the observed data. As the data is counts of traffic, a poisson, quasi-poisson or negative binomial regressions can be used (Zeileis et al., 2008). Recently, Ibarra-Espinosa et al. (2017a) compared quasi-poisson and negative binomial regresions predicting hourly traffic data, with better results for a quasi-poisson approach (correlation of 0.72).

Newer approaches involve GPS data from smartphones and cars.

4.1.3 Generating traffic flows from Origin-Destination-Surveys (ODS)

The origin destination survey (ODS) is an important tool which quantifies the amount of trips generated in the study area. ODS studies started decades ago. The oldest ODS paper on Google Scholar is entitles "FUNCTIONS OF A HIGHWAY-PLANNING SURVEY DEPARTMENT" by W. J. Sapp in 1938 at the TWENTY-FOURTH ANNUAL ROAD SCHOOL (Sapp, 1938). In this paper the importance of information for the traffic engineer is discussed: "The engineer must have the supporting data available to substantiate his decisions."

Another study of 1942 shows the importance of traffic counts, disucssing the elaboration of an origin destination survey where 8000 Boy Scouts of America participated in counting traffic. The method for analyzing the data consisted in counting the vehicles identifying the licence plate in order to determine the origin (the first time the vehicle was recorded), the route of vehicles, the destination and the approximate time for the trip.

After those pioneer studies many many other studies went deeper into the subject. And after that, with the irruption of new technologies, new software, use of smarthphones with GPS, satellites and big technological centers owned by companies such as Google (`http://www.google.com`), new ways for characterizing trips were developed. In this section i will briefly mention the Google Distance Matrix (`https://developers.google.com/maps/documentation/distance-matrix/`), the pgRouting library (Patrushev, 2007) for postGIS and will expand with two R packages, googleway (Cooley, 2018) and dodgr (Padgham and Peutschnig, 2018).

TABLE 4.1: Matrix OD for motorized indivitual trips between 06:30 and 08:30 MASP 2007

	V101	V102	V103	V104	V105	V106	V107	V108	V109	V110
101	42	0	0	83	0	84	42	0	0	318
102	49	0	10	0	0	20	0	10	0	0
103	0	10	0	19	0	81	17	0	0	54
104	0	35	86	40	0	170	40	35	35	0
105	0	0	0	13	0	0	0	0	0	0
106	94	0	72	87	24	196	15	0	0	27
107	0	0	13	64	13	28	44	0	0	0
108	0	0	0	0	0	0	0	3525	885	0
109	0	0	0	0	0	206	0	3916	975	0
110	954	0	18	954	0	0	0	652	939	2928

The ODS will provide us the matrix of pairs of zones origin and destinations by mode of transport. Then, we can use any of the mentioned softwares to find the shortest path between each zone. The table 4.1 shows an extraction of the OD matrix for the Metropolitan Area of São Paulo (MASP) in 2007 for motorized individual trips. The fig @ref(fig.zod) shows a map with the location of the zones OD.

Now, as we know the the trips between each pair of OD zones, we can find the routes that connects them. Algorithms are used to find the shortest path. It connects two nodes minimizing the total travel time. There are several algorithms, including Dijkstra (1959).

4.1.3.1 Google Distance Matrix API

This service allows to "retrieve duration and distance values based on the recommended route between start and end points." It returns durations and distance and it is possible to choose modes of transport as well as to choose between current or historical times. The first step is to get a KEY.

If you browse

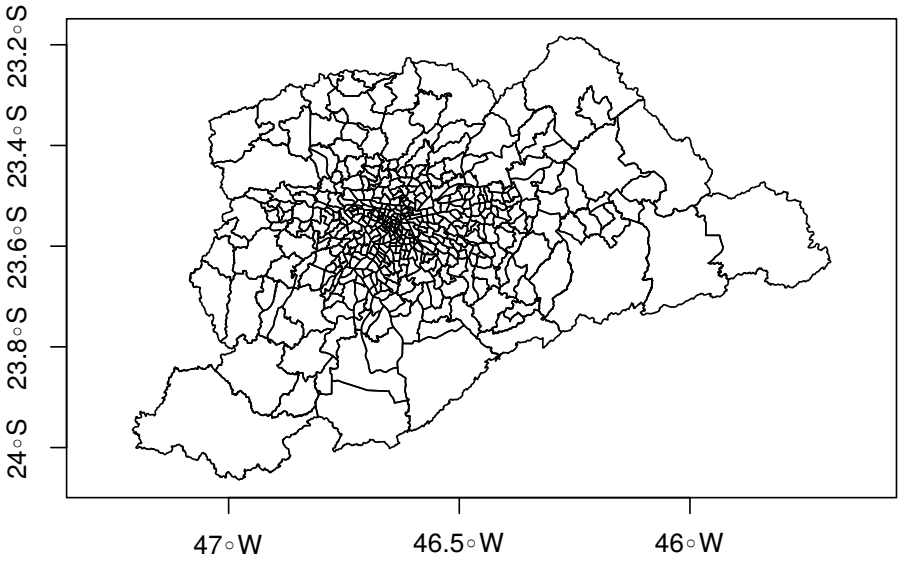


FIGURE 4.2: Zones OD for MASP 2007

```
https://maps.googleapis.com/maps/api/distancematrix/json?units=imperial&origins=Washington,DC&
```

and replace YOUR_API_KEY you will see (my brower is in portuguese):

```
{
  "destination_addresses" : [ "Nova York, NY, EUA" ],
  "origin_addresses" : [ "Washington, D.C., Distrito de Columbia, EUA" ],
  "rows" : [
    {
      "elements" : [
        {
          "distance" : {
            "text" : "225 mi",
            "value" : 361972
          },
          "duration" : {
            "text" : "3 horas 53 minutos",
            "value" : 13964
```

```
          },
          "status" : "OK"
        }
        ]
    }
    ],
  "status" : "OK"
}
```

The modes of transport covered are **driving** using the road network, **walking** via pedestrian paths & sidewalks, **bicycling** via bicycle paths and **transit** via public transit routes. For more information read the documentation.

4.1.3.2 pgRouting for postGIS

pgRouting (`http://pgrouting.org/`) is an open source routing library for postGIS. It provides many routing algorithms and it can be run via QGIS (`https://www.qgis.org`). This library is very extensive. A good resource is the book "pgRouting: A Practical Guide" (`http://locatepress.com/pgrouting`).

4.1.3.3 The R package googleway

googleway (Cooley, 2018) R package allows to access Goolge Maps API `https://developers.google.com/maps/`. The API functions are:

- Directions - `google_directions()`
- Distance Matrix - `google_distance()`
- Elevation - `google_elevation()`
- Geocoding - `google_geocode()`
- Reverse Geocoding - `google_reverse_geocode()`
- Places - `google_places()`
- Place Details - `google_place_details()`
- Time zone - `google_timezone()`
- Roads - `google_snapToRoads()` and `google_nearestRoads()`

This package allows to plot over Google Maps.

```
library(googleway)
## not specifying the api will add the key as your 'default'
key <- "my_api_key"
set_key(key = key)
google_keys()
```

```
## Google API keys
##  -  default : my_api_key
##  -  map :
##  -  directions :
##  -  distance :
##  -  elevation :
##  -  geocode :
##  -  places :
##  -  find_place :
##  -  place_autocomplete :
##  -  place_details :
##  -  reverse_geocode :
##  -  roads :
##  -  streetview :
##  -  timezone :
```

From zone Luz 7, coordinates long -46.63461 and lat -23.53137 to zone 8 Bom Retiro coordinates -46.64482 -23.52204 there are 133 LDV trips between 6:30 and 08:30. We first create the data-frame. This data is based on OD from São Paulo.

```
mydf <- data.frame(region = 1,
                   from_lat = -23.53137,
                   from_long = -46.634613,
                   to_lat = -23.52204,
                   to_long = -46.64482)
```

Then we use the package `googleway` to create the points between origin and destination and maptools to transform points to lines.

```
library(maptools, quietly = T)
library(googleway)
foo <- google_directions(origin = unlist(mydf[1, 2:3]),
                         destination = unlist(mydf[1, 4:5]),
                         key = mykey,
                         mode = "driving",
                         simplify = TRUE)
pl <- decode_pl(foo$routes$overview_polyline$points)
df <- sf::st_as_sf(pl, coords = c("lon", "lat"), crs = 4326)
streets <- list(x = pl$lon, y = pl$lat)
streets <- map2SpatialLines(streets)
plot(streets, axes = T, main= "Route of 133 LDV trips")
```

```
knitr::include_graphics(path = "figuras/gway.png")
```

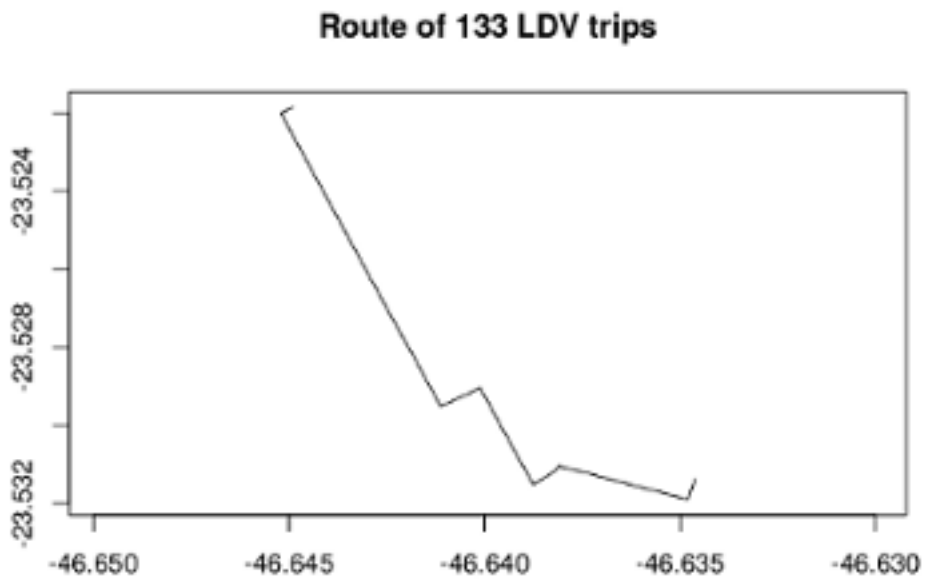


FIGURE 4.3: Driving route between zones 'Luz' and 'Bom Retiro' in São Paulo

4.1.3.4 The R package dodgr

dpdgr(Padgham and Peutschnig, 2018) is a new R package with great capbilities. It calculates the distance on dual-weight graphs using priority-queue shortest paths. In order to calculate the traffic flows it is necessary to have the matrix OD for the desired mode of transport and the coorodinates of centroids of the OD zones.

The function `dodgr_streetnet` uses the osmdata r package to download street network data from Open Street Map (contributors, 2017) for the points of the centroids of zones OD. Depending on the spatial extent of the data, the resulting data can be large. The function `weight_streetnet` weight the lines from OSM road network according to a specific profile of traffic: "psv" for Public Service Vehicle. "bicycle", nd others. The weights are profile values for the OSM type of roads based on this webpage: `https://www.routino.org/xml/routino-profiles.xml`. The function `dodgr_vertices` extract the vertices pf thegraph including the coordinates. Finally, the function `dodgr_flowmap` reads the graph and plots the flows. Below is an example for São Paulo using the data of ODS (Metro, 2017).

4.1.4 Top-down approach

VEIN was designed with traffic flow at street leve on mind, however, it is possible that user might want or need to use a top-down approach. Here are some possible causes:

1. Bottom-up approach can demand more computatonal resources for a country or a continent.
2. Another possibility is that the emissions inventory is going to be used solely for air quality modelling purposes, where the proportion of grid spacing and street is such that spatial detail would be lose, for instance with resolution of 10 km.
3. Also, it is possible that there is no way of obtaining traffic information at street level.
4. Limited resources, time, funding, human resources, etc.
5. Lastly, due to simplism. It is also possible that the objective sim-

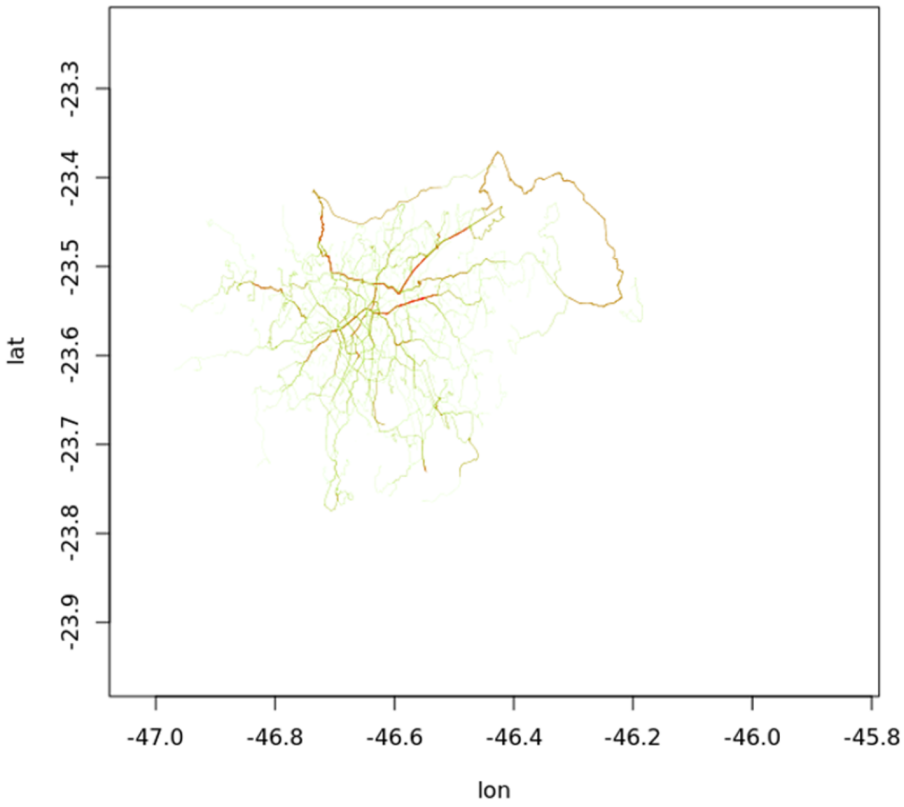


FIGURE 4.4: Daily trips of Light Duty Vehicles in São Paulo

ply is to estimate an emissions inventory using a top-down approach.

Under these circumstances a top-down approach would be better suited for some users. As VEIN is a toolkit for estimating emissions, it is reasonable to use all VEIN resources with a top-down approach.

In this case, the user must follow some considerations:

- Use `inventory` functions in the same way as shown on section 3.
- Create a network, but instead of using a road network with spatial lines, use spatial polygons. The Spatial polygon might represent some area where the amount of vehicles is known.

- The age functions shown in following sections, show that it is possible to apply age distributions to each street, in this case, to each area.

The Fig. 4.5 shows the emissions of PM for each state Brazil and prepared for a congress using VEIN as a top-down tool (Ibarra-Espinosa et al., 2018a).

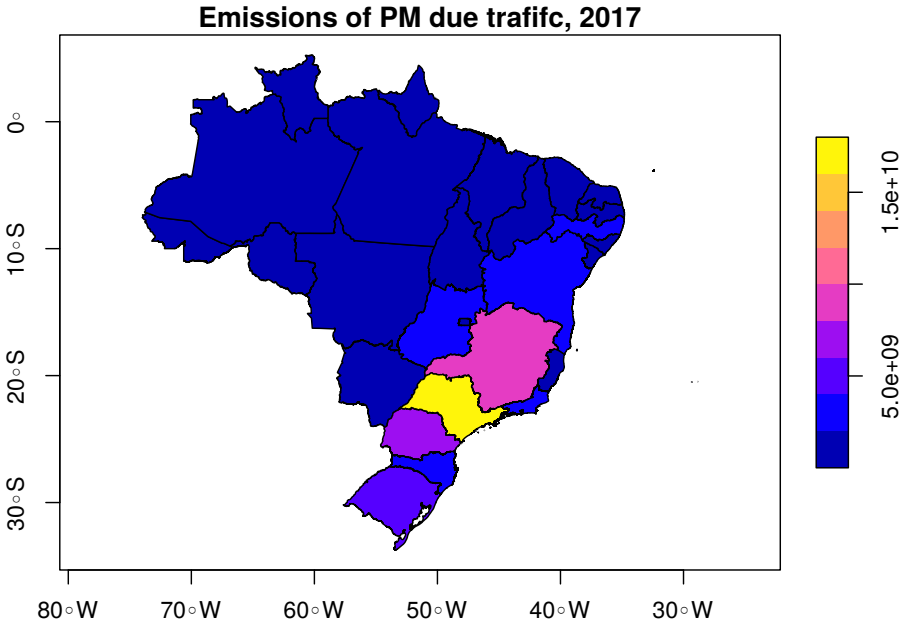


FIGURE 4.5: Emissions of PM due trafifc, 2017

4.2 Main functions

The Fig.(3.1) shows a complete diagram with the steps for elaborating an emissions inventory. Also, the function `inventory` shown on sub-section (3.1) shows the functions to structure an inventory. This and the following subsection of application shows respective the part of the diagram Fig.(4.6) and how to run VEIN as well as storing the results in the directories shown in Fig. (3).

The first element that the user must have is the traffic at street level. This is

shown as a green circle with the word 'traffic' on Fig. (4.6). The user must use any `age` function which produces objects of class `Vehicles`. The function `netspeed` produces an object of class `Speed`. This objects are required by the `emis` function.

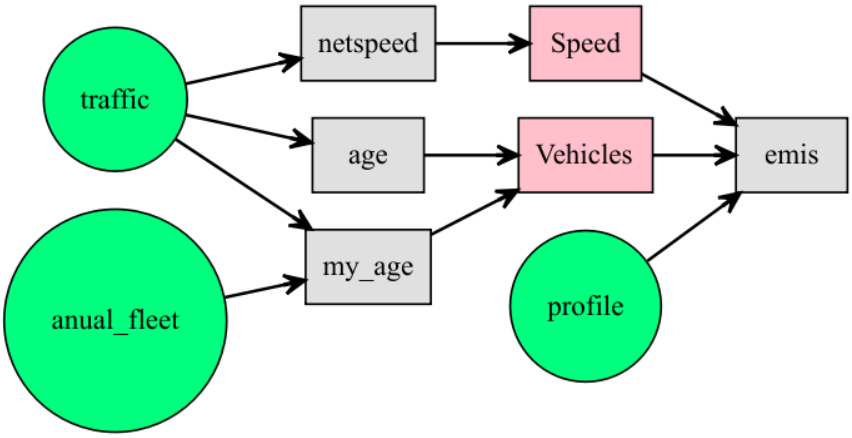


FIGURE 4.6: Structuring an emissions inventories with VEIN

4.2.1 Expanding traffic data with the function `temp_fact`

Traffic data must be temporally extrapolated because it is usually available only for the morning rush hour. Traffic data can be estimated from short period traffic count datasets, then expanded to represent longer timespan, such as Annual Average Daily Traffic (AADT; (Wang and Kockelman, 2009, lam2000estimation)). The next step is to extrapolate the vehicular flow at street link i, vehicle type j, and age of use k, to obtain the vehicular flow for hour of the week l ($F_{i,j,k,l}$; see equation (4.2).

$$F_{i,j,k,l} = F^*_{i,j,k} \cdot TF_{j,l} \tag{4.2}$$

where $TF_{j,l}$ are the temporal factors varying according to each hour of l and type of vehicle j. For instance, TF is defined as a matrix with 24 lines and numbers of columns to each day considered, from Monday to Sunday. In order to expand traffic to other hours, TF matrices must be

normalized to the hour that represents the traffic data. It means that TF values at morning peak hour must be 1 and the respective proportion must be assigned to the other hours. For example, TF values can be obtained from automatic traffic count stations.

The function `temp_fact` return $F_{i,j,k,l}$ as an object with class `Vehicles`. The arguments are:

- `q` is a data-frame of traffic flow to each hour (veh/h) at each street.
- `pro` s a matrix or data-frame to extrapolate .

4.2.2 Calculating speed at other hours with the function `netspeed`

The average speed of traffic flow is very important and it must be determined for each link and hour. Once the vehicular flow is identified for each hour, the average speed is then identified for each hour. This was accomplished by employing curves from the Bureau of Public Roads (BPR; (Bureau of Public Roads, 1964)), as shown in Eq. (4.3). The process involves calculating speed by dividing the length of road by the time. The time is calculated using the total traffic expanded to each street link i and hour l.

$$T_{i,l} = To_i \cdot \left(1 + \alpha \cdot \left(\frac{Q_{i,l}}{C_i}\right)^{\beta}\right) \tag{4.3}$$

The function `netspeed` do this calculations. The arguments of this function are:

```
args(netspeed)
```

```
## function (q = 1, ps, ffs, cap, lkm, alpha = 0.15, beta = 4, net,
##     scheme = FALSE, distance = "km", time = "h", isList)
## NULL
```

`netspeed` allows basically creates two types of speeds data-frames which depends on the availability of data by the user. If the user has `q`, `ps`, `ffs` and `cap` the user can use the argument `scheme = FALSE`, or when the user only has `ps` and `ffs` the user can use the argument `scheme = TRUE`.

- `q` is a data-frame of traffic flow to each hour (veh/h) at each street.

TABLE 4.2: speeds for scheme = T

Period	Speed
00:00-06:00	ffs (Free flow speed)
06:00-07:00	average between ffs and ps
07:00-10:00	ps (Peakspeed)
10:00-17:00	average between ffs and ps
17:00-20:00	ps (Peak speed)
20:00-22:00	average between ffs and ps
22:00-00:00	ffs (Free flow speed)

- `ps`is the Peak speed (km/h) at each street.
- `ffs` Free flow speed (km/h) at each street.
- `cap` Capacity of link (veh/h) at each street.
- `lkm` Distance of link (km) of each street.
- `alpha` Parameter of Bureau of Public Roads (1964) curves.
- `beta` Parameter of Bureau of Public Roads (1964) curves.
- `scheme` Logical to create a Speed data-frame with 24 hours and a default profile. It needs `ffs` and `ps` at each street:

4.2.3 Distribution of vehicles by age of use with the functions `age_ldv`, `age_hdv` and `age_moto`

These functions reads traffic data at each street and return an object of class `Vehicles`, which is a data-frame with the number of vehicles at each street and the number of columns represent the amount of vehicles at each age. The functions `age_moto` and `age_hdv` are identical. These functions apply survival equations into the fleet from Ministerio do Meio Ambiente (2011). The arguments are:

- `x`numerical vector of vehicles at each street.
- `name` word of vehicle assigned to columns of dataframe.
- `a` parameter of survival equation. The default value for `age_ldv` is 1.698 and for `age_hdv` and `age_moto` is 0.2.
- `b` parameter of survival equation. The default value for `age_ldv` is -0.2 and for `age_hdv` and `age_moto` is 17.

- `agemin` age of newest vehicles for that category. The default value is 1, however it can be bigger than one when it is a vehicle that is not circulating more then a year ago.
- `agemax` age of oldest vehicles for that category. The default value is 50 assuming that the oldest vehicle in circulation has 50 years of use. However, new type of vehicles will be newer.
- `k` multiplication factor. This factor helps to split the traffic `x` in the vehicular composition.
- `bystreet` when TRUE it is expecting that `a` and `b` are numeric vectors with length equal to `x`. In other words, the values of `a` and `b` varies in each street.
- `message` message with average age and total number of vehicles.

4.2.4 The function `my_age`

These functions also reads traffic data at each street and returns an object of class `Vehicles`, which is a data-frame with the number of vehicles at each street and the columns represent the amount of vehicles at each age. However, it is based on data the user has and not by parameters. Therefore, using this function with own data should produce more representative results. The arguments are:

```
args(my_age)
```

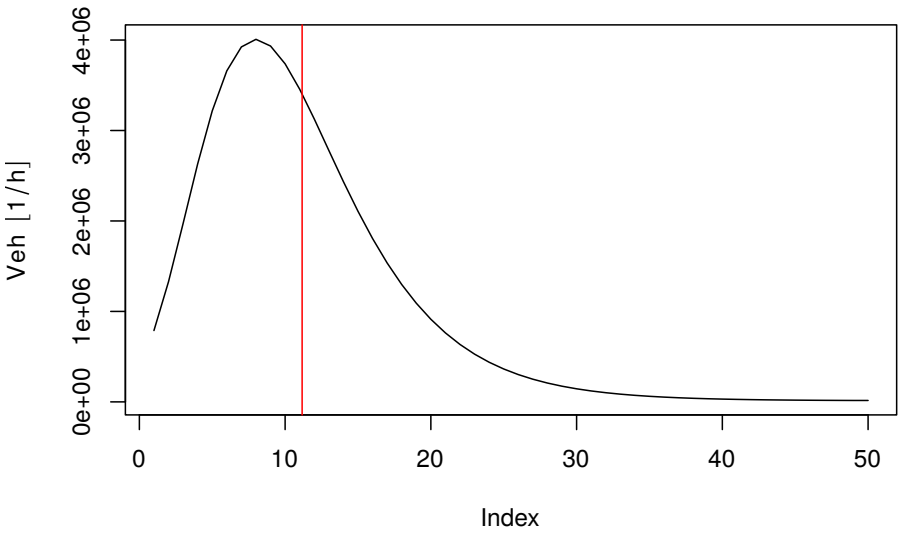
```
## function (x, y, name = "age", k = 1, pro_street, net, message = TRUE)
## NULL
```

- `x` numerical vector of vehicles at each street.
- `y` Age distribution of vehicles. This parameter can be annual sales or annual registry for the category of vehicle.
- `name` of vehicle assigned to columns of dataframe.
- `k` multiplication factor. This factor helps to split the traffic `x` in the vehicular composition.
- `message` message with average age and total number of vehicles.

4.2.5 The class `Vehicles`

`Vehicles` is a class in VEIN, shown in on Fig. (4.6). This class includes the methods `print`, `plot` and `summary`. This means that, `Vehicles` objects presents customized versions of `print`, `plot` and `summary` in order to make easier to the user to use VEIN. The figure @ref(fig.plotpc) shows a simple plot of a `Vehicles` object, followed by the `head` of this object. The plot shows the sum of each type of vehicle by age of use, with a vertical red line indicating the average age, 11.17 years of use.

```
library(vein)
data(net)
PC_E25 <- age_ldv(x = net$ldv,name = "PC_E25", k = 75/100*37.25, message = F)
plot(PC_E25)
```




```
##
## Average =  11.17
```

```
head(PC_E25[, 1:4]) # The first 4 columns
```

```
## Result for Vehicles
##                  V1               V2               V3               V4
## 1 1761.92888 [1/h] 2968.78285 [1/h] 4404.60761 [1/h] 5877.97812 [1/h]
```

```
## 2  591.76508 [1/h]  997.10155 [1/h] 1479.34063 [1/h] 1974.18989 [1/h]
## 3  240.18939 [1/h]  404.70994 [1/h]  600.44421 [1/h]  801.29679 [1/h]
## 4  341.44967 [1/h]  575.32964 [1/h]  853.58258 [1/h] 1139.11162 [1/h]
## 5   22.27726 [1/h]   37.53633 [1/h]   55.69044 [1/h]   74.31926 [1/h]
## 6 1163.27810 [1/h] 1960.07916 [1/h] 2908.05358 [1/h] 3880.81682 [1/h]
```

4.2.6 Other traffic functions

Another function is `adt` which calculates average daily traffic (ADT) from hourly traffic data. This function reads numeric vectors with the amount of vehicles at each street and expands the traffic with temporal factors for each type of vehicle. The arguments are:

```
args(adt)
```

```
## function (pc, lcv, hgv, bus, mc, p_pc, p_lcv, p_hgv, p_bus, p_mc,
##     expanded = FALSE)
## NULL
```

- `pc` numeric vector for passenger cars
- `lcv` numeric vector for light commercial vehicles
- `hgv` numeric vector for heavy good vehicles or trucks
- `bus` numeric vector for bus
- `mc` numeric vector for motorcycles
- `p_pc` data-frame profile for passenger cars
- `p_lcv` data-frame profile for light commercial vehicles
- `p_hgv` data-frame profile for heavy good vehicles or trucks
- `p_bus` data-frame profile for bus
- `p_mc` data-frame profile for motorcycles

4.3 Vehicular composition

4.4 Application

As mentioned above, the application consists in using the travel demand model for west part of São Paulo city, present in VEIN. This script reads traffic data and expands it applying an age function. It uses the `inventory` function with the default vehicular composition, shown on section (@red(st)). Please, use the scripts in the extra material of this book. The base year is 2015 and the extended example is available in appendix 1.

```
library(vein)
inventory(file.path(tempdir(), "YourCity"))
setwd("YourCity")
data(net) # Loads the traffic demand simulation for west São Paulo
data(net)
data(pc_profile)
pc_week <- temp_fact(net$ldv+net$hdv, pc_profile)
speed <- netspeed(pc_week, net$ps, net$ffs, net$capacity, net$lkm)
saveRDS(net, file = "network/net.rds")
saveRDS(speed, file = "network/speed.rds")
```

5

Emission Factors

An emission factor is the amount of mass of pollutant generated by activities (Pulles and Heslinga, 2010). In the case of vehicles, the emission factors are generally known as the mass of pollutant per traveled distance $g \cdot km^{-1}$ in metric units. The distance unit could be different, like miles for instance. The type of units depends on measurement used when developing the emission factors.

There are hot and cold exhaust emisions. *Hot* exhaust emissions are produced by a vehicle when its engine and exhaust after-treatment system are at their normal operational temperatures and *Cold* during the vehicle warm-up phase (P et al., 2009).

The emission factors come from measurements of pollutants emitted by the sources. In the case of vehicles, the dynanometer measurements of the emission factors are the mass of pollutant collected during the distance traveled by a vehicle following a specific driving cycle. The Federal Test Procedure (FTP) is a test to certify the vehicle emissions under the driving cycles such as FTP-75. This driving cycle has a duration of 1874 s for a distance of 17783 m and an average speed of 34.12 $km \cdot h^{-1}$ (Barlow, 2009).

In the literature it is possible to find different type of emission factors. For instance, in Europe, during the development of the project Assesment of Reliability of Transport Emission Models and Inventory Systems (ARTEMIS), the *traffic situation model* was developed. The model concept consists in the combination of parameters that affects vehicle kinematics and engine operation: type of road, sinuosity and gradient, trafffic conditions or level of service (free-flow, heavy, saturated and stop and go) and average speed by speed limit of the road (Boulter and Barlow, 2009). Measurements of vehicular emissions under each traffic situation lead to emission factors by traffic situation, used in the Handbook of Emission Factors (HBEFA, www.hbefa.net).

There is another approach based on 1 Hz measurement of emissions. Here, the pollutants are measured on real live traffic driving. Emission factors can be derived here using mainly two approaches. One approach is applying the Vehicular Specific Power (VSP) (Jimenez et al., 1999). This method is used in the Motor Vehicle Emission Simulator (MOVES) (Koupal et al., 2003) and the International Vehicle Emissions model (IVE) (Davis et al., 2005). Another approach is to apply the Passenger car and Heavy-duty Emission Model (PHEM), which is based on instantaneous engine power demand and engine speed developed during the ARTEMIS project (Barlow, 2009, Boulter and Barlow (2009)).

Perhaps the most used approach to obtain emission factors are speed functions. As emissions tests on driving cycles are valid for only one average speed, measuring emissions of different driving cycles at different average speeds, allows to obtain point clouds where a regression is applied, obtaining an emission factor as a speed function. The literature shows experiments in diffferent parts of the world, such as in Chile (Corvalán et al., 2002) and Europe (Ntziachristos and Samaras, 2000). However, probably the most used source of emission factors as speed functions are the European emission guidelines developed by the European Monitoring and Evaluation Programme (EMEP, `http://www.emep.int/`) and published by the European Environment Agency (EEA, `https://www.eea.europa.eu/themes/air/emep-eea-air-pollutant-emission-inventory-guidebook/emep`) (Ntziachristos and Samaras, 2016). These emission factors are included in the VEIN model.

Another aspect important in vehicular emissions is the degradation of the emissions of aged vehicles. Over the time, different part of the vehicles suffer deterioration, increasing the emissions. Therefore, approaches have been developed to account for this effect in inventories. One approach consists in determining functions that increment the emissions by accumulated mileage, such as studies of Corvalán and Vargas (2003).

In Brazil, the emission factors are reported by the Environmental Protection Agency of São Paulo CETESB (2015), in their vehicular emissions inventory report. Light vehicles emission factors come from average measurements of the FTP75 driving cycle, motorcycle emission factors come from average measurements of World Motorcycle Test Cycle (WMTC) and HDV from the European Stationary Cycle (ETC).

As the VEIN model was developed in Brazil, but users of other parts of the world may be intereted in using the model, the approach in VEIN has to allow flexibility to the user. Therefore, the emission factors approach in VEIN consists in three options, as shown on Fig. (5.1). The first approach consists in local emissions factors by age of use, such as the one from CETESB (2015), denoted as local_ef in the green circle. The second approach consists in selecting speed functions from Ntziachristos and Samaras (2016), availabe in VEIN and denoted as the grey box as speed_ef. The third approach conists in incorporating speed variation from the speed function into the local emission factors by age of use. In any case, VEIN uses a function to account for the degradation of emissions due to accumulated mileage (denoted in grey box as emis_det). These emissions are entered into the emission estimation function.

The following sections show how to do these calculation in VEIN, step by step.

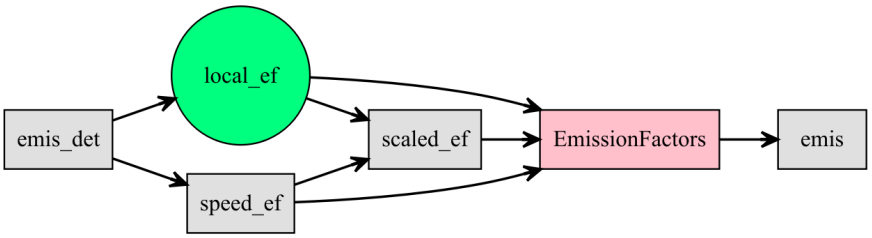


FIGURE 5.1: Structuring an emissions inventories with VEIN

5.1 Speed functions `ef_ldv_speed` and `ef_hdv_speed`

The estimation of emissions in VEIn is shown the equation (5.1):

$$EH_{i,j,k,l,m} = F_{i,j,k,l} \cdot L_i \cdot EF(V_{i,l})_{j,k,m} \cdot DF_{j,k} \tag{5.1}$$

where $EH_{i,j,k,l,m}$ is the emission for each street link i, vehicle category

from composition k, hour l and pollutant m, $F_{i,j,k,l}$ is the vehicular flow calculated in Eq. 1. L_i is the length of the street link i. $EF(V_{i,l})_{j,k,m}$ is the emission factor of each pollutant m. $DF_{j,k}$ is the deterioration factor for vehicle of type j and age of use k, explained in detail in section 5.5.

These functions return speed functions as $f(V)$. The functions come from the EMEP/EEA emissions guidelines (Ntziachristos and Samaras, 2016) and are available in PDF reports. The equations and their parameters were translated to spreedsheets and loaded internally in VEIN. Therefore, the user only must enter the required parameters obtaining the desired function. The functions respect the assumptions and speed limits.

5.1.1 Emission factors of LDV depending on speed with the function `ef_ldv_speed`

The arguments for `ef_ldv_speed` are:

- `v`: Category of vehicle: "PC", "LCV", "Motorcycle" or "Moped".
- `t`: Sub-category of vehicle: PC: "ECE_1501", "ECE_1502", "ECE_1503", "ECE_1504" , "IMPROVED_CONVENTIONAL", "OPEN_LOOP", "ALL", "2S" or "4S". LCV: "4S", Motorcycle: "2S" or "4S". Moped: "2S" or "4S".
- `cc`: Size of engine in cc: PC: "<=1400", ">1400", "1400_2000", ">2000", "<=800", "<=2000". Motorcycle: ">=50" (for "2S"), "<=250", "250_750", ">=750". Moped: "<=50". LCV : "<3.5" for gross weight.
- `f`: Type of fuel: "G", "D", "LPG" or "FH" (Full Hybrid: starts by electric motor).
- `eu`: Euro standard: "PRE", "I", "II", "III", "III+DPF", "IV", "V", "VI" or "VIc".
- `p`: Pollutants: **Criteria**: "CO", "NOx", "HC", "PM", "CH4", "NMHC", "CO2", "SO2", "Pb", "FC" (Fuel Consumption).- **PAH and POP**: "indeno(1,2,3-cd)pyrene", "benzo(k)fluoranthene", "benzo(b)fluoranthene", "benzo(ghi)perylene", "fluoranthene", "benzo(a)pyrene", "pyrene", "perylene", "anthanthrene", "benzo(b)fluorene", "benzo(e)pyrene", "triphenylene", "benzo(j)fluoranthene", "dibenzo(a,j)anthacene", "dibenzo(a,l)pyrene", "3,6-dimethyl-phenanthrene", "benzo(a)anthracene", "acenaphthylene", "acenapthene", "fluorene", "chrysene", "phenanthrene", "napthalene", "anthracene", "coronene", "dibenzo(ah)anthracene" **Dioxins and Furans**: "PCDD", "PCDF", "PCB". **Metals**: "As", "Cd", "Cr", "Cu", "Hg", "Ni", "Pb", "Se", "Zn". **NMHC**: - *ALKANES*: "ethane",

TABLE 5.1: Most used combinations for emission factors for LDV

Argument	Value
v	PC LCV Motorcycles
t	4S
cc	<=1400 1400_2000 >2000
f	G D
eu	PRE I II III IV V VI
p	CO NOx HC FC PM

"propane", "butane", "isobutane", "pentane", "isopentane", "hexane", "heptane", "octane", "TWO_methylhexane", "nonane", "TWO_methylheptane", "THREE_methylhexane", "decane", "THREE_methylheptane", "alcanes_C10_C12", "alkanes_C13". *CYCLOALKANES*: "cycloalcanes". *ALKENES*: "ethylene", "propylene", "propadiene", "ONE_butene", "isobutene", "TWO_butene", "ONE_3_butadiene", "ONE_pentene", "TWO_pentene", "ONE_hexene", "dimethylhexene". *ALKYNES*:"ONE_butine", "propine", "acetylene". *ALDEHYDES*: "formaldehyde", "acetaldehyde", "acrolein", "benzaldehyde", "crotonaldehyde", "methacrolein", "butyraldehyde", "isobutanaldehyde", "propionaldehyde", "hexanal", "i_valeraldehyde", "valeraldehyde", "o_tolualdehyde", "m_tolualdehyde", "p_tolualdehyde". KETONES: "acetone", "methylethlketone". *AROMATICS*: "toluene", "ethylbenzene", "m_p_xylene", "o_xylene", "ONE_2_3_trimethylbenzene", "ONE_2_4_trimethylbenzene", "ONE_3_5_trimethylbenzene", "styrene", "benzene", "C9", "C10", "C13".

- `k`: Multiplication factor.
- `show.equation`: Option to see (or not) the equation parameters.

It is very important that the user enters the right values into the arguments because the final category must match. If the user enters values that do not match, the resulting speed function will be wrong. There are 146 matchs. The probably most used combinations are:

The returning speed function represents how a type of vehicle emits pollutants on average. Fig. (5.2) shows the emissions of CO by Passenger Cars with with technologies Pre Euro and Euro I from Ntziachristos and

Samaras (2016). Higher emissions occure at low average speeds and older vehicles with technologies pre Euro emit more than vehicles with Euro I. Even more, the average emissions of Pre Euro are 29.31 $g \cdot km^{-1}$ and Euro I 2.61 $g \cdot km^{-1}$, meaning that, on average, a vehicle Pre euro is 14 times higher than a vehicle with euro I.

The Fig. (5.2) shows the plot using the package ggplot2 (Wickham, 2009). This package requires that the data must be in long format.

```
library(vein)
library(ggplot2)
ef1 <- ef_ldv_speed(v = "PC", cc = "<=1400", f = "G",
                    eu = "PRE", p = "CO", show.equation = F)
ef2 <- ef_ldv_speed(v = "PC", cc = "<=1400", f = "G",
                    eu = "I", p = "CO", show.equation = F)
V <- 0:110
df <- data.frame(EF = c(ef1(V), ef2(V)))
df$V = V
df$Euro <- factor(c(rep("PRE", 111), rep("I", 111)),
                  levels = c("PRE", "I"))
ggplot(df, aes(V, EF, colour = Euro)) + geom_point(size = 3) +
  geom_line() + theme_bw()+
  labs(y = "CO[g/km]", x = "[km/h]")
```

5.1.2 Emission factors of HDV depending on speed with the function `ef_hdv_speed`

The arguments for `ef_hdv_speed` are:

```
args(ef_hdv_speed)
```

```
## function (v, t, g, eu, x, gr = 0, l = 0.5, p, k = 1, show.equation = FALSE)
## NULL
```

- `v` Category of vehicle: "Coach", "Trucks" or "Ubus"
- `t` Sub-category of vehicle: "3Axes", "Artic", "Midi", "RT,"Std" and "TT"
- `g` Gross weight of each category: "<=18", ">18", "<=15", ">15 & <=18", "<=7.5",

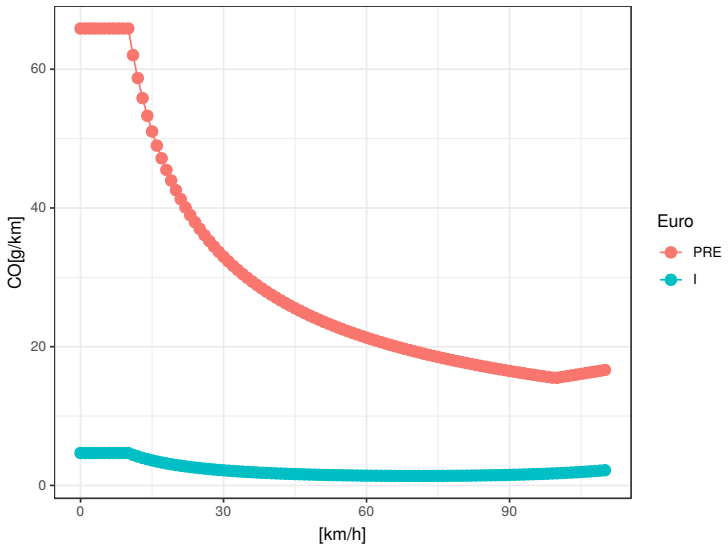


FIGURE 5.2: Emission factor as a speed function

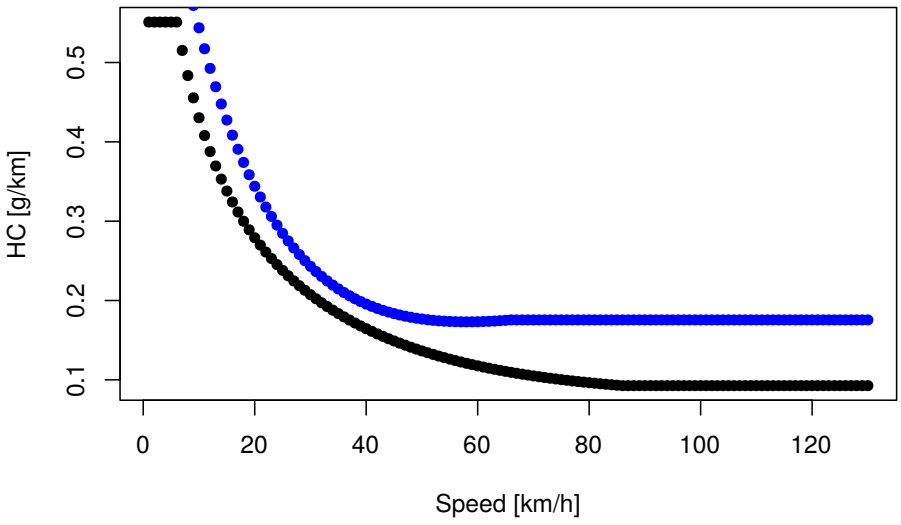
- “>7.5 & <=12”, “>12 & <=14”, “>14 & <=20”, “>20 & <=26”, “>26 & <=28”, “>28 & <=32”, “>32”, “>20 & <=28”, “>28 & <=34”, “>34 & <=40”, “>40 & <=50” or “>50 & <=60”

- ‘eu Euro emission standard: “PRE”, “I”, “II”, “III”, “IV” and “V”
- ‘gr Gradient or slope of road: -0.06, -0.04, -0.02, 0.00, 0.02. 0.04 or 0.06
- `l` Load of the vehicle: 0.0, 0.5 or 1.0
- `p` Pollutant: **Criteria**: “CO”, “NOx”, “HC”, “PM”, “CH4”, “NMHC”, “CO2”, “SO2”, “Pb”, “FC” (Fuel Consumption).- **PAH and POP**: “indeno(1,2,3-cd)pyrene”, “benzo(k)fluoranthene”, “benzo(b)fluoranthene”, “benzo(ghi)perylene”, “fluoranthene”, “benzo(a)pyrene”, “pyrene”, “perylene”, “anthanthrene”, “benzo(b)fluorene”, “benzo(e)pyrene”, “triphenylene”, “benzo(j)fluoranthene”, “dibenzo(a,j)anthacene”, “dibenzo(a,l)pyrene”, “3,6-dimethyl-phenanthrene”, “benzo(a)anthracene”, “acenaphthylene”, “acenapthene”, “fluorene”, “chrysene”, “phenanthrene”, “napthalene”, “anthracene”, “coronene”, “dibenzo(ah)anthracene” **Dioxins and Furans**: “PCDD”, “PCDF”, “PCB”. **Metals**: “As”, “Cd”, “Cr”, “Cu”, “Hg”, “Ni”, “Pb”, “Se”, “Zn”. **NMHC**: - *ALKANES*: “ethane”, “propane”, “butane”, “isobutane”, “pentane”, “isopentane”, “hexane”, “heptane”, “octane”, “TWO_methylhexane”, “nonane”, “TWO_methylheptane”, “THREE_methylhexane”, “decane”, “THREE_methyl-

heptane", "alcanes_C10_C12", "alkanes_C13". *CYCLOALKANES*: "cycloalcanes". *ALKENES*: "ethylene", "propylene", "propadiene", "ONE_butene", "isobutene", "TWO_butene", "ONE_3_butadiene", "ONE_pentene", "TWO_pentene", "ONE_hexene", "dimethylhexene". *ALKYNES*:"ONE_butine", "propine", "acetylene". *ALDEHYDES*: "formaldehyde", "acetaldehyde", "acrolein", "benzaldehyde", "crotonaldehyde", "methacrolein", "butyraldehyde", "isobutanaldehyde", "propionaldehyde", "hexanal", "i_valeraldehyde", "valeraldehyde", "o_tolualdehyde", "m_tolualdehyde", "p_tolualdehyde". KETONES: "acetone", "methylethlketone". *AROMATICS*: "toluene", "ethylbenzene", "m_p_xylene", "o_xylene", "ONE_2_3_trimethylbenzene", "ONE_2_4_trimethylbenzene", "ONE_3_5_trimethylbenzene", "styrene", "benzene", "C9", "C10", "C13".

- `k`: Multiplication factor.
- `k` Multiplication factor
- `show.equation` Option to see or not the equation parameters

```
V <- 0:130
ef1 <- ef_hdv_speed(v = "Trucks",t = "RT", g = "<=7.5",
                    e = "II", gr = 0,
l = 0.5, p = "HC", show.equation = FALSE)
ef2 <- ef_hdv_speed(v = "Trucks",t = "RT", g = "<=7.5",
                    e = "II", gr = 0.06,
l = 0.5, p = "HC", show.equation = FALSE)
plot(1:130, ef1(1:130), pch = 16, type = "b",
     ylab = "HC [g/km]", xlab = "Speed [km/h]")
lines(1:130, ef2(1:130), pch = 16, type = "b", col = "blue")
```



5.2 Local emission factors by age of use. The functions `EmissionFactors` and `EmissionFactorsList`

The functions `EmissionFactors` and `EmissionFactorsList` create the classes with same names. The class `EmissionFactors` is also a data-frame with numeric columns with units of $g \cdot km^{-1}$. This class is not used in critical steps of VEIN, and it has a purpose of creating a data-frame with numeric columns and units. The function is applied to a numeric vector and it just converts it to `units` adding units to it.

In the case of `EmissionFactorsList`, this class is a list of functions $f(V)$. This is usefull because the `emis` function, seen in detail on chapter 6, requires that the emission factors are functions of velocity $f(V)$, regardless $f(V)$ if it is constant or not. When this function is applied to a data-frame or to a matrix, it returns a list and each column of the data-frame or matrix is another list. Also, each row of the original data-frame is converted to a $f(V)$.

The arguments or `EmissionFactorsList` and `EmissionFactors` are:

-`x`: Object with class “data.frame”, “matrix” or “numeric”

The following lines of code show examples using `EmissionFactors`. Firstly, it is loaded the dataset of emission factors *fe2015* for CO and the vehicles PC using gasoline PC_G and Light Trucks LT. The class of fe2015 is data-frame. The subset of the data is named DF_CO. The first 6 elemens of the data-frame are numbers without units.

```
library(vein)
data(fe2015) #CETESB Emission factors
DF_CO <- fe2015[fe2015$Pollutant=="CO", c("PC_G", "LT")]
head(DF_CO)
```

```
##    PC_G    LT
## 1 0.171 0.027
## 2 0.216 0.012
## 3 0.237 0.012
## 4 0.273 0.005
## 5 0.275 0.379
## 6 0.204 0.416
```

The object EF_CO is of class `EmissionFactors` and "data-frame" and each observation has the units $g \cdot km^{-1}$.

```
EF_CO <- EmissionFactors(DF_CO)
head(EF_CO)
```

```
## EmissionFactors:
##           PC_G           LT
## 1 0.171 [g/km] 0.027 [g/km]
## 2 0.216 [g/km] 0.012 [g/km]
## 3 0.237 [g/km] 0.012 [g/km]
## 4 0.273 [g/km] 0.005 [g/km]
## 5 0.275 [g/km] 0.379 [g/km]
## 6 0.204 [g/km] 0.416 [g/km]
```

```
class(EF_CO)
```

```
## [1] "EmissionFactors" "data.frame"
```

The plot of an object of class EmissionFactors shows maximum 9 emission factors. Fig. (5.3) shows the emission factors of both categories, where newer vehicles emit less and older vehicles emit more.

```
plot(EF_CO, xlab = "Age of use")
```

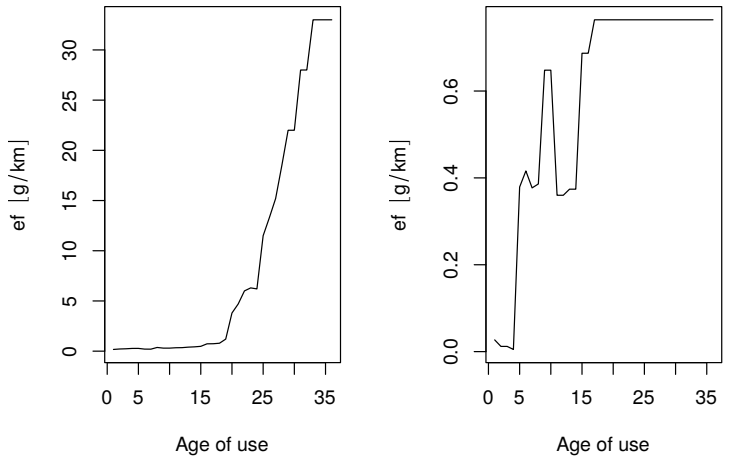


FIGURE 5.3: Emission factor of PC and LT by age of use

Regarding the class EmissionFactorsList, the print and summary methods are very simple, only showing a description of the object. The example of the following lines of code also uses the same set of Emission Factors from CETESB (2015). The resulting object, EF_COL, is of class EmissionFactorsList and list. The print of the object shows only a description of the first and last member of the list object.

```
EFL_CO <- EmissionFactorsList(DF_CO)
class(EFL_CO)
```

```
## [1] "EmissionFactorsList" "data.frame"
```

```
EFL_CO
```

```
## This EmissionFactorsList has  2  lists
## First has  36  functions
```

```
## Last has  36  functions
```

Indeed, if we want to see the content of the `EmissionFactorsList` we have to extract the elements of the list. EFL_CO has two lists; one for PC and one for LT. Then, each list has 36 functions, the command `class(EFL_CO[[1]][[1]])` shows the object is a function $f(V)$.

```
EFL_CO[[1]][[1]]
```

```
## function (V)
## x[j, i]
## <bytecode: 0x558540824a38>
## <environment: 0x55855ce2a240>
```

Also, as the speed functions are constant, there is no need to add values of V.

```
EFL_CO[[1]][[1]](100) # constant speed function
```

```
## [1] 0.171
```

```
EFL_CO[[1]][[1]](0)   # constant speed function
```

```
## [1] 0.171
```

Finally, after extracting the value, Fig. (5.4) shows the same figure as Fig. (5.3)

```
efco1 <- sapply(1:36, function(i) EFL_CO[[1]][[i]]())
efco2 <- sapply(1:36, function(i) EFL_CO[[2]][[i]]())
df <- EmissionFactors(cbind(efco1, efco2))
plot(df, xlab = "Age of use")
```

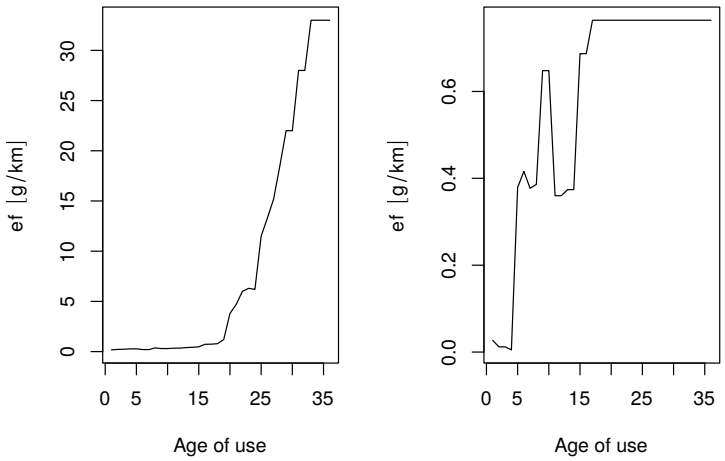


FIGURE 5.4: Emission factor of PC and LT

5.3 Incorporating speed variation with the functions `ef_ldv_scaled` and `ef_hdv_scaled`

The functions in section 5.1 and 5.2 showed the speed and local emission factors respectively. However, the user might have local and constant emission factors depending only on the age of use, but also, outputs from a traffic demand model which includes speed. Under those circumstances, it would be interesting to investigate the effects of the average speed of traffic flow. VEIN includes functions to transform a constant emission factor by age of use into a speed dependent function.

These functions are called `ef_ldv_scaled` and `ef_hdv_scaled`. The concept is explained in detail in my Ph.D thesis (Ibarra-Espinosa, 2017). The idea comes from revisiting the nature of the local emission factors. The Brazilian emission factors consist of average measurements for emissions certification tests which use the driving cycles Federal Test Procedure FTP-75 for LDV, World Motorcycle Test Cycle (WMTC) for motorcycles, and also the European Stationary Cycle (ESC) for HDV (CETESB, 2015). The average speed of FTP-75 and WMTC are known, being 34.2 $km \cdot h^{-1}$ and 54.7 $km \cdot h^{-1}$ based on the reference report on driving cycles from the Transport and Research Laboratory (TRL) (Barlow, 2009). In the case of

ESC, the user might search on literature a way to relate this cycle with an average speed.

Coming back to the CETESB (2015) emission factors, these are annual average values of emissions for the different technologies to accomplish Brazilian emission standards, which are valid only for a specific average speed.If two vehicles have similar technology but different emission factors, one constant and other speed function, it would be possble to relate them. These functions use the speed to relate both emission factors. The condition to transform a contant emission factor into a speed dependent function is that, the new speed dependent function must be of the same value at the speed which is representative for the local factor, and the values at other speeds are the incorporation of the speed variation. The equation (5.2) shows the procedure:

$$EF_{scaled}(V_{i,l})_{j,k,m} = EF(V_{i,l})_{j,k,m} \cdot \frac{EFlocal_{j,k,m}}{EF(Vdc_{i,l})_{j,k,m}} \qquad (5.2)$$

Where $EF_{scaled}(V_{i,l})_{j,k,m}$ is the scaled emission factor and $EF(V_{i,l})_{j,k,m}$ is the Copert emission factor for each street link i, vehicle from composition k, hour l and pollutant m. $EFlocal_{j,k,m}$ represents the constant emission factor (not as speed functions). $EF(Vdc_{i,l})_{j,k,m}$ are Copert emission factors with average speed value of the respective driving cycle for the vehicular category j.

The functions `ef_ldv_scaled` and `ef_hdv_scaled` return scaled emissions factors automatically. The arguments are:

- `df`: Data-frame with emission factors (Deprecated in 0.3.10).
- `dfcol`: Numeric vector with the emission factors constant by age of use. These emission factors are the target to incorporate speed variation.
- `SDC`: A number with the speed of the driving cycle of the emission factors from the argument `dfcol`. The resulting speed functions will return the same values of dfcol at the speed `SDC`. The default is 34.12 "km/h".
- `v`. Category of vehicle: "PC", "LCV", "Motorcycle" or "Moped".
- `t`. Character; sub-category of vehicle: PC: "ECE_1501", "ECE_1502", "ECE_1503", "ECE_1504" , "IMPROVED_CONVENTIONAL", "OPEN_LOOP", "ALL", "2S" or "4S". LCV: "4S", Motorcycle: "2S" or "4S". Moped: "2S" or "4S". The default is `4S`.

- `cc`. Character; size of engine in cc: PC: "<=1400", ">1400", "1400_2000", ">2000", "<=800", "<=2000". Motorcycle: ">=50" (for "2S"), "<=250", "250_750", ">=750". Moped: "<=50". LCV : "<3.5" for gross weight.
- `f`: Character; type of fuel: "G", "D", "LPG" or "FH" (Full Hybrid: starts by electric motor).
- `eu`: Character; euro standard: "PRE", "I", "II", "III", "III+DPF", "IV", "V", "VI" or "VIc".
- `p`: Character; pollutant: "CO", "FC", "NOx", "HC" or "PM".

And the argument of `ef_hdv_scaled` are: !! something is missing here!!

5.4 Cold Starts

Cold start emissions are produced during engine startup, when the engine and/or catalytic converter system has not reached its normal operational temperature. Sev- eral studies have shown the significant impact for these types of emissions (Chen et al., 2011, Weilenmann et al. (2009)). Under this condition emissions will be higher, and if the atmospheric temperature decreases, cold start emissions will increase regardless of whether the catalyst has reached its optimum temperature for functioning (Boulter and Barlow, 2009). VEIN also considers cold start emissions using the approach outlined in Copert (Ntziachristos and Samaras, 2016), as shown in equation (5.3).

$$EC_{i,j,k,l,m} = \beta_j \cdot F_{i,j,k,l} \cdot L_i \cdot EF(V_{i,l})_{j,k,m} \cdot DF_{j.k} \cdot \Big(EF_{\text{cold}}(ta_n, V_{i,l})_{j,k,m} - 1\Big) \tag{5.3}$$

This approach adds two terms to Eq. 5.1. The first term $EF_{cold}(ta_n, V_{i,l})_{j,k,m} - 1$ is the emission factors for cold start conditions at each street link i, vehicle category from composition k, hour l and pollutant m and monthly average temperature n. (Ntziachristos and Samaras, 2016) suggest using monthly average temperature. This is an important aspect that will be reviewed in future versions of VEIN.

The second term β_j is defined as the fraction of mileage driven with a

cold engine/catalyst (Ntziachristos and Samaras, 2016). The VEIN model incorporates a dataset of cold starts recorded during the implementation of the International Vehicle Emissions (IVE) model (Davis et al., 2005) in São Paulo (Lents et al., 2004), which provides the hourly mileage driven with cold start conditions.

The function for cold start emission factors is `ef_ldv_cold` and its arguments are:

```
args(ef_ldv_cold)
```

```
## function (v = "LDV", ta, cc, f, eu, p, k = 1, show.equation = FALSE)
## NULL
```

where:

- `v`: Category of vehicle: "LDV".
- `ta`: Ambient temperature. Monthly mean can be used.
- `cc`: Size of engine in cc: "<=1400", "1400_2000" or ">2000".
- `f`: Type of fuel: "G", "D" or "LPG".
- `eu`: Euro standard: "PRE", "I", "II", "III", "IV", "V", "VI" or "VIc".
- `p`: Pollutant: "CO", "FC", "NOx", "HC" or "PM".
- `k`: Multiplication factor.
- `show.equation`: Option to see or not the equation parameters.

```
ef1 <- ef_ldv_cold(ta = -5, cc = "<=1400", f ="G", eu = "I", p = "CO")
ef2 <- ef_ldv_cold(ta = 0, cc = "<=1400", f ="G", eu = "I", p = "CO")
ef3 <- ef_ldv_cold(ta = 5, cc = "<=1400", f ="G", eu = "I", p = "CO")
ef4 <- ef_ldv_cold(ta = 10, cc = "<=1400", f ="G", eu = "I", p = "CO")
```

There is another function called `ef_ldv_cold_list` which will be deprecated soon.

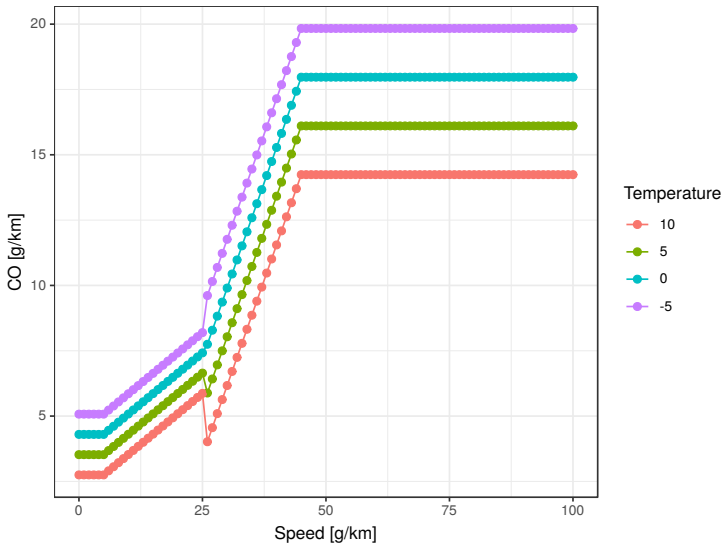


FIGURE 5.5: Cold Emission factor of PC CO (g/km)

5.5 Deterioration

By default, VEIN includes deterioration factors from Copert (Ntziachristos and Samaras, 2016). However, it is possible to include other sources, such as from (Corvalán and Vargas, 2003) or include deteriorated local emission factors. This aspesct is faced in VEIN with the function `emis_det`. This function returns deteriorated factors, as numeric vectors, which must be multiplied with the emission factors of vehicles with 0 mileage.

The arguments of this functions are:

```
args(emis_det)
```

```
## function (po, cc, eu, km)
## NULL
```

where:

- `p`: Pollutant.

- `cc`: Size of engine in cc.
- `eu`: Euro standard: "PRE", "I", "II", "III", "III", "IV", "V", "VI".
- `km`: mileage in km. VEIN includes a dataset of mileage function named "fkm".

```
data(fe2015)
data(fkm)
pckma <- cumsum(fkm$KM_PC_E25(1:24)) #only vehicles with catalizer
x1 <- fe2015[fe2015$Pollutant == "CO", ]
x1E3 <- subset(x1, x1$Euro_LDV %in% c("III", "IV", "V"))$PC_G
x1E1 <- subset(x1, x1$Euro_LDV %in% c("I", "II"))$PC_G
det_E3 <- emis_det(po = "CO", cc = 1000, eu = "III",
                   km = pckma[1:length(x1E3)])
det_E1 <- emis_det(po = "CO", cc = 1000, eu = "III",
                   km = pckma[(length(x1E3) + 1):23 ])
original_EF <- x1$PC
deteriorated_EF <- x1$PC * c(det_E3, det_E1, rep(1, 13))
plot(x = 1:36, y = original_EF, type = "b", pch = 15, col = "blue",
     ylab = "CO[g/km]", xlab = "Age of use")
#     main = "Deteriorated (red) and not-deteriorated (blue) EF CO")
lines(x = 1:36, y = deteriorated_EF,  type = "b", pch = 16, col = "red")
```

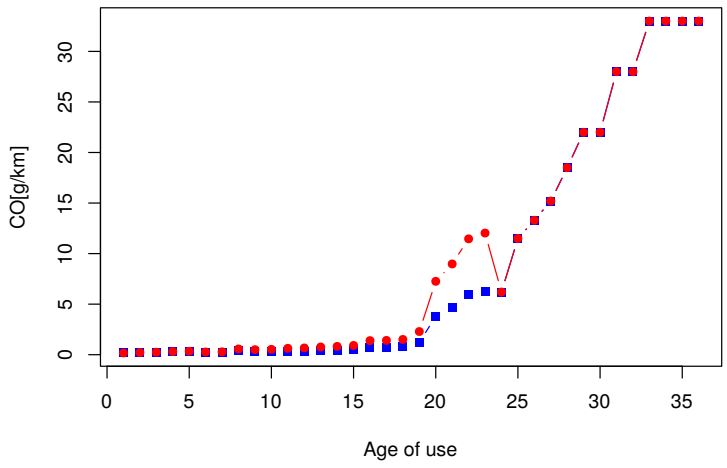


FIGURE 5.6: Deteriorated (red) and not-deteriorated (blue) EF CO

5.6 Evaporative emissions `ef_evap`

Evaporative emissions are important sources of hydrocarbons and these emissions are produced by vaporization of fuel due to variations in ambient temperatures (Mellios and Ntziachristos, 2016, Andrade et al. (2017)). There are three types of emissions: **diurnal emissions**, due to increases in atmospheric temperature, which lead to thermal expansion of vapor fuel inside the tank; **running losses**, when the fuel evaporates inside the tank due to normal operation of the vehicle; and **hot soak** emissions, which occur when the hot engine is turned off. These methods implemented in VEIN were sourced from the evaporative emissions methods of Copert Tier 2 (Mellios and Ntziachristos, 2016). In VEIN it is also possible to use local emission factors. Here I'm showing both approaches:

a) Tier 2 copert approach

$$EV_{j,k} = \sum_{s} D_s \cdot \sum_{j} F_j \cdot (HS_{j,k} + de_{j,k} + RL_{j,k}) \tag{5.4}$$

where EV_j are the volatile organic compounds (VOC) evaporative emissions due to each type of vehicle j. D_s is the "seasonal days" or number of days when the mean monthly temperature is within a determined range: [-5°,10°C], [0°, 15°C], [10°, 25°C] and [20°, 35°C]. $F_{j,k}$ is the number of vehicles according to the same type j and age of use k. $HS_{j,k}$, $de_{j,k}$ and $RL_{j,k}$ are average hot/warm soak, diurnal and running losses evaporative emissions ($\mathrm{g} \cdot \mathrm{day}^{-1}$), respectively, according to the vehicle type j and age of use k. $HS_{j,k}$ and $RL_{j,k}$ are obtained using equations also sourced from (Mellios and Ntziachristos, 2016):

$$HS_{j,k} = x_{j,k} \cdot (c \cdot (p \cdot e_{shc} + (1-p) \cdot e_{swc}) + (1-c) \cdot e_{shfi}) \tag{5.5}$$

where: x is the number of trips per day for the vehicular type j and age of use k. c is the fraction of vehicles with fuel return systems. p is the fraction of trips finished with hot engine, for example, an engine that has reached its normal operating temperature and the catalyst has reached

its light-off temperature (Ntziachristos and Samaras, 2016). The light-off temperature is the temperature at the point when catalytic reactions occur inside a catalytic converter. e_{shc} and e_{swc} are average hot-soak and warm-soak emission factors for gasoline vehicles with carburettor or fuel return systems ($\mathrm{g} \cdot \mathrm{parking}^{-1}$). e_{shfi} is the average hot-soak emission factors for gasoline vehicles equipped with fuel injection and non-return fuel systems ($\mathrm{g} \cdot \mathrm{parking}^{-1}$).

The Eq. (5.6) shows the procedure.

$$RL_{j,k} = x_{j,k} \cdot (c \cdot (p \cdot e_{rhc} + (1-p) \cdot e_{rwc}) + (1-c) \cdot e_{rhfi}) \quad (5.6)$$

where: x and p have the same meanings of Eq. (5.5). e_{rhc} and e_{rwc} are average hot and warm running losses emission factors for gasoline vehicles with carburettor or fuel return systems ($\mathrm{g} \cdot \mathrm{trip}^{-1}$) e_{rhfi} are average hot running losses emission factors for gasoline vehicles equipped withfuel injection and non-return fuel systems ($\mathrm{g} \cdot \mathrm{trip}^{-1}$).

It is recommended to estimate the number of trips per day (Mellios and Ntziachristos, 2016), x, as the division between the mileage and 365 times the length of trip: $x = \frac{mileage_j}{(365 \cdot ltrip)}$.

However, the mileage of a vehicle is not constant throughout the years. Therefore, VEIN incorporates a dataset of equations to estimate mileage of different types of vehicles by age of use (Bruni and Bales, 2013).

The function for evaporative emission factors is `ef_evap` and it arguments are :

```
args(ef_evap)
```

```
## function (ef, v, cc, dt, ca, k = 1, show = FALSE)
## NULL
```

where: - `ef`: Name of evaporative emission factor as *eshotc* ($g \cdot proced^{-}1$): mean hot-soak with carburator, *eswarmc* ($g \cdot proced^{-}1$): mean cold and warm-soak with carburator, *eshotfi*: mean hot-soak with fuel injection, *erhotc* ($g \cdot trip^{-}1$): mean hot running losses with carburator, *erwarmc* ($g \cdot trip^{-}1$) mean cold and warm running losses, *erhotfi* ($g \cdot trip^{-}1$) mean hot

running losses with fuel injection. - `v`: Type of vehicles, "PC", "Motorcycles", "Motorcycles_2S" and "Moped" - `cc`: Size of engine in cc. PC "<=1400", "1400_2000" and "2000" Motorcycles_2S: "<=50". Motorcyces: ">50", "<250", "250_750" and ">750" - `dt`: Average daily temperature variation: "-5_10", "0_15", "10_25" and "20_35" - `ca`: Size of canister: "no" meaning no canister, "small", "medium" and "large" - `k`: multiplication factor - `show`: when TRUE shows row of table with respective emission factor.

Example:

```
library(vein)
library(ggplot2)
library(cptcity)
dt <- c("-5_10", "0_15", "10_25", "20_35")
ef <- sapply(1:4, function(i){
  ef_evap(ef = "erhotc",v = "PC", cc = "<=1400",
                dt = dt[i], ca = "no",
                show = TRUE)
})
```

```
##        ef  units veh     cc    dt canister    g
## 28 erhotc g/trip  PC <=1400 -5_10       no 1.67
##        ef  units veh     cc   dt canister    g
## 21 erhotc g/trip  PC <=1400 0_15       no 2.39
##        ef  units veh     cc    dt canister    g
## 14 erhotc g/trip  PC <=1400 10_25       no 3.25
##       ef  units veh     cc    dt canister    g
## 7 erhotc g/trip  PC <=1400 20_35       no 5.42
```

```
df <- data.frame(ef = ef, temp = c(0, 10, 20, 30))
source("theme_black.R")
ggplot(df, aes(x = temp, y = ef)) +
  geom_bar(stat = "identity", fill = cpt(n = 4), col = "white") +
  labs(x = "Temperature[C]", y = "RL Evaporative NMHC [g/trip]") +
  theme_black()
```

b) Alternative approach

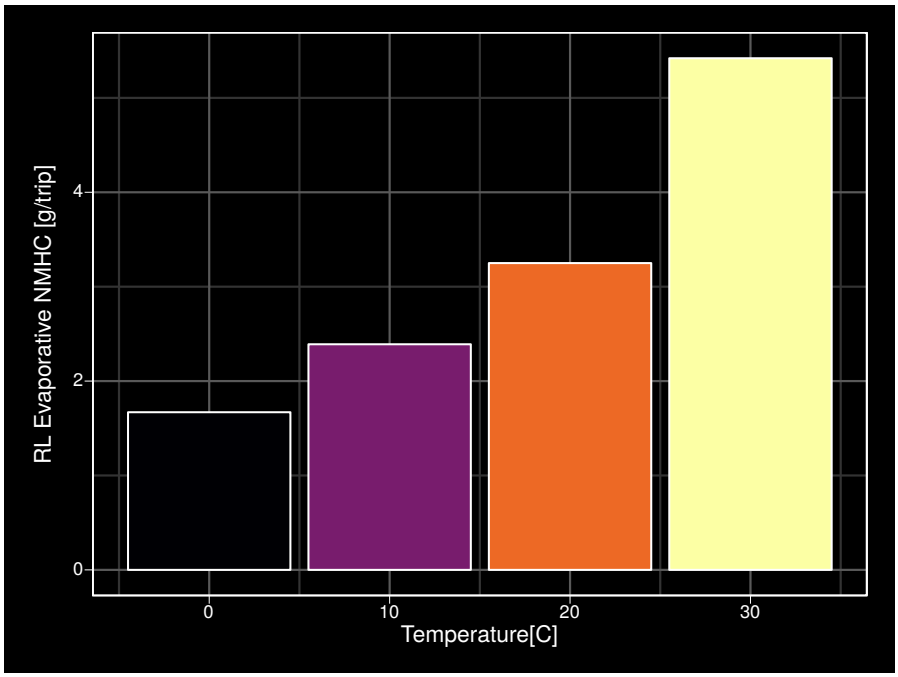


FIGURE 5.7: Running losses evaporative emission actors (g/trip)

The evaporative emission factors mentioned before are suitable for top-down estimations. That approach also requires knowledge of the 'procedure' and 'trips'. In this section it is introduced an alternative which consists in transform the emission factors into $g \cdot km^{-}1$ and then do a bottom-up estimation.

In order to do that, we need to follow some assumptions. First, we consider that the number of procedures is equal to trips. Then we estimate how many trips per day are produced each day and then we estimate how many kilometers are driven each day and convert these to emission factors as shown on Eq. (5.7).

$$EF_{ev}(\frac{g}{km}) = EF(_{ev})(\frac{g}{trip}) \cdot A(\frac{trips}{day}) \cdot B(\frac{km}{day})^{-1} \tag{5.7}$$

Clearly, we need to know A $(\frac{trips}{day})$ and B$(\frac{km}{day})^{-1}$. Diurnal evaporative

emissions factors are expressed as $(\frac{g}{day})$. To convert to $(\frac{g}{km})$ we only need the kilometers driven each day $\frac{km}{day}^{-1}$.

Now, it will be shown an example with the evaporative emission factors from CETESB (2015). These emission factors are based on the methodology Tier 2 from -@Mellios and Ntziachristos (2016). If we consider evaporative emission factors of Passenger Cars using Gasoline (blended with 25% of Ethanol) (CETESB, 2015) and 4.6 $(\frac{trips}{day})$ (Ibarra-Espinosa, 2017).

```
##   year ed_20_35 eshot_20_35 erhot_20_35
## 1 2015     0.06        0.09        0.03
## 2 2014     0.10        0.10        0.04
## 3 2013     0.12        0.13        0.05
## 4 2012     0.19        0.16        0.06
## 5 2011     0.19        0.17        0.14
## 6 2010     0.08        0.08        0.06
```

The variable ed_20_35 are diurnal evaporative emission factors in $g \cdot day^{-1}$ and eshot_20_35 and erhot_20_35 $g \cdot trip^{-1}$.

```
library(vein)
data(fkm)
evap$ed_20_35_gkm <- evap$ed_20_35 / fkm$KM_PC_E25(1:41)/365
evap$eshot_20_35_gkm <- evap$eshot_20_35 * 4.6/ fkm$KM_PC_E25(1:41)/365
evap$erhot_20_35_gkm <- evap$erhot_20_35  * 4.6/ fkm$KM_PC_E25(1:41)/365
plot(x = 1:41, y = evap$eshot_20_35_gkm, col = "blue",
     type = "b", pch = 16,
     xlab = "Age of use", ylab = "EV NMHC [g/km]")
lines(x = 1:41, y = evap$ed_20_35_gkm, col = "red",
      type = "b", pch = 15)
lines(x = 1:41, y = evap$erhot_20_35_gkm, col = "green",
      type = "b", pch = 17)
```

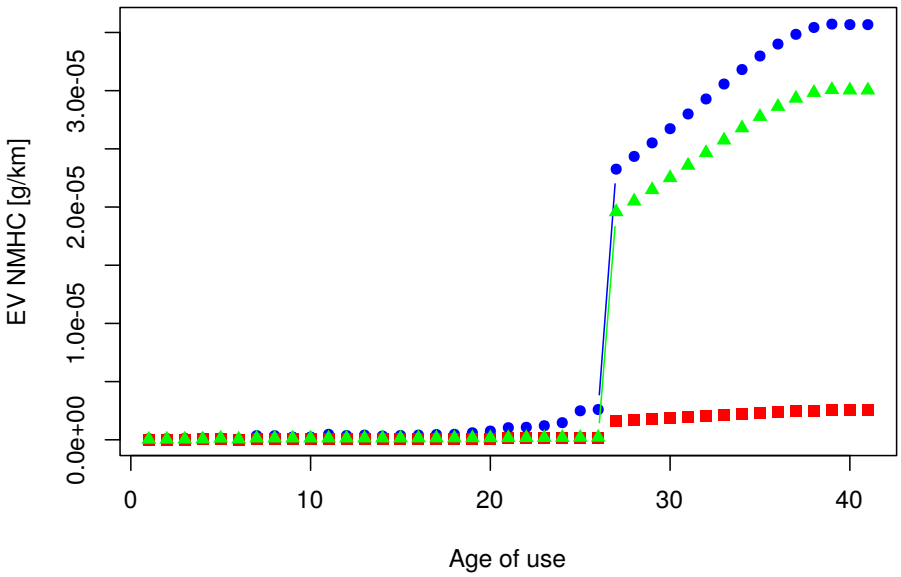


FIGURE 5.8: Hot Soak (blue), Diurnal (green) and Running Losses (red) EF (g/km)

5.7 Emission factors of wear `ef_wear`

Wear emissions are very important because they contribute with an important fraction of PM from tyre and break wear. VEIN includes these functions from Ntziachristos and Boulter (2009) which include wear emission factors form tyre, break and road abrasion.

The arguments are:

```
args(ef_wear)
```

```
## function (wear, type, pol = "TSP", speed, load = 0.5, axle = 2)
## NULL
```

- `wear`: Character; type of wear: "tyre", "break" and "road"
- `type`: Character; type of vehicle: "2W", "PC", "LCV", 'HDV"
- `pol`: Character; pollutant: "TSP", "PM10", "PM2.5", "PM1" and "PM0.1"

TABLE 5.2: Emission factors from tunnels in São Paulo 2014

	CO	NOx
LDV	5.8 [g/km]	0.3 [g/km]
HDV	3.6 [g/km]	9.2 [g/km]

- `speed`: List of speeds
- `load`: Load of the HDV
- `axle`: Number of axle of the HDV

```
library(vein)
?ef_wear
```

5.8 Emission factors from tunnel studies

With VEIN you can choose three type of emissions factors, speed functions, local emission factors or scaled factors. In this section I will show how to expand the use of local emission factors considering tunnel emission factors (Pérez-Martinez et al., 2014), from the International Vehicle Emissions (IVE) Model (Davis et al., 2005) applied in Colombia (González et al., 2017).

Pérez-Martinez et al. (2014) measured air pollutant concentrations in two tunnels in São Paulo city, one with predominant use of LDV vehicles and another with more HDV. The resulting emission factors for the fleet are shown on Table 5.2.

If we want to compare these with the CETESB (2015) emission factors, we would have to weight these factors with the fleet. The weight mean emission factor of CO and Passenger Cars (PC) is 1.40 $g \cdot km^{-1}$ and for Light Trucks (LT) is 0.60 $g \cdot km^{-1}$. In the case of NOx, Passenger Cars (PC) is 0.16 $g \cdot km^{-1}$ and for Light Trucks (LT) is 3.24 $g \cdot km^{-1}$. The emission factors from the example are for vehicles with 0 kilometers without dete-

rioration. Anyways, tunnel emission factors are higher that the weighted emission factors from CETESB.

```
library(vein)
data(fe2015)
fecoPC <- fe2015[fe2015$Pollutant == "CO", "PC_G"]
fecoLT <- fe2015[fe2015$Pollutant == "CO", "LT"]
fenoxPC <- fe2015[fe2015$Pollutant == "NOx", "PC_G"]
fenoxLT <- fe2015[fe2015$Pollutant == "NOx", "LT"]
PC <- age_ldv(x = 1, name = "PC", agemax = 36, message = FALSE)
LT <- age_hdv(x = 1, name = "LT", agemax = 36, message = FALSE)
weighted.mean(fecoPC, PC)  # PC CO
```

```
## [1] 1.40355
```

```
weighted.mean(fecoLT, LT)  # LT CO
```

```
## [1] 0.5971173
```

```
weighted.mean(fenoxPC, PC) # PC NOx
```

```
## [1] 0.1699646
```

```
weighted.mean(fenoxLT, LT) # LT NOx
```

```
## [1] 3.241522
```

If the user wants to use tunnel emission factors from Pérez-Martinez et al. (2014) in VEIN, the user would have to use the same value for all respective categories of the vehicular composition. For instance, after running `inventory`, include tunnel emission factors in each `*input.R`.

5.9 Emission factors from International Vehicle Emissions (IVE)

The IVE model is calculates emission factors by correcting BASE emission factors with the vehicle specific power (VSP) methodology to predict emissions (Jimenez et al., 1999). The formula is shown on Eq. (5.8).

$$VSP = v \cdot (1.1 \cdot a + 9.81(atan(sin(grade))) + 0.132) + 0.000302v^3 \tag{5.8}$$

where: v is velocity $(m \cdot s^{-1})$, a is the second by second acceleration $(m \cdot s^{-2})$ and grade the second by second change in height defined as $\frac{(h_{t=0} - h_{t=-1})}{v}$; being h as altitude m. This method requires that the user measures the activity Global Position System (GPS) recordings second by second and/or emissions measurements with Portable Emissions Measurement Systems (PEMS).

González et al. (2017) measure the vehicular activity in the city of Manizales, Colombia. In this case, there were no PEMS measurements, but IVE allows to produce emission factors from the GPS recordings based on Mobile EPA emissions model(Arbor, 2003, Davis et al. (2005)).

VEIN includes all the BASE IVE emission factors covering:

- "VOC_gkm", "CO_gkm", "NOx_gkm", "PM_gkm", "Pb_gkm", "SO2_gkm", "NH3_gkm", "ONE_3_butadiene_gkm", "formaldehyde_gkm", "acetaldehyde_gkm", "benzene_gkm", "EVAP_gkm", "CO2_gkm", "N20_gkm", "CH4_gkm"
- "VOC_gstart", "CO_gstart", "NOx_gstart", "PM_gstart", "Pb_gstart", "SO2_gstart", "NH3_gstart", "ONE_3butadiene_gstart", "formaldehyde_gstart","acetaldehyde_gstart", "benzene_gstart", "EVAP_gstart", "CO2_gstart", "N20_gstart", "CH4_gstart"

5.10 Emission factors from the Environmental Agency of São Paulo

It has been mentioned that the model includes already some emission factors from the Environmental Agency of São Paulo CETESB for year 2015. However, a new feature alredy present in VEIN is incorporation of all CETESB emission factors for 2016 (CETESB, 2016), covering the following list of pollutants:

- "COd", "HCd", "NMHCd", "CH4", "NOxd", "CO2" "PM", "N2O", "KML", "FC", "NO2d", "NOd", "gCO2/KWH", "RCHOd", "CO", "HC", "NMHC", "NOx", "NO2" ,"NO", "RCHO"

The letter 'd' means deteriorated factor. I added the pollutants "NO", "NO2" based on the speciation of the Ntziachristos and Samaras (2016) guidelines.

The following vehicular categories are covered:

- "PC_G", "PC_FG", "PC_FE", "PC_E" "LCV_G", "LCV_FG", "LCV_FE", "LCV_E", "LCV_D", "SLT", "LT", "MT", "SHT" "HT", "UB", "SUB", "COACH", "ARTIC", "M_G_150", "M_G_150_500", "M_G_500" "M_FG_150", "M_FG_150_500", "M_FG_500". "M_FE_150", "M_FE_150_500", "M_FE_500", "CICLOMOTOR", "GNV".

I also added the categiry "ARTIC" for articulated buses, based on the proportion of Articulated buses to standard urban buses on Ntziachristos and Samaras (2016) guidelines, which is apporximatly 1.4 times the standard emission factor.

6

Estimation of emissions

The emissions estimation process was shown on Eq. (5.1) on chapter 5. In this equation, it was shown that how the emissions are obtained by multiplying the traffifc flow with the distance that each car travels (length of the road if it is a road network), and emissions and deterioration factors.

In this chapter I will show how VEIN interprets this and other emission equations to estimate emissions. At the end of each section The Fig. 6.1 showsa diagram with the estimation process. The pink boxes hows VEIN classes, the circle data and the grey boxes functions. The object `Vehicles` is a class consisting in a matrix of vehicles with untis $1 \cdot h^{-1}$, as shown on chapter 4, however, *the units in `Vehicles` is not a requirement for estimating emissions*. The object of class `Speed` is a matrix of speeds with the number of columns as the calculated speeds at different hours at each row. This object can be present or not, depending on the type of emission factor considered, for instant, emission factors not depending on speed. The object class of `EmissionFactorsList` are list of functions depending on speed as $f(V)$. Each function can depend on speed or not as shown on chapter 5, section 5.2. Lastly, the object lkm is the length of the road expressed in lkm.

The function `emis` reads the inputs and estimates the emissions producing an object with class `EmissionsArray` which has 4 dimensions, number of streets, ages of use of vehicle, number of hours and number of days.

The estimation process is done with the emissions functions. The emissions estimations functions are:

- `emis` for hot emissions,
- `emis_cold` for cold start emissions,
- `emis_evap` for evaporative emissions,
- `emis_paved` for resuspension emissions on paved roads, and
- `emis_wear` for wear of breakes, tyres and roads.

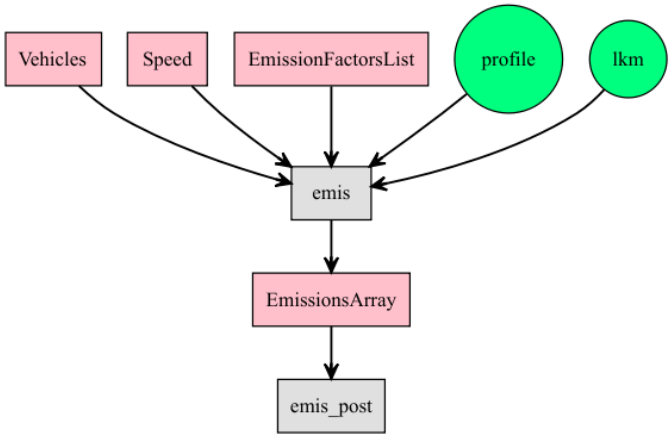


FIGURE 6.1: Emissions estimation process with VEIN

These functions perform internal checks for ensuring that the length lkm has the unit of km. This means that, if `lkm` has units different than km, the function will not run. These function runs internally `lapply` which are faster `for` written in C. Despite that these functions are fast, i will try to make them faster with some RCPP implementation in future.

6.1 The `emis` function

The arguments of `emis` are:

```
args(vein::emis)
```

```
## function (veh, lkm, ef, speed = 34, agemax = ifelse(is.data.frame(veh),
##     ncol(veh), ncol(veh[[1]])), profile, hour = nrow(profile),
##     day = ncol(profile), array = T)
## NULL
```

- `veh`: "Vehicles" data-frame or list of "Vehicles" data-frame. Each data-

frame has number of columns matching the age distribution of that type of vehicle. The number of rows is equal to the number of streets link.
- `lkm`: Length of each link that must in km. As consequence, emission factors must be in $g \cdot km^{-1}$.
- `ef`: "EmissionFactorsList". A list of emission factors as speed functions. Each element has the form $f(V)$. The implicit unit is $g \cdot km^{-1}$.
- `speed`: "Speed" object. A Speed data-frame with number of columns as hours.
- `agemax`: Age of oldest vehicles of the vehicles veh. The information of this argument can be obtained from the `veh` argument Therefore, this argument will be deprecated.
- `profile`: Numerical or dataframe or matrix with nrows equal to the hours and cols to each day. This is traffic data normalized to the hour of the input traffic data.
- `hour`: Number of considered hours in estimation. As this information can be derived form the argument `profile`, the default value is the number of rows of the matrix profile.
- `day`: Number of considered days in estimation. As this information can be derived form the argument `profile`, the default value is the number of coluns of the matrix profile.
- `array`: When FALSE produces a dataframe of the estimation. When TRUE expects a profile as a dataframe producing an array with dimensions (streets x columns x hours x days)

When the only arguments present in the function are **veh**, **lkm** and **ef** assumes a *top-down* and shows a message.

6.2 The `emis_cold` function

The arguments of `emis_cold` are:

```
args(vein::emis_cold)
```

```
## function (veh, lkm, ef, efcold, beta, speed = 34, agemax = if (!inherits(x = veh,
```

```
##     what = "list")) {
##     ncol(veh)
## } else {
##     ncol(veh[[1]])
## }, profile, hour = nrow(profile), day = ncol(profile), array = TRUE)
## NULL
```

The arguments are similar with `emis` with the difference that it is added two arguments:

- `efcold`: List of functions of cold start emission factors of vehicular categories. Technically, each function is also of the form $f(V)$.
- `beta`: Datraframe with the hourly cold-start distribution to each day of the period. Number of rows are hours and columns are days. It represents the fraction of mileage driven under cold-start conditions.

The equation for estimating cold-start emissions is on Eq. (5.3).

6.3 The `emis_evap` function

The estimation of evaporative emissions applies Tier 2 from Mellios and Ntziachristos (2016). The approach followed in VEIN was very simply, consisting in only adding elements of a data-frame.

```
args(vein::emis_evap)
```

```
## function (veh, name, size, fuel, aged, nd4, nd3, nd2, nd1, hs_nd4,
##     hs_nd3, hs_nd2, hs_nd1, rl_nd4, rl_nd3, rl_nd2, rl_nd1, d_nd4,
##     d_nd3, d_nd2, d_nd1)
## NULL
```

- `veh`: this are the number of vehicles at each age of use and for each street. It is a `Vehicles` object.
- `name`: Character indicating the name of the vehicle.
- `size`: Character indicating the size of the vehicle.
- `fuel`: Character indicating the fuel of the vehicle.

- `age`: Numeric vector with the age distribution, for instance, 1:40 for vehicles between 1 and 40 years of use.
- `nd4`: Number of days of your perdiof of study with monthly average temperature between 20 and 35 celcius degrees. If the period of time is a year, this is the annual number of days under that condition.
- `nd3`: Number of days of your perdiof of study with monthly average temperature between 10 and 25 celcius degrees.
- `nd2`: Number of days of your perdiof of study with monthly average temperature between 0 and 15 celcius degrees.
- `nd1`: Number of days of your perdiof of study with monthly average temperature between -5 and 10 celcius degrees.
- `hs_nd4`: Number of average daily hot-soak evaporative emissions for days with temperature between 20 and 35 celcius degrees
- `hs_nd3`: Number of average daily hot-soak evaporative emissions for days with temperature between 10 and 25 celcius degrees
- `hs_nd2`: Number of average daily hot-soak evaporative emissions for days with temperature between 0 and 15 celcius degrees
- `hs_nd1`: Number of average daily hot-soak evaporative emissions for days with temperature between -5 and 10 celcius degrees
- `rl_nd4`: Number of average daily running losses evaporative emissions for days with temperature between 20 and 35 celcius degrees
- `rl_nd3`: Number of average daily running losses evaporative emissions for days with temperature between 10 and 25 celcius degrees
- `rl_nd2`: Number of average daily running losses evaporative emissions for days with temperature between 0 and 15 celcius degrees
- `rl_nd1`: Number of average daily running losses evaporative emissions for days with temperature between -5 and 10 celcius degrees
- `d_nd4`: Number of average daily diurnal evaporative emissions for days with temperature between 20 and 35 celcius degrees
- `d_nd3`: Number of average daily diurnal evaporative emissions for days with temperature between 10 and 25 celcius degrees
- `d_nd2`: Number of average daily diurnal evaporative emissions for days with temperature between 0 and 15 celcius degrees
- `d_nd1`: Number of average daily diurnal evaporative emissions for days with temperature between -5 and 10 celcius degrees

6.4 The `emis_paved` function

Evaporative emissions are emissions of resuspended dust due to traffic circulating ober paved or non-paved roads. These emissions can be an important source of mass particulate matter, and several cities programs that aims to improve air quality by diminishing these emissions (Amato et al., 2010). However, these emissions are not considered by in the European emissions guidelines, where their focus is on primary particles and not those resulting from the resuspension of previously deposited material (Ntziachristos and Boulter, 2009).

The method adopted in VEIN comes from the USEPA (USA-EPA, 2016) which presents equations for annual, daily and hourly estimations:

$$EF_{paved} = k \cdot sL^{0.91} \cdot W^{1.02} \tag{6.1}$$

Where

- EF_{paved} is the emission factor of particulate matter.
- k particle size splitter.
- sL road surface silt loading $g \cdot m^{-2}$.
- W average weight.

Equation (6.1) can be extrapolated to consider natural mitigation of rainy periods of time with daily basis:

$$EF_{anual} = EF_{paved} \cdot (1 - \frac{P}{4 \cdot N}) \tag{6.2}$$

Where

- EF_{anual} anual or long term emission factor.
- P number of days with accumulated rain above 0.254 mm.
- N total number of days.

or hourly

$$EF_{hourly} = EF_{paved} \cdot (1 - \frac{1.2 \cdot P}{N}) \tag{6.3}$$

Where

- EF_{annual} annual or long term emission factor.
- P number of hours with accumulated rain above 0.254 mm.
- N total number of hours. For instance, 8760 for 1 year.

The function `emis_paved` has the arguments:

```
args(vein::emis_paved)
```

```
## function (veh, lkm, k = 0.62, sL1 = 0.6, sL2 = 0.2, sL3 = 0.06,
##     sL4 = 0.03, W)
## NULL
```

Where,

-`veh`: It is an array with dimenssions number of streets x hours of day x days of week. - `lkm`: Length of each link. - `k`: K_PM30 = 3.23, K_PM15 = 0.77, K_PM10 = 0.62 and K_PM2.5 = 0.15. - `sL1`: Silt loading (g/m2) for roads with ADT <= 500. - `sL2`: Silt loading (g/m2) for roads with ADT > 500 and <= 5000. - `sL3`: Silt loading (g/m2) for roads with ADT > 5000 and <= 1000. - `sL4`: Silt loading (g/m2) for roads with ADT > 10000. - `W`: array of dimensions of veh. It consists in the hourly averaged weight of traffic fleet in each road.

For instance, Lets create an array of vehicles. The funcion `adt` calculates the amount pf vehicles at all hours. Lets use the `data(net)` asumming no buses. Let's calculate the total traffic for only 24 hours with the same profile. For simplicity, let's assume that all vehicle are expressed in *vehicle equivalent* and it is a dry period.

```
library(vein)
data(net)
data(profiles)
vkpc  <- vkm(net$ldv*0.75, 1, matrix(profiles$PC_JUNE_2012[, 1]))
vklcv  <- vkm(net$ldv*0.1, 1, matrix(profiles$LCV_JUNE_2012[, 1]))
vkmc  <- vkm(net$ldv*0.15, 1, matrix(profiles$MC_JUNE_2012[, 1]))
vkhgv  <- vkm(net$hdv, 1, matrix(profiles$HGV_JUNE_2012[, 1]))
vk <- vkpc + vklcv + vkmc + vkhgv
dim(vk)
```

```
## [1] 1505   24
```

`W` is the average hourly fleet weight. It ahs the same dimensions of `adt2`. Let's assume an individual weight of PC is 1, LCV 1.5, HGV = 10 and MC 0.5. This example is a simplification, `adt` should be calculated with full characterization of the fleet.

```
wpc  <- vkm(net$ldv*0.75, 1, profiles$PC_JUNE_2012[, 1])*1
wlcv  <- vkm(net$ldv*0.1, 1, profiles$LCV_JUNE_2012[, 1])*1.5
wmc  <- vkm(net$ldv*0.15, 1, profiles$MC_JUNE_2012[, 1])*0.5
whgv  <- vkm(net$hdv, 1, profiles$HGV_JUNE_2012[, 1])*10
W <- (wpc + wlcv + wmc + whgv)/vk
W[is.na(W)] <- 0
dim(W)
```

```
## [1] 1505   24
```

and now we estimate the emissions with the default values form PM10.

```
emi <- emis_paved(veh = vk, lkm = net$lkm, W = W)
emi[1:4, 1:4]
```

```
## Result for Emissions
##                h1              h2              h3              h4
## 1 28.492378 [g/h] 41.326236 [g/h] 27.987685 [g/h] 30.978253 [g/h]
## 2 48.704190 [g/h] 31.257192 [g/h] 27.139666 [g/h] 34.919757 [g/h]
## 3  4.360828 [g/h]  2.327479 [g/h]  1.576257 [g/h]  1.744684 [g/h]
## 4 10.371056 [g/h]  5.535283 [g/h]  3.748702 [g/h]  4.149262 [g/h]
```

6.5 The `emis_wear` function

Wear emissions can be very important, in fact, these are second most important source of particulate matter in Europe (Lükewille et al., 2017). These methods in VEIN comes from Ntziachristos and Boulter (2009) which include wear of "tyre", "break" and "road".

The arguments of the function `emis_wear` are:

```
args(vein::emis_wear)
```

```
## function (veh, lkm, ef, what = "tyre", speed, agemax = ncol(veh),
##     profile, hour = nrow(profile), day = ncol(profile))
## NULL
```

Where,

- `veh`: Object of class "Vehicles".
- `lkm`: Length of the road.
- `ef`: list of emission factor functions class "EmissionFactorsList", length equals to hours.
- `agemax`: Age of oldest vehicles for that category
- `profile`: Dataframe or matrix with nrows equal to hours and ncol as days of the week
- `hour`: Number of considered hours in estimation, with default value as number of rows of profile.
- `day`: Number of considered days in estimation, with default value as number of columns of profile.

Let's estimate wear emissions!

First, we get the emission factor with the `ef_wear` function:

```
library(vein)
data(net)
data(profiles)
pro <- profiles$PC_JUNE_2012[, 1] # 24 hours
pc_week <- temp_fact(net$ldv+net$hdv, pro)
df <- netspeed(pc_week, net$ps, net$ffs, net$capacity, net$lkm, alpha = 1)
ef <- ef_wear(wear = "tyre", type = "PC", pol = "PM10",
                            speed = df)
```

Then we estimate emissions

```
emi <- emis_wear(veh = age_ldv(net$ldv, name = "VEH"), speed = df,
                 lkm = net$lkm, ef = ef, profile =  pro)
```

```
## Average age of VEH is 11.17
```

```
## Number of VEH is 1946.95 * 10^3 veh
```

```
df <- emis_post(emi, pollutant = "PM", by = "streets_wide")
df[1:4, 1:4]
```

```
## Result for Emissions
##                 V1              V2               V3               V4
## 1 2.0689049 [g/h] 1.0160833 [g/h] 0.56468672 [g/h] 0.52486176 [g/h]
## 2 0.7614073 [g/h] 0.3743085 [g/h] 0.20803274 [g/h] 0.19336135 [g/h]
## 3 0.1116298 [g/h] 0.0548773 [g/h] 0.03049965 [g/h] 0.02834868 [g/h]
## 4 0.2768287 [g/h] 0.1360872 [g/h] 0.07563435 [g/h] 0.07030028 [g/h]
```

7

Post estimation with `emis_post`

Once the emissions are estimated we obtained `EmissionsArray` objects, which as mentioned before, they are arrays with the dimensions streets x age distribution of vehicles x hours x days.

Now the function `emis_post` reads the `EmissionsArray` and and convert it to data-frames that are easier to manage.

The arguments of `emis_post` are:

```
args(vein::emis_post)
```

```
## function (arra, veh, size, fuel, pollutant, by = "veh", net)
## NULL
```

Where,

- `arra`: `EmissionsArray` obtained with the `emis` functions. It is an array of emissions 4d: streets x category of vehicles x hours x days or 3d: streets x category of vehicles x hours
- `veh`: Character indicating the type of vehicle , for instance: "PC".
- `size`: Character indicating the size or weight, for instance: "<1400", "1400<cc<2000", "GLP", "Diesel".
- `fuel`: Character indicating fuel, for instance: "Gasoline", "E_25", "GLP", "Diesel".
- `pollutant`: Character indicating the pollutant, for instance "CO", "NOx", etc.
- `by`: Character indicating type of output, "veh" for total vehicular category , "streets_narrow" or "streets_wide". This is the most important argument of this function. "streets_wide" returns a dataframe with rows as number of streets and columns the hours as days*hours considered, e.g. 168

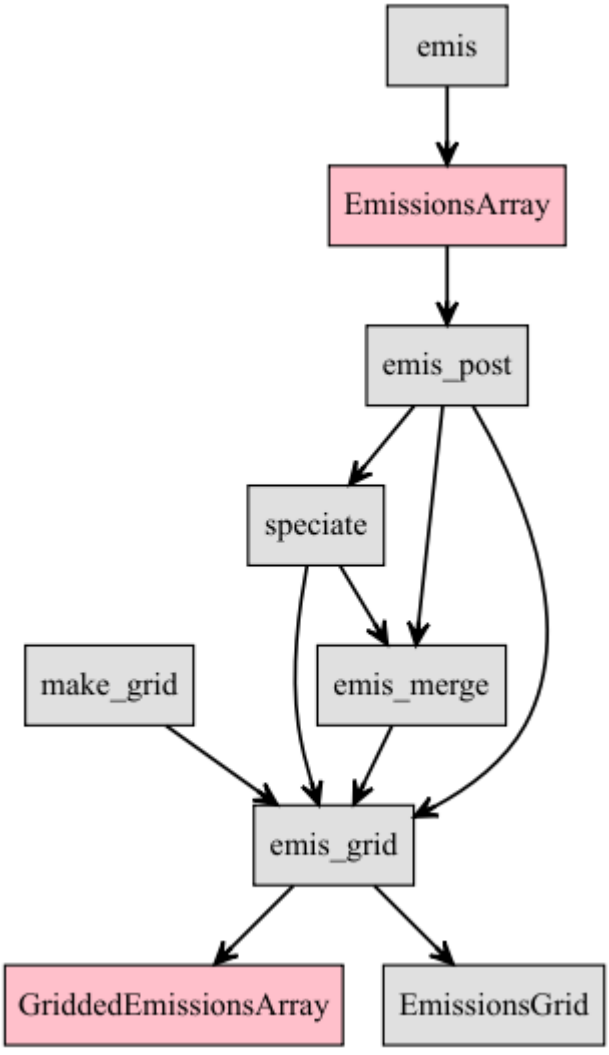


FIGURE 7.1: Post-emissions

columns as the hours of a whole week and “streets_wide repeats the row number of streets by hour and day of the week

Lets create some objects

7.1 Emissions by street

From previous chapters we worked with `Vehicles`, `EmissionFactors` and estimate emissions generating `EmissionsArray`. Now let’s create an `EmissionsArray` object.

```
library(vein)
library(veinreport)
library(cptcity)
library(ggplot2)
data(net)
data(profiles)
data(fe2015)
PC_G <- age_ldv(x = net$ldv, name = "PC")
```

```
## Average age of PC is 11.17
```

```
## Number of PC is 1946.95 * 10^3 veh
```

```
# Estimation for 168 hour and local factors
pcw <- temp_fact(net$ldv, profiles$PC_JUNE_2014)
# June is not holliday in southern hemisphere
hdvw <- temp_fact(net$hdv, profiles$HGV_JUNE_2014)
speed <- netspeed(pcw + hdvw, net$ps, net$ffs, net$capacity, net$lkm, alpha = 1)
lef <- EmissionFactorsList(fe2015[fe2015$Pollutant=="CO", "PC_G"])
E_CO <- emis(veh = PC_G,lkm = net$lkm, ef = lef, speed = speed,
             profile = profiles$PC_JUNE_2014)
```

```
## Number of columns of 'veh' is different than length of 'ef'
```

```
## adjusting length of ef to the number of colums of 'veh'
```

```
## 187546.38 kg emissions in 24 hours and 7 days
```

Now that we have our EmissionsArray E_CO, we can process it with the function emis_post. The emissions by street are obtained with the argument by = "streets_wide":

```
E_CO_STREETS <- emis_post(E_CO, by = "streets_wide")
E_CO_STREETS[1:6, 1:3]
```

```
## Result for Emissions
##                 V1               V2              V3
## 1 676.629408 [g/h] 349.068278 [g/h] 206.13032 [g/h]
## 2 259.924802 [g/h] 134.093349 [g/h]  79.18423 [g/h]
## 3  38.107534 [g/h]  19.659404 [g/h]  11.60919 [g/h]
## 4  90.628506 [g/h]  46.754599 [g/h]  27.60933 [g/h]
## 5   3.884417 [g/h]   2.003943 [g/h]   1.18336 [g/h]
## 6 378.775340 [g/h] 195.407492 [g/h] 115.39120 [g/h]
```

In the version 0.3.17 it was added the capability of returning an spatial object class 'sf' with 'LINESTRING':

```
E_CO_STREETS <- emis_post(E_CO, by = "streets_wide", net = net)
class(E_CO_STREETS)
```

```
## [1] "sf"         "data.frame"
```

```
ggplot(E_CO_STREETS) + geom_sf(aes(colour = as.numeric(V9))) +
  scale_color_gradientn(colours = rev(cpt())) + theme_bw()+
  ggtitle("CO emissions at 08:00 (g/h)")
```

Now, if we estimate the NOx emissions of Light Trucks we will a slight different pattern of emissions:

```
LT <- age_hdv(x = net$hdv, name = "LT")
```

```
## Average age of LT is 17.12
```

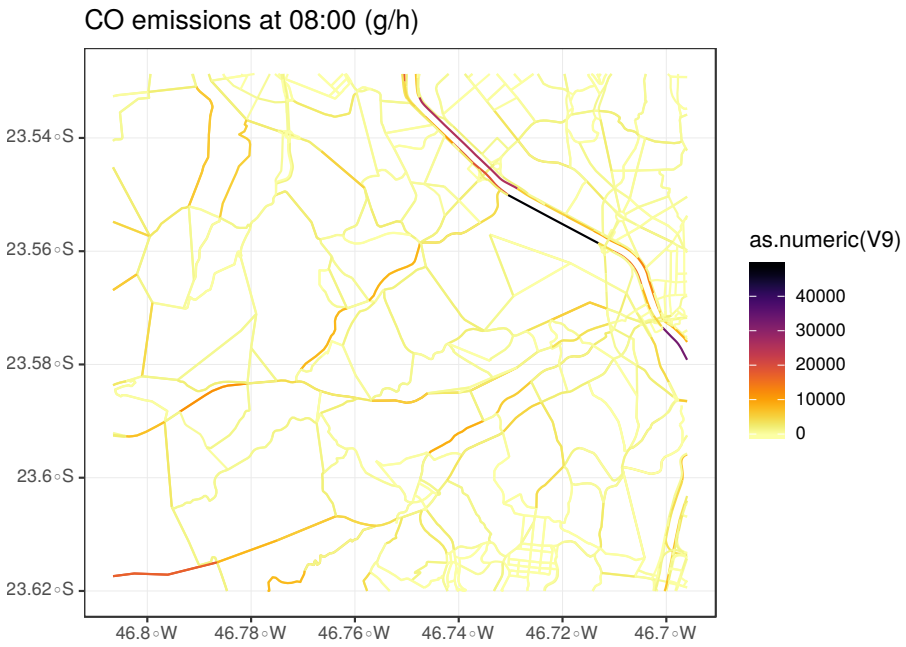


FIGURE 7.2: CO emisions of PC (g/h)

```
## Number of LT is 148.12 * 10^3 veh
```

```
lef <- EmissionFactorsList(fe2015[fe2015$Pollutant==”NOx”, ”LT”])
E_NOx <- emis(veh = LT, lkm = net$lkm, ef = lef, speed = speed,
              profile = profiles$PC_JUNE_2014)
```

```
## Number of columns of 'veh' is different than length of 'ef'

## adjusting length of ef to the number of colums of 'veh'

## 34029.87 kg emissions in 24 hours and 7 days
```

```
E_NOx_STREETS <- emis_post(E_NOx, by = ”streets_wide”, net = net)
ggplot(E_NOx_STREETS) + geom_sf(aes(colour = as.numeric(V9))) +
  scale_color_gradientn(colours = rev(cpt())) + theme_bw()+
  ggtitle(”NOX emissions at 08:00 (g/h)”)
```

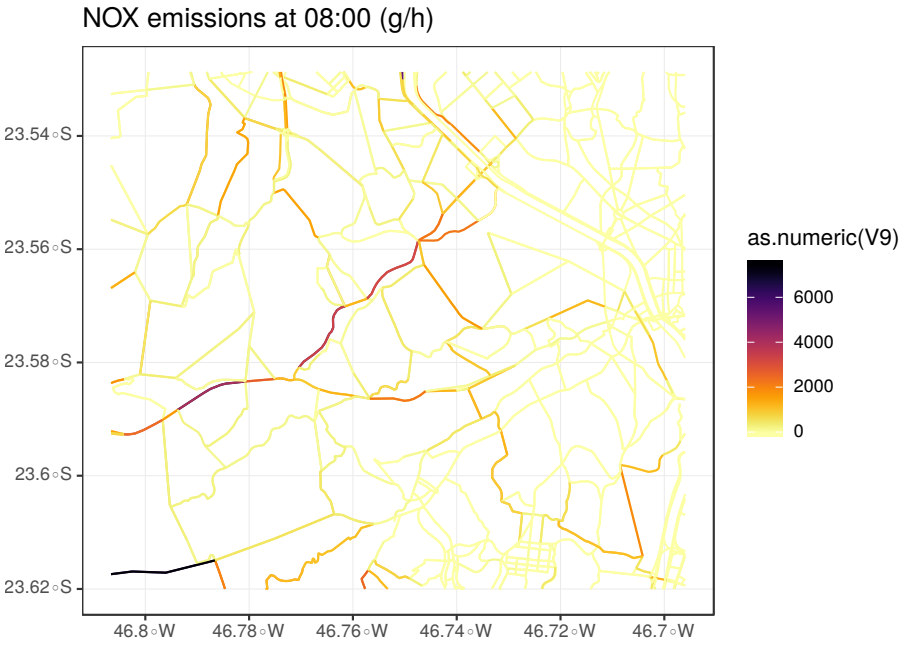


FIGURE 7.3: NOx emisions of LT (g/h)

7.2 Total emissions in data-frames

In order to obtain the total emissions in data-frame, the same function `emis_post` is used, but in this case, with the argument `by` = "veh". We also need to add arguments of `veh` for the type of vehicle, `size` the size or gross weight, `fuel` and `pollutant`. The argument `net` is not required in this case.

```
E_NOx_DF <- emis_post(arra = E_NOx, veh = "LT", size = "Small", fuel = "B5",
                      by = "veh", pollutant = "NOx")
head(E_NOx_DF)
```

```
##     E_NOx              g veh  size fuel pollutant age hour
## 1 E_NOx_1 182.5943 [g/h]  LT Small   B5       NOx   1    1
## 2 E_NOx_2 163.2499 [g/h]  LT Small   B5       NOx   2    1
## 3 E_NOx_3 177.5608 [g/h]  LT Small   B5       NOx   3    1
```

```
## 4 E_NOx_4 208.5892 [g/h]  LT Small   B5       NOx   4    1
## 5 E_NOx_5 765.7001 [g/h]  LT Small   B5       NOx   5    1
## 6 E_NOx_6 885.6223 [g/h]  LT Small   B5       NOx   6    1
```

The resulting object is a data-frame with the name of the input array, then it has the g/h. Also, the name of the vehicle, the size, fuel, pollutant, age and hour. This is interesting because we can now what are the most pollutatn vehicle and at which hour this emissions ocurres.

```
E_NOx_DF[E_NOx_DF$g == max(E_NOx_DF$g), ]
```

```
##         E_NOx              g veh  size fuel pollutant age hour
## 517 E_NOx_17 29139.51 [g/h]  LT Small   B5       NOx  17   11
```

The highest emissions by hour are of Light Trucks of 17 years of use at hour 11 on local time. However, it is possible to get more interesting insights of the data. The datra can be aggregated by age, hour or plot all together as shown on Fig. 7.6. The highest emissions ocurre between 17 and 27 years of use. This figure also shows the effect of emissions standards introduced in different years.

```
df <- aggregate(E_NOx_DF$g, by = list(E_NOx_DF$hour), sum)
plot(df, type = "b", pch = 16, xlab = "hour", ylab = "NOx (g/h)")
```

```
library(ggplot2)
library(veinreport) # theme_black
df <- aggregate(E_NOx_DF$g, by = list(E_NOx_DF$age), sum)
names(df) <- c("Age", "g")
ggplot(df, aes(x = Age, y = as.numeric(g), fill = as.numeric(g))) +
  geom_bar(stat = "identity") +
  scale_fill_gradientn(colours = cpt()) + theme_black() +
  labs(x = "Age of use", y = "NOx (g/h)")
```

```
library(ggplot2)
library(veinreport) # theme_black
ggplot(E_NOx_DF, aes(x = age, y = as.numeric(g), fill = hour)) +
```

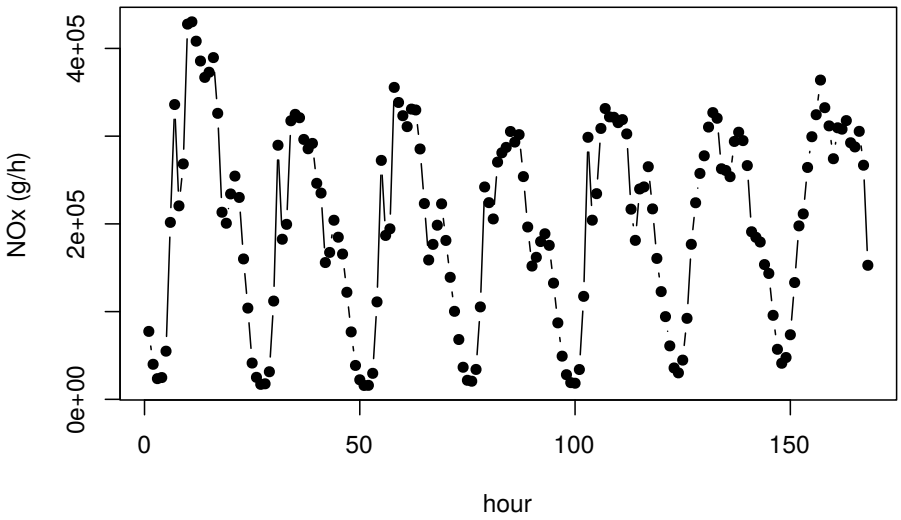


FIGURE 7.4: NOx emissions of LT by hour

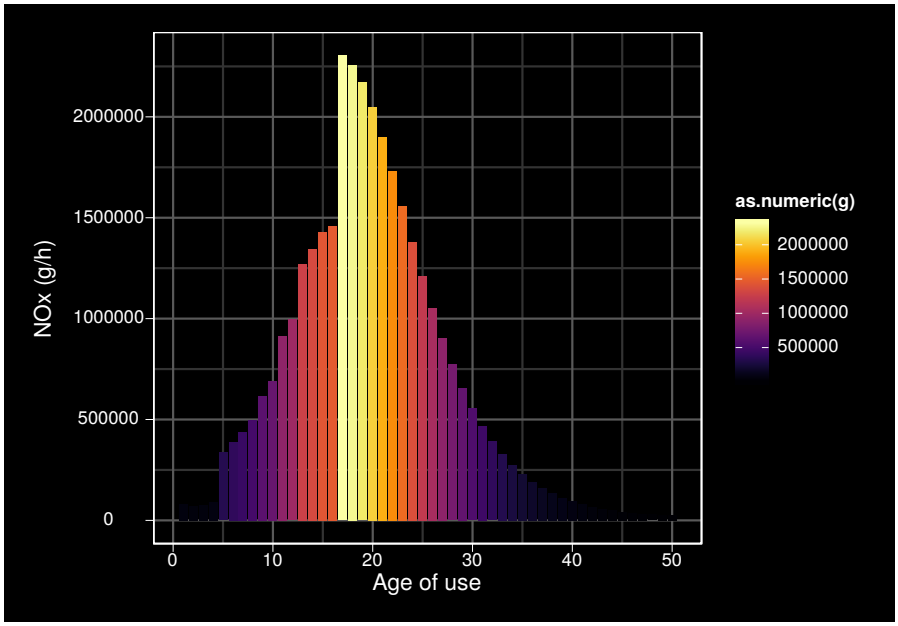


FIGURE 7.5: NOx emissions of LT by age

```
  geom_bar(stat = "identity") +
  scale_fill_gradientn(colours = cpt()) + theme_black() +
  labs(x = "Age of use", y = "NOx (g/h)")
```

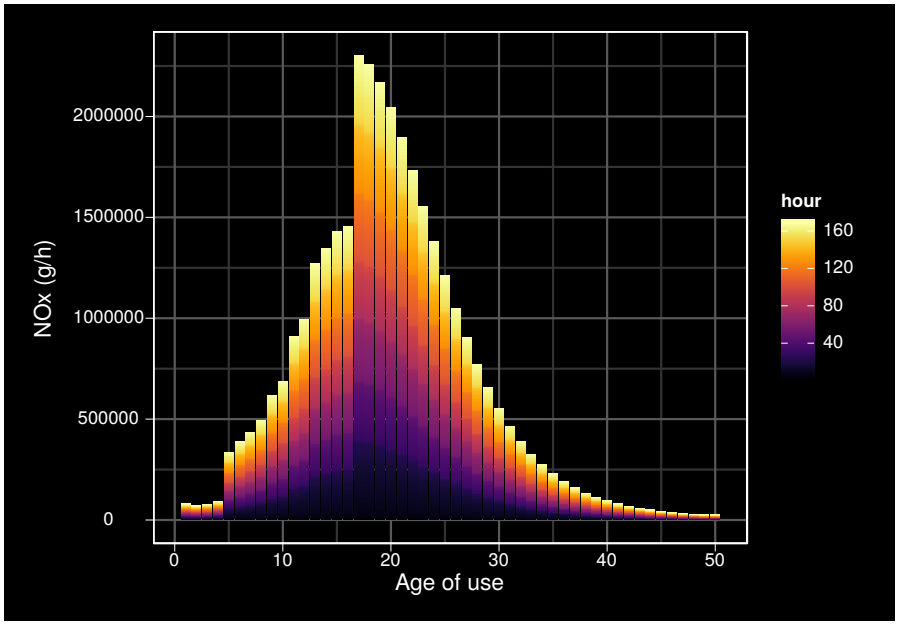


FIGURE 7.6: NOx emissions of LT

7.3 Merging emissions

The function `inventory` was designed to store the emissions of each type of vehicle in each directory. Hence, it was necessary to create a function that read and merge the emissions that are in each directory, returning a data-frame os a spatial feature data-frame. The function is `emis_merge`. As it can be seen on Fig. 7.1, `emis_merge` comes after `emis_post` or `speciate`. The arguments of `emis_merge` are:

```
args(vein::emis_merge)
```

```
## function (pol = "CO", what = "STREETS.rds", streets = T, net,
##     path = "emi", crs, under = "after", as_list = FALSE)
## NULL
```

Where,

- pol: Character. Pollutant.
- what: Character. Word to search the emissions names, "STREETS", "DF" or whatever name. It is important to include the extension .'rds'
- streets: Logical. If true, emis_merge will read the street emissions created with emis_post by "streets_wide", returning an object with class 'sf'. If false, it will read the emissions data-frame and rbind them.
- net: 'Spatial feature' or 'SpatialLinesDataFrame' with the streets. It is expected #'that the number of rows is equal to the number of rows of street emissions. If #' not, the function will stop.
- path: Character. Path where emissions are located
- crs: coordinate reference system in numeric format from http://spatialreference.org/ to transform/project spatial data using sf::st_transform

In order to see how this functions works, let's run the example in the inventory function. First, lets create a project, or in other words a directory named "YourCity", into the temporary directory. In this part you can place your project wherever you want with the actual name of your city. Then run inventory with the default configuration.

```
name = file.path(tempdir(), "YourCity")
vein::inventory(name = name)
```

```
## files at /tmp/RtmpJQp9lK/YourCity
```

```
## Directories:
##  [1] "/tmp/RtmpJQp9lK/YourCity"
##  [2] "/tmp/RtmpJQp9lK/YourCity/ef"
##  [3] "/tmp/RtmpJQp9lK/YourCity/emi"
##  [4] "/tmp/RtmpJQp9lK/YourCity/emi/BUS_01"
```

```
##  [5] "/tmp/RtmpJQp9lK/YourCity/emi/HGV_01"
##  [6] "/tmp/RtmpJQp9lK/YourCity/emi/LCV_01"
##  [7] "/tmp/RtmpJQp9lK/YourCity/emi/MC_01"
##  [8] "/tmp/RtmpJQp9lK/YourCity/emi/PC_01"
##  [9] "/tmp/RtmpJQp9lK/YourCity/est"
## [10] "/tmp/RtmpJQp9lK/YourCity/images"
## [11] "/tmp/RtmpJQp9lK/YourCity/network"
## [12] "/tmp/RtmpJQp9lK/YourCity/post"
## [13] "/tmp/RtmpJQp9lK/YourCity/post/df"
## [14] "/tmp/RtmpJQp9lK/YourCity/post/grids"
## [15] "/tmp/RtmpJQp9lK/YourCity/post/streets"
## [16] "/tmp/RtmpJQp9lK/YourCity/profiles"
## [17] "/tmp/RtmpJQp9lK/YourCity/veh"
```

In my case, the files are in directory /tmp/RtmpJQp9lK/YourCity. Now, if you open the file file main.R, you will see:

```r
setwd('/tmp/RtmpXS55Un/YourCity')
library(vein)
# 1) Network ####
data(net)
net <- sf::st_as_sf(net)
net <- sf::st_transform(net, 31983)
saveRDS(net, 'network/net.rds')
## Are you going to need Speed?
data(pc_profile)
pc_week <- temp_fact(net$ldv+net$hdv, pc_profile)
speed <- netspeed(pc_week, net$ps, net$ffs, net$capacity, net$lkm, alpha = 1)
saveRDS(speed, 'network/speed.rds')
# 2) Traffic ####
source('traffic.R') # Edit traffic.R
# 3) Estimation ####
inputs <- list.files(path = 'est', pattern = 'input.R',
                     recursive = TRUE, full.names = TRUE)
for (i in 1:length(inputs)){
  print(inputs[i])
  source(inputs[i])
}
# 4) Post-estimation ####
g <- make_grid(net, 1000)
source('post.R')
```

This script starts with `setwd` function, Then the first section is the network, where user reads and prepares the traffic information. Then the second section runs a script whichruns the age functions for the deault vehicular composition of the `inventory` function. The third section estimates the emissions by running each input.R file inside the directory *est* The fourth section, creates a grid and run the script post.R is shown below:

```
1  # streets ####
2  CO <- emis_merge('CO', net = net)
3  saveRDS(CO, 'post/streets/CO.rds')
4
5  # grids ####
6  gCO <- emis_grid(CO, g)
7  print(plot(gCO['V1'], axes = TRUE)) # only an example
8
9  saveRDS(gCO, 'post/grids/gCO.rds')
10
11 # df ####
12 dfCO <- emis_merge('CO', what = 'DF.rds', FALSE)
13 saveRDS(dfCO, 'post/df/dfCO.rds')
14 aggregate(dfCO$g, by = list(dfCO$veh), sum, na.rm = TRUE) # Only an example
```

The function `emis_merge` shown in line 2 is designed to read the all the files with names CO and the default argument `what` is "STREETS.rds", for instance, PC_GASOLINE_CO_STREETS.rds. Hence, this function reads all the files under that condition. The other argument is `streets` with defailt value of `TRUE`, meaning that the function now knows that the resulting object must be an spatial network, and the `net` argument is already calling the net object part of the VEIN data, the function will merge all the objects summing the emissions of all vehicle street by street. The resulting object is a spatial "LINESTRING" class of `sf`. This function assumes that emissons files are data.frames and non tests have been made to see if this function would read work `sf` objects.

On the other hand, the line 12 also runs all the emissions files whose names includes the word CO, but also including the words "DF.rds", which are the files from `emis_post` with argument `by` equals to "veh". In this case, it reads and merge the data-frames and prints the sum emissions by pollutant.

If the user source he file main.R, it will calculate the emissions and produce some plots.

```
source(paste0(name, "/main.R"))
```

7.4 Creating grids

Once we have processed our emissions array with `emis_post` and/or we have spatial emissions, we can then create grids and allocate our emissions into the grids. Lets check the function `make_grid` first:

```
args(vein::make_grid)
```

```
## function (spobj, width, height = width, polygon, crs = 4326,
##     ...)
## NULL
```

This function originally used an `sp` approach. However, now uses an `sf` approach for creating the grid. Actually, the arguments are pretty much the same with the `sf::st_make_grid` with the exeption that is focused in returning polygons with coordinates at centroids of each cell. Therefore, the arguments height and polygon are deprecated. Lets create grid for our net.

```
library(vein)
library(sf)
data(net)
net <- st_transform(st_as_sf(net), 31983)
g <- make_grid(spobj = net, width = 500)
```

```
## Number of lon points: 23
## Number of lat points: 21
```

```
class(g)
```

```
## [1] "sf"         "data.frame"
```

```
plot(g$geometry, axes = TRUE)
plot(net$geometry, add = TRUE)
```

The class of `net` is `SpatialLinesDataFrame`, which is converted to `sf`. Then, as the coordinte reference system of net is WGS84 with epsg 4326, we are transforming to UTM to create a grid with grid spacing of 500 mts. The class of the grid object, `g` is "sf data.frame".

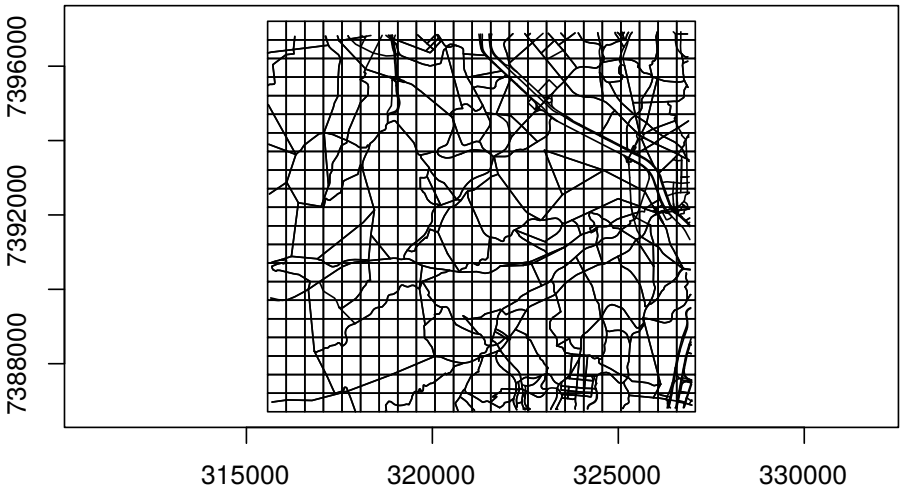


FIGURE 7.7: Grid with spacing of 500 mts

7.5 Gridding emissions with `emis_grid`

The function`emis_grid` allocates emissions proportionally to each grid cell. The process is performed by intersection between geometries and the grid. It means that requires "sr" according with your location for the projection. It is assumed that spobj is a spatial*DataFrame or an "sf" with the pollutants in data. This function return an object class "sf".

Before `sf` era, i tried to use`raster::intersect` which imports `rgeos` and took **ages**. Then I started to use QGIS Development Team (2017) (`https://www.qgis.org`), and later the R package Muenchow et al. (2018) which takes 10 minutes for allocating emissions of the mega-city of São Paulo and a grid spacing of 1 km. *10 min is not bad*. However, when `sf` appeared and also, included the Spatial Indexes (`https://www.r-spatial.org/r/2017/06/22/spatial-index.html`), it changed the game. A new era started. It took **5.5 seconds**. I could not believe it. But there also some i could accelerate this process importing some `data.table` aggregation functions. Now `emis_grid` can aggegate big spatial extensions. I havent tried yet at continental scale, but I will try. Anyways, let's go see the arguments:

```
args(vein::emis_grid)
```

```
## function (spobj, g, sr, type = "lines")
## NULL
```

Where,

- spobj : A spatial dataframe of class "sp" or "sf". When class is "sp" it is transformed to "sf".
- g: A grid with class "SpatialPolygonsDataFrame" or "sf".
- sr: Spatial reference e.g: 31983. It is required if spobj and g are not projected. Please, see http://spatialreference.org/.
- type: type of geometry: "lines" or "points".

```
data(net)
net@data <- data.frame(hdv = net[["hdv"]])
g <- make_grid(spobj = net, width = 1/102.47/2)
```

```
## Number of lon points: 23
## Number of lat points: 19
```

```
netg <- emis_grid(net, g)
```

```
## Sum of street emissions 148118

## although coordinates are longitude/latitude, st_intersection assumes that they are planar

## Sum of gridded emissions 148118
```

```
head(netg)
```

```
## Simple feature collection with 6 features and 2 fields
## geometry type:  POLYGON
## dimension:      XY
## bbox:           xmin: -46.8066 ymin: -23.62 xmax: -
46.77732 ymax: -23.61512
## epsg (SRID):    4326
```

```
## proj4string:    +proj=longlat +datum=WGS84 +no_defs
##   id      hdv                          geometry
## 1  1 201.8275 POLYGON ((-46.8066 -23.62, ...
## 2  2 200.6097 POLYGON ((-46.80172 -23.62,...
## 3  3 205.6319 POLYGON ((-46.79684 -23.62,...
## 4  4 224.1988 POLYGON ((-46.79196 -23.62,...
## 5  5 770.9490 POLYGON ((-46.78708 -23.62,...
## 6  6   0.0000 POLYGON ((-46.7822 -23.62, ...
```

```
plot(netg["hdv"], axes = TRUE)
```

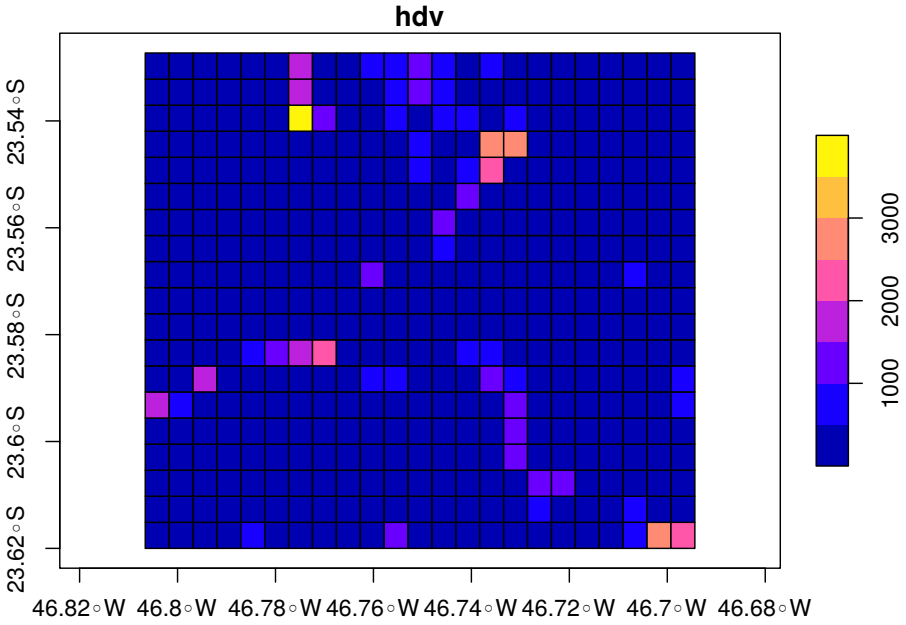


FIGURE 7.8: Spatial grid of HDV traffic 500 mts

The example in this case, showed the allocation of traffic. The resulting object is a `sf` with the sum of the attributes inside each grid cell. This means that, when the input are street emissions at different hours, it will return gridded emissions at each hour:

```
E_NOx_STREETS <- emis_post(E_NOx, by = "streets_wide", net = net)
NOxg <- emis_grid(E_NOx_STREETS, g)
```

```
## Sum of street emissions 34029872.64

## although coordinates are longitude/latitude, st_intersection assumes that they are planar

## Sum of gridded emissions 34029872.64
```

```
plot(NOxg["V1"], axes = TRUE)
```

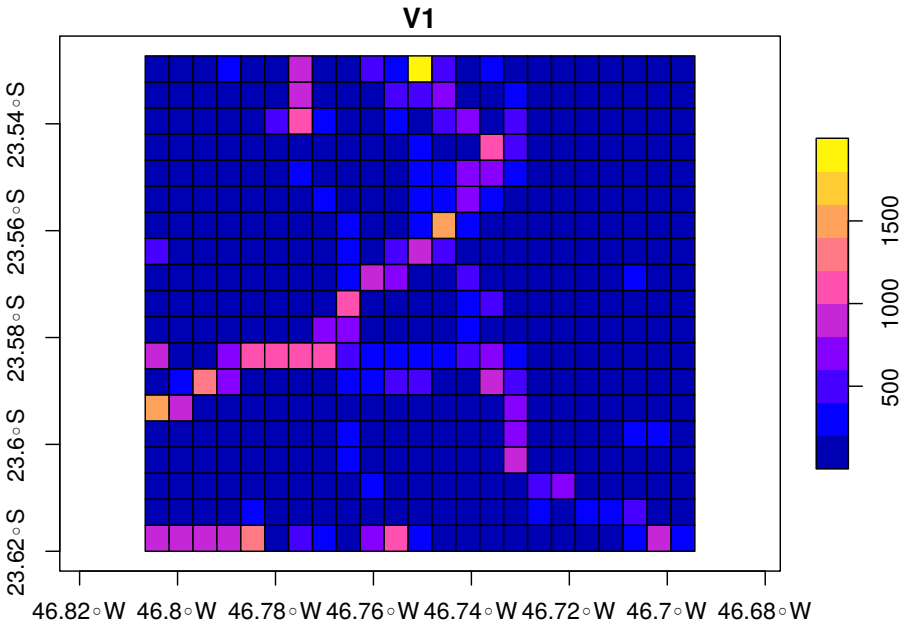


FIGURE 7.9: NOx emissions for 00:00 [g/h]

8

Speciation

The speciation for emissions is a very important part that deserves a only chapter on this book. VEIN initially covered speed functions emission factors of CO, HC, NOx, PM and Fuel Consumption (FC). But currently, the the pollutants covered are:

- **Criteria**: "CO", "NOx", "HC", "PM", "CH4", "NMHC", "CO2", "SO2", "Pb", "FC" (Fuel Consumption).
- **Polycyclic Aromatic Hydrocarbons (PAH) and Persisten Organic Pollutants (POP)**: "indeno(1,2,3-cd)pyrene", "benzo(k)fluoranthene", "benzo(b)fluoranthene", "benzo(ghi)perylene", "fluoranthene", "benzo(a)pyrene", "pyrene", "perylene", "anthanthrene", "benzo(b)fluorene", "benzo(e)pyrene", "triphenylene", "benzo(j)fluoranthene", "dibenzo(a,j)anthacene", "dibenzo(a,l)pyrene", "3,6-dimethylphenanthrene", "benzo(a)anthracene", "acenaphthylene", "acenapthene", "fluorene", "chrysene", "phenanthrene", "napthalene", "anthracene", "coronene", "dibenzo(ah)anthracene"
- **Dioxins and Furans**: "PCDD", "PCDF", "PCB".
- **Metals**: "As", "Cd", "Cr", "Cu", "Hg", "Ni", "Pb", "Se", "Zn".
- **NMHC**:
- *ALKANES*: "ethane", "propane", "butane", "isobutane", "pentane", "isopentane", "hexane", "heptane", "octane", "TWO_methylhexane", "nonane", "TWO_methylheptane", "THREE_methylhexane", "decane", "THREE_methylheptane", "alcanes_C10_C12", "alkanes_C13".
- *CYCLOALKANES*: "cycloalcanes".
- *ALKENES*: "ethylene", "propylene", "propadiene", "ONE_butene", "isobutene", "TWO_butene", "ONE_3_butadiene", "ONE_pentene", "TWO_pentene", "ONE_hexene", "dimethylhexene".
- *ALKYNES*:"ONE_butine", "propine", "acetylene".
- *ALDEHYDES*: "formaldehyde", "acetaldehyde", "acrolein", "benzaldehyde", "crotonaldehyde", "methacrolein", "butyraldehyde", "isobutanalde-

hyde", "propionaldehyde", "hexanal", "i_valeraldehyde", "valeraldehyde", "o_tolualdehyde", "m_tolualdehyde", "p_tolualdehyde".
- KETONES: "acetone", "methylethlketone".
- *AROMATICS*: "toluene", "ethylbenzene", "m_p_xylene", "o_xylene", "ONE_2_3_trimethylbenzene", "ONE_2_4_trimethylbenzene", "ONE_3_5_trimethylbenzene", "styrene", "benzene", "C9", "C10", "C13".

Also, some Brazilian emission factors and speciations for WRF-Chem, mechanisms: "e_eth", "e_hc3", "e_hc5", "e_hc8", "e_ol2", "e_olt", "e_oli", "e_iso", "e_tol", "e_xyl", "e_c2h5oh", "e_ald", "e_hcho", "e_ch3oh", "e_ket", "E_SO4i", "E_SO4j", "E_NO3i", "E_NO3j", "E_MP2.5i", "E_MP2.5j", "E_ORGi", "E_ORGj", "E_ECi", "E_ECj", "H2O".

By the end of this book, more emission factors will be added.

Because VEIN has the capabilities to produce species from this pollutants including volatile organic compunds (VOC) and particulate matter compounds.

The speciation of emissions in VEIN can be done with three ways, by selecting the pollutants in ef_speed* functions, other way explicit and the other implicit. The explicit way is by usint the function `speciate` for the specific available speciation. The implicit way is by adding a percentage value in the argument `k` in any of the functions of emission factors. The implicit way requires that the user must know the percentage of the species of pollutant.

8.1 Speed functions of VOC species

As mentioned before, the speed function emission factors, currently covers several pollutants. We firstly focus on som PAH and POP. They way to select them is just:

```
library(vein)
pol <- c("indeno(1,2,3-cd)pyrene", "benzo(k)fluoranthene",
         "benzo(b)fluoranthene", "benzo(ghi)perylene", "fluoranthene",
         "benzo(a)pyrene")
df <- lapply(1:length(pol), function(i){
  EmissionFactors(ef_ldv_speed("PC", "4S", "<=1400", "G", "PRE",
                               pol[i], x = 10)(10))
})
names(df) <- pol
df
```

```
## $`indeno(1,2,3-cd)pyrene`
## 1.03e-06 [g/km]
##
## $`benzo(k)fluoranthene`
## 3e-07 [g/km]
##
## $`benzo(b)fluoranthene`
## 8.8e-07 [g/km]
##
## $`benzo(ghi)perylene`
## 2.9e-06 [g/km]
##
## $fluoranthene
## 1.822e-05 [g/km]
##
## $`benzo(a)pyrene`
## 4.8e-07 [g/km]
```

These pollutants comes from Ntziachristos and Samaras (2016) and in this case, are not dependent on speed. I used lapply to iterate in each pollutant at 10 km/h. Now I will show the same for dioxins and furans.

```
library(vein)
pol <- c("PCDD", "PCDF", "PCB")
df <- lapply(1:length(pol), function(i){
```

```
  EmissionFactors(ef_ldv_speed("PC", "4S", "<=1400", "G", "PRE",
                               pol[i], x = 10)(10))
})
names(df) <- pol
df
```

```
## $PCDD
## 1.03e-11 [g/km]
##
## $PCDF
## 2.12e-11 [g/km]
##
## $PCB
## 6.4e-12 [g/km]
```

In the case of nmhc, the estimation is:

```
library(vein)
pol <- c("ethane", "propane", "butane", "isobutane", "pentane")
df <- lapply(1:length(pol), function(i){
  EmissionFactors(ef_ldv_speed("PC", "4S", "<=1400", "G", "PRE",
                               pol[i], x = 10)(c(10,20,30)))
})
names(df) <- pol
df
```

```
## $ethane
## Units: [g/km]
## [1] 0.09934632 0.06062781 0.04524681
##
## $propane
## Units: [g/km]
## [1] 0.02829865 0.01726974 0.01288849
##
## $butane
## Units: [g/km]
## [1] 0.1746087 0.1065580 0.0795247
```

```
##
## $isobutane
## Units: [g/km]
## [1] 0.07767076 0.04739993 0.03537478
##
## $pentane
## Units: [g/km]
## [1] 0.10717361 0.06540455 0.04881171
```

Now the same example for one pollutant and several euro standards.

```
library(vein)
euro <- c("V", "IV", "III", "II","I", "PRE")
df <- lapply(1:length(euro), function(i){
  EmissionFactors(ef_ldv_speed("PC", "4S", "<=1400", "G", euro[i],
                               "benzene")(c(10, 30, 50)))
})
names(df) <- euro
df
```

```
## $V
## Units: [g/km]
## [1] 0.0003928819 0.0002194495 0.0001597751
##
## $IV
## Units: [g/km]
## [1] 0.0004864655 0.0004872061 0.0005276205
##
## $III
## Units: [g/km]
## [1] 0.0017465678 0.0008206890 0.0005928019
##
## $II
## Units: [g/km]
## [1] 0.013332523 0.004133087 0.002363304
##
## $I
## Units: [g/km]
```

```
## [1] 0.025656752 0.010921829 0.006979341
##
## $PRE
## Units: [g/km]
## [1] 0.4112336 0.1872944 0.1287895
```

8.2 Speciate function

The arguments of the function `speciate` are:

```
args(vein::speciate)
```

```
## function (x, spec = "bcom", veh, fuel, eu, show = FALSE, list = FALSE,
##     dx)
## NULL
```

Where,

- `x`: Emissions estimation
- `spec`: speciation: The speciations are: "bcom", tyre","break","road","iag","nox" and "nmhc". 'iag' now includes a speciation for use of industrial and building paintings. "bcom" stands for black carbon and organic matter.
- `veh`: Type of vehicle: When spec is "bcom" or "nox" veh can be "PC", "LCV", HDV" or "Motorcycle". When spec is "iag" veh can take two values depending: when the speciation is for vehicles veh accepts "veh", eu "Evaporative", "Liquid" or "Exhaust" and fuel "G", "E" or "D", when the speciation is for painting, veh is "paint" fuel or eu can be "industrial" or "building" when spec is "nmhc", veh can be "LDV" with fuel "G" or "D" and eu "PRE", "I", "II", "III", "IV", "V", or "VI". when spec is "nmhc", veh can be "HDV" with fuel "D" and eu "PRE", "I", "II", "III", "IV", "V", or "VI". when spec is "nmhc" and fuel is "LPG", veh and eu must be "ALL"
- `fuel`: Fuel. When spec is "bcom" fuel can be "G" or "D". When spec is "iag" fuel can be "G", "E" or "D". When spec is "nox" fuel can be "G", "D", "LPG",

"E85" or "CNG". Not required for "tyre", "break" or "road". When spec is "nmhc" fuel can be G, D or LPG.

- `eu`: sEuro emission standard: "PRE", "ECE_1501", "ECE_1502", "ECE_1503", "I", "II", "III", "IV", "V", "III-CDFP","IV-CDFP","V-CDFP", "III-ADFP", "IV-ADFP","V-ADFP" and "OPEN_LOOP". When spec is "iag" accept the values "Exhaust" "Evaporative" and "Liquid". When spec is "nox" eu can be "PRE", "I", "II", "III", "IV", "V", "VI", "VIc", "III-DPF" or "III+CRT". Not required for "tyre", "break" or "road"
- `show`: when TRUE shows row of table with respective speciation
- `list`: when TRUE returns a list with number of elements of the list as the number species of pollutants

As shown before, there are currently 8 type of speciations. Now, i will show examples for most of them.

8.3 Black carbon and organic matter

Let's use the data inside the vein and estimate emissions. The vehicles considered are Light Trucks, assuming all HGV. We are using the 4 stage estimation with the first part arranging traffic data

```
library(vein)
# 1 Traffic data
data(net)
data(profiles)
data(fe2015)
lt <- age_hdv(net$ldv)
```

```
## Average age of age is 17.12
```

```
## Number of age is 1946.95 * 10^3 veh
```

```
vw <- temp_fact(net$ldv, profiles$PC_JUNE_2014) +
  temp_fact(net$hdv, profiles$HGV_JUNE_2014)
```

```
speed <- netspeed(vw, net$ps, net$ffs, net$capacity, net$lkm, alpha = 1)
# 2 Emission factors
euro <- c("V", rep("IV", 3),
          rep("III", 7), rep("II", 7), rep("I", 5), rep("PRE", 27))
lefd <- lapply(1:50, function(i) {
  ef_hdv_speed(v = "Trucks", t = "RT", g = ">32", gr = 0,
               eu = euro[i], l = 0.5, p = "PM",
               show.equation = FALSE) })
# 3 Estimate emissions
pmd <- emis(veh = lt, lkm = net$lkm, ef = lefd, speed = speed,
            profile = profiles$HGV_JUNE_2014)
```

```
## 32714.53 kg emissions in 24 hours and 7 days
```

```
# 4 process emissions
# Agreggating emissions by age of use
df <- apply(X = pmd, MARGIN = c(1,2), FUN = sum, na.rm = TRUE)
euro
```

```
##  [1] "V"   "IV"  "IV"  "IV"  "III" "III" "III" "III" "III" "III" "III"
## [12] "II"  "II"  "II"  "II"  "II"  "II"  "II"  "I"   "I"   "I"   "I"
## [23] "I"   "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE"
## [34] "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE" "PRE"
## [45] "PRE" "PRE" "PRE" "PRE" "PRE" "PRE"
```

```
dfbcom <-   rbind(speciate(df[, 1], "bcom", "PC", "D", "V"),
                  speciate(rowSums(df[, 2:4]), "bcom", "PC", "D", "IV"),
                  speciate(rowSums(df[, 5:11]), "bcom", "PC", "D", "III"),
                  speciate(rowSums(df[, 12:18]), "bcom", "PC", "D", "II"),
                  speciate(rowSums(df[, 19:23]), "bcom", "PC", "D", "I"),
                  speciate(rowSums(df[, 24:50]), "bcom", "PC", "D", "PRE"))
dfbcom$id <- 1:1505
bc <- aggregate(dfbcom$BC, by = list(dfbcom$id), sum)
om <- aggregate(dfbcom$OM, by = list(dfbcom$id), sum)
net$BC <- bc[, 2]
net$OM <- om[, 2]
```

Now we have spatial objects of Back Carbon

```
sp::spplot(net, "BC", scales = list(draw = T), main = "Black Carbon [g/168h]",
           col.regions = rev(cptcity::cpt()))
```

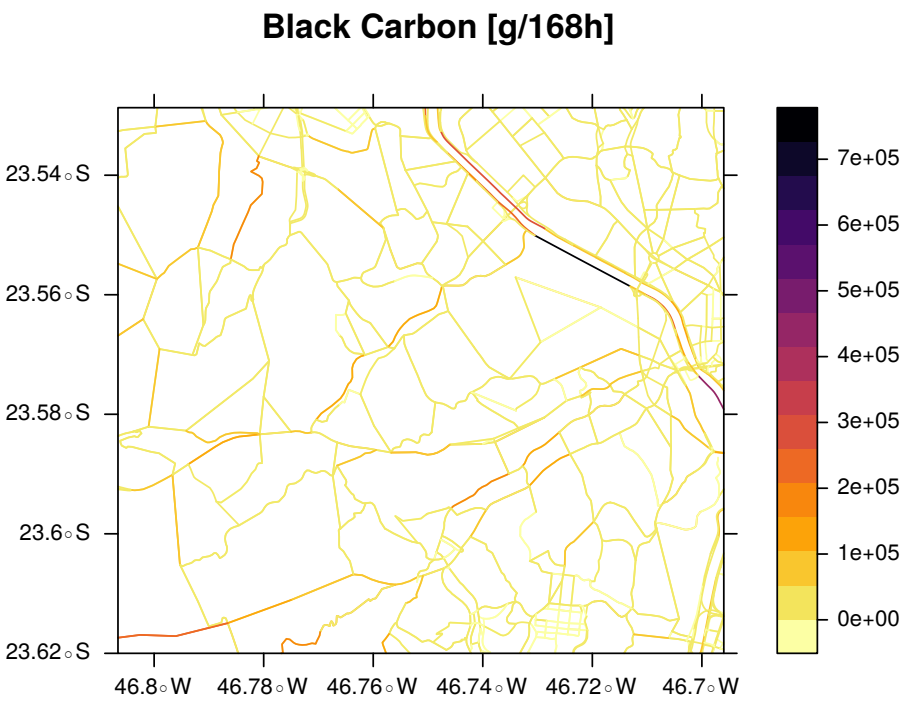


FIGURE 8.1: Black Carbon [g/168h]

and Organic Matter

```
sp::spplot(net, "OM", scales = list(draw = T), main = "Organic Matter [g/168h]",
           col.regions = rev(cptcity::cpt()))
```

If you are interested in speciate total emissions by age of use not spatial emissions, you could use `emis_post` with `by = "veh"` and then aggregate the emissions by standard. Then speciate PM by standard:

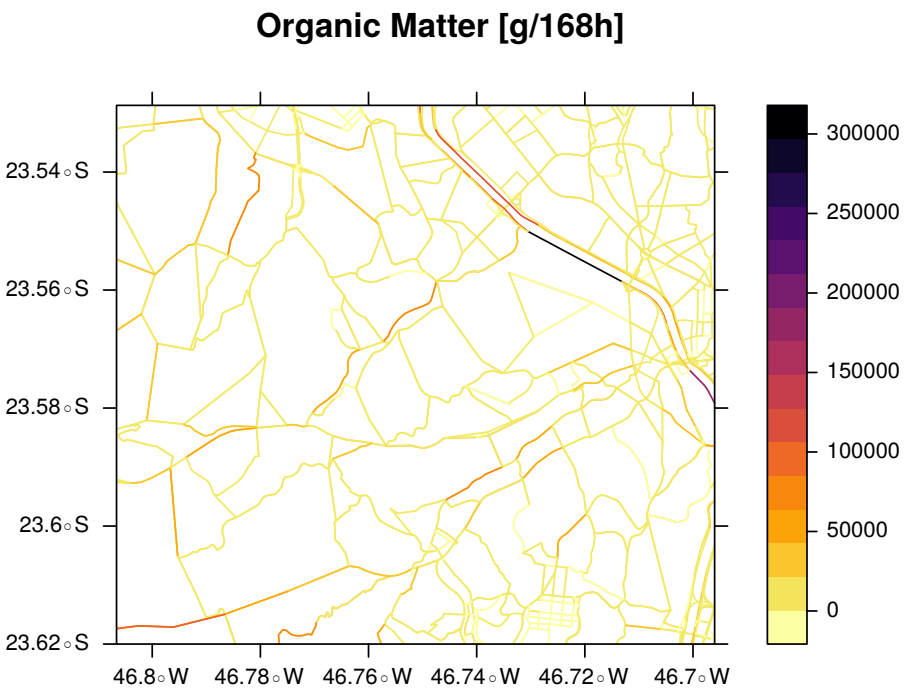


FIGURE 8.2: Organic Matter [g/168h]

```
dfpm <- emis_post(arra = pmd,  veh = "LT", size = "small", fuel = "D",
                  pollutant = "PM", by = "veh")
dfpm$euro <- euro
dfpmeuro <- aggregate(dfpm$g, by = list(dfpm$euro), sum)
names(dfpmeuro) <- c("euro", "g")
bcom <- as.data.frame(sapply(1:6, function(i){
  speciate(dfpmeuro$g[i], "bcom", "PC", "D", dfpmeuro$euro[i])
}))
names(bcom) <- dfpmeuro$euro
```

And the resulting speciation is:

TABLE 8.1: Black Carbon and Organic Matter [g/168h]

	I	II	III	IV	PRE
BC	6826527.37503195	5313757.92745243	3321183.01325297	155078.69338865	6700527.8093088
OM	2730610.95001278	1222164.32331406	498177.451987945	20160.2301405245	4690369.46651618

8.4 Tyre wear, breaks wear and road abrassion

Tyre, break and road abrassions comes from Ntziachristos and Boulter (2009). Tyres consist in a complex mixture of rubber, which after the use starts to degradate. In deed, when the driving cycle ismore aggresive, higher is tyre mass emitted from tyre, with tyre wear emission factors higher in HDV than LDV. Break wear emits mass and with more aggresive driving, more emissions.

The input are wear emissions in Total Suspended Particles (TSP) ,as explained in section @ref(#ew). The speciation consists in 60% PM10, 42% PM2.5, 6% PM1 and 4.8% PM0.1. Now, a simple example for TP adspeciation:

```
library(vein)
data(net)
data(profiles)
pro <- profiles$PC_JUNE_2012[, 1] # 24 hours
pc_week <- temp_fact(net$ldv+net$hdv, pro)
df <- netspeed(pc_week, net$ps, net$ffs, net$capacity, net$lkm, alpha = 1)
ef <- ef_wear(wear = "tyre", type = "PC", speed = df)
emit <- emis_wear(veh = age_ldv(net$ldv, name = "VEH"), speed = df,
                  lkm = net$lkm, ef = ef, profile =  pro)
```

```
## Average age of VEH is 11.17
```

```
## Number of VEH is 1946.95 * 10^3 veh
```

```
emib <- emis_wear(what = "break", veh = age_ldv(net$ldv, name = "VEH"),
                  lkm = net$lkm, ef = ef, profile =  pro, speed = df)
```

```
## Average age of VEH is 11.17
## Number of VEH is 1946.95 * 10^3 veh
```

```
emit
```

```
## This EmissionsArray has
##  1505 streets
##  50 vehicle categories
##  24 hours
##  1 days
## [1] 0.0499920404 0.0183982869 0.0026973699 0.0066891571 0.0002749512
## [6] 0.0212774028
```

```
emib
```

```
## This EmissionsArray has
##  1505 streets
##  50 vehicle categories
##  24 hours
##  1 days
## [1] 0.0528581237 0.0153135442 0.0022451163 0.0070774117 0.0002288516
## [6] 0.0271699850
```

```
emitp <- emis_post(arra = emit, veh = "PC", size = "ALL", fuel = "G",
                   pollutant = "TSP", by = "veh")
emibp <- emis_post(arra = emib, veh = "PC", size = "ALL", fuel = "G",
                   pollutant = "TSP", by = "veh")
```

The estimation covered 24 hours and for simplicity, we are assuming a year with 365 similar days and dividing by 1 million to have t/y. Hence,the speciation is:

```
library(ggplot2)
tyrew <- speciate(x =  unclass(emitp$g), spec = "tyre")
breakw <- speciate(x =  unclass(emibp$g), spec = "brake")
df <- data.frame(Emis = c(sapply(tyrew, sum), sapply(breakw, sum))*365/1000000)
df$Pollutant <- factor(x = names(tyrew), levels = names(tyrew))
df$Emissions <- c(rep("Tyre", 4), rep("Brake", 4))
ggplot(df, aes(x = Pollutant, y = Emis, fill = Emissions)) +
  geom_bar(stat = "identity", position = "dodge")+
  labs(x = NULL, y = "[t/y]")
```

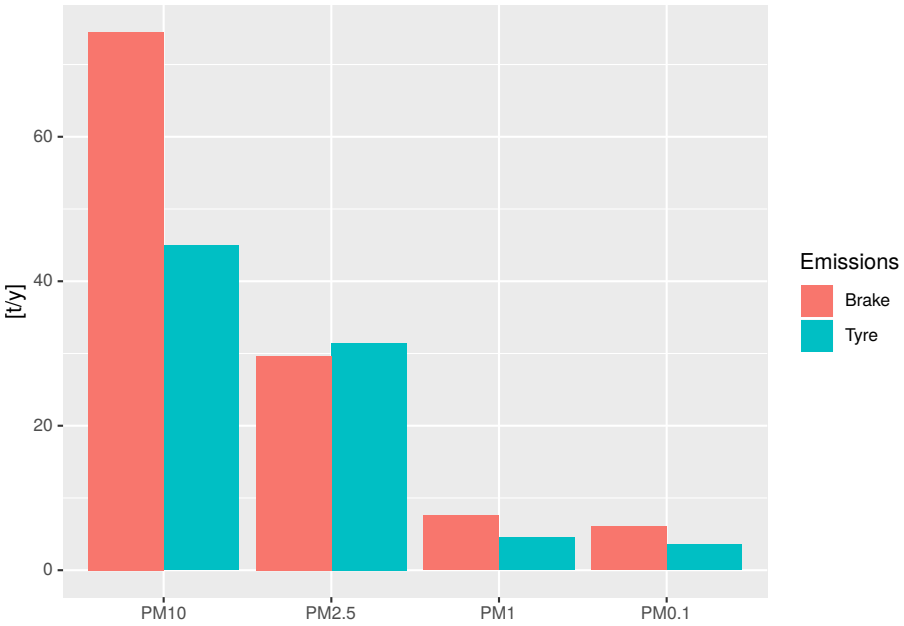


FIGURE 8.3: Break and Tyre emissions (t/y)

It is interesting to see that break emissions are higher than tyre wear emissions, and the smalle the diameter, higher the difference, as shows:

The procudure can be used with `emis_post` with `by = streets_wide` to obtain the spatial speciation.

TABLE 8.2: Ratio between break and tyre wear emissions

	x
PM10	1.6593167
PM2.5	0.9433433
PM1	1.6931803
PM0.1	1.6931803

8.5 NO and NO_2

The speciation of NO_X into NO and $NO2$ depends on the type of vehicle, fuel and euro standard. The following example will consists in comparing a Gasoline passenger car and a Diesel truck.

```
library(vein)
data(net)
data(profiles)
propc <- profiles$PC_JUNE_2012[, 1] # 24 hours
prolt <- profiles$PC_JUNE_2012[, 1] # 24 hours
pweek <- temp_fact(net$ldv+net$hdv, pro)
df <- netspeed(pc_week, net$ps, net$ffs, net$capacity, net$lkm, alpha = 1)
euro <- c("V", rep("IV", 3),
          rep("III", 7), rep("II", 7), rep("I", 5), rep("PRE", 27))
lefpc <- lapply(1:50, function(i) {
  ef_ldv_speed(v = "PC", t = "4S", cc = "<=1400", f = "G",
               eu = euro[i], p = "NOx", show.equation = FALSE) })
leflt <- lapply(1:50, function(i) {
  ef_hdv_speed(v = "Trucks", t = "RT", g = ">32", gr = 0,
               eu = euro[i], l = 0.5, p = "NOx", show.equation = FALSE) })
emipc <- emis(veh = age_ldv(net$ldv),lkm = net$lkm, ef = lefpc, speed = df,
              profile = profiles$PC_JUNE_2014[, 1])*365/1000000
```

```
## Average age of age is 11.17
```

```
## Number of age is 1946.95 * 10^3 veh
```

```
## 4097.62 kg emissions in 24 hours and 1 days
```

```
emilt <- emis(veh = age_ldv(net$hdv),lkm = net$lkm, ef = leflt, speed = df,
              profile = profiles$HGV_JUNE_2014[, 1])*365/1000000
```

```
## Average age of age is 11.17

## Number of age is 148.12 * 10^3 veh

## 14612.67 kg emissions in 24 hours and 1 days
```

Then, once the emissions are estimated, we will speciate the emissions by euro standard. The estimation covered 24 hours and for simplicity, we are assuming a year with 365 similar days and dividing by 1 million to have t/y.

```
df <- rowSums(apply(X = emipc, MARGIN = c(2,3), FUN = sum, na.rm = TRUE))
dfpc <-   rbind(speciate(df[1], "nox", "PC", "G", "V"),
                speciate(df[2:4], "nox", "PC", "G", "V"),
                speciate(df[5:11], "nox", "PC", "G", "V"),
                speciate(df[12:18], "nox", "PC", "G", "V"),
                speciate(df[19:23], "nox", "PC", "G", "V"),
                speciate(df[24:50], "nox", "PC", "G", "V"))
df <- rowSums(apply(X = emipc, MARGIN = c(2,3), FUN = sum, na.rm = TRUE))
dfhdv <-   rbind(speciate(df[1], "nox", "HDV", "D", "V"),
                 speciate(df[2:4], "nox", "HDV", "D", "V"),
                 speciate(df[5:11], "nox", "HDV", "D", "V"),
                 speciate(df[12:18], "nox", "HDV", "D", "V"),
                 speciate(df[19:23], "nox", "HDV", "D", "V"),
                 speciate(df[24:50], "nox", "HDV", "D", "V"))

df <- data.frame(rbind(sapply(dfpc, sum), sapply(dfhdv, sum)))
row.names(df) <- c("PC", "HGV")
knitr::kable(df, caption = "NO2 and NO speciation (t/y)")
```

TABLE 8.3: NO2 and NO speciation (t/y)

	NO2	NO
PC	44.8689	1450.761
HGV	179.4756	1316.154

8.6 Volatile organic compounds: `nmhc`

nmhc were shown earluier in this chapter, but they can be also used to speciate objects, resulting in all species at once. The speciation of NMHC must be applied to NMHC. However, the emission guidelines of Ntziachristos and Samaras (2016) does not show explicit emission factor of NMHC and the suggeted procedure is substract the CH_4 from the HC. This was done on VEIN and now, ef_speed* functions returns NMHC directly. This makes easier to produce speciation.

```
library(vein)
data(net)
data(profiles)
propc <- profiles$PC_JUNE_2012[, 1] # 24 hours
pweek <- temp_fact(net$ldv+net$hdv, propc)
df <- netspeed(pweek, net$ps, net$ffs, net$capacity, net$lkm, alpha = 1)
euro <- c("V", rep("IV", 3),
          rep("III", 7), rep("II", 7), rep("I", 5), rep("PRE", 27))
lefpc <- lapply(1:50, function(i) {
  ef_ldv_speed(v = "PC", t = "4S", cc = "<=1400", f = "G",
               eu = euro[i], p = "NMHC", show.equation = FALSE)})
```

```
euro <- c("V", rep("IV", 3),
          rep("III", 7), rep("II", 7), rep("I", 5), rep("PRE", 27))
lefpc <- lapply(1:length(euro), function(i) {
  ef_ldv_speed(v = "PC", t = "4S", cc = "<=1400", f = "G",
               eu = euro[i], p = "HC", show.equation = FALSE) })
```

```
enmhc <- emis(veh = age_ldv(net$ldv), lkm = net$lkm, ef = lefpc, speed = df,
              profile = profiles$PC_JUNE_2014[, 1])
```

```
## Average age of age is 11.17
```

```
## Number of age is 1946.95 * 10^3 veh
```

```
## 3030.65 kg emissions in 24 hours and 1 days
```

```
df_enmhc <- emis_post(arra = enmhc, veh = "PC", size = "ALL", fuel = "G",
                      pollutant = "NMHC", by = "veh")
# assuming all euro I
spec <- speciate(x = as.numeric(df_enmhc$g), spec = "nmhc", veh = "LDV",
                 fuel = "G", eu = "I")
names(spec)
```

```
##  [1] "ethane"                "propane"
##  [3] "butane"                "isobutane"
##  [5] "pentane"               "isopentane"
##  [7] "hexane"                "heptane"
##  [9] "octane"                "TWO_methylhexane"
## [11] "nonane"                "TWO_methylheptane"
## [13] "THREE_methylhexane"    "decane"
## [15] "THREE_methylheptane"   "alcanes_C10_C12"
## [17] "alkanes_C13"           "cycloalcanes"
## [19] "ethylene"              "propylene"
## [21] "propadiene"            "ONE_butene"
## [23] "isobutene"             "TWO_butene"
## [25] "ONE_3_butadiene"       "ONE_pentene"
## [27] "TWO_pentene"           "ONE_hexene"
## [29] "dimethylhexene"        "ONE_butine"
## [31] "propine"               "acetylene"
## [33] "formaldehyde"          "acetaldehyde"
## [35] "acrolein"              "benzaldehyde"
## [37] "crotonaldehyde"        "methacrolein"
## [39] "butyraldehyde"         "isobutanaldehyde"
## [41] "propionaldehyde"       "hexanal"
```

```
## [43] "i_valeraldehyde"           "valeraldehyde"
## [45] "o_tolualdehyde"            "m_tolualdehyde"
## [47] "p_tolualdehyde"            "acetone"
## [49] "methylethlketone"          "toluene"
## [51] "ethylbenzene"              "m_p_xylene"
## [53] "o_xylene"                  "ONE_2_3_trimethylbenzene"
## [55] "ONE_2_4_trimethylbenzene" "ONE_3_5_trimethylbenzene"
## [57] "styrene"                   "benzene"
## [59] "C9"                        "C10"
## [61] "C13"
```

8.7 The speciation `iag`

The Carbon Bond Mechanism Z (1999) is an lumped-structure mechanism.

Citing:

"it is currently unfeasible to treat the organic species individually in a regional or global chemistry model for three major reasons:

- (1) limited computational resources, - (2) lack of detailed speciated emissions inventories, and - (3) lack of kinetic and mechanistic information for all the species and their reaction products.

Thus there exists a need for a condensed mechanism that is capable of describing the tropospheric hydrocarbon chemistry with reasonable accuracy, sensitivity, and speed at regional to global scales.

The research in this aspect is intense and out of the scope of this book. However, it is important that the user who intends to performs atmospheric simulation to understand this why it is important to speciate the emissions and what represent each group.

A popular air quality model nowedays is the Weather Research and Forecasting model coupled to Chemistry (WRF-Chem) (Grell et al., 2005) `https://ruc.noaa.gov/wrf/wrf-chem/and` the **Emissions Guide** (`https://ruc.noaa.gov/wrf/wrf-chem/Emission_guide.pdf`).

The speciation iag splits the NMHC into the lumped groups for the mechanism CMB-Z. The name iag comes from the Institute of Astronomy, Geophysics and Atmospheric Sciences (IAG, http://www.iag.usp.br/) from the University of São Paulo (USP). The Departament of Atmospheric Sciences (DAC) of IAG has measure and model air quality models for several years. There are several scientific production such as: Nogueira et al. (2015), Hoshyaripour et al. (2016), Andrade et al. (2017), Freitas et al. (2005), Martins et al. (2006), Pérez-Martinez et al. (2014), Ulke and Andrade (2001), Vivanco and de Fátima Andrade (2006), Boian and Andrade (2012), de Fatima Andrade et al. (2012), Andrade et al. (2015), Vara-Vela et al. (2016), Rafee (2015), Ibarra-Espinosa et al. (2017c). The following figure, shows an air quality simulation over South Easth Brazil from DAC/IAG/USP.

Some of these papers show measurements in tunnels, fuel, etc. The speciation iag it is based on these experiments, and the last versions, covers an update during 2015 so that the exhaust emissions speciation is more representative of brazilian gasoline. This means that:

- ** THE SPECIATION IAG IS BASED ON BRAZILIAN MEASUREMENTS**.

and the user who wants to applt it outside Brazil, should be ensure, that the fleet and fuel are compatible. As that will be hard to accomplish, I can say that this speciation is for and to be used in Brazil, even more, in São Paulo.

The currently speciation iag is:

The arguments of the function speciate take the following form:

- x: Emissions estimation, it is recommended that x are griddded emissions from NMHC.
- spec: iag. Alternatively, you can put any name of the following: “e_eth”, “e_hc3”, “e_hc5”, “e_hc8”, “e_ol2”, “e_olt”, “e_oli”, “e_iso”, “e_tol”, “e_xyl”, “e_c2h5oh”, “e_hcho”, “e_ch3oh”, “e_ket”
- veh: When spec is “iag” veh can take two values depending: when the speciation is for vehicles veh accepts “veh”, eu “Evaporative”, “Liquid” or “Exhaust”
- fuel: “G”, “E” or “D”.
- eu: “Exhaust” “Evaporative” or “Liquid”.

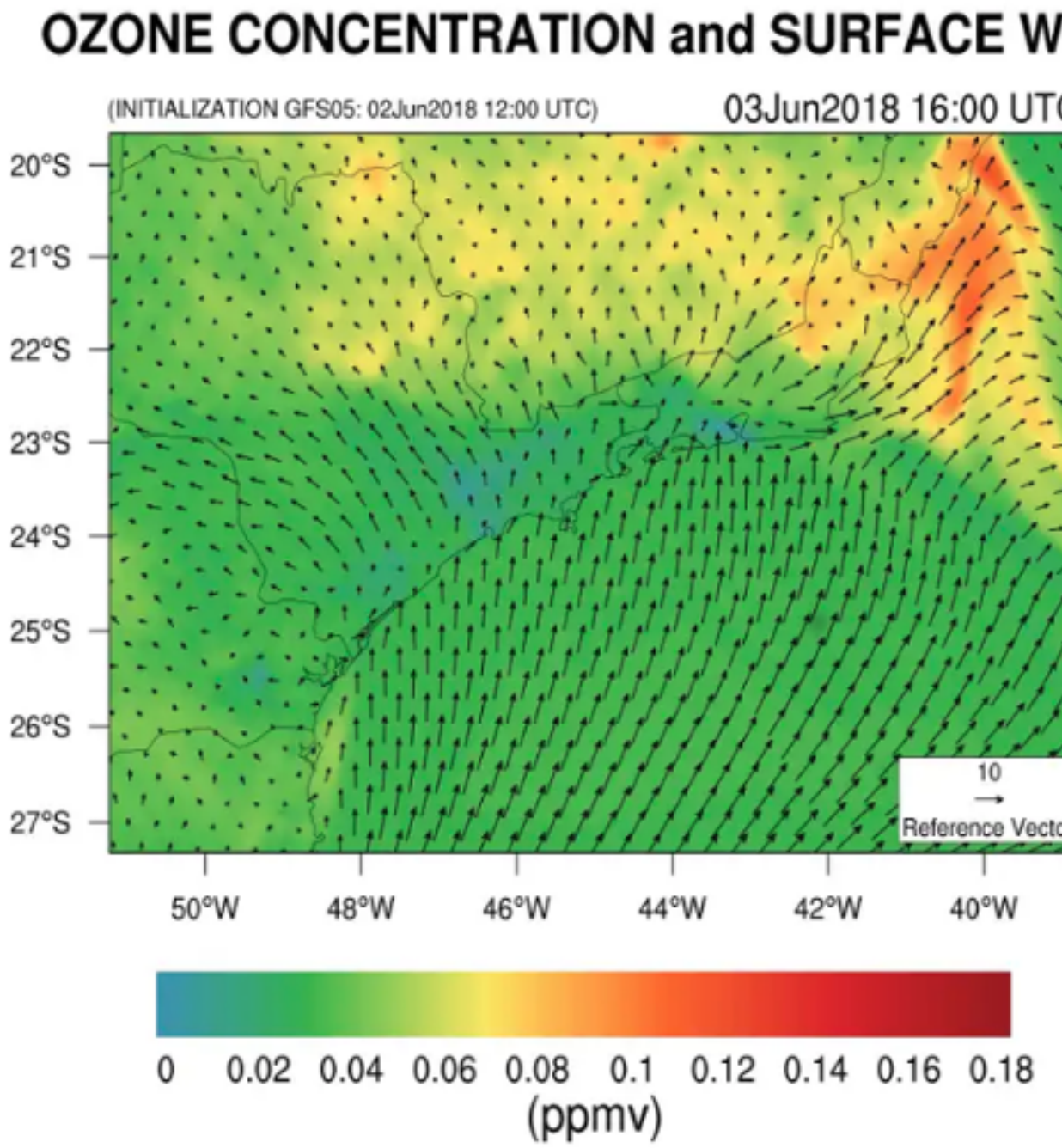


FIGURE 8.4: http://www.lapat.iag.usp.br/aerossol/wrf9/index.php

		NMHC with E25			NMHC
NMHC	MIR	Exhaust	Evap	Liq	Exhaust
ETH	0.28	0.2826	0.2317	0.0250	0
HC_3	1.33	0.4352	0.3567	0.2400	0
HC_5	1.58	0.1586	0.1300	0.4500	0
HC_8	1.01	0.0765	0.0627	0	0.0490
OL_2	9.07	0.5807	0.2800	0.0382	0.1260
OLT	8.91	0.2434	0.1174	0.200	0.0018
OLI	1.94	0.1614	0.1323	0.4600	0.0013
ISO	10.68	0.0077	0.0037	0	0
TOL	2.5	0.1405	0.1152	0.0850	0.0050
XYL	8.15	0.2677	0.1291	0	0.0149
C_2H_5OH	1.69	0.3082	0.3082	0.3500	1.5226
$HCHO$	6.98	0.1127	0.0508	0	0.3605
ALD	8.96	0.0864	0.0663	0	0.1317
CH_3OH	0.65	0	0	0	0
KET	1.65	0	0	0	0

FIGURE 8.5: Speciation for NMHC by type of fuel and process mol/100g (Ibarra-Espinosa, S., 2017)

- `show`: Let this FALSE.
- `list`: Let this TRUE so that the result is a list, and each element of the list a lumped specie.

Example:

```
# Do not run
x <- data.frame(x = rnorm(n = 100, mean = 400, sd = 2))
```

```
dfa <- speciate(x, spec = "e_eth", veh = "veh", fuel = "G", eu = "Exhaust")
head(dfa)
```

```
##       e_eth
## 1 0.9266105
## 2 0.9261302
## 3 0.9241043
## 4 0.9280154
## 5 0.9129768
## 6 0.9303943
```

```
df <- speciate(x, spec = "iag", veh = "veh", fuel = "G",
               eu = "Exhaust", list = TRUE)
names(df)
```

```
##  [1] "e_eth"    "e_hc3"    "e_hc5"    "e_hc8"    "e_ol2"    "e_olt"
##  [7] "e_oli"    "e_iso"    "e_tol"    "e_xyl"    "e_c2h5oh" "e_ald"
## [13] "e_hcho"   "e_ch3oh"  "e_ket"
```

```
for(i in 1:length(df)){
  print(df[[i]][1:3, ]) # Firt three lines of each element of the list
}
```

```
## Units: [mol/h]
## [1] 0.9266105 0.9261302 0.9241043
## Units: [mol/h]
## [1] 1.426859 1.426119 1.422999
## Units: [mol/h]
## [1] 0.5200474 0.5197779 0.5186409
## Units: [mol/h]
## [1] 0.2509360 0.2508059 0.2502573
## Units: [mol/h]
## [1] 1.903939 1.902952 1.898790
## Units: [mol/h]
## [1] 0.7982062 0.7977924 0.7960473
## Units: [mol/h]
```

TABLE 8.4: Speciation of PM2.5

E_SO4i	E_SO4j	E_NO3i	E_NO3j	E_MP2.5i	E_MP2.5j	E_ORGi	E_ORGj	E_ECi	E_ECj	E
0.0077	0.0623	0.00247	0.01053	0.1	0.3	0.0304	0.1296	0.056	0.024	0

```
## [1] 0.5291831 0.5289088 0.5277519
## Units: [mol/h]
## [1] 0.02538359 0.02537043 0.02531494
## Units: [mol/h]
## [1] 0.4606613 0.4604225 0.4594154
## Units: [mol/h]
## [1] 0.8776344 0.8771795 0.8752607
## Units: [mol/h]
## [1] 1.232777 1.232138 1.229443
## Units: [mol/h]
## [1] 0.3455650 0.3453859 0.3446304
## Units: [mol/h]
## [1] 0.4506896 0.4504560 0.4494707
## Units: [mol/h]
## [1] 0 0 0
## Units: [mol/h]
## [1] 0 0 0
```

8.8 The speciation `pmiag`

The speciation `pmiag`is also based on IAG studies and applied only for PM2.5 emissions. The speciation splits the PM2.5 in percentages as follow:

When running this speciation, the only two required arguments are `x` and `spec`. Also, There is a message that this speciation applies **only in gridded emissions, because the unit must be in flux** $g/km^2/h$, and internally are transformed to the required unit $ μg/m^2/s$ as:

$$\frac{g}{(km)^2 * h} * \frac{10^6 \mu g}{g} * (\frac{km}{1000m})^2 * \frac{h}{3600s} \frac{1}{dx^2}$$

dx is the length of the grid cell. Example:

```
library(vein)
data(net)
pm <- data.frame(pm = rnorm(n = length(net), mean = 400, sd = 2))
net@data <- pm
g <- make_grid(net, 1/102.47/2) # 500 m
```

```
## Number of lon points: 23
## Number of lat points: 19
```

```
gx <- emis_grid(net, g)
```

```
## Sum of street emissions 601988.04
## although coordinates are longitude/latitude, st_intersection assumes that they are planar
## Sum of gridded emissions 601988.04
```

```
df <- speciate(gx, spec = "pmiag", veh = "veh", fuel = "G",
               eu = "Exhaust", list = FALSE, dx = 0.5)
```

```
## To be used in emissions grid only, emissions must be in g/(Xkm^2)/h
## PM.2.5-10 must be calculated as substraction of PM10-
PM2.5 to enter this variable into WRF
```

```
names(df)
```

```
##  [1] "e_so4i"   "e_so4j"   "e_no3i"   "e_no3j"   "e_pm2.5i" "e_pm2.5j"
##  [7] "e_orgi"   "e_orgj"   "e_eci"    "e_ecj"    "h2o"
```

```
head(df)
```

```
##                  e_so4i     e_so4j       e_no3i      e_no3j   e_pm2.5i
## 1 0.001448040 [g/m^2/s] 0.01171596 0.0004645010 0.001980241 0.01880571
## 2 0.001439303 [g/m^2/s] 0.01164527 0.0004616984 0.001968293 0.01869224
```

```
## 3 0.001475335 [g/m^2/s] 0.01193680 0.0004732569 0.002017569 0.01916020
## 4 0.002549542 [g/m^2/s] 0.02062811 0.0008178400 0.003486581 0.03311093
## 5 0.005804243 [g/m^2/s] 0.04696160 0.0018618804 0.007937490 0.07537977
## 6 0.000000000 [g/m^2/s] 0.00000000 0.0000000000 0.000000000 0.00000000
##     e_pm2.5j      e_orgi     e_orgj      e_eci       e_ecj        h2o
## 1 0.05641712 0.005716935 0.02437220 0.01053120 0.004513370 0.05209181
## 2 0.05607673 0.005682442 0.02422515 0.01046766 0.004486138 0.05177751
## 3 0.05748060 0.005824700 0.02483162 0.01072971 0.004598448 0.05307375
## 4 0.09933280 0.010065724 0.04291177 0.01854212 0.007946624 0.09171728
## 5 0.22613932 0.022915451 0.09769219 0.04221267 0.018091146 0.20880198
## 6 0.00000000 0.000000000 0.00000000 0.00000000 0.000000000 0.00000000
```

9

Inputs for atmospheric models

This last chapter of this book is about generating inputs for atmospheric models, specifically, **WRF-Chem** (Grell et al., 2005). As the Pacific Northwest National Laboratory (PNNL, `https://www.pnnl.gov/atmospheric/research/wrf-chem/`) defines:

The Weather Research and Forecasting (WRF) model is a next generation meteorological model being developed collaboratively among several agencies (NOAA/NCEP, NOAA/ESRL, NCAR). WRF-Chem is a version of WRF that also simultaneously simulates the emission, turbulent mixing, transport, transformation, and fate of trace gases and aerosols.

Initially, VEIN counted with the function `emis_wrf` which created a data.frame object of hourly gridded emissions with each pollutant as a column, from the first cell to the last. The data-frame extendend in long format to each hour. This data.frame was designed to be used with script Another Asimilation System for WRF (AS4WRF) (Vara-Vela et al., 2016) written in NCL (Boulder, 2017).

This approach was effective and already tested for some Latinamerican cities (Ibarra et al., 2015a), (Ibarra et al., 2015b). However, this function depends on external software which may not be available. Therefore, me andsome collegues developed the package `eixport` (Ibarra-Espinosa et al., 2018b), (Ibarra-Espinosa et al., 2017b), which is an R package to read and export emissions to atmospheric models. `eixport` currently covers the models WRF-Chem (Grell et al., 2005), SPM-BRAMS (Freitas et al., 2005) and R-LINE (Snyder et al., 2013), but only the WRF-Chem interface has been fully implemented. Therefore, this chapter covers only this model.

The concept of connecting VEIN and Wrf-Chem via eixport is quite simple with two approaches:

1. Generating `GriddedEmissionsArray` for the wrfinput grid and inputting this emissions into the wrfchemi input file..
2. Generating gridded emissions data-frame for AS4WRF.

9.1 WRFChem input with wrfinput and `GriddedEmissionsArray`

The process for generation WRF-Chem input files with `GriddedEmissionsArray` is shown on Fig. 9.1. Pink boxes are classes, grey boxes are `vein` functions, green functions are `eixport` functions and white boxes, external objects. Here, the external input file is the **wrfinputd_0x** file, where the **x** is for the domain. This file is inputted into the function `make_grid` which creates a polygon grid needed by `emis_grid`. The main characteristic of this grid, is that it has the resolution of the wrfinput file.

The wrfinpiut_d0x file isalso used by the `eixport` function `wrf_create` to create a wrfchemi input file with zeroes.

The objects with class `EmissionsArray` for each type of vehicle and pollutant are processed by the function `emis_post` which create street emissions. Then, the function `emis_merge` merges all the street emissions files from `emis_post_ into one street emissions by pollutant ehich is inputted into function`emis_grid`to create a polygon grid of emissions, class Spatial Feature`sf`[@sf], [@RJ-2018-009]. Then, the spatial gridded emissions are inputted into the contructor function`GriddedEmissionsArray‘ to create an object of that class, and the dimensions of the wrfinput file, that is, the sanem number of spatial rows and columns.

Finally, the `GriddedEmissionsArray` objects are inputted into the wrfchemi file with the `eixport` function `wrf_put`.

Example

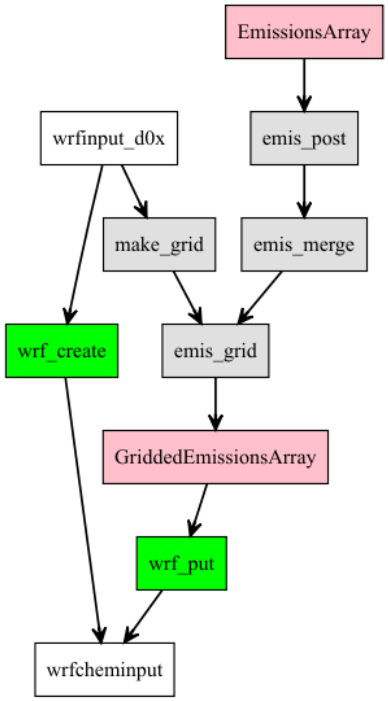


FIGURE 9.1: Generation of wrfchem inputs using GriddedEmissionsArray

9.1.1 Creating a WRF-Chem input file

The emission file will be generated with traffic simulation from the Traffic Engineering Company (CET) for 2012, which consists in traffic flow for morning rush hour of Light Duty Vehicles (LDV). The emission factors will be the data `fe2015` and the wrfinput comes from the `eixport` package. Let's go:

9.1.1.1 0) Network

The object net has a class `SpatialLinesDataFrame`, we transform it into a `sf`object. The length of the road is the field 'lkm' in the object net, which are in km but has no units. We must add the right units in order to use `vein`

```
require(vein)
require(sf)
require(units)
net <- readRDS("figuras/net.rds")
class(net)
net <- sf::st_as_sf(net)
net[1, ]
net$lkm <- units::set_units(st_length(net), km) # ensure right units
```

9.1.1.2 1) Vehicular composition

In this case, the vehicular composition consits in only to vehicles, Passenger Cars using Gasoline with 25% of Ethanol and Light Trucks consuming Diesel with 5% od biodiesel. Also, the emission factors cover CO. The temporal distribution will cover only one hour.

```
PC_E25 <- age_ldv(net$ldv)
```

9.1.1.3 2) Emission factors

The emission factors used comes from CETESB (2015), which are constant by age of use. In practice, this data.frame is like an Excel spreadsheet. Then, the constructor function `EmissionFactorsList` convert our numeric vector, which is the column of our data.frame, into required type of object of the `emis` function. Parenthesis were added in order to print the objects in one line.

```
data(fe2015)
(EF_CO_PC_E25 <- EmissionFactorsList(fe2015[fe2015$Pollutant == "CO", "PC_G"]))
```

9.1.1.4 3) Estimation of emissions

The estimation of emissions is shown in the following code chunk in a simplified way. The emissions array are aggregated.

```
data(profiles)
emi <- emis(veh = PC_E25, lkm = net$lkm, ef = EF_CO_PC_E25,
            profile = profiles$PC_JUNE_2012)
```

9.1.1.5 4) Post-estimations

The resulting emissions array `emi` is now processed with `emis_post`.

```
co_street <- emis_post(arra = emi, by = "streets_wide", net = net)
```

9.1.1.5.1 4a WRFChem input file with `eixport`

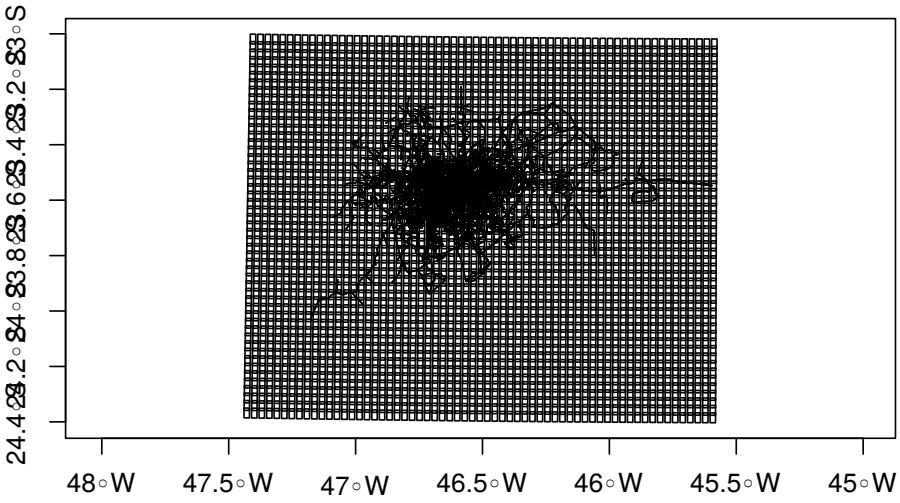
Now it is time generate the emissions grid. In order to create a wrfchem input file, we need a wrfinput file. In this case, the wrfinput coversa wider area of the emissions, located in São Paulo, Brazil. The wrfinput file is available from the R package `eixport`.

```
wrf <- paste(system.file("extdata", package = "eixport"),
             "/wrfinput_d02", sep="")
g  <- make_grid(wrf)
```

```
## path to wrfinput

## using grid info from: /home/sergio/R/x86_64-pc-linux-gnu-
library/3.5/eixport/extdata/wrfinput_d02
## Number of lat points 51
## Number of lon points 63
```

```
plot(st_geometry(g), axes = TRUE)
plot(st_geometry(co_street), add = TRUE)
```



Notice that weh we create grid from the path to wrfinput, there is a message with *Number of lat points 51* and *Number of lon points 63*. This information is crytical for later conversions. Now that we have the street emissions and the grid, we can obtain our gridded emissions:

```
gCO <- emis_grid(spobj = co_street, g = g)
```

```
## Sum of street emissions 1845699895.43

## although coordinates are longitude/latitude, st_intersection assumes that they are planar

## Sum of gridded emissions 1845699895.43
```

```
names(gCO)
```

```
##   [1] "id"      "V1"      "V2"      "V3"      "V4"      "V5"
##   [7] "V6"      "V7"      "V8"      "V9"      "V10"     "V11"
##  [13] "V12"     "V13"     "V14"     "V15"     "V16"     "V17"
##  [19] "V18"     "V19"     "V20"     "V21"     "V22"     "V23"
##  [25] "V24"     "V25"     "V26"     "V27"     "V28"     "V29"
##  [31] "V30"     "V31"     "V32"     "V33"     "V34"     "V35"
##  [37] "V36"     "V37"     "V38"     "V39"     "V40"     "V41"
##  [43] "V42"     "V43"     "V44"     "V45"     "V46"     "V47"
##  [49] "V48"     "V49"     "V50"     "V51"     "V52"     "V53"
```

```
##  [55] "V54"      "V55"      "V56"      "V57"      "V58"      "V59"
##  [61] "V60"      "V61"      "V62"      "V63"      "V64"      "V65"
##  [67] "V66"      "V67"      "V68"      "V69"      "V70"      "V71"
##  [73] "V72"      "V73"      "V74"      "V75"      "V76"      "V77"
##  [79] "V78"      "V79"      "V80"      "V81"      "V82"      "V83"
##  [85] "V84"      "V85"      "V86"      "V87"      "V88"      "V89"
##  [91] "V90"      "V91"      "V92"      "V93"      "V94"      "V95"
##  [97] "V96"      "V97"      "V98"      "V99"      "V100"     "V101"
## [103] "V102"     "V103"     "V104"     "V105"     "V106"     "V107"
## [109] "V108"     "V109"     "V110"     "V111"     "V112"     "V113"
## [115] "V114"     "V115"     "V116"     "V117"     "V118"     "V119"
## [121] "V120"     "V121"     "V122"     "V123"     "V124"     "V125"
## [127] "V126"     "V127"     "V128"     "V129"     "V130"     "V131"
## [133] "V132"     "V133"     "V134"     "V135"     "V136"     "V137"
## [139] "V138"     "V139"     "V140"     "V141"     "V142"     "V143"
## [145] "V144"     "V145"     "V146"     "V147"     "V148"     "V149"
## [151] "V150"     "V151"     "V152"     "V153"     "V154"     "V155"
## [157] "V156"     "V157"     "V158"     "V159"     "V160"     "V161"
## [163] "V162"     "V163"     "V164"     "V165"     "V166"     "V167"
## [169] "V168"     "geometry"
```

```
gCO$geometry
```

```
## Geometry set for 3213 features
## geometry type:  POLYGON
## dimension:      XY
## bbox:           xmin: -47.43966 ymin: -24.4031 xmax: -
45.57575 ymax: -23.00105
## epsg (SRID):    4326
## proj4string:    +proj=longlat +datum=WGS84 +no_defs
## First 5 geometries:
## POLYGON ((-47.41831 -24.35009, -47.41831 -24.38...
## POLYGON ((-47.38871 -24.35053, -47.38871 -24.38...
## POLYGON ((-47.35907 -24.35097, -47.35907 -24.38...
## POLYGON ((-47.32947 -24.35143, -47.32947 -24.38...
```

```
## POLYGON ((-47.29984 -24.35187, -47.29984 -24.38...
```

This function requires the package `lwgeom` when the data is in latitude and longitude degrees. There are some messages about the total emissions of street and grid. This was made in order to ensure that emis_grid is conservative. The resulting object `gCO` is an `sf` object of POLYGON. In order to plot the emissions, i selected the emissions above 1, because it is easier to see the plot. If we plot the gridded emissions, we will see:

```
gCO$V9 <- gCO$V9*(12 + 16)^-1
plot(gCO[gCO$V9 >1, "V9"], axes = TRUE,  nbreaks = 50,
     pal = cptcity::cpt(colorRampPalette = T),
     main = "Emissions of CO at 08:00 (mol/h)")
```

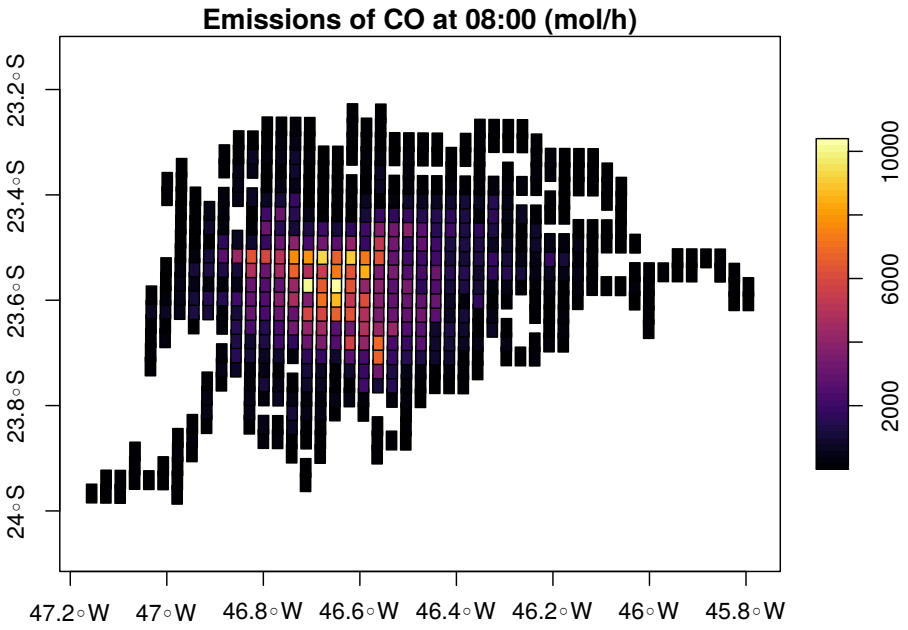


FIGURE 9.2: Gridded emissions (mol/h)

The emissions are mostly distributed into main roads, as expected. The next step is create the `GriddedEmissionsArray` that will be inputted into the `eixport` functions. The `GriddedEmissionsArray` is a contructor function that reads class, `SpatialPolygonDataFrame`, `sf` of POLYGONs, a `data.frame` or a `matrix` to create an Array of the gridded emissions. The dimensions

are lat, lon, mass and time. Therefore, it is important to know the number of lat and lon points!

```
gCOA <- GriddedEmissionsArray(x = gCO, cols = 63, rows = 51, times = 168)
```

```
## This GriddedEmissionsArray has:
##  51 lat points
##  63 lon points
##  168 hours
```

```
plot(gCOA, col = cptcity::cpt())
```

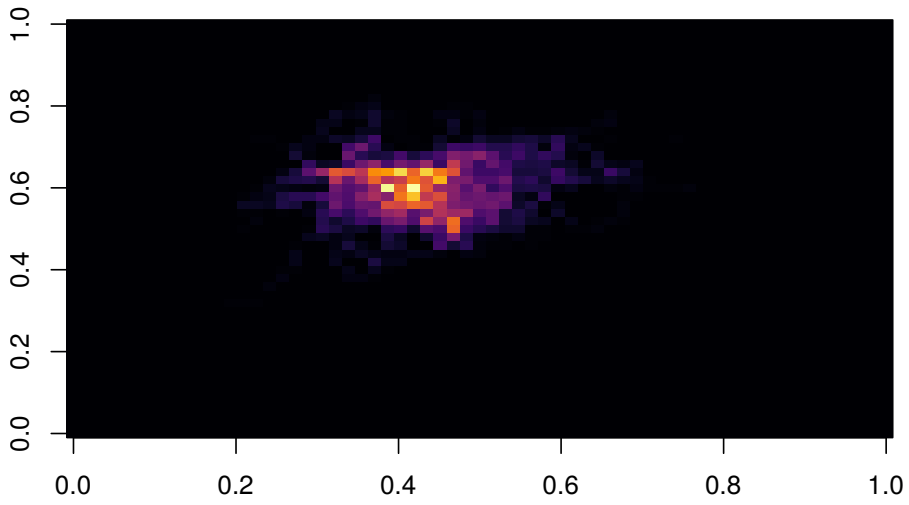


FIGURE 9.3: GriddedEmissionsArray (mol/h)

The image is similar to the plot of the gridded emissions, which means that it is correct. Now we can input the our new created object `gCOA` into the wrfchem input file, but first, we need to create it. This is done using the `eixport` functions.

We first load the library `eixport`. Then load the data `emis_opt` which has the emissions options for WRFchem. In this case, we are creating an wrfchem input file with 40 pollutants, with 0.

```
library(eixport)
data(emis_opt)
emis_opt[["ecb05_opt1"]]
wrf_create(wrfinput_dir = system.file("extdata", package = "eixport"),
           wrfchemi_dir = tempdir(),
           frames_per_auxinput5 = 168,
           domains = 2,
           variaveis = emis_opt[["ecb05_opt1"]],
           verbose = F)
```

The wrfchemi input file was created on a temporal directory with the function `tempdir`. Now we can input our `GriddedEmissionsArray` into our new wrfchem input file.

```
f <- list.files(path = tempdir(), full.names = T, pattern = "wrfchemi_d02")
f
wrf_put(file = f, name = "E_CO", POL = gCOA)
```

Then, we just check our resulting NetCDF file plotting the emissions we just put.

```
wrf_plot(f, "E_CO")
```

9.1.1.5.2 4b WRFChem input file with `emis_wrf`

`emis_wrf` creates a `data.frame` with columns lat, long, id, pollutants, local time and GMT time. This dataframe has the proper format to be used with WRF assimilation system: "ASimilation System 4 WRF (AS4WRF, Vara-Vela (2013))

```
args(emis_wrf)
```

```
## function (sdf, nr = 1, dmyhm, tz, crs = 4326, islist, utc)
## NULL
```

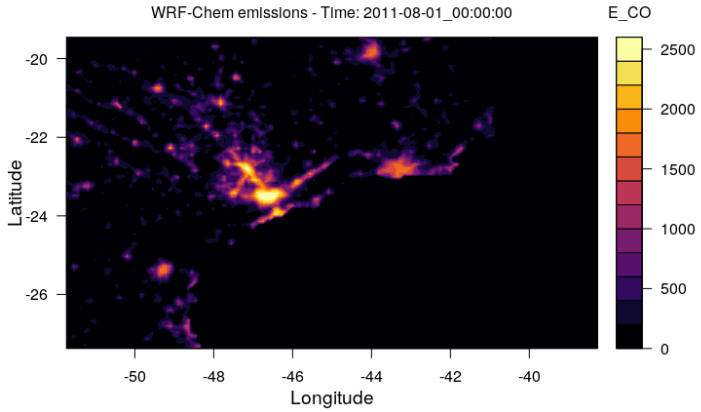


FIGURE 9.4: Wrfchem input file (NetCDF) (mol/h)

where:

- `sdf`: Gridded emissions, which can be a SpatialPolygonsDataFrame, or a list of SpatialPolygonsDataFrame, or a sf object of "POLYGON". The user must enter a list with 36 SpatialPolygonsDataFrame with emissions for the mechanism CBM-Z.
- `nr`: Number of repetitions of the emissions period
- `dmyhm`: String indicating Day Month Year Hour and Minute in the format "d-m-Y H:M" e.g.: "01-05-2014 00:00" It represents the time of the first hour of emissions in Local Time
- `tz`: Time zone as required in for function as.POSIXct
- `crs`: Coordinate reference system, e.g: "+init=epsg:4326". Used to transform the coordinates of the output
- `islist`: logical value to indicate if sdf is a list or not
- `utc`: ignored.

In this case, we can use our gridded emissions directly here:

```
gCO$id <- NULL
df <- emis_wrf(sdf = gCO, dmyhm = "06-10-2014 00:00",
               tz = "America/Sao_Paulo", islist = FALSE)

## You can create wrchem inputs directly with
## eixport::create and eixport::wrf_put
```

```
## https://CRAN.R-project.org/package=eixport
```

```
head(df)
```

```
##    id      long       lat pollutant    time_lt            time_utc dutch
## 1   1 -47.41831 -24.35009         0 2014-10-06 2014-10-
06 03:00:00   600
## 6   2 -47.38871 -24.35053         0 2014-10-06 2014-10-
06 03:00:00   600
## 11  3 -47.35907 -24.35097         0 2014-10-06 2014-10-
06 03:00:00   600
## 16  4 -47.32947 -24.35143         0 2014-10-06 2014-10-
06 03:00:00   600
## 21  5 -47.29984 -24.35187         0 2014-10-06 2014-10-
06 03:00:00   600
## 26  6 -47.27024 -24.35230         0 2014-10-06 2014-10-
06 03:00:00   600
```

Then you must export this `data.frame` into a .txt file. You must include the number of columns to match your luped species and also take out the columns time_lt, time_utc and dutch. These three columns are just informative.

```
df <- df[,1:4]
write.table(x = df, file = tempfile(), sep = "\t",
            col.names = TRUE, row.names = FALSE)
```

Finally, in order to generate the wrfchem input file, you must have the resulting .txt file, a wrfinput file with the same grid spacing, the NCL script AS4WRF and a namelist. AS4WRF and the namelist can be obtained contacting `angel.vela@iag.usp.br`[1] and `alvv1986@gmail.com`[2].

[1] mailto:angel.vela@iag.usp.br
[2] mailto:alvv1986@gmail.com

10

Quality check and errors

This last chapter of this book presents to aspestcs fthat must be considered for any practicioner interested in developing emissions inventories. The first part covers a summary of the EMEP/EEA air pollutant emission inventory guidebook 2016, Technical guidance to prepare national emission inventories (McGlade and Vidic, 2009), based on the Intergovernmental Panel on Climate Change (IPCC) 2006 Good Practice Guidance [Change (2006). The second part consists in advices and specific considerations for avoinding errors when runnign VEIN in each part of the inventory.

10.1 Guidance from EMEP/EEA air pollutant emission inventory guidebook

I believe that this part of this capter delivers knowledge that you really will gain with experience. But even with experience you can get lost, and returning to this part would save you. This part is based on the EMEP/EEA air pollutant emission inventory guidebook (McGlade and Vidic, 2009).

10.1.1 Key categories

Key categories are the most important **source** categories. This section is based on the chapter Key category analysis and methodological choice (J, 2013) of the EMEP/EEA air pollutant emission inventory guidebook 2013. They are important because they are responsabile for most of pollution in a determined region. For instance, it has been described that vehicles are the most important source of pollution in mega-cities (Molina and Molina, 2004). Evenmore, in the case of São Paulo, the official emissions inventory

informs that vehicles are responsabiel for mor than 97 % of CO, 79 % of HC, 68 % of NO_X, and only 29 % of PM and 22 % of SO_X (CETESB, 2015). This shown another characteristics of key categories: they depend of specific pollutants.

For another example, consider a city which suffers cold weather with use bio-mass burning for cooking and heating. The main source of $PM_{2.5}$ will be certainly bio-mass burning.

Now consider an industrial region with industrial process that emit too much SO_X. The key-cateogries might be industrial sources.

And one more example, consider a huge mega-city with electric mobility. However, the main source of electricity are thermoelectric based on carbon (the key).

This implies that it should be a nomemclature for categorizing and naming sources. IPCC, has a nomenclature for instance.

The ideia behind key categories, is that most efforts must be applied in this categories, obtainging the highest level of detail with less uncertainty. Hence, the emissions guidelines (McGlade and Vidic, 2009) proposes three levels of complexity estimation methods, known as Tier Methods. The complexity increases from level 1, 2 and 3. The VEIN tier is 3, which is that the most complex function of vehicular emissions estimations are incporated, with the exception of evaporative. I need to improve that part.

- Tier 1: a simpler method which include available activity and emissions factors.
- Tier 2: Similar to Tier 1, but includes more specific emission factors.
- Tier 3: Most complex methodologies with higher level of detail, temporal and spatial.

10.1.2 Uncertainty

This is a very important part in any emissions inventory and a dedicated chapter or section should be made in any report/paper. This section is based on the chapter Uncertainties (Pulles T, 2013) of the EMEP/EEA air pollutant emission inventory guidebook 2013.The 2006 IPCC Guidelines

chapter states that estimating the uncertainty of an inventory is needed (Change, 2006).

It is recommended to use 95% confidence interval. This means that:

- there is a 95% of probability that the actual value of the quantity estimates is within the interval defined by the confidence interval.
- The probability of the actual value will be outside the range it is 5%.

The general form for estimating emissions was shown on Eq. (1.1) (Pulles T, 2013). This equation will be the base for calculating the uncertainty. This section is applied when measurements are made, for the case of activity or emission factors. In those case, it is possible calculate the required confiden intervals.

10.1.2.1 Default uncertainty ranges

Activity data

The following table is taking directly form McGlade and Vidic (2009) and propose indicative ranges that could be applies in cases where no independed data are available.

- National official statistics: - .
- Update of last year's statistics using Gross Economic Growth factors: 0 - 2%.
- International Energy Agency (IEA) statistics: OECD: 2 - 3%, non-OECD 5-10%.
- United Nation data bases: 5 - 10%.
- Default values, other sources: 30 - 100%.

Emission factors

The following table is taking directly form McGlade and Vidic (2009) and propose rating definitions for emission factors(McGlade and Vidic, 2009).

- A: An estimate based on a large number of measurements made at a large number of facilities that fully represent the sector. Error: 10 o 30%.
- B: An estimate based on a large number of measurements made at a large number of facilities that represent a large part of the sector. Error: 20 to 60%

TABLE 10.1: Precision indicators (Ntziachristos and Samaras 2016)

Category	NOx	CO	NMHC	CH4	PM	N2O	NH3	CO2
PC G w/o Catalyst	A	A	A	A	-	C	C	A
PC G w Catalyst	A	A	A	A	-	A	A	A
PC D	A	A	A	A	A	B	B	A
PC LPG	A	A	A	-	-	-	-	A
PC LPG w/o Catalyst	A	A	A	A	D	C	C	A
PC LPG w Catalyst	D	D	D	D	D	D	D	A
PC 2 strokes	B	B	B	D	-	D	D	B
LCV G	B	B	B	C	-	B	B	A
LCV D	B	B	B	C	A	B	B	A
HDV G	D	D	D	C	-	D	D	D
HDV D	A	A	A	D	A	B	B	A
MC cc <50	A	A	A	B	-	B	B	A
MC cc > 50 2 strokes	A	A	A	B	-	B	B	A
MC cc > 50 4 strokes	A	A	A	B	-	B	B	A
Cold-start PC G Pre Euro	B	B	B	-	-	-	-	B
Cold-start PC G Euros	B	B	B	A	-	-	-	A
Cold-start PC D Pre Euro	C	C	C	-	C	-	-	B
Cold-start PC D Euros	A	A	A	A	A	-	-	A
Cold-start PC LPG	C	C	C	-	-	-	-	B
Cold-start LCV G	D	D	D	-	-	-	-	D
Cold-start LCV F	D	D	D	-	D	-	-	D

- C: An estimate based on a number of measurements made at a small number of representative facilities, or an engineering judgement based on a number of relevant facts. Error: 50 to 200%.
- D: An estimate based on single measurements, or an engineering calculation derived from a number of relevant facts. Error: 100 to 300%.
- E: An estimate based on an engineering calculation derived from assumptions only. Error: Order of magnitude.

In McGlade and Vidic (2009) appears ratings for road transport emission factors that differ from the ratings that appear in Ntziachristos and Samaras (2016). To preserve consistenty in this book, here is presented the precision indicators, Table 4-1 of Ntziachristos and Samaras (2016) report.

Uncertainties can be aggregated with two approaches

- *Rule A*: uncertainties are combined by *addition*, as shown in Eq. (10.1):

$$U_{total} = \frac{\sqrt{\sum_{i=1}^{n}(U_i \cdot x_i)^2}}{\sum_{i=1}^{n}} \tag{10.1}$$

Where, x are the quantities, U_i are the uncertain quantities and the percentage uncertainties (half the 95% confidence interval) associated with them, respectivly. U_{total} is the percentage uncertinti in the sum of the quantites (half the 95% confidence interval divided by the total (i.e. mean) and expressed as percentage).

- *Rule B*: uncertainties are combined by *multiplication*, as shown on Eq. (10.2):

$$U_{total} = \sqrt{\sum_{i=1}^{n}(U_i)^2} \tag{10.2}$$

Where, U_i are the percentage quantities (hal the 95% confidence interval) associated with each of the quantities. U_{total} is the percentage in the product of the quantities (half the 95% confidence interval divided by the total and expressed as percentage).

Alternatively, a Monte Carlo simulation can be done.

10.1.3 Quality Assurance and Quality Check

This section is mostly based on the chapter Inventory management, improvement and QA/QC (Goodwin et al., 2013) of the EMEP/EEA air pollutant emission inventory guidebook 2013.

According to Wikipedia:

- **Quality assurance (QA)** is a way of preventing mistakes and defects in manufactured products and avoiding problems when delivering solutions or services to customers (Wikipedia contributors, 2018b).
- **Quality control (QC)** is a process by which entities review the quality of all factors involved in production (Wikipedia contributors, 2018c).

The main reference in QA/QC are the International Organization for Standardization ISO 9000 (Wikipedia contributors, 2018a).

The idea is to avoid errors in the development of the inventory. Hence, it is very important that the objective of the inventory, frequency and spatial and temporal resolution must be very clear. As mentioned before, the inventory can have a purpose of policy application or scientific. In any case, the QAQC procedures should be explicitly stated covering five data quality objectives **transparency**, **consistency**, **comparability**, **completeness** and **acccuracy**.

This means that another researcher/practicioner should be able to reproduce the results. However, this is not always the case. Evenmore, it has been shown that there are currently a crisis of reproducibility in science, where 'more than 70% of researchers have tried and failed to reproduce another scientist's experiments, and more than half have failed to reproduce their own experiments' (Baker, 2016). I believe that emissions inventories should guarantee the reproducibility of results, in scientific and policy application inventories.

10.1.4 Inventory managment cycle

Another important aspect is the inventory managment cycle. The inventory manager is responsabile for institutional arrangments, meet deadlines and for the inventory managment cycle. The inventory complier gets the data and estimate the emissions with the respective Tier.

The cycle is:

1. Priorization of improvements: As the resources are limited, priorization must be given to key categories.
2. Data-collection: It is important to stablish formal agreements needs with data providers using protocols. The protocols must cleary show the data needed, its format, content and dates of delivery.
3. Inventory compilation. The inventory compiler estimate the emissions.
4. Consolidation. The inventory manager consolidates all the emis-

sions ensuring quality in data and methods for estimating emissions.
5. Data Quality Review.
6. Reporting.
7. Lessons learned and improvement review.
8. Inventory Managment Report.
9. Quality Assurance and Quality Control Plan.

10.2 Avoiding errors with VEIN

The first part of this chapter covered some fundamental aspects in emissions inventory managment for quality assurance and quality control. This part covers typical erros that I've faced using VEIN and I hope it help users how to avoid them.

Currently, VEIN does not have grafical user interface (GUI) and runs on R (R Core Team, 2017), which can be intimidating for new users. Also, even experienced users can do mistakes. If you find a mistake, write it down to abooid it in future. Be organized. I recommend to code your inventory keeping in mind that you will have to check your scripts in the future, so it would be nice if in the first try your code looks nice. And also, don't panic.

10.2.1 Traffic flow

One of the first inputs of it is the traffic flow data. You must have an agreement with data providers to get the data. Also, the compiler must understand the format of the data. In my experience, data providers comes from government agencies with limitated resources and few time. This means that, if there is not a formal agreement, they won't speed too much time for processing their data to meet your needs (because it is not part of their jobs). And even, if there was a formal agreement, the data processing must be done by the data compiler.

The data provided in this book covers a travel demand output for Metropoli-

tan Are ofSão Paulo (MASP) made by the Traffic Company Engineering of São Paulo, for the year 2012. The has the same content inside VEIN package, with the exception that covers the whole MASP. The data originally is in format MAPINFO. Therefore, the package **sf** must be used to read the data.

```
library(sf)
net <- st_read("data/masp.TAB")
```

The section @ref(#traffic) shows details about this data.

- Have a meeting with data delivers to check and solve any doubt regarding the data.
- Check if your data is projected or not. The data probably will be projected with a UTM zone, for instance code 31983 `http://spatialreference.org/ref/epsg/sirgas-2000-utm-zone-23s/`. VEIN imports functions from `sf` and `lwgeom` which depend on GEOS libraries. This means that VEIN can work with data projected or not. Nevertheless, I suggest to work with projected data for your location.
- Ensure that the data is correctly read and that there are no objects of class `factor` in the columns.
- Make sure that of what are the units of the traffic flow and remember that most of VEIN functions are designed to work with hourly traffic flow.
- Plot the data. Check if the data looks fine or have some mistakes.
- Calculate the length of each road. Make proper transformations and **make sure that resulting length of road as `units` km**. I suggest to use the name lkm. This can be easily done with in R with packages `sf` and `units` installed. Let's say that your data is named *net* and your data is already projected. Also, that your traffic flow is named *ldv* for light duty vehicles and *hdv* for heavy duty vehicles.

```
plot(net["ldv"], axes = T)
plot(net["hdv"], axes = T)
net$lkm <- sf::st_length(net) #returns distance in meters
net$$lkm <- units::set_units(net$lkm, km) #transform meters in km
```

Despite that this transformation can be done by dividing lkm by 1000, this would be wrong because the `units` wouldn't change and they must be `km`. Hence, using the functions of the `units` package is the recommended way.

10.2.2 Vehicular composition

The vehicular composition is a critical part in the emissions inventories for vehicles. It consists in the percentage of each type of vehicle and technology. Despite that it seems pretty straightforward, making a mistake in this part of the emissions inventories would cost lots of time. **Developing an emissions inventory is a complex task, you must take great care in simple calculations, because if the resutls are not consistent, it can take LOTS of time, to find the error, usually when the dealines are dead**.

The function `inventory` needs the vehicular composition to create the respective directories to run VEIN. I have the feeling that most of model users like structured models with clear input and outputs. VEIN is not like that, and this is in part due to the nature of the emissions inventories. I could design a model that works perfectly with one type of input, but in real life, a desired input is not always easy to get. For instance, the traffic simulation used inside the model is not easy to get, even in cities of developed countries. Hence, the inventory compiler must struggle to do their job. Therefore, VEIN was designed with flexibility and verstility on mind.

Anyways, the vehicular composition are the number of each type the following vehicles: PC, LCV, HGB, BUS, MC. Then, each sub category will be divided by type of age of use. For instance, the vehicular emissions inventory for São Paulo State considers 4 type of vehicles:

- Particulate Cars using gasohol (Gasoline with 25% of ethanol, PC_25).
- Particulate Cars Flex using gasohol (Gasoline with 25% of ethanol, PC_F25).
- Particulate Cars Flex using ethanol (Gasoline with 25% of ethanol, PC_FE100).
- Particulate Cars using ethanol (Gasoline with 25% of ethanol, PC_E100).

This means that the number of PC is 4.

Then each of this vehicles is divided by age of use. As consecuence, we must know when each of these vehicle entered and went out of the market. Again, for São Paulo conditions, Flex engines entered into market in 2003 and nowadays must of new cars are flex. Vehicles with engines designed for burning ethanol had a peak in early 80s, but they went of the market in 2006. Gasoline vehicles have been in circulation from the beginning and CETESB inventory considers a life span of 40 years of use.

The same analyses must be done with each of the vehicle categories.

The distribution by age of use indirectly shows the technology associated with emission standards by age of use.

10.2.3 Units

Currently, VEIN checks that the variable lkm (length) must be in km. This is to avoid that the user wrongly enter length in meters or without units. As a result, the emissions woult be huge and wrong.

In the case of vehicles, currently there are not designed a unit of "vehicles" in VEIN. In transportation studies, it is used the unit "equivalent vehicle" which standarize each type of vehicle by its size. For instance, LCV are sometimes equivalent of 1.2 vehicles. Buses or HGV can be equuvalent to 2 or more vehicles. however, there are no such typeof this things in VEIN and units managment is designed to control emission factors and length.

The temporal dimension is also an aspect difficult to handle regarding the units. This is because, sometimes mileage are correctly in km, but the timespan is in one year. Threfore, the units magament is degined to avoid errors with emission factors and calculation of emissions. This means that a future version of VEIN will erradicate all temporal dimensions ensure right calculation of mass only. This means that VEIN will not chech if the data is hourly or anunual.

10.2.4 Emission factors

When I started this book, VEIN contained few emission factors. Now, the version 0.5.2 has all the 2016 emission factors of CETESB, almost

100 emisision factors from the European Emission guidelines the all the BASE emission factors from the International Vehicle Model (IVE). The functions to access this data are:

- ef_cetesb.
- ef_ldv_speed.
- ef_hdv_speed.
- ef_ive.

I will be working to import emission factors from HBEFA model which are based traffic situation (very cool).

10.2.5 Deterioration

VEIN currently cover the deterioration emission factors from the Euroepan emission guidelines. This values results in a simply numeric vector depending on standard, mileage, type of vehicle and pollutant. However, it would be possible to use any other deterioation factors.

Ensure to use correctly the data and cite respective literature.

10.2.6 Fuel evaluation

It is a good practice to ensure that the mass of fuel consumed of vehicle in your study area, matchs the fuel sale son your area. If not, calibrate your emissions by number of vehicles (if bottom-up) or a combination of vehicles and mileage (if top-down) to match fuel sales.

10.2.7 Emissions estimation

Most of emission functions returns an array of emissions, which means a matrix of matrices. The idea was that each dimension has a meaning but I've been thinking that it is not necessary and each dimension should have different nature, for instance, it is not necessary two dimensions for time, despite that one indicates hour and the other days. So I mght change that in future. Dont panic, I'm always trying to change the functions without breaking older code.

I hope you liked this book.

Appendix A: Fast Example of VEIN

```
library(vein)
inventory(name = file.path(tempdir(), "YourCity"),
          show.dir = TRUE,
          show.scripts = TRUE)
source(paste0(file.path(tempdir(), "YourCity"), "main.R"))
```

Appendix B: Detailed Example of VEIN

.1 Network

```
inventory(file.path(tempdir(), "YourCity"))
setwd("YourCity")
data(net) # Loads the traffic demand simulation for west São Paulo
data(net)
data(pc_profile)
pc_week <- temp_fact(net$ldv+net$hdv, pc_profile)
speed <- netspeed(pc_week, net$ps, net$ffs, net$capacity, net$lkm)
saveRDS(net, file = "network/net.rds")
saveRDS(speed, file = "network/speed.rds")
```

.2 Vehicular composition (CETESB, 2015)

The vehicular composition `vehcomp` has 5 types of vehicles: Passenger Carss (PC), Light Commercial Vehicles (LCV), Heavy Good Vehicles or trucks (HGV), Buses (BUS), and Motorcycles (MC). The default value of this argument is: `c(PC = 4, LCV = 5, HGV = 5, BUS = 3, MC = 9)`, which means that there are 4 types of PC, 5 of LCV, 5 of trucks, 3 of buses and 9 types of motorcycles. This composition comes from the vehicular emissions inventory of the Environmental Agency of São Paulo, Brazil (CETESB, 2015). In Brazil, the fuel used in vehicles is blended with ethanol with and biodiesel. The user can use **any** vehicular composition that representes its fleet with

up-to 99 type of vehicles per category. The default composition according Brazilian emissions inventory is:

Passenger Cars (PC)

1. Passenger Cars using Gasoline blended with 25% of ethanol (E25).
2. Passenger Cars with Flex engine using Gasoline blended with 25% of ethanol (FE25).
3. Passenger Cars with Flex engine using 100% of ethanol (FE100).
4. Passenger Cars with engines that uses only ethanol (E100).

Light Commercial Vehicles (LCV)

1. Light Commercial Vehicles with gross weight (GW) less than 3.8 t using Gasoline blended with 25% of ethanol (E25).
2. Light Commercial Vehicles with GW less than 3.8 t with Flex engine using Gasoline blended with 25% of ethanol (FE25).
3. Light Commercial Vehicles with GW less than 3.8 t with Flex engine using 100% of ethanol (FE100).
4. Light Commercial Vehicles with GW less than 3.8 t with engines that uses only ethanol (E100).
5. Light Commercial Vehicles with GW less than 3.8 t with engines that uses only ethanol (E100).

Heavy Good Vehicles (HGV) or Trucks

1. Semi Light Trucks (SLT) with 3.8 t < GW < 6 t using Diesel blended with 5% of biodiesel (B5).
2. Light Trucks (LT) with 6 t < GW < 10 t using Diesel blended with 5% of biodiesel (B5).
3. Medium Trucks (MT) with 10 t < GW < 15 t using Diesel blended with 5% of biodiesel (B5).
4. Semi Heavy Trucks (SHT) with 15 t < GW on a Rigid Truck (RT) and GW < 40 on an Articulated Truck (AT) using Diesel blended with 5% of bodiesel (B5).
5. Heavy Trucks (HT) with 15 t < GW on a RT and GW >= 40 on an AT using Diesel blended with 5% of bodiesel (B5).

Buses

1. Urban Bus (UB) using Diesel blended with 5% of biodiesel (B5).
2. Small Urban Bus (SUB) using Diesel blended with 5% of biodiesel (B5).
3. Motorway Bus (MB) or Coach using Diesel blended with 5% of biodiesel (B5).

Motorcycles (MC)

1. Motorcycles with engine cc < 150 using Gasoline blended with 25% of ethanol (E25).
2. Motorcycles with engine 150 < cc < 500 using Gasoline blended with 25% of ethanol (E25).
3. Motorcycles with engine cc > 500 using Gasoline blended with 25% of ethanol (E25).
4. Motorcycles with engine cc < 150 with Flex engine using Gasoline blended with 25% of ethanol (FE25).
5. Motorcycles with engine 150 < cc < 500 with Flex engine using Gasoline blended with 25% of ethanol (FE25).
6. Motorcycles with engine cc > 500 with Flex engine using Gasoline blended with 25% of ethanol (FE25).
7. Motorcycles with engine cc < 150 with Flex engine using 100% of ethanol (FE100).
8. Motorcycles with engine 150 < cc < 500 with Flex engine using 100% of ethanol (FE100).
9. Motorcycles with engine cc > 500 with Flex engine using 100% of ethanol (FE100).

.3 Traffic data

The vehicular composition will split the traffic simulation as shown on next table. The simulation has traffic for Light Duty Vehicles and Heavy Good

TABLE .2: Vehicular composition of PC for applied in this book

Vehicles	Composition
PC_E25	37.25%
PC_FE25	22.26%
PC_FE100	37.97%
PC_E100	2.44%

Vehicles, therefore, the vehicular composition must split this categories and considerations:

- Passenger Cars (PC) = 75% of Light Duty Vehicles (LDV) of traffic simulation.
- Light Commercial Vehicles (LCV) = 10% of LDV of traffic simulation.
- Motorcycles (MC) = 15% of LDV on traffic simulation.
- Heavy Good Vehicles (HGV) = 75% of Heavy Duty Vehicles (HDV).
- Buses = = 25% of Heavy Duty Vehicles (HDV).
- LCV and PC have vehicles with flex engines capable to run with any mixture of gasoline and ethanol (Giroldo et al., 2005).
- Type of fuel consumed consists in gasoline blended with 25% of ethanol (E25).
- The vehicular composition consists in type of vehicles and type of fuel. Optionally, the user could have a wider vehicular composition considering more sizes, gross weight, etc.
- The percentages in composition apply for each type of vehicle PC, LCV, HGV, BUS and MC.

Passenger Cars

The vehicular composition consisted in PC using E25, PC with Flex engines using E25 and E100, and OC with engines for consuming only E100. The PC with Flex engines entered into Brazilian market in 2003, therefore, at year 2015 flex vehicles has 13 years of use. On the other case, PC with engines for E100 went out of the market in 2007, therefore, the newest PC with E100 engine has 9 years of use.

TABLE .3: Vehicular composition of LCV for applied in this book

Vehicles	Composition
LCV_E25	39.13%
LCV_FE25	15.21%
LCV_FE100	25.90%
LCV_E100	1.18%
LCV_B5	18.58%

```
PC_E25 <- age_ldv(x = net$ldv,name = "PC_E25",
                  k = 75/100*37.25)
PC_FE25 <- age_ldv(x = net$ldv, name = "PC_FE25", agemax = 13,
                   k = 75/100*22.26)
PC_FE100 <- age_ldv(x = net$ldv, name = "PC_FE100", agemax = 13,
                    k = 75/100*37.97)
PC_E100 <- age_ldv(x = net$ldv, name = "PC_E100", agemin = 9,
                   k = 75/100*2.44)
saveRDS(PC_E25, file = "veh/PC_E25.rds")
saveRDS(PC_FE25, file = "veh/PC_FE25.rds")
saveRDS(PC_FE100, file = "veh/PC_FE100.rds")
saveRDS(PC_E100, file = "veh/PC_E100.rds")
```

Light Commercial Vehicles

The engine/fuel type affects in the same way to LCV with PC vehicles. However, this category has a fraction of vehicles being driven with diesel. In Brazil, all diesle is blended with approximatly 5% of biodiesel, then it is named as B5. The categorization of the names in LCV is similar with PC.

```
LCV_E25 <- age_ldv(x = net$ldv,name = "LCV_E25",
                   k = 10/100*39.13)
LCV_FE25 <- age_ldv(x = net$ldv, name = "LCV_FE25", agemax = 13,
                    k = 10/100*15.21)
LCV_FE100 <- age_ldv(x = net$ldv, name = "LCV_FE100", agemax = 13,
                     k = 10/100*25.90)
```

TABLE .4: Vehicular composition of HGV for applied in this book

Vehicles	Composition
SLT	8.38%
LT	25.50%
MT	15.28%
SHT	24.98%
HT	25.85%

```
LCV_E100 <- age_ldv(x = net$ldv, name = "LCV_E100", agemin = 9,
                    k = 10/100*1.18)
LCV_B5 <- age_ldv(x = net$ldv, name = "LCV_B5",
                  k = 10/100*18.58)
saveRDS(LCV_E25, file = "veh/LCV_E25.rds")
saveRDS(LCV_FE25, file = "veh/LCV_FE25.rds")
saveRDS(LCV_FE100, file = "veh/LCV_FE100.rds")
saveRDS(LCV_E100, file = "veh/LCV_E100.rds")
saveRDS(LCV_B5, file = "veh/LCV_B5.rds")
```

Heavy Good Vehicles

HGV uses diesel which is blended with approximatly 5% of biodiesel from sugar- cane.

```
HGV_SLT_B5 <- age_hdv(x = net$hdv,name = "HGV_SLT_B5",
                      k = 75/100*8.38)
HGV_LT_B5 <- age_hdv(x = net$hdv, name = "HGV_SLT_B5",
                     k = 75/100*25.50)
HGV_MT_B5 <- age_hdv(x = net$hdv, name = "HGV_SLT_B5",
                     k = 75/100*15.28)
HGV_SHT_B5 <- age_hdv(x = net$hdv, name = "HGV_SLT_B5",
                      k = 75/100*24.98)
HGV_HT_B5 <- age_hdv(x = net$hdv, name = "HGV_SLT_B5",
                     k = 75/100*25.85)
saveRDS(HGV_LT_B5, file = "veh/HGV_SLT_B5.rds")
```

TABLE .5: Vehicular composition of BUS for applied in this book

Vehicles	Composition
UB	77.43%
SUB	9.07%
MB	13.5%

```
saveRDS(HGV_SLT_B5, file = "veh/HGV_LT_B5.rds")
saveRDS(HGV_MT_B5, file = "veh/HGV_MT_B5.rds")
saveRDS(HGV_SHT_B5, file = "veh/HGV_SHT_B5.rds")
saveRDS(HGV_HT_B5, file = "veh/HGV_HT_B5.rds")
```

Buses

In Brazil there are many type of buses, but in this book we are focussing in the most abundandt: Urban Buses, Small Urban Buses and Motoreway Buses ro Coach. According to the Secretary or Urban Mobility of São Paulo (Sptrans, `http://www.sptrans.com.br/`), the fleet has an average age of use of 5 years and 5 monthts. To achieve this average age, the agemax of this vehicles is 10 years of use.

```
UB_B5 <- age_hdv(x = net$ldv,name = "UB_B5", agemax = 10,
                 k = 25/100*77.43)
SUB_B5 <- age_hdv(x = net$ldv, name = "SUB_B5",
                  k = 25/100*9.07)
MB_B5 <- age_hdv(x = net$ldv, name = "MB_B5",
                 k = 25/100*13.5)
saveRDS(HGV_LT_B5, file = "veh/HGV_SLT_B5.rds")
saveRDS(HGV_SLT_B5, file = "veh/HGV_LT_B5.rds")
saveRDS(HGV_MT_B5, file = "veh/HGV_MT_B5.rds")
```

Motorcycles

The vehicular composition consisted in Motorcycles using E25, and recnetly, in year 2010, entered into the market flex motorcycles, which can

TABLE .6: Vehicular composition of MC for applied in this book

Vehicles	Composition
MC_150_E25	72.97%
MC_150_500_E25	11.28%
MC_500_E25	3.15%
MC_150_FE25	3.93%
MC_150_500_FE25	0.57%
MC_500_FE25	0.16%
MC_150_FE100	6.69%
MC_150_500_FE100	0.98%
MC_500_FE100	0.27%

use gasoline E25 or ethano E100. Therefore, the oldest flex MC is 6 years old.

```
MC_150_E25 <- age_hdv(x = net$ldv,name = "MC_150_E25",
                      k = 15/100*72.97)
MC_150_500_E25 <- age_hdv(x = net$ldv, name = "MC_150_500_E25",
                          k = 15/100*11.28)
MC_500_E25 <- age_hdv(x = net$ldv, name = "MC_500_E25",
                      k = 15/100*3.15)

MC_150_FE25 <- age_hdv(x = net$ldv,name = "MC_150_FE25", agemax = 6,
                       k = 15/100*3.93)
MC_150_500_FE25 <- age_hdv(x = net$ldv, name = "MC_150_500_FE25", agemax = 6, k = 15/100*0.57)
MC_500_FE25 <- age_hdv(x = net$ldv, name = "MC_500_FE25", agemax = 6,
                       k = 15/100*0.16)

MC_150_FE100 <- age_hdv(x = net$ldv,name = "MC_150_FE100", agemax = 6,
                        k = 15/100*6.69)
MC_150_500_FE100 <- age_hdv(x = net$ldv, name = "MC_150_500_FE100", agemax = 6,
                            k = 15/100*0.98)
MC_500_FE100 <- age_hdv(x = net$ldv, name = "MC_500_FE100", agemax = 6,
                        k = 15/100*0.27)
```

```
saveRDS(MC_150_E25, file = "veh/MC_150_E25.rds")
saveRDS(MC_150_500_E25, file = "veh/MC_150_500_E25.rds")
saveRDS(MC_500_E25, file = "veh/MC_500_E25.rds")

saveRDS(MC_150_FE25, file = "veh/MC_150_FE25.rds")
saveRDS(MC_150_500_FE25, file = "veh/MC_150_500_FE25.rds")
saveRDS(MC_500_FE25, file = "veh/MC_500_FE25.rds")

saveRDS(MC_150_FE100, file = "veh/MC_150_FE100.rds")
saveRDS(MC_150_500_FE100, file = "veh/MC_150_500_FE100.rds")
saveRDS(MC_500_FE100, file = "veh/MC_500_FE100.rds")
```

Appendix B

Bibliography

Amato, F., Querol, X., Johansson, C., Nagl, C., and Alastuey, A. (2010). A review on the effectiveness of street sweeping, washing and dust suppressants as urban pm control methods. *Science of The Total Environment*, 408(16):3070 – 3084.

Andrade, M. d. F., Kumar, P., de Freitas, E. D., Ynoue, R. Y., Martins, J., Martins, L. D., Nogueira, T., Perez-Martinez, P., de Miranda, R. M., Albuquerque, T., et al. (2017). Air quality in the megacity of são paulo: Evolution over the last 30 years and future perspectives. *Atmospheric Environment*, 159:66–82.

Andrade, M. d. F., Ynoue, R. Y., Freitas, E. D., Todesco, E., Vara Vela, A., Ibarra, S., Martins, L. D., Martins, J. A., and Carvalho, V. S. B. (2015). Air quality forecasting system for southeastern brazil. *Frontiers in Environmental Science*, 3:1–12.

Anselin, L. (1995). Local indicators of spatial association—lisa. *Geographical analysis*, 27(2):93–115.

Arbor, A. (2003). User's guide to mobile 6.1 and mobile 6.2. *Assessment and Standard Division, Office of Transportation and Air Quality, USEPA, Mich*.

Baker, M. (2016). Is there a reproducibility crisis? a nature survey lifts the lid on how researchers view the'crisis rocking science and what they think will help. *Nature*, 533(7604):452–455.

Barlow (2009). A reference book of driving cycles for use in the measurement of road vehicle emissions. Technical report, Transport Research Lalboratory.

Boian, C. and Andrade, M. d. F. (2012). Characterization of ozone transport among metropolitan regions. *Revista Brasileira de Meteorologia*, 27(2):229–242.

Boulder, C. U. (2017). The ncar command language (ncl)(version 6.4. 0).

Boulter and Barlow (2009). Artemis: Assessment and reliability of transport emission models and inventory systems final report. Technical report, Transport Research Lalboratory.

Bruni, A. D. C. and Bales, M. P. (2013). Curvas de intensidade de uso por tipo de veículo automotor da frota da cidade de são paulo. Technical report, CETESB. http://veicular.cetesb.sp.gov.br/wp-content/uploads/sites/35/2013/12/curvas-intensidade-uso-veiculos-automotores-cidade-sao-paulo.pdf.

Bureau of Public Roads (1964). Traffic and assignment mannual. Technical report, Dept. of Commerce, Urban Planning Division, Washington D.C.

CETESB (2015). Emissões veiculares no estado de são paulo 2014. http://veicular.cetesb.sp.gov.br/relatorios-e-publicacoes/.

CETESB (2016). Emissões veiculares no estado de são paulo 2016. http://veicular.cetesb.sp.gov.br/relatorios-e-publicacoes/.

Change, I. (2006). 2006 ipcc guidelines for national greenhouse gas inventories.

Chen, R.-H., Chiang, L.-B., Chen, C.-N., and Lin, T.-H. (2011). Cold-start emissions of an si engine using ethanol–gasoline blended fuel. *Applied Thermal Engineering*, 31(8):1463–1467.

contributors, O. (2017). Planet dump retrieved from https://planet.osm.org. Accessed on 18-07-2017.

Cooley, D. (2018). *googleway: Accesses Google Maps APIs to Retrieve Data and Plot Maps*. R package version 2.5.0.

Corvalán, R. M., Osses, M., and Urrutia, C. M. (2002). Hot emission model for mobile sources: application to the metropolitan region of the city of santiago, chile. *Journal of the Air & Waste Management Association*, 52(2):167–174.

Corvalán, R. M. and Vargas, D. (2003). Experimental analysis of emission deterioration factors for light duty catalytic vehicles case study: Santiago, chile. *Transportation Research Part D: Transport and Environment*, 8(4):315–322.

Davis, N., Lents, J., Osses, M., Nikkila, N., and Barth, M. (2005). Part 3: Developing countries: development and application of an international vehicle emissions model. *Transportation Research Record: Journal of the Transportation Research Board*, 8(1939):155–165.

de Fatima Andrade, M., de Miranda, R. M., Fornaro, A., Kerr, A., Oyama, B., de Andre, P. A., and Saldiva, P. (2012). Vehicle emissions and pm2. 5 mass concentrations in six brazilian cities. *Air Quality, Atmosphere & Health*, 5(1):79–88.

Dijkstra, E. W. (1959). A note on two problems in connexion with graphs. *Numerische mathematik*, 1(1):269–271.

Dowle, M. and Srinivasan, A. (2017). *data.table: Extension of 'data.frame'*. R package version 1.10.4-3.

EJ-JRC/PBL (2016). Emission database for global atmospheric research (edgar), release edgar v4.3.1_v2 (1970 - 2010).

Eom, J., Park, M., Heo, T.-Y., and Huntsinger, L. (2006). Improving the prediction of annual average daily traffic for nonfreeway facilities by applying a spatial statistical method. *Transportation Research Record: Journal of the Transportation Research Board*, 1(1968):20–29.

Freitas, E., Martins, L., Silva Dias, P., and Andrade, M. d. F. (2005). A simple photochemical module implemented in rams for tropospheric ozone concentration forecast in the metropolitan area of são paulo, brazil: Coupling and validation. *Atmospheric Environment*, 1(39):6352–6361.

Giroldo, M. B., Werninghaus, E., Coelho, E., and Makant, W. (2005). Development of 1.6l flex fuel engine for brazilian market. In *SAE Technical Paper*. SAE International.

González, C., Gómez, C., Rojas, N., Acevedo, H., and Aristizábal, B. (2017).

Relative impact of on-road vehicular and point-source industrial emissions of air pollutants in a medium-sized andean city. *Atmospheric Environment*, 152:279–289.

Goodwin, T, P., J, A., L, T., and K, R. (2013). Emep/eea air pollutant emission inventory guidebook 2013: Inventory managment, improvement and qa/qc. Technical report, Technical report 2013, EEA, Copenhagen, Denmark.

Grell, G. A., Peckham, S. E., Schmitz, R., McKeen, S. A., Frost, G., Skamarock, W. C., and Eder, B. (2005). Fully coupled "online" chemistry within the wrf model. *Atmospheric Environment*, 39(37):6957–6975.

Hoshyaripour, G., Brasseur, G., Andrade, M., Gavidia-Calderón, M., Bouarar, I., and Ynoue, R. (2016). Prediction of ground-level ozone concentration in são paulo, brazil: Deterministic versus statistic models. *Atmospheric Environment*, 145:365 – 375.

Ibarra, S., Rehein, A., Vara-Vela, A., and Ynoue, R., editors (2015a). *Simulation For The Metropolitan Region Of Porto Alegre*.

Ibarra, S., Ynoue, R., and Vara-Vela, A., editors (2015b). *Emissions inventory and atmospheric simulation of 58 urban centers of South America*.

Ibarra-Espinosa, S. (2017). *Air pollution modeling in São Paulo using bottom-up vehicular emissions inventories*. PhD thesis, University of São Paulo.

Ibarra-Espinosa, S., Freitas, E., Ynoue, R., de Fátima Andrade, M., and Schuch, D. (2018a). Towards a vectorial global vehicular emissions inventory. In *2018 Joint 14th iCACGP Quadrennial Symposium/15th Igac Science Conference*.

Ibarra-Espinosa, S., O'Sullivan, S., Osses, M., and Ynoue, R. (2017a). Negative binomial and quasi-poisson regressions of hourly traffic data with openstreetmap. *Journal of Computers, Environment and Urban Systems*. Under Review.

Ibarra-Espinosa, S., Schuch, D., and de Freitas, E. D. (2017b). *eixport: An R package to export emissions to atmospheric models*. R package version 0.3.4.

Ibarra-Espinosa, S., Schuch, D., and Dias de Freitas, E. (2018b). eixport: An r package to export emissions to atmospheric models. *The Journal of Open Source Software*.

Ibarra-Espinosa, S., Ynoue, R., O'Sullivan, S., Pebesma, E., Andrade, M. D. F., and Osses, M. (2017c). Vein v0.2.2: an r package for bottom-up vehicular emissions inventories. *Geoscientific Model Development Discussions*, 2017:1–29.

Ibarra-Espinosa, S., Ynoue, R., O'Sullivan, S., Pebesma, E., Andrade, M. D. F., and Osses, M. (2018c). Vein v0.2.2: an r package for bottom–up vehicular emissions inventories. *Geoscientific Model Development*, 11(6):2209–2229.

Ihaka, R. and Gentleman, R. (1996). R: a language for data analysis and graphics. *Journal of computational and graphical statistics*, 5(3):299–314.

J, G. (2013). Emep/eea air pollutant emission inventory guidebook 2013: Key category analysis and methodological choice. Technical report, Technical report 2013, EEA, Copenhagen, Denmark.

Jimenez, J. L., McClintock, P., McRae, G., Nelson, D. D., and Zahniser, M. S. (1999). Vehicle specific power: A useful parameter for remote sensing and emission studies. In *Ninth CRC On-Road Vehicle Emissions Workshop, San Diego, CA*.

Koupal, J., Cumberworth, M., Michaels, H., Beardsley, M., and Brzezinski, D. (2003). Design and implementation of moves: Epa's new generation mobile source emission model. *Ann Arbor*, 1001:48105.

Lam, W. H. and Xu, J. (2000). Estimation of aadt from short period counts in hong kong—a comparison between neural network method and regression analysis. *Journal of Advanced Transportation*, 34(2):249–268.

Lents, J., Davis, N., Nikkila, N., and Osses, M. (2004). São paulo vehicle activity study. Technical report, International Sustainable System Research Center, 605 South Palm Street, Suite C, La Habra, CA 90631, USA.

Lowry, M. (2014). Spatial interpolation of traffic counts based on origin–destination centrality. *Journal of Transport Geography*, 36:98–105.

Lükewille, A., Tista, M., and Hoenders, R. (2017). European union emission inventory report 1990–2010 under the unece convention on long-range transboundary air pollution (lrtap). Technical report, EEA technical report.

Martins, L. D., Andrade, M. F., Freitas, E. D., Pretto, A., Gatti, L. V., Albuquerque, É. L., Tomaz, E., Guardani, M. L., Martins, M. H., and Junior, O. M. (2006). Emission factors for gas-powered vehicles traveling through road tunnels in são paulo, brazil. *Environ. Sci. Technol.*, 40(21):6722–6729.

Matloff, N. (2011). *The art of R programming: A tour of statistical software design*. No Starch Press.

McGlade, J. and Vidic, S. (2009). Emep/eea air pollutant emission inventory guidebook 2009: Technical guidance to prepare national emission inventories. Technical report, Technical report 9/2009, EEA, Copenhagen, Denmark.

Mellios, G. and Ntziachristos, L. (2016). Emep/eea emission inventory guidebook; gasoline evaporation from vehicles. Technical report, European Environment Agency, Copenhagen.

Metro (2017). Pesquisa origem e destino. Accesed on 10-08-2017.

Ministerio do Meio Ambiente (2011). Primeiro inventario nacional de emissoes atmosféricas por veiculos automotores rodoviarios.

Molina, M. J. and Molina, L. T. (2004). Megacities and atmospheric pollution. *Journal of the Air & Waste Management Association*, 54(6):644–680.

Muenchow, J., Schratz, P., and Brenning, A. (2018). Rqgis: Integrating r with qgis for statistical geocomputing. *R Journal*. Accepted for publication on 2017-12-04.

Nogueira, T., de Souza, K. F., Fornaro, A., de Fatima Andrade, M., and de Carvalho, L. R. F. (2015). On-road emissions of carbonyls from vehicles powered by biofuel blends in traffic tunnels in the metropolitan area of sao paulo, brazil. *Atmospheric Environment*, 108:88–97.

Ntziachristos, L. and Boulter, P. (2009). Emep/eea emission inventory guidebook; road transport: Automobile tyre and break wear and road abrasion. *European Environment Agency, Copenhagen*.

Ntziachristos, L. and Samaras, Z. (2000). Speed-dependent representative emission factors for catalyst passenger cars and influencing parameters. *Atmospheric Environment*, 34(27):4611–4619.

Ntziachristos, L. and Samaras, Z. (2016). Emep/eea emission inventory guidebook; road transport: Passenger cars, light commercial trucks, heavy-duty vehicles including buses and motorcycles. *European Environment Agency, Copenhagen*.

Ortuzar, J. d. D. and Willumsen, L. G. (2002). *Modelling transport*, volume 3. Wiley.

P, B., T, B., S, L., and I, M. (2009). Emission factors 2009 report 1. a review of methods for determining hot exhaust emission factors for road vehicles. Technical report, Transport Research Lalboratory.

Padgham, M. and Peutschnig, A. (2018). *dodgr Distances on Directed Graphs*. R package version 0.1.0.

Patrushev, A. (2007). Shortest path search in real road networks with pgrouting. *Free and Open Soruce Software For Geospatial FOSS*.

Pebesma, E. (2017). *sf: Simple Features for R*. R package version 0.5-5.

Pebesma, E., Mailund, T., and Hiebert, J. (2016). Measurement units in R. *The R Journal*, 8(2):486–494.

Pebesma, E. J. and Bivand, R. S. (2005). Classes and methods for spatial data in R. *R News*, 5(2):9–13.

Peng, R. D. (2015). *R programming for data science*. Leanpub.com.

Pérez-Martinez, P., Miranda, R., Nogueira, T., Guardani, M., Fornaro, A., Ynoue, R., and Andrade, M. (2014). Emission factors of air pollutants from vehicles measured inside road tunnels in s
ao paulo: case study comparison. *Int. J. Environ. Sci. Te.*, 11(8):2155–2168.

Pierce, D. (2017). *ncdf4: Interface to Unidata netCDF (Version 4 or Earlier) Format Data Files*. R package version 1.16.

Pulles, T. and Heslinga, D. (2010). The art of emission inventorying. *TNO, Utrecht*.

Pulles T, K. J. (2013). Emep/eea air pollutant emission inventory guidebook 2013: Uncertainties. Technical report, Technical report 2013, EEA, Copenhagen, Denmark.

QGIS Development Team (2017). *QGIS Geographic Information System*. Open Source Geospatial Foundation.

R Core Team (2017). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria.

Rafee, S. A. A. (2015). *Estudo numerico do impacto das emissões veiculares e fixas da cidade de Manaus nas concentrações de poluentes atmosféricos da região amazônica*. PhD thesis, Londrina: Universidade Tecnologica Federal do Parana.

Réquia Jr, W. J., Koutrakis, P., and Roig, H. L. (2015). Spatial distribution of vehicle emission inventories in the federal district, brazil. *Atmospheric Environment*, 112:32–39.

Sapp, W. (1938). Runctions of a highway-planning survey department. *Annual Road School*.

Selby, B. and Kockelman, K. M. (2013). Spatial prediction of traffic levels in unmeasured locations: applications of universal kriging and geographically weighted regression. *Journal of Transport Geography*, 29:24–32.

Snyder, M. G., Venkatram, A., Heist, D. K., Perry, S. G., Petersen, W. B., and Isakov, V. (2013). Rline: A line source dispersion model for near-surface releases. *Atmospheric Environment*, 77:748 – 756.

Ulke, A. G. and Andrade, M. F. (2001). Modeling urban air pollution in sao paulo, brazil: sensitivity of model predicted concentrations to different turbulence parameterizations. *Atmospheric Environment*, 35(10):1747–1763.

UNFCCC (2017). *Greenhouse Gas Inventory Data*.

USA-EPA (2016). Ap42 compilation of emission factors; resuspenssion emissions from paved roads. *Environment Protection Agency, USA*.

Vara-Vela, A. (2013). *Avaliação do impacto da mudança dos fatores de emissão veicular na formação de ozônio troposférico na Região Metropolitana de São Paulo(RMSP)*. PhD thesis, Instituto de Astronomia, Geofísica e Ciências Atmosféricas, Universidade de São Paulo, São Paulo, Brazil.

Vara-Vela, A., Andrade, M. F., Kumar, P., Ynoue, R. Y., and Muñoz, A. G. (2016). Impact of vehicular emissions on the formation of fine particles in the são paulo metropolitan area: a numerical study with the wrf-chem model. *Atmos. Chem. and Phys.*, 16:777–797.

Vivanco, M. G. and de Fátima Andrade, M. (2006). Validation of the emission inventory in the sao paulo metropolitan area of brazil, based on ambient concentrations ratios of co, nmog and nox and on a photochemical model. *Atmospheric Environment*, 40(7):1189–1198.

Wang, X. and Kockelman, K. (2009). Forecasting network data: Spatial interpolation of traffic counts from texas data. *Transportation Research Record: Journal of the Transportation Research Board*, 1(2105):100–108.

Weilenmann, M., Favez, J.-Y., and Alvarez, R. (2009). Cold-start emissions of modern passenger cars at different low ambient temperatures and their evolution over vehicle legislation categories. *Atmospheric environment*, 43(15):2419–2429.

Wickham, H. (2009). *ggplot2: elegant graphics for data analysis*. Springer New York.

Wickham, H. (2015). *R packages: organize, test, document, and share your code*. " O'Reilly Media, Inc.".

Wickham, H. and Bryan, J. (2017). *readxl: Read Excel Files*. R package version 1.0.0.

Wickham, H. and Chang, W. (2017). *devtools: Tools to Make Developing R Packages Easier*. R package version 1.13.4.

Wickham, H. and Henry, L. (2018). *tidyr: Easily Tidy Data with 'spread()' and 'gather()' Functions*. R package version 0.8.0.

Wikipedia contributors (2018a). Iso 9000 — Wikipedia, the free encyclopedia. [Online; accessed 16-July-2018].

Wikipedia contributors (2018b). Quality assurance — Wikipedia, the free encyclopedia. [Online; accessed 16-July-2018].

Wikipedia contributors (2018c). Quality control — Wikipedia, the free encyclopedia. [Online; accessed 16-July-2018].

Zaveri, R. A. and Peters, L. K. (1999). A new lumped structure photochemical mechanism for large-scale applications. *Journal of Geophysical Research: Atmospheres*, 104(D23):30387–30415.

Zeileis, A., Kleiber, C., and Jackman, S. (2008). Regression models for count data in r. *Journal of statistical software*, 27(8):1–25.

Zhao, F. and Chung, S. (2001). Contributing factors of annual average daily traffic in a florida county: exploration with geographic information system and regression models. *Transportation Research Record: Journal of the Transportation Research Board*, 1(1769):113–122.