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Interactive comment on "Street-in-Grid modeling of gas-phase pollutants in Paris city" *by* Lya Lugon et al.

Anonymous Referee #2

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General comments:

This manuscript presents recent developments of the multi-scale modelling system Street-in-Grid (SinG) which dynamically couples the mesoscale chemistry transport model Polair3D and the street network model MUNICH with two-way feedback. A new non-stationary numerical scheme is implemented in MUNICH that avoids the time step dependency in the partitioning of NO and NO2 chemistry. The new approach is used to evaluate SinG during May 2014 over Paris city and discuss the benefit of the two-way coupling between MUNICH and Polair3D when modelling NOx, NO and NO2. The SinG model adopts an elegant solution to avoid the double-counting of traffic emissions and is one of the few street-scale models that solve complex gas-phase chemistry based on Carbon Bond 2005 chemical mechanism. As stated by the Authors at the

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Discussion paper

end of the Conclusions, it will be extended in the near future to solve condensed phase chemistry. All these characteristics make SinG an excellent modelling tool to advance research on urban chemistry.

I have some general comments. The first one is about the title, which, in my opinion, is too generic and does not reflect the content of the manuscript. I suggest the Authors consider a reformulation of the title that better describes the main objective of the work. The main focus is on NOx/NO/NO2 representation, and the two-way feedback addressed in SinG. Regarding the new numerical scheme implemented in MUNICH and SinG, the discussion would benefit with some quantification of the computational time used in a stable stationary configuration compared with the new non-stationary solution presented in the manuscript. Is there any overhead added with the non-stationary approach? Are other gases apart from NOx sensitive to the old numerical scheme that makes the solution unstable or with a small enough time step the stationary solution is still accurate? The two-way feedback implemented in SinG is very elegant to avoid the double-counting of emissions at the urban scale, but it is somehow counter-intuitive the results compared with MUNICH alone which indeed has double-counting emissions from Polair3D background. One would expect MUNICH results to be overestimated due to the double-counting effect, but this is not the case. Both SinG and MUNICH evaluations with measurements are very similar. Some elaboration on the possible reasons for this result and the implications for other modelling systems that may still have double-counting of emissions in their urban solutions would be desired. Finally, some discussion about the impact of the Street-in-Grid at the regional scale downwind the city is missing. It is clear that the two-way coupling will improve the skills of SinG at the regional scale if it is evaluated with urban sites, but does this result also in an improvement of the mesoscale model photochemistry downwind Paris? Is there any sensitivity in NOx and other reactive gases like O3 in some rural areas affected by the pollution plume of Paris?

The results of the manuscript are novel and have an interest in the scientific community. However, I have the impression that the material presented is more suited for the "Geoscientific Model Development" than "Atmospheric Chemistry and Physics" journal. Overall, the manuscript is well written but deserves some English editing. I recommend the authors to address the general comments and improve the manuscript following the specific and technical comments detailed below.

Specific comments:

- Line 1: Quantify or provide a range for "coarse spatial resolution".

- Line 15: I suggest to explicitly mention in the abstract that SinG implements a two-way feedback. The Authors could use "two-way dynamical coupling" or "a dynamical coupling between the regional and local scales with a two-way feedback."

- Line 74: The concept of dynamic coupling defined here is confusing. In multi-scale or nested domain models, the dynamic coupling can be one-way or two-way. The latter means that the feedback from the smaller scale to the coarser scale is allowed, which is the case of SinG. For the sake of clarity, I recommend using the concept of "two-way dynamic coupling" or "dynamic coupling with two-way feedback".

- Line 108: The sentence explaining how the multi-scale concentrations are obtained in Stocker et al. (2012) is not clear. What is the difference between the "gridded concentration" and the "regional-scale concentration"?

- Line 113: The objective is very well presented here; part of this sentence could be used to improve the current manuscript Title. I think that the novel contribution of the work is the discussion on the role of the two-way feedback between scales.

- Line 124: Is SinG a model or an interface? The Authors could clarify how MUNICH and Polair3D are integrated into SinG. Is SinG a version of Polair3D with an urban component that runs MUNICH internally as a subroutine providing meteorological and chemistry inputs?

- Line 128: A one-way formulation is still a dynamic coupling. As suggested before, the use of "two-way feedback" may help the reader understand the added value of SinG compared with other modelling systems.

- Line 147: What are the implications of assuming the concentrations uniform within the street segments? What is the maximum length of a street segment allowed in MUNICH?

- Line 172: How is the standard deviation of the vertical wind speed computed from WRF variables?

- Line 174: The CB05 is a gas-phase mechanism. Please, replace "concentration of pollutants" for "concentration of gases" and "module" for "mechanism".

- Line 184: In equation 9, is the parameter triangle sub-zero the same as triangle sub-one but for time n? Please, clarify the meaning of the notation used to define triangle sub one.

- Line 193: What is the computational overhead of running MUNICH coupled to Polair3D in SinG compared with running only Polair3D?

- Line 195: Clarify in the text that "cell i" is the cell of the regional model.

- Line 203: From equation 11, SinG does not perform an average but a sum of the mass of background and the street. Please, amend. Why the authors use Vcell instead of (Vcell-Vbuild)? This is the exact volume from where equation 11 derives the mass.

- Line 206: I guess there is an error in the numbers of sub-Sections 2.4, 2.5, 2.6 and 2.7. sub-Section 2.4 should be a new Section 3, and the following sub-sections the new 3.1, 3.2 and 3.3.

- Line 208: Did the authors perform any spin-up in the chemistry?

- Line 210: Please clarify if SinG runs the 4 Polair3D domains or it is a decoupled run? Is Polair3D using two-way nesting?

- Line 240: Not many streets are used in the local-scale domain. What are the implications in the total traffic emissions of Paris ingested in the models then? Can the Authors quantify the percentage of emissions that the main streets used in the simulations represent from the total? How are the rest of the streets treated SinG during the two-way coupling? Are all the streets still used in eq 10 for Vbuild_i or only the main streets?

- Line 268: What is the temporal resolution of the background concentrations used in MUNICH? This may explain part of the differences seen between SinG and MUNICH. SinG may use background conditions with higher temporal variability compared with MUNICH set up.

- Line 292: Why the authors consider that some of the results are not stable numerically? None of the runs shows numerical instabilities, at least from what can be seen in Figure 7 and 8. The solution using 600s is quite similar to the one with 100s. Which are the criteria to identify numerical instabilities in SinG or MUNICH?

- Line 293: Please, show the observations in Figure 7 and 8. Why do the Authors not show SinG and MUNICH results in the same station both figures? It is difficult to appreciate the differences between methodologies using different sites.

- Line 295: Why a time step of 100s is selected with the non-stationary approach? Figure 7 and 8 show the same results with 600s, which imply that the model should be much faster with the same accuracy with 600s.

- Line 304: Please, provide MUNICH results in Table 5 or clarify if MUNICH results are the same as the background concentration of Polair3D in open-areas.

- Line 325: Figure 11 shows a better agreement of SinG and MUNICH during the morning peak than the evening one. Do the Authors have an explanation for this behaviour?

- Line 330: The Polair3D shows a substantial underestimation of NO as most CTMs. It appears a significant drawback for MUNICH and SinG to reproduce NO in open areas within the city. Can the Authors elaborate on approaches to overcome this limitation?

- Line 441: Results of SinG at the regional scale over the Paris area show higher NOx concentrations than Polair3D. What is the impact downwind Paris area in some urban background or rural sites using SinG or Polair3D? Does this increase of NOx in SinG results in a positive effect on the model downwind Paris (i.e., O3)? If this is the case, it would be relevant to elaborate on this because it has implications in the way how urban-cities are modeled in mesoscale models.

- Line 452: As mentioned before, equation 11 does not define SinG regional scale concentration as an average but a sum of masses.

- Line 480: I suggest to add a last sentence highlighting that NO is less sensitive to this coupling and why.

- Line 481: Do the Authors have any plan to evaluate other gases at street-level in the future? One of the most important capabilities of SinG is solving complex chemistry at street-scale. Understand the dynamics of other reactive gases in the urban environment deserves future research efforts.

Technical comments:

- Figure and Table captions: all captions should be self-explanatory. Several Tables and Figures present information that is not described in the caption (i.e., name of variables, units, the meaning of acronyms or abbreviations.)

- Equations: There are several equations with the definition of terms in the same line. Please, split those cases in separate equations. This occurs in Eq 3, 7, 8, 9, 11.

- Line 2: Delete "i.e."

- Line 15: Amend the format of the World Health Organization reference. Use "WHO (2016)" or "World Health Organization (2016)". It has not much sense to define an acronym that will not be used anymore in the text.

- Line 25: Add a comma after "e.g." or "i.e.".

- Line 25: Follow the appropriate style used by ACP when using references between parentheses. To simplify the text, I suggest using only the references, not the model acronyms.

- Line 44: Use the same style to introduce acronyms throughout the text, first the complete name followed by the acronym in parentheses.

- Line 44: Avoid opening a parenthesis just after a closing one, and use similar style format if several references are provided. In particular, "(CALINE4; Bensons, 1984; Sharma, et al.). Check and unify the reference format used in the text.

- Line 44: The reference "Sharma et al." is incomplete. Please, provide the year here and in the reference section.

- Line 52: Define the acronym SIRANE, as done previously with other models.

- Line 136: Amend the use of references. In this case should be like "at different locations (e.g., Sartelet et al., 2012; Abdallah et al., 2018; ...)."

- Line 137: Remove "including Greater Paris" from the middle of the list of references.

- Line 150, Equation 2: The use of Q and Qinflow are confusing. Q is a mass variable while Qinflow, Qemis, Qoutflow, ..., Qdep are mass fluxes. I suggest using another letter for the fluxes, e.g., Finflow.

- Line 153: Amend "each of this term" with "each term".

- Line 158: Please, define what is Qair and Cst like is done with H, W and Ust.

- Line 161: Together with the reference of equation 8 from Kim et al. (2018), add the reference to equation 7 of this manuscript.

- Line 194: Amend "details" with "detailed".

- Line 220: Specify the version of WRF model used.

- Line 222: Is the top of the atmosphere in WRF set at 5000m? If not, amend.

- Line 225: Delete "and chemical".

- Line 228: Specify the version of MEGAN model used.

- Line 233: Amend the link provided. It is not working.

- Line 236: Specify the period of average used in Figure 4.

- Line 284: Figure 6 and Figure 5 could be combined in a single figure. I recommend using two different colours to differentiate urban and traffic measurement stations (i.e., red and black dots).

- Line 358: Please, clarify how relative difference is computed. Which is the reference value?

- Line 361: It would be desirable to use the same range and colour scale in both panels of Figure 14.

- Line 389: Amend "daily mass fluxes" with "daily weighted mass fluxes".

- Line 396: In the legends of Figure 16, use the same notation as equation 12. Instead of Qinflow should be qf_inflow.

- Line 401: Check the use of the hyphen. Sometimes is used and others not (e.g., daily weighted, daily-weighted).

- Line 439: Detailed the meaning of the colour in the Figure by adding "Percentage of streets (purple colour). Add a % at the top of the colour scale.

- Line 460: Re-word "coupling finely".

- Line 467: Use "appropriate" instead of "verified".

- Line 497: Correlation is never used in the manuscript. Please, remove the statistic from the Annex.

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