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Geoscientific Model Development
Discussions

Interactive comment on "Simulation of O_3 and NO_X in Sao Paulo street urban canyons with VEIN (v0.2.2) and MUNICH (v1.0)" *by* Mario E. Gavidia-Calderón et al.

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Dear reviewer and editor,

Thanks for your accurate observations, time, and dedication in reviewing this manuscript. We covered all your points shown below.

Many thanks

Comment 1

The paper assumes that the pollutant concentration is mainly contributed by the local sources, not regional sources. In a lot of cases, just the local emission amount may

not be accurate. What about regional emission? In particular, O3 typically is a regional source that can be transported from a far way. Without quantifying the ratio between local and regional sources, it is difficult to evaluate the reliability of the model.

Reply: Thank you for this important observation. Previous studies in SPMA identify the vehicular fleet as the main source of air pollution (Andrade et al 2015, 2017). According to Sao Paulo Environmental Agency (CETESB), in 2014 the vehicular fleet was responsible for emitting 97% of CO, 82 % of VOCs, 78 % of NOX, and 40% of particulate matter (PM) emissions in SPMA (CETESB, 2015). To clarify the importance of the local sources, we include the following paragraph in section 2.3.1 Emissions and street link coordinates: "The vehicular fleet is the principal source of air pollution in SPMA (Andrade et al., 2015, 2017). The particularity of this fleet is the extensive use of biofuels (i.e. gasohol, ethanol, and biodiesel). During 2014, vehicular emissions were responsible for emitting 97 % of CO, 82 % of VOCs, 78 % of NOX, and 40 % of particulate matter (CETESB, 2015)."

On the other hand, as we described in section 2.3.4, background concentration in air quality modeling in street canyons accounts for the proportion of air pollutants that aren't emitted in the simulated street-network (Vardoulakis et al., 2003). In our case, we used concentrations of O3, NO2, NO from the Ibirapuera air quality station as background concentration. To explicitly state the air pollutants used as background concentrations, we add the following sentences in section 2.3.4: "In this work, measurements of O3, NO2, and NO in Ibirapuera AQS were used as background concentrations."

Comment 2

2.2 VEIN emission model Line 140-142: "Therefore, if we consider the mean emission factor ratio times the mentioned traffic flow ratio results that the NOX emissions should be approximately 2.37 higher." Is the suggested ratio of 2.37 considering contributions from both light vehicles and heavy vehicles?

Reply: Thank you for your comment. The answer is yes. As we detected less traffic flow by comparing GPS with travel demand models' outputs of light and heavy-duty vehicles, it should be less emissions. That paragraph was reformulated and we recalculated the ratios between real-world and laboratory emission-factors to produce adjustment factors, already implemented in a newer version of the VEIN model (https://atmoschem.github.io/vein/reference/ef_cetesb.html). Specifically, the real-world emissions factors for light-duty vehicles and trucks 1.11 and 1.38 times higher than the emission factors reported by the environmental authority (CETESB, 2015).

We rephrase the paragraph as follows: "The emissions dataset presents two aspects that need to be discussed. The first one is that there are some differences between the traffic flow from travel demand model outputs (TDM) and GPS (Ibarra-Espinosa et al., 2019, 2020). The ratio between traffic flows from TDM and GPS for our study area is 2.22. Regarding the emissions factors used to estimate the emissions, they are based on the average measurement of emissions certification tests (CETESB, 2015), therefore, they may underestimate real-drive emissions (Ropkins et al., 2009). For instance, the real-world emission factors derived from tunnel measurements in São Paulo for NOX were 0.3 g km-1 for light vehicles and 9.2 g km-1for heavy vehicles (Pérez-Martínez et al., 2014), while the respective fleet-weighted CETESB (2015) emission factors are 0.26 g km-1 and 6.68 g km-1, as shown in Fig. S1 in Supplement, resulting in ratios of 1.11 and 1.38. Then, if we consider the mean emission-factor ratio (1.11 + 1.38)/2, times the mentioned traffic flow ratio (2.22) results that the NOX emissions might be approximately 2.73 higher than the estimated using pure CETESB (2015) data. Consequently, we expect that air quality simulations for NOx might be lower than observations."

Comment 3

Line 145: "We choose Wednesday emission as a typical weekday and Saturday emission for the weekend." How much difference between typical Saturday and Sunday traffic in SPMA?

Reply: Thank you for your comment. One of the advantages of VEIN is the use of vehicle GPS data that allows a traffic estimation and therefore a better temporal and spatial emission profile. Figure 1 shows the mean emission from all street links from the Pinheiros neighborhood for NOX and VOCs. In the case of NOx emissions, Sunday total emissions are 25 % lower than Saturday total emissions, while in the case of VOC the values are almost the same. According to Ibarra et al. (2020), the difference between NOX emission during the weekday and the weekend is explained by the Buses contribution, which is lower during the weekend, and even lower during Sunday. Figure 1 is added to Supplement. This is an important point to explain NOX and NO overestimation during Sunday for both Pinheiros and Paulita Avenue urban canyons.

Comment 4

2.3.3 Building height and street width Line 176 "Building height is retrieved from the World Urban Database and Access Portal Tools project (WUDAPT) for SPMA (Fig. 3)." How well is WUDAPT describing building height? Especially, LCZ1, "compact high-rise", is having a description of "height of roughness elements >25m". It is also mentioned in line 226 that "Paulista Avenue domain is more uniform, presenting urban canyons with a mean building height of 45 meters (LCZ1 - Compact high rise).", how is the value of 45 meters obtained? How sensitive is the model to these building height values?

Reply: Thank you for noticing this. We explain this point by adding the following paragraph in section 2.2.3: "We retrieve the building height from the updated URBPARM.TBL file from WRF-Chem simulations in Pellegati et al. (2019). This file was built with the information described in Stewart et al. (2014), and contains the geomorphological and radiative parameters for each WUDAPT LCZ to be used in the Building Environment Parameterization (BEP) simulation in Pellegati et al. (2019)."

We believe that WUDAPT offers a good reference building height value rather than use a constant building height value. Certainly, this information needs to be improved by comparing it with other data sources as Google Earth or by in-situ measurements. We rephrased line 399 in the Discussion and Conclusions section as the following: "On the other hand, now Google Earth allows new features like 3D view, that together with in-situ measurements, can improve WUDAPT building heights estimates."

Furthermore, we also ran a test with different constant building heights (i.e. 30 m, 50 m, 70 m). MUNICH is coherent with previous results where dispersion is restricted in deep urban canyon leading to higher pollutants concentrations (Afiq et al. 2012). As shown in Fig. 2 higher concentrations of NOX are produced inside the urban canyon when we increase the building height, this leads to a decrease of O3, by its reaction with the NOx. As we can see, background concentration and emission rates have a higher impact than the building height in air quality simulation with MUNICH.

Comment 5

2.3.4 Background concentration Line 195-198 "With that in mind, by using the mean wind field from WRF simulation for the study period, we select Ibirapuera AQS (83 shown in Fig. 4) measurement as background concentration, which, according to the wind field, advect pollutants to Pinheiros station (99) and Cerqueira Cesar (83) as can be seen in Fig. 4." Is the difference of wind direction from mean during the study period justifying the choice of a single AQS at upwind to provide background concentration. Surely, that single station cannot be upwind for all year round?

Reply: Thanks for bringing this important question. When we analyzed the wind fields generated by WRF simulations we can see that there is a different behavior during the daylight (Fig 3.a) and nighttime (Fig 3.b). During daylight, there is the advection from Ibirapuera AQS to Pinheiros and Cerqueira Cesar AQS, whereas during night time west winds are predominant. As ozone concentrations during the night are low, it is more important to use information from air quality stations that measure the ozone upwind Pinheiros and Cerqueira Cesar AQS during daylight, when ozone concentrations are higher. For that reason, we chose Ibirapuera AQS. Still, as noted in the discussion sec-

tion, it could be better to use air quality model results as background concentration for MUNICH, not only for a better background concentration estimate but also to address this wind direction implication. Figure 2 is added to Supplement, and we clarify that this assumption is valid during daylight.

Comment 6

Figure 4 Minor: in figure Cerqueira Cesar (red diamond) has number 91 instead of 83 as in line 197 and caption. Typo?

Reply: Thank you for noticing this. Yes, Red diamond should have the number 83. It is now corrected in the manuscript.

Comment 7

2.5 Model set up Line 215 "VEIN calculates the emissions for the whole SPMA" Line 219-220 "The red lines are the street links used by VEIN to calculate the emissions, and the yellow rectangle the urban canyon selected for comparison against observation." I am not quite sure what this means. Are red lines in figure 5(a), (b) all street links in the domain? If there are street links that are not used by VEIN to calculate the emission? If so, how is their emission calculated?

Reply: Thanks for bringing this up. As detailed in section 2.3.1, VEIN produces emissions for all the street links in SPMA. This information is a simple feature (sf) class object that contains a column with the Municipality/Neighborhood name of each street link. For this work, we subset the street links for Pinheiros neighborhood, and for the neighborhoods that contain the Paulista Avenue urban canyon. Therefore, the red lines in figure 5(a), (b) in the manuscript are a selection of the original VEIN output for SPMA. We clarify this in section 2.5 by adding the following sentence: "VEIN produces emissions for all the street links in SPMA. This information can be filtered by the neighborhood name of the street links. We subset that information for Pinheiros neighborhood, and for the neighborhoods that contain the Paulista Avenue urban canyon."

Comment 8

3.2 Emission adjustment Line 263-264 “We ran different scenarios with increased NOX and VOCs emission from VEIN. The best results were produced when doubled the NOX and VOC emissions. This scenario is called MUNICH-Emiss.” If there is any reason picking 2x as the adjusted emission? Would it perform better if higher emission, e.g., 2.5x, is used?

Reply: Thank you for your comment. We performed sensitivity tests with different emissions increment scenarios: the original emissions (original VEIN output), doubled emissions, tripled emissions, and quadrupled emissions. We noticed that the increment of emissions improves ozone simulation. Nevertheless, the increment could lead to unreasonable NOX concentrations, as in the case of the quadrupled emission scenario. The tripled emission scenario presented less error in magnitude than the doubled emission scenario, but it presented a lower Pearson correlation coefficient than the doubled emission scenario for NO, NO2, and NOX. To decide the better scenario, we used the index of agreement statistic (IOA). The doubled emission scenario presented higher IOA values for NO, NO2, and NOX. For that reason, we chose the doubled emission scenario as MUNICH-Emiss. We didn’t test for 2.5x as the MUNICH-Emiss scenario already provided good results and reached Hanna and Chang (2012) performance criteria.

Comment 9

4 Discussion and conclusions Line 396 “calibrated emissions.” What does this mean? Is it the MUNICH-Emiss? Or is it calibrated in some way?

Reply: Yes, in this case, “calibrated emissions” refers to the scenario where emissions are doubled. We have explicitly stated on the manuscript by adding “(i.e. MUNICH-Emiss scenario)” on line 396.

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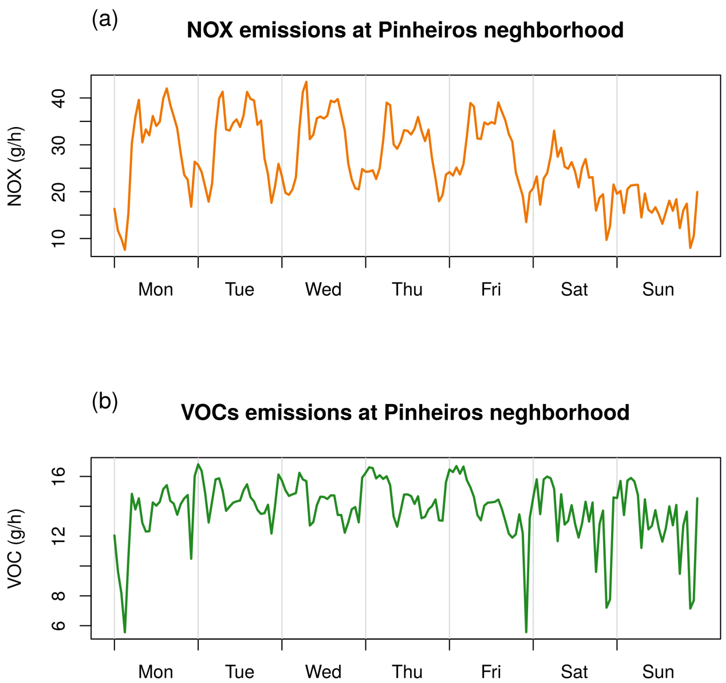

Fig. 1. Mean emission from all street links from the Pinheiros neighborhood for (a) NOX and (b) VOCs for a typical week.

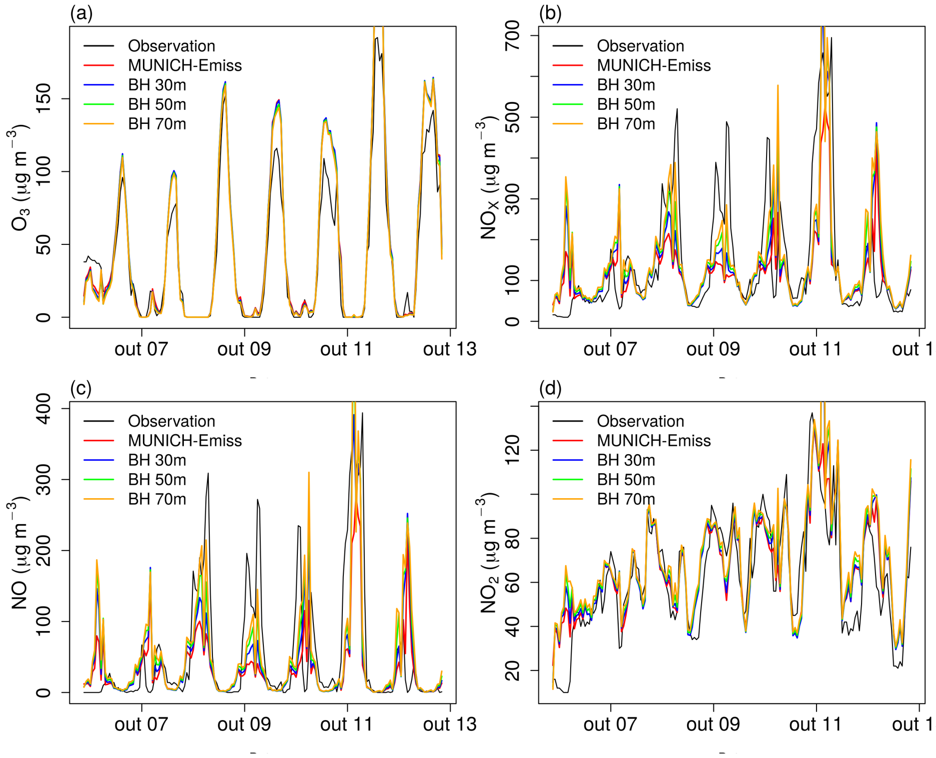

Fig. 2. Effect of different building heights on MUNICH air quality simulations.

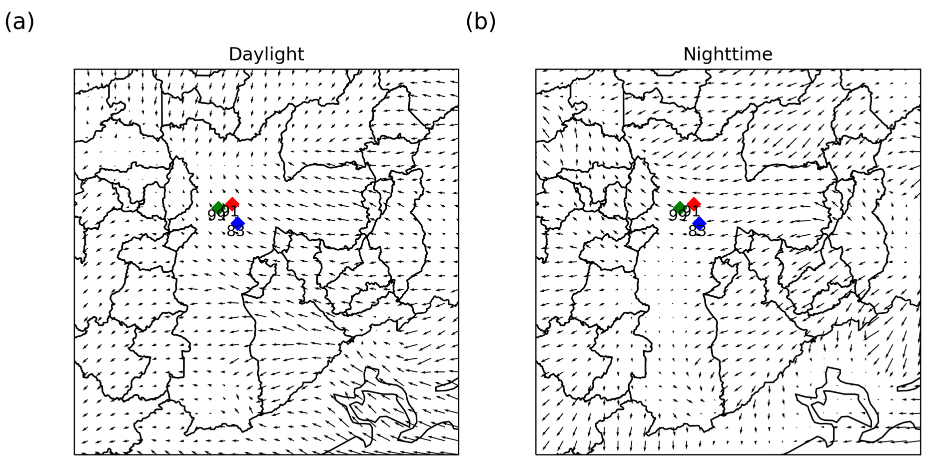

Fig. 3. WRF averaged wind field for daylight and nighttime during the simulation period. Pinheiros AQS is number 99; Cerqueira Cesar AQS, 91; and Ibirapuera AQS, 99.