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AIR POLLUTANTS MODELING USING BOTTOM-UP VEHICULAR EMISSIONS INVENTORY

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Abstract. *Urban air quality is directly associated to vehicle emissions. Although technology of fuel, engines and abatement have improved, the incessant increase of the size of the urban fleet promotes further increase in the pollutants by two reasons: more sources and degenerated circulating conditions. In this work, the impacts of different scenarios of Passenger Cars (PC) fleet on hot exhaust emissions were estimated. A bottom-up vehicle emissions inventory was made for five routes in Curitiba, for CO,* CO_2*,* CH_4 *and NOx. The calculations were performed through an open source software called VEIN (Vehicular Emissions Inventories). The inventory aggregates information from the composition of vehicular fleet (by the distribution of age, fuel and engine size), traffic activity (speed, hourly flow) and emission factors. Five scenarios of PC fleet were considered, namely, current (age distribution limited to 40 years), and 20 and 30 years limited age distribution, increase and decrease of total PC. The results indicates that the main contributors are older vehicles (30-40 years), for most of inventoried pollutants. Increasing or reducing the PC fleet, for a fixed distribution of age of 40 years, contributes proportionally for the emissions. The results indicate that the model can be an important tool for evaluating vehicle emissions under different urban mobility scenarios.*

Keywords: *VEIN, Air Pollution, Vehicular Emissions.*

1. INTRODUCTION

Transportation emissions are the main source of air pollution in urban areas, specially in developing countries (Molina and Molina, 2004). The increase of atmospheric pollution is related to respiratory, cardiovascular diseases (Xiping *et al.*, 1995; Zhang *et al.*, 2000) and higher rates of mortality (Zhang *et al.*, 2000). Although several technological improvements on vehicle engines have been made over the years, the ongoing rates of urbanization, associated with the chronic deficiency of high-quality public transportation, has lead to an expressive increase of individual motorization rate, resulting in a challenge to maintain the levels of air quality in urban areas.

One important tool for air quality management is the emissions inventory, which is defined as the compilation of all pollutants released by activities for a defined area and time-lapse (Ntziachristos and Samaras, 2016). For vehicle emission studies, once known the local data, regarding fleet characteristics, spatial and temporal trip patterns, inventories can be used for evaluating the distribution of emissions throughout urban areas. Origin-Destination Surveys (ODS), mostly applied in big cities, produces important information regarding the patterns of trips by mode of transportation, that can be incorporated into vehicle emission inventories models (Armstrong and Khan, 2004; Barla *et al.*, 2011).

The Brazilian current policies, such as the National Policy of Urban Mobility, address mechanisms for sustainable mobility. Among its guidelines are the "identification of the environmental, social and economic costs of moving passengers and goods", the "priority of non-motorized modes of transport on motorized vehicles and public transport services on individual motorized transport". It also considers guidelines regarding the encouragement of scientific and technological development and the use of renewable energy in non-polluting.

In this context, the objective of this work is to evaluate the emissions for carbon monoxide (CO), nitrogen oxides (NOx), methane (CH_4) and carbon dioxide (CO_2) for five trips by passenger car (PC) in Curitiba-PR, considering different scenarios of vehicles age and fleet.

2. METHODOLOGY

We adopted the VEIN model (Version 0.7.0), a new model, which presents inventory of vehicle emissions with high spatial and temporal resolution for different applications (Ibarra-Espinosa *et al.*, 2017). The main methods of this section are divided into Traffic Data, Emissions Factors and Hot Exhaust Emissions. The parameters considered in the model are incorporated as traffic data, vehicular composition and emission factors (Tab. 1).

Table 1. Summary of the main VEIN classes and data.

Description	Source
Distribution of PC by age of use	Ministério do Meio Ambiente (2014)
Traffic flow temporal factor	IPPUC (2019)
Share of population without routine trips	IPPUC (2019)
Street capacity	IPPUC (2019)
Distance and Speed of the trip	Dorman *et al.* (2019); Google Maps Plataform (2019)
PC emission factors	Ntziachristos and Samaras (2016); CETESB (2016)
Data of mileage functions by vehicle	Bruni and Bales (2013)
Vehicular composition by fuel and age	DETRAN-PR (2019); Ministério do Meio Ambiente (2014)
Vehicular composition by engine size	ANFAVEA (2018)
Deterioration factor	Ntziachristos and Samaras (2016)

2.1 Traffic Data

The origin-destination survey (ODS) of Curitiba-PR aimed to identify and quantify the main behavioral patterns of trips throughout the city territory. The survey provided information to estimate an origin-destination matrix by each censitary zone (as defined by the IBGE). An average trip from zone A to B was considered as the average preferential direction between each centroid. The expression of total trips from A to B, T_a^b, is given by

$$T_a^b = Sample_a^b \times Pop_a \times \overline{Tx} \times \overline{Pm}, \tag{1}$$

where $Sample_a^b$ indicates the proportion of ODS interviews that travels from A to B; Pop_a population of zone A; $\overline{Tx}$ rate of trips per commuter and $\overline{Pm}$ percentage of population that travels everyday (66%, according to IPPUC (2019)).

The driving route and speed between zones was defined by using the "mapsapi" package (R language), that allows accessing Google Maps Directions API — a service that calculates directions between locations using an HTTP request (Dorman *et al.*, 2019). The free-flow speed[1], daily traffic volume and routes are shown in Figure 1.

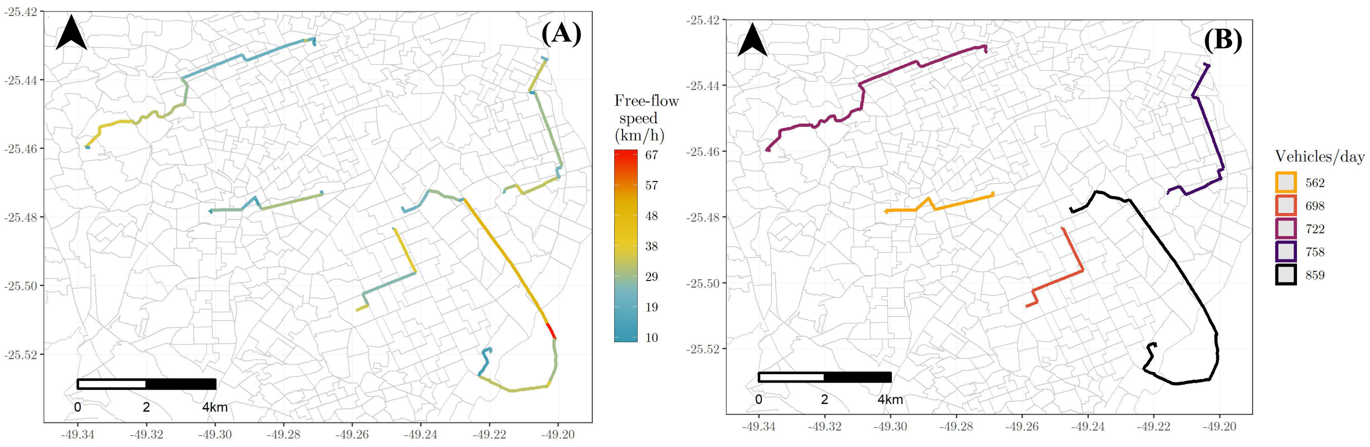

Figure 1. (A) Free-flow speed generated by Google Maps Plataform (2019). (B) total PC trips considered in the study.

The average age of Brazilian PC fleet is 10.4 years, and its emissions varies according to fuel. Since flex-fuel PC can adopt ethanol, gasoline or a mixture of both, we considered the proportion of use based on fuel prices, according to Sena (2015). Figure 2-A shows the normalized fleet by fuel and age, and Fig. 2-B the PC flow by hour — indicating the rush hours at 8 a.m. and 6 p.m.. Also, PC categories were divided by size of the engine cc (cm^3), according to sales statistics of ANFAVEA (2018), by: 35.3% of $cc <= 1400\ \text{cm}^3$, 62.4% of $1400 < cc <= 2000$ and 2.3% of $cc > 2000\ \text{cm}^3$.

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[1] Speed when the demand is lower than the road capacity.

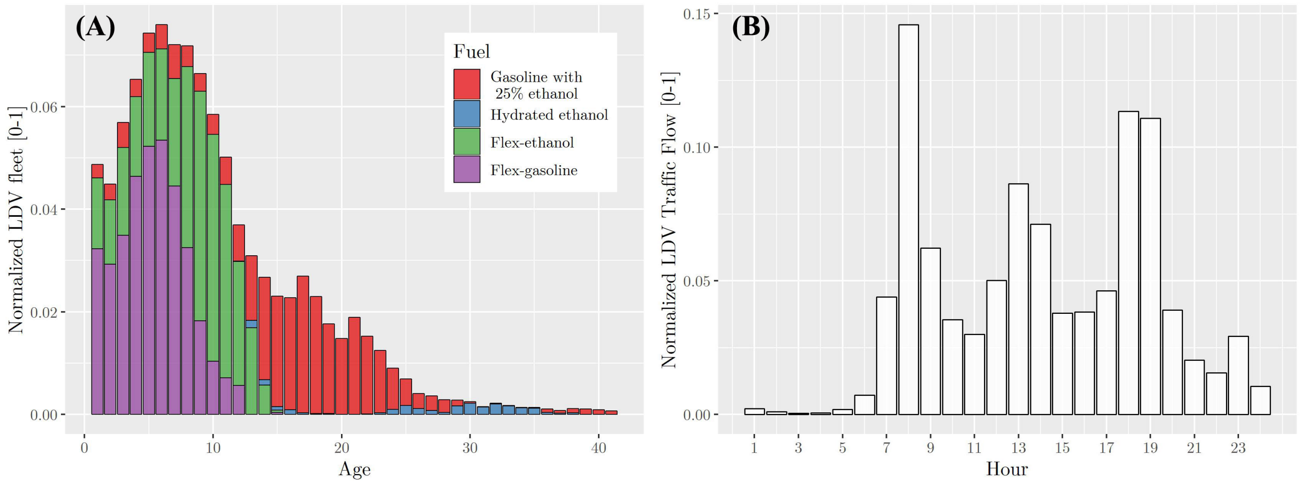

Figure 2. (A) Fleet composition considered in the study (CETESB, 2016); (B) Traffic flow index (IPPUC, 2019).

The average speed is estimated for each street link i and week hour l. The VEIN model adopts the Bureau of Public Roads (BPR) function for estimating the speed at different time periods (BUREAU OF PUBLIC ROADS, 1964), that has been widely applied in transportation and planning guides. The relation is given by

$$T_{i,l} = T_{Oi} \cdot \left(1 + \alpha \cdot \left(\frac{Q_{i,l}}{C_i}\right)^{\beta}\right), \tag{2}$$

where $T_{i,l}$ is the time travel per street link i and hour l (s); T_{Oi} is the travel time under free flow conditions where the speed is on its maximum (s); $Q_{i,l}$ é the traffic volume per street link i and hour l (veh/h); C_i is the street capacity (veh/h); and α, β are adjusted parameters, where 0.15 and 4 are the default values, respectively. The travel mean speed, $V_{i,l}$, is further determined since the travelled distance is known and fixed.

2.2 Emissions factors

The emission factors is based on recordings of a chassis dynamometer, that simulates the resistive power imposed on the wheels of a vehicle. According to Franco *et al.* (2013), the dynamometer is coupled via gearboxes to drive lines that are directly connected to the wheel hubs of the vehicle. In Brazil, the measurements follows the Federal Test Procedure (FTP-75), that consist of driving cycle for PC with an average speed V^{dc} of 34.12 km/h (Daemme, 2017). The EF adopted by VEIN model are speed-dependent for PC using gasoline, and its function is adjusted to the driving cycle average speed. The local emission factor are related to speed by the expression

$$EF_{scaled}(V_{i,l})_{j,k,m} = EF^{local}_{j,k,m} \cdot \frac{EF(V_{i,l})_{j,k,m}}{EF(V^{dc}_{i,l})_{j,k,m}}, \tag{3}$$

where $V_{i,l}$ is the speed for each street link i and hour l; $EF_{scaled}(V_{i,l})_{j,k,m}$ is the scaled emission factor for speed $V_{i,l}$, vehicle type j, age k, and pollutant m; $EF(V_{i,l})_{j,k,m}$ is the COPERT emission factor; $EF^{local}_{j,k,m}$ represents the constant emission factor (not speed dependent); $EF(V^{dc}_{i,l})_{j,k,m}$ are COPERT emission factors with average speed value of the respective driving cycle dc for the vehicular category j. For PC using ethanol, the EF as functions of speed are unavailable, so the EF are not speed-dependent.

The use of COPERT model for estimating speed-dependent EFs are important to verify the potential impacts of increasing or decreasing speed (e.g. periods of free flow or congestion). Errera *et al.* (2010) evaluated the magnitude of congestion effects with the introduction of zero emission vehicles (ZEVs), showing that, in order to stabilize the yearly total emission when only ZEVs is recruited in the fleet, an additional amount of conventional vehicles would have to be replaced by ZEVs in order to compensate marginal effects — emissions increase due to a drop of mean travelling speed.

2.3 Hot exhaust emission

The estimation of hot exhaust emissions is given by

$$EH_{i,j,k,l,m} = F_{i,j,k,l} \cdot L_i \cdot EF_{scaled}(V_{i,l})_{j,k,m} \cdot DF_{j,k}, \tag{4}$$

where $EH_{i,j,k,l,m}$ is the emission for street link i, vehicle category j from age k, hour l and pollutant m $(\mathrm{g} \cdot \mathrm{h}^{-1})$; $F_{i,j,k,l}$ is traffic flow on street link i, by vehicle category j, age k and hour l $(\mathrm{veh} \cdot \mathrm{h}^{-1})$; L_i is the length of the street link

i (km); $EF_{scaled}(V_{i,l})_{j,k,m}$ is the scaled emission factor from Eq. (3)($\mathrm{g} \cdot \mathrm{km}^{-1}$); $DF_{j,k}$ is the deterioration factor for each pollutant m $[-]$. Deterioration factors are emission degradation functions of gasoline vehicles using catalysts due to accumulated mileage based on European measurements (Ntziachristos and Samaras, 2016).

2.4 Scenarios

In Curitiba, 44.9% of the total trips is made by passanger cars (IPPUC, 2019). For future scenarios, an increase (decrease) to 50% (34.9%) were considered. Also, in order to evaluate the contribution of old vehicles emissions, two scenarios of age limited to 20 and 30 years were adopted. The five scenarios of fleet is summarized in Tab. 2.

Table 2. Modeling scenarios.

Scenarios	PC relative share (%)	Total PC	Maximum age of fleet (years)
Current	44.9%	3599	40
Limited age (20 years)	44.9%	3599	20
Limited age (30 years)	44.9%	3599	30
Increase car share	50.0%	4008	40
Decrease car share	34.9%	2797	40

The category of each PC for the current scenario is shown in Tab. 5, where: E25, E100, FE25 and FE100 represents Gasoline using 25% hydrated ethanol, Ethanol, Flex engines using gasoline and ethanol, respectively; 1400, 1400_2000 and 2000 represents engines sizes lower than 1400, between 1400 and 2000, and higher than 2000 cm^3, respectively. The average age for PC using ethanol is higher since its commercialization were limited to a shorter range of years, and were interrupted after the introduction of flex-engines vehicles on market.

Table 3. Vehicle composition for the current scenario.

PC type	Percentage[1]	Average age	Maximum age
PC_E100_1400_2000	1.4	26.83	40
PC_E100_2000	0.05	26.83	40
PC_E100_1400	0.79	26.83	40
PC_E25_1400_2000	17.73	16.72	40
PC_E25_2000	0.65	16.72	40
PC_E25_1400	10.05	16.72	40
PC_FE100_1400_2000	20.28	8.1	15
PC_FE100_2000	0.74	8.1	15
PC_FE100_1400	11.49	8.1	15
PC_FE25_1400_2000	22.92	6.63	15
PC_FE25_2000	0.83	6.63	15
PC_FE25_1400	12.99	6.63	15

[1] For the 2017 composition. Source: ANFAVEA (2018); Sena (2015); CETESB (2016).

3. RESULTS AND DISCUSSION

The Figure 3 shows the emissions by age of fleet. Although the old fleet is not significant (Figure 2), the emission factors and deterioration associated is generally high. For instance, the CO emission factor for PC of age 40 using gasoline is 33 $\mathrm{g/km}$, while for age 1 is 0.114 $\mathrm{g/km}$. For ethanol, the EF is 0.67 $\mathrm{g/km}$ for age 11, and 18 $\mathrm{g/km}$ for age 36 (CETESB, 2016). Also, the emissions order of magnitude changes according to the pollutant, whereas CO_2 represents 98% of total emissions. CO_2 is directly associated to fuel consumption (Fontaras *et al.*, 2017), having not decreased significantly its EF for newer PC. Although CO_2 and CH_4 are not regulamented pollutants for vehicle emissions, it has major impacts for greenhouse effects. NOx consists on nitric oxide (NO) and nitrogen dioxide (NO_2), where approximately 97–99% corresponds to NO (CETESB, 2016).

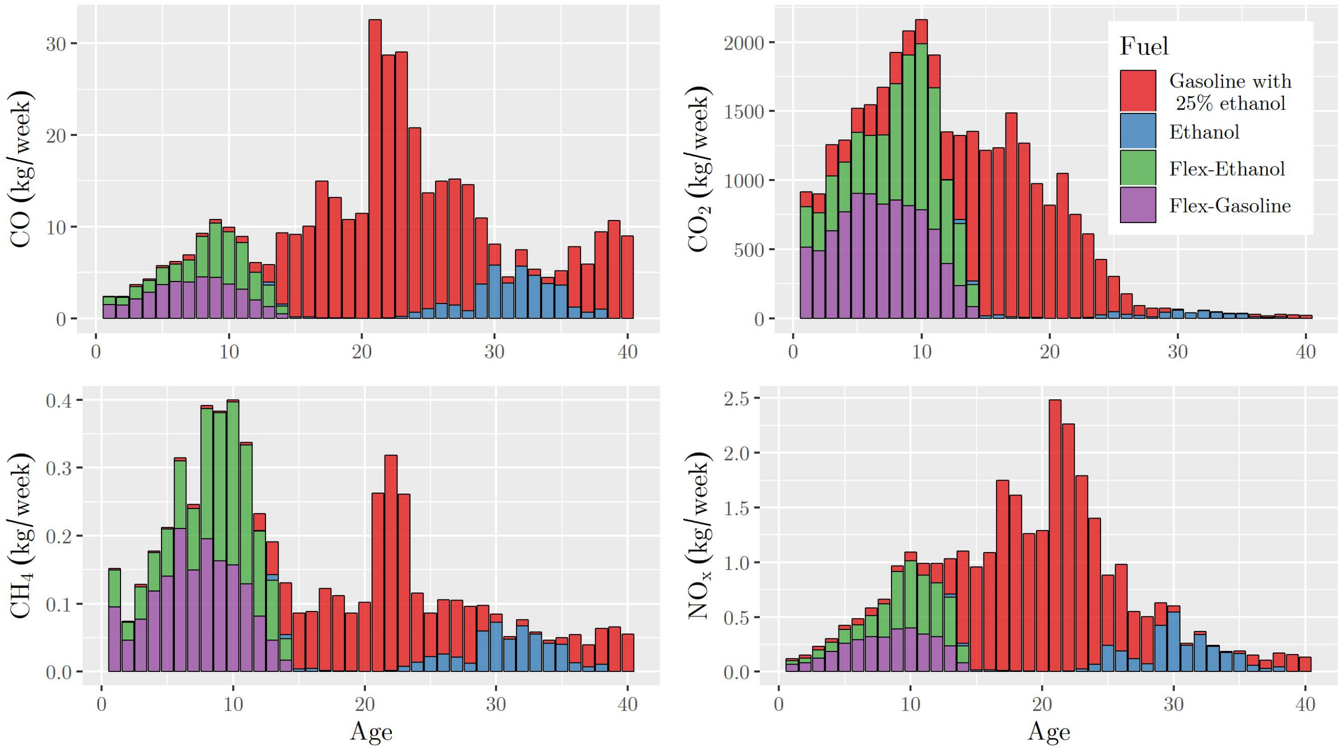

Figure 3. Hot exhaust emissions for the current scenario, according to fuel and fleet age.

Table 4 shows the pollutants emissions according to fuel and scenario, expressed in kg/week. Only PC using gasoline and ethanol had its emissions reduced for limited age scenarios, since flex engines fleet has been on market for up to 15 years ago. Comparing to the current scenario, CO_2 emissions increases for the 20 and 30 years scenario, primarily due to a variation of EF for ages of 3–10 years. As mentioned, the EF does not decrease according to PC age. However, CO, CH_4 and NOx indicates significant reduction for the 20-years scenario, since its CO_2 EFs has decreased for newer vehicles.

Table 4. Total emissions of CO, CO_2, CH_4, NOx per fuel and scenario, in a typical week (five working days).

		CO (kg/week)						**CH$_4$** (kg/week)			
Scenario \ Fuel	Gasoline	Ethanol	Flex-Ethanol	Flex-Gasoline	Total	Scenario \ Fuel	Gasoline	Ethanol	Flex-Ethanol	Flex-Gasoline	Total
Current	302.25	40.73	37.76	39.1	419.84	Current	2.34	0.55	1.54	1.63	6.06
20 years	112.88	4.54	37.76	39.1	194.29	20 years	1.04	0.14	1.54	1.63	4.35
30 years	260.91	26.23	37.76	39.1	364.01	30 years	2.1	0.43	1.54	1.63	5.7
Increase car share	336.58	45.36	42.05	43.54	467.53	Increase car share	2.61	0.61	1.72	1.81	6.75
Decrease car share	234.93	31.66	29.35	30.39	326.34	Decrease car share	1.82	0.43	1.2	1.27	4.71
		CO$_2$ (kg/week)						**NOx** (kg/week)			
Scenario \ Fuel	Gasoline	Ethanol	Flex-Ethanol	Flex-Gasoline	Total	Scenario \ Fuel	Gasoline	Ethanol	Flex-Ethanol	Flex-Gasoline	Total
Current	14628.64	590.57	8053.96	8858	32131.16	Current	20.87	3.08	3.78	3.41	31.13
20 years	15058.21	562.29	8053.96	8858	32532.46	20 years	13.22	0.52	3.78	3.41	20.92
30 years	14752.14	586.01	8053.96	8858	32250.1	30 years	20.51	2.9	3.78	3.41	30.59
Increase car share	16290.25	657.65	8968.78	9864.14	35780.8	Increase car share	23.24	3.43	4.2	3.79	34.67
Decrease car share	11370.59	459.04	6260.21	6885.17	24975	Decrease car share	16.22	2.4	2.93	2.65	24.2

Table 5 shows the comparison between scenarios. The increase and decrease of PC fleet, presented on Table 2, impacts proportionally on emissions as expected — since all scenarios had the same fuel distribution (shown in Fig. 2).

Table 5. Total emissions of CO, CO_2, CH_4, NOx and the comparison with the current scenario emission.

Pollutant \Scenario	Current (kg/week)	Limited age (20 years)		Limited age (30 years)		Increase car share		Decrease car share	
		(kg/week)	%	(kg/week)	%	(kg/week)	%	(kg/week)	%
CO	419.84	194.29	46.3	364.01	86.7	467.53	111.4	326.34	77.7
CO_2	32131.16	32532.46	101.2	32250.1	100.4	35780.8	111.4	24975	77.7
CH_4	6.06	4.35	71.8	5.7	94.1	6.75	111.4	4.71	77.7
NOx	31.13	20.92	67.2	30.59	98.3	34.67	111.4	24.2	77.7

Figure 4 indicates the total emissions by hour. The total fleet, shown in Fig. 1(B), is distributed along the day, according to the traffic flow index (Fig. 2). The emissions per hour indicated an adequate model response, with higher emissions on rush hours.

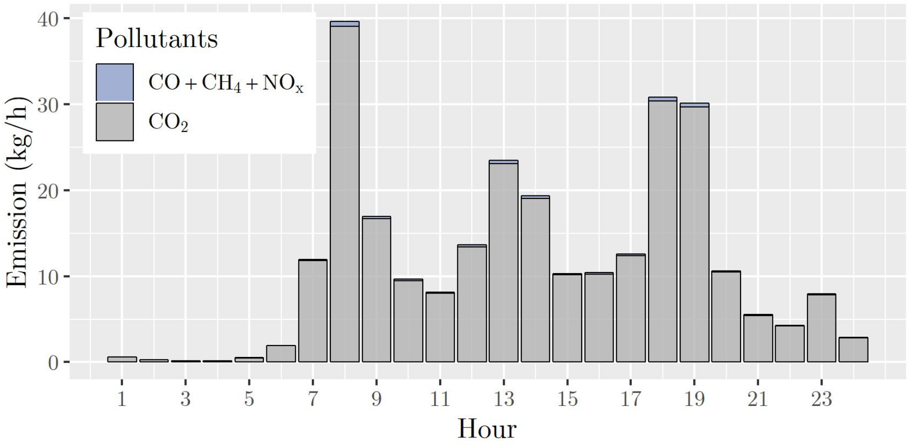

Figure 4. Total emissions per hour for the current scenario, in a typical week (five working days).

Figure 5 shows the total emissions distributed spatially. The reason for such differences on emissions is due to the number of PC on each route. Once all trips between zones were completed, not only for PC, but also for motorcycles and buses, the emissions can be added on space and time. Such results are an important tool for estimating the distributed emissions and for serving as input for air quality models.

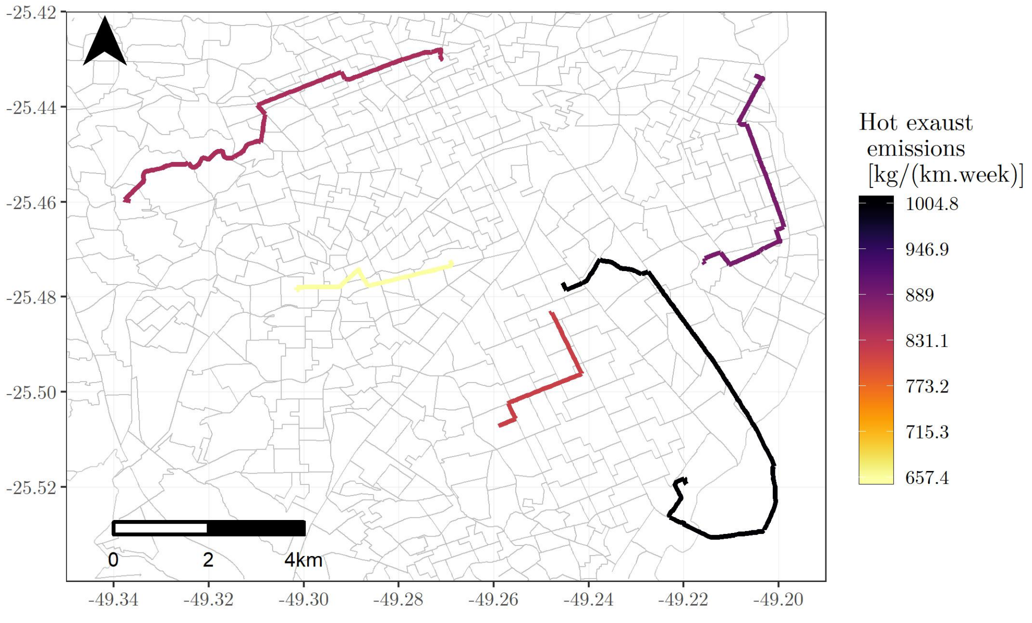

Figure 5. Total emissions distributed spatially.

4. CONCLUSIONS

This work aimed at modelling air pollutants emissions in Curitiba using bottom-up vehicle emissions inventory. For the city of Curitiba, there are some available data, such as traffic activity, fleet characteristics and trip patterns from ODS data, as shown in Tab. 1. The emission factors are functions of these characteristics but are also dependent on the vehicle speed. The results were summarized in Tab. 4, Fig. 4 and 5. It shows an important contribution for total emissions on rush hours, especially from the old fleet and for scenarios of increase PC.

Finally, the paper shows that ODS data, adopted for transportation policies in many cities, can be used for producing vehicles emissions inventory. The model can be further improved when considering more local data, all the existing trips between zones and therefore the effect of changes on mean traveling speed.

5. ACKNOWLEDGEMENTS

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