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Interactive comment on "VEIN v0.2.2: an R package for bottom-up Vehicular Emissions Inventories" *by* Sergio Ibarra-Espinosa et al.

Sergio Ibarra-Espinosa et al.

sergio.ibarra@usp.br

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Response to comments of Referee 2: Thank you for your comments. Please see our revised draft of the manuscript, in the attached file vein3.pdf, with changes marked in blue with the number representing each of your comments between parentheses. This manuscript also includes the replies for Referee 1 in red and some replies for editor in brown.

Comment 1: The relationship between hourly average speed and traffic flow is given by equation 4, which includes the parameters alfa and beta. The authors suggest default values but allow the users of the model to choose local data. Perhaps with a

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better explanation about the variable Capacity this issue will be clarify but, in any case, the explanation on how these default values were established is needed, and to what extent they depend on the local type of fleet / circulation circumstances.

Reply 1: We added descriptions between line 33-34 of page 4 and line 1-7 of page 5. We added cited definitions of capacity from the Highway Capacity Manual. We also cited manuscripts of authors that fitted the BPR parameters alpha and beta based on local recordings of speed and traffic to represent the local characteristics of traffic fleet and circulation.

Comment 2: In the Emission Factors options explained in item 2.2, it is not clear the difference between the option 2) Emission factors from local sources (line 31, page 4) and the $EFlocal_{j,k,m}$ that represents the constant emission factor (not speed functions). If they represent the same (i.e. the EFs measured in any place, on the basis of dynamometer?s experiments) the authors should explain why the option 2) is given. In the case to have other experiments, such as on-road measurements or tunnel studies, how these numbers are included? This item has to be expanded in order to give more details about the use of local EFs data..

Reply 2: We added descriptions between lines 22-26 of page 5 for item 2 relating to local emission factors. We also added the Appendix B, which shows examples about how to estimate emissions with VEIN using COPERT, local and scaled emission factors.

Comment 3: The authors does not mention the difference in the emissions regarding the type of fuel used, which is particularly relevant for example in Brazil where almost all new cars sold can run on any combination of gasoline and ethanol. This deserve clarifications in several parts of the manuscript:

a) Deterioration factors: The model includes an emission factor database (fe2015) that does not include this factor. Nevertheless the authors report the use of deterioration factors from Ntziachristos and Samaras (2016), who said that these factors should not be used to provide the deterioration of emissions where an older fuel is used in a newer technology (e.g. use of Fuel 2000 in Euro 4 vehicles) and, therefore, cannot be used for other type of fuels. This reviewer agrees that it is necessary to make some consideration in this regard, and that the availability of these numbers is scarce, so that considering European values (due to the lack of better ones) is a valid option. However, it is necessary to prevent end users of the model about this assumption including a comment in the manuscript because it is known that the use of ethanol accelerates the deterioration of the engine

b) Speciation schemes dependence with fuel composition. An unknown set of schemes from Rafee (2015), whose reference is in Portuguese, has been considered. It is necessary to include a brief explanation about this work including, for example, which type of fuels these ses include..

Reply 3a): Great obvervation. Yes Ntziachristos and Samaras (2016) show that new technologies associated with newer standards need fuel with proper quality. For instance, as on page 52 of Ntziachristos and Samaras (2016, https://www.eea.europa.eu/publications/emep-eea-guidebook-2016/part-b-sectoral-guidance-chapters/1-energy/1-a-combustion/1-a-3-b-i/view), the subsection on **Fuel effects**, quoting: "emission standards of Euro 3 technology (introduced 2000) are achieved with Fuel 2000, and the more stringent emission standards of Euro 4 and 5 with Fuel 2005". This refers to the effect that, older vehicles started to consume the new and better fuel, which also led to diminishing emissions also in these types of vehicles. To take into account this effect, the Equation (24):

$$FCeHOT_{i,k,r} = FCor_r i, k, Fuel/FCorr_{i,k,Base} * eHOTi, k, r$$

cannot be used to account for deterioration. This means that

$FCorr_{Fuel}/FCorr_{Base}$

is restricted to values below or equal to 1. Currently, there are no fuel correction functions in VEIN on CRAN repository. However, we didincluded the function $fuel_corr$ on GitHub repository.

On the other hand, the section about **Emission degradation due to vehicle age** on page 51, presents the deterioration factors depending on accumulated mileage and technology of vehicles with 3-way catalizers. To our knowledge, there are not available deterioration factors for vehicles consuming bio-fuels. Hence, we agree that, in the absence of better data, using COPERT deterioration factors in a Brazilian fleet is valid. We included the information between lines 24-30 of page 16 to warn users of COPERT factors, by mentioning that users must include deterioration and fuel effects factors.

Reply 3 b): The reference of Rafee (2015) was replaced with an Ph.D thesis in english of the author of this manuscript Ibarra S. (2017), which is included in the references. The new speciation updates the exhaust speciation of NMHC which is based on other studies. We added the information in between lines 28-32 of page 8 and pages 1-3 of page 9.

Comment 4: The data of vehicle start pattern taken from the IVE experience in Brazil, how can be extrapolated to other cities/regions? Please, clarify the variability of this parameter, and its dependence on the type of technologies used in the different countries.

Reply 4: The data of start patterns should be generated by users by using local data. For instance Gonzalez et al (2017) generated a start pattern using surveys to estimate vehicular emissions using IVE. However, the user eventually could use the start pattern available in VEIN only in the absence of other data. This pattern is β parameter by type of vehicle on equation (7). The function ef_ldv_cold covers this type of emissions, based on Ntziachristos and Samaras (2016), which depends on the type of vehicle, temperature, size of engine, fuel, euro standard and pollutant. As consequence, this function can be used in other countries by identifying the equivalence between local and Euro standard, as shown on Table 2 for the Brazilian case. We added explanations on page 7, between lines 19-21.

Minor comments 5.a. : Page 5 line 28 ? studies report that when ambient temperature is -7C, emissions are one order of magnitude higher than at 22C (Ludykar et al., 1999)?, please clarify the corresponding pollutant (the numbers are totally different between compounds).

Reply 5a: Great observation. We specified the change in each pollutant by citing Table 1 of the same study between lines 4-7 of page 7.

Minor comments 5.b: In Page 4 line 25 the authors define the meaning of Emission factor, referring to Tinus Pulles definition, but for the manuscript define ?an emission factor is the mass of pollutant emitted by the vehicular type, technology and years of use?, but the activity data was not included in the definition (km travelled).

Reply 5b: In Page 5, line 16, we added the phrase: "by traveled distance, as mass of pollutant / distance", representing the travelled distance of the activity.

Minor comments 5.c: Page 5 lines 8 to 11: Mileage driven with a cold engine/catalyst: the authors said that they included in the model the cold starts recorded during the implementation of the International Vehicle Emissions (IVE) model, but is not enough clear if the data from COPERT are also included. Please, also clarify if other data about this parameter may be included by other modelers.

Reply 5.c: Equation 7 shows the approach for estimating cold start emissions. The incorporation of the start pattern from the IVE study was meant to bse used as the β, the fraction of mileage driven with cold engine/catalyst. This approximation represents the percentage of distance driven under cold conditions. The user could also follow Ntziachristos and Samaras (2016) approach for estimating $\beta = 0.6474 - 0.02545 * lengthtrip - (0.00974 - 0.000385 * lenthtrip) * ta$. We added an explanation between lines 21-23 on page 7.

Minor comments 5.d: 5.d. Page 6 line 5: ?This is an important aspect that will be reviewed in future versions of VEIN?. Please, clarify the intention.

Reply 5.d: We removed that line which you have highlighted. We intended to imply that start patterns used in β would need to be tested, but this has already been tested in IVE inventories.

Minor comments 5.e:It is not clear the input data needed to estimate the daily cycle, (1) rush hours during the morning pick or (2) the available data in each country/city, combining with a TF matrix accordingly, with a value of 1 for the maximum flow, at the time that it occurs.

Reply 5.e.:We added further explanations on page 4, lines 16-18, 21-22.

Minor comments 5.f:Please, clarify if it would be possible to include other speciation schemes.

Reply 5.f: Very important comment. Currently, the chemical mechanisms in VEIN includes the COV speciation 'iag' which splits the VOC emissions for the mechanism Carbon Bond Mechanism Z. If the user intends to use other mechanisms, needs to know how to speciate the COV and PM based on the user's own data. This means that the user must know the percentages to split the pollutants. In this case, the user could use that percentage in the argument k for any VEIN function of emission factor for the respective type of vehicle. The user could then use this to estimate the emissions for that fraction of vehicles. For example, if the user knows that 5% of COV emissions of LDVs consuming diesel are Xylenes, then the user must use the function ef_ldv_speed or ef_ldv_scaled (or its own local emission factors) with the argument k = $5/100$. The argument k is just a factor added to the resulting emission function. Finally, the user must aggregate the emissions by pollutant. We added this explanation on page 22, lines 29-33 and and page 23, lines 1-3. Moreover, users can contribute to the development of the model with the pull requests on GitHub repository https://github.com/atmoschem/vein (previously https://github.com/ibarraespinosa/vein).

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VEIN v0.2.2: an R package for bottom-up Vehicular Emissions Inventories

Sergio Ibarra-Espinosa[1], Rita Ynoue[1], Shane O'Sullivan[2], Edzer Pebesma[3], Maria de Fátima Andrade[1], and Mauricio Osses[4]

[1]Department of Atmospheric Sciences, Universidade de São Paulo, Rua do Matão 1226, São Paulo, SP, Brazil
[2]Department of Pathology, Faculdade de Medicina, Universidade de São Paulo, Av. Dr. Arnaldo 455, São Paulo, SP, Brazil
[3]Institute for Geoinformatics, Westfälische Wilhelms-Universität Münster, Heisenbergstraße 2, 48149 Münster, Germany
[4]Department of Mechanical Engineering, Universidad Técnica Federico Santa María, Vicuña Mackenna 3939, Santiago, Chile

Correspondence to: Sergio Ibarra-Espinosa (zergioibarra@gmail.com)

Abstract.
Emission inventories are the quantification of pollutants from different sources. They provide important information not only for climate and weather studies, but also for urban planning and environmental health protection. We developed an open source model (named VEIN v0.2.2) that provides high resolution vehicular emissions inventories for different fields of studies. We focused on vehicular sources at street and hourly levels due to the current lack of information about these sources, mainly in developing countries. The type of emissions covered by VEIN are: exhaust (hot and cold) and evaporative considering the deterioration of the factors. VEIN also performs speciation and incorporates functions to generate and spatially allocate emissions databases. It allows users to load their own emissions factors, but it also provides emissions factors from the road transport model (Copert), the United States Environmental Protection Agency (EPA) and Brazilian databases. The VEIN model reads, distributes by age of use and extrapolates hourly traffic data, and estimates hourly and spatially emissions. Based on our knowledge, VEIN is the first bottom-up vehicle emissions software that allows input to the WRF-Chem model. Therefore, the VEIN model provides an important, easy and fast way of elaborating or analyzing vehicular emissions inventories, under different scenarios. The VEIN results can be used as an input for atmospheric models, health studies, air quality standardizations and decision making.

1 Introduction

Emissions inventory is a quantification of pollutants discharged into the atmosphere by different sources (Pulles and Heslinga, 2010). This quantification is vital for regulatory and scientific purposes, because it allows to monitor the state of the Earth's atmosphere and climate. It also allows to create air quality standards, which will protect ecosystems and human health. For instance, the Intergovernmental Panel on Climate Change (IPCC) includes a dedicated task force, separated from the other three working groups, only for the purpose of greenhouse gas emissions inventory issues (Paustian et al., 2006).

In this instance, there are several emissions inventories that use different input data and approaches for different scales. One of the most frequently used inventories is the Emission Database for Global Atmospheric Research (EDGAR; Olivier

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Fig. 1.

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