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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Development and application of a reactive plume-in-grid model: evaluation over Greater Paris" *by* I. Korsakissok and V. Mallet

Anonymous Referee #1

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General comments

The paper focuses on an important scientific issue: the representation of the unresolved subgrid scale variability in Chemistry Transport Models. However, the aims of this paper are not clearly defined. The title suggests that the authors have two major objectives: 1) the development of a new modeling approach; and 2) evaluation of the model over a case-study in Paris. In my opinion, the paper focuses more on the implementation of an existing approach rather than development of a new modeling approach, and the main objective of the paper is the demonstration of the application of the coupled puff and grid model and evaluation of the model over a case study. I think

the readability of the paper could be improved by clearly describing the objectives and reorganizing the structure of the paper accordingly. For example, Section 1 would be better presented as an Introduction section, and subtitles 1.1 and 1.2 removed. Also, Section 2 of the paper should be omitted and replaced by appropriate references, or moved to an Appendix, if necessary. The rest of the paper should also be re-organized to improve its readability. I also have some specific comments (see below). Overall, this is a good paper, it is novel and scientifically sound, and I think it would be of interest to your readers. I support publication after authors have addressed my comments.

Specific comments

I think that the authors should be more quantitative when they refer to the spatial and temporal scales through out the paper. Combining three characteristic time scales of the vertical diffusion, the injection time, and the chemical reaction rates is critical for this modeling effort. I suggest that the authors become more explicit when referring to these critical scales. For example: Section 1 lines 5-10 "First, a point emission is assumed to immediately mix within the cell volume, whereas a typical point-source plume does not expand to the size of the grid cell for a substantial time period." Here "grid cell size" and "substantial time period" merit evaluation. Also, in Section 2.1.1 line $\sim$20 "A continuous plume is well represented if ...." "sufficient" and "large enough" are too general in this context. Another example: Conclusions, Section 7, lines 20-25: "Using a plume-in-grid treatment for point ....", I suggest that the authors provide a more quantitative measure.

Abstract, lines 15-20 In my opinion, the numbers provided as model scores here (RMSE) are not representative for this application, when a Gaussian puff model is embedded in the CTM and the authors should justify their use. I expect that the improvement in model results should be higher than the one represented by the numbers provided in the abstract (I find the results surprisingly low for NO I wonder if the author's shouldn't also study the sum NO+NO2 that is less reactive as a family of species).

Section 1 I think this part of the text needs re-organization in order to clearly set the goals of the study. The authors should explain why they decided to consider this complicated issue. I would rather expect to find here a list of the problems encountered previously when such a coupling technique was applied and in what way the authors overcame these problems.

Section 2 The section starts by saying that this study couples two previously developed models (Gaussian Puff, Korsakissok and Mallet 2009, and Polair3D, Boutahar et al. 2004). As far as the dynamic coupling of the two models is concerned the authors cite their previous paper (Korsakissok and Mallet 2010) (lines $\sim$5). However the spatial scales between this study and the present differ significantly (i.e. continental to regional) with resolution increase by a factor of almost 10. What refinement has been done in meteorology, land-use data, topography etc. in order to assess the finer scale?

Section 2.1.2 Also there are some important assumptions that are not discussed. For example, the interpolation of concentrations (lines 5-10). This issue is not a trivial one (especially for reactive species) and several approaches have been developed through time in order to render defendable such interpolations (land-use regression, krigging etc.). More details should be given (i.e. what kind of interpolation has been used (linear, bilinear??) is it justified in this context?)

Section 2.1.3 It is not clear what criteria on the injection time was finally used; please add a conclusive sentence at the end of the paragraph. It seems like the "tinj" scale is one of the more critical parameters in the paper. I suggest that the authors be very clear when describing the assumptions for the determination. The authors should also discuss how the results based on sensitivity tests conducted on a continental scale may be extrapolated to the present study where grid-cells are smaller by 10 times (lines $\sim$25). An issue that is not discussed in the paper is that for time steps (I am referring to the Polair3D model here) between two "injections" the Polair3D model is running with a mass deficit compared to what would be the case if emissions were handled by the Polair3D model as is the common procedure. I assume that for species

such as SO2 for which point emissions represent up to 60% of the total emitted mass (Section 3.2 ln 15) this will affect also advection and diffusion within the Eulerian model. Shouldn't a part of the difference between the "reference" simulation and the coupled version be also due to this effect? I don't imply that this is a bad assumption but I suggest that it should be listed as a modeling assumption and discussed as it should. The authors have already run a simulation where all point sources are "switched off" (the "background" version). This simulation could be a possible way to show how this effect impacts model results.

Section 2.2 It is unclear to what extent the authors had to make some assumptions in the implementation of the chemical scheme or they used the same scheme as in Karamchandani et al. Even though the description of the chemistry treatment is well presented I think the authors should be more clear what is new and what has already been used.

Section 3.1 Here is another issue: if the results are to be presented as improvement relative to the performance of the 'state-of-the-art Polair3D' model then more information is required on how well Polair3D predicts pollutant concentrations. For example, it appears here that meteorological data for the regional CTM simulation are directly interpolated from a global meteorological model (ECMWF). Usually, regional scale CTMs use meteorological input from meso-scale models such as MM5 or WRF over regional domains; please discuss.

Section 3.3 I think that it would have helped a lot to have already an idea of the order of magnitude of the ratio between Dtpuff and Dtinj. The numbers provided here suggest that for 12 time steps $\sim$ 20 minutes the Eulerian model runs without the selected point sources. This is typically the characteristic time of turbulence in the CBL.

Section 4.2 Since the authors are investigating small scale variations in pollutant concentrations by trying to represent local effects, attention should be paid to the averaging in space and time to avoid the effect of smoothing the variability produced by the model.

Averaging the results too much, could defeat the purpose of the study. Also, it invokes doubt on how model errors are compensated between pollution events and downwind or upwind stations rather than provide evidence of the model's improvement.

Section 4.3.2 The authors suggest that ozone's photochemical production is in general governed by a VOC-sensitive regime over the specific area affects the rate of O3 titration (lines 20-25). However this argument applies to ozone's formation rate at longer time scales and not locally at the time scale of the interaction between the Eulerian and the local model put together by the authors. I wonder if that argument shouldn't simply be omitted.

Section 6 I find that this section of the analysis is very important because it is where the authors discuss for the first time the problems of trying to couple the two different representations of the Advection Diffusion Equation coupled together (i.e. the Eulerian and the Gaussian models). However, it seems that the analysis presented here is quite preliminary. First, it only applies to the Eulerian model and so it provides a very indirect (if any) insight to the presented application which is based on the feedback between a local dispersion model and an Eulerian model. The authors do not explain their choice to vary this specific parameter (Kzmin) among others used in the Troen-Marht parameterization. No physical interpretation has been given to this parameter other than to ensure minimum vertical diffusion, which is a rather loose physical interpretation. Also, the range of variability of this parameter in this "sensitivity study" is too small (i.e. 3) to allow the derivation of any conclusion. The difference in the response of NO compared to O3 could be also explained by the fact that there is more ozone in the upper atmospheric levels and therefore the vertical mixing brings more ozone from the top to the surface level whereas the opposite is true for a primary species such as NO (low levels at the upper air and high concentrations at the surface). I suggest that the authors emphasize this part of the study by fitting it into the general context of how the vertical diffusion of surface emissions within the Eulerian model or the Gaussian plume model is treated and what assumptions could be made.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 5091, 2010.