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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

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We thank the reviewer for his/her useful and detailed comments. His suggestions helped making the paper clearer by highlighting several important issues.

1 General comments

Objectives The reviewer claims that the paper's objectives are not clearly defined. The reviewer correctly assumes that the general modeling approach used in this paper is

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not new. However, the model is a new model, and, in this viewpoint, it is useful to give information about the parameterizations and approaches implemented in this model. Thus, one of the aims of this paper is to present this model. The main objectives of the study are, as we state in the introduction:

> (1) to determine the plume-in-grid impact, in terms of statistics as well as spatial variability, in the case of a high number of point sources well distributed over an urban area, and (2) to give insights on the sensitivity to various parameters, and on the relevant spatial and temporal scales.

Paper's organization The title of section 1 has been changed to "Introduction" and subsections have been removed, as suggested. We kept Section 2, where the formulas and parameterizations used in the model are described, since there is no other publication to refer to about the chemical part of the model. However, we have drastically shortened the description of the non-reactive part of the model (for which we refer to Korsakissok and Mallet (2010)), and focused on the description of spatial and temporal scales of the model. We kept the chemistry part, which we think is very important in this paper, but moved part of it to the appendix. We reorganized the paper as follows:

1. *Introduction* (the subsections titles have been removed),
2. *Model overview*, with a focus on spatial and temporal scales, and on chemical interactions with the background,
3. *Application* : description of the application over Paris region, and the simulations set-up (some subsections have been merged),
4. *Impact of the plume-in-grid treatment*, with two subsections focusing on the impact on statistics, and on the spatial variability,

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5. *Sensitivity analysis*, with the analysis of the vertical diffusion, then the sensitivity to local-scale parameters (same as in the previous version of the article),

6. *Conclusions*.

2 Specific comments

Spatial and temporal scales The reviewer's point is that we should define precisely the spatial and temporal scales of the phenomena we describe. This is indeed a crucial point in our study. We would like to point out that a comprehensive study about spatial and temporal scales in the plume-in-grid model was presented in Korsakissok and Mallet (2010). We agree that the scales differ significantly from the previous study (continental scale and regional scale), so we added a section to better explain the choices of temporal scales (time step between two puffs and injection time) in the plume-in-grid model (Section 2.2). In addition, we added a few lines about the implications of these choices in terms of computational time and number of puffs (Section 3.2):

> The plume-in-grid simulations are carried out with $t_{\text{inj}} = 20$ minutes and $\Delta t_{\text{puff}} = 100$ s, as explained in Section 2.2. This ensures that the puffs are injected after 12 time steps, which corresponds to 1068 puffs handled by the model. The computational time using the plume-in-grid model with this number of puffs and full gaseous chemistry is between 2 and 3 times the time for the Eulerian simulations.

We would also like to stress out that the sensitivity to these temporal scales is addressed in Section 5.2.

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Abstract and model's scores The RMSE improvement presented in the abstract corresponds to the RMSE on stations, given in Section 4. We agree that the model's performance cannot be summarized by this mild improvement, and we should insist more on the better representation of the spatial variability. As the reviewer states, the results for NO in terms of total RMSE are "surprisingly low" when given in the abstract without the general context. As explained in the paper, this is due to the low impact of point sources in total NO_x emissions (about 20%, since most emissions are due to traffic). In this regard, using a plume-in-grid model for point sources cannot have a very high impact on the global statistics, for this case-study. We removed the RMSE scores from the abstract.

Using NO_x We also addressed the reviewer's interesting suggestion, to use NO_x instead of NO. The RMSE results are similar (the part of point sources in total emissions is still low), and are therefore not shown. We also used NO_x in the sensitivity study, and we thought interesting to complete the results with a figure which summarizes the sensitivity to each parameters (diffusion, time step between puffs and injection time) of SO_2, NO_x and O_3 (Section 5.1.2, new Fig.13, and attached figures). It represents the RMSE difference (Polair3D - plume-in-grid, $\mu g\ m^{-3}$) for the base case, and for three sensitivity simulations. It emphasizes the parameter to which each species is the most sensitive (green bar on the figures).

Comment on Section 1 See general comments. Previous applications of such coupled models on photochemistry focused on how to model chemical interactions. In this study, we chose to apply the up-to-date chemical model of SCICHEM model, which gives good results, and to focus on other aspects, mainly the influence of diffusion and local-scale modeling. The application also differs from previous uses of plume-in-grid models, as we explain in the introduction.

Comment on Section 2 See the part about temporal and spatial scales. The critical issue is how to extrapolate the findings of the plume-in-grid study at continental scale to the present study. This is mainly done by scaling the time parameter (injection time) to the puff travel time to cross a grid cell. Concerning the other input data (meteorology, land use...), they are processed as usual for an Eulerian simulation at regional scale. Except meteorological data (see below, comment on Section 3.1), other data (emissions and land use) are given at a finer resolution than the grid cell size.

Comment on Section 2.1.2 – Interpolation The interpolations used in the model are always bilinear. This is done for input data interpolated on simulation grid (e.g. meteorological data), and for output concentrations interpolated on stations. It is therefore consistent to also use a bilinear interpolation to get data (meteorological data and concentrations) at a puff's center. A possible alternative is to directly use the averaged cell concentration as a background value. We preferred to interpolate the values, which should be more consistent with the puff's location within the cell, and ensures that background values do not abruptly change when the puff moves from one cell to another.

Comment on Section 2.1.3 – Mass deficit The reviewer states that the Polair3D model runs with a mass deficit, due to the lacking point sources (handled by the puff model). This does not influence the advection-diffusion part which is linear. For instance, running two Polair3D non-reactive simulations with half the sources and adding the results should produce the same results as one simulation with all the sources—except for purely numerical issues due to flux limiting. The only non-linearity in the model equations comes from chemical interactions, which are handled by our model.

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Comment on Section 2.2 – Chemical scheme The main assumptions made in the chemical scheme are (1) the way concentrations in the overlap volume are distributed between the puffs and (2) the way non-linear background interactions are treated. In this study, we chose to use the same assumptions as in Karamchandani et al. (2000), and we clearly stated this when describing these two assumptions.

Comment on Section 3.1 – Polair3D performance The aim of this study is to present the improvement due to adding a subgrid-scale treatment for point sources, all other data being the same. Thus, we compare results between Polair3D with/without subgrid treatment, without focusing on how well the model Polair3D itself predicts the pollutants. Polair3D performance is shown by the statistics given in this part, and a detailed evaluation of the model on a similar case is given in Tombette and Sportisse (2007). Here, ECMWF fields are used, and the resolution is $0.36°$. Results may have been improved by using a better resolution for meteorological data, with MM5 model for instance. However, it was considered sufficient since the Paris Basin is characterized by a non-hilly terrain and rather homogeneous fronts. Using aerosol chemistry would also improve the results, but would not be possible here, since it has not yet been implemented in the Gaussian model.

Comment on Section 3.3 The two timescales are given in the new part 2.2 about spatial and temporal scales of the model.

Comment on Section 4.2 – Averaging The reviewer points out that averaging too much the results smooths the spatial variability, whereas the use of the plume-in-grid model is to improve the modeling of the small-scale variability. We totally agree with this statement. The impact on averaged results on stations is not very large, because of the relatively small impact of point sources, but also due to this averaging effect. The plume-in-grid effect cannot be reduced to these results. This is why we show not

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only global results, but also results on particular days and stations. However, this was also interesting to have a look at the global results, in order to see whether the use of a local-scale model is relevant in such a case (six-months results), or should be devoted to particular episodes.

Comment on Section 4.3.2 – Ozone production regime The reviewer suggests to omit the argument about photochemical ozone production regimes, since it is not relevant at the scale of the in-plume chemistry. This is perfectly true, and we followed the reviewer's recommendation.

Comment on Section 6.1 – Vertical diffusion We agree with the reviewer that the title "sensitivity study" may not be appropriate for the part discussing vertical diffusion. Indeed, changing the minimal value for the vertical diffusion coefficient in Troen and Mahrt parameterization was not done specifically for the purpose of a sensitivity analysis. We decided to adapt this value to urban areas, since we have seen in previous applications that urban diffusion was often underestimated during stable cases, leading to an overestimation of the concentrations. The reviewer suggests that NO response to this change comes from the vertical repartition of NO (strong gradient, and higher concentrations on the surface than in the upper levels). We totally agree with this explanation, and modified the article accordingly:

> As in the case of plume-in-grid, the secondary pollutants, especially O_3, are less sensitive to the model configuration than the primary pollutants, since vertical gradients are smaller. The most impacted species is NO, which can be explained by the strong vertical concentration gradient for this species, with higher concentration at ground level due to traffic emissions. Thus, increasing the vertical diffusion tends to lower NO ground concentrations.

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The comparison between vertical diffusion in Eulerian and Gaussian models was extensively made in Korsakissok and Mallet (2010). The conclusions can be applied to the present study, since they do not depend on the grid resolution, or on the application domain : the comparison was carried out in the vicinity of the source, and the evolution of σ_z was compared for several parameterizations up to a few hours after the puff emission. The case-study presented in Korsakissok and Mallet (2010) had the advantage of dealing with only one point emission and one meteorological situation, which allowed to infer direct conclusions about the effect on the global results. With many point sources of various heights scattered over the domain, such a sensitivity study would be more difficult on the present case. We added a paragraph which replaces this study in the general context of Eulerian/Gaussian comparisons for vertical diffusion, referring to the former paper for more details. The two conclusions that we draw are, in summary : (1) that improving vertical diffusion is not as efficient (in terms of resulting concentrations and comparison to observations) for elevated sources, which stay aloft for a longer time period, as for ground sources and (2) that in all cases (Eulerian and Gaussian diffusion), primary species and especially NO are the most impacted by a change in the vertical diffusion, which may be explained by a strong vertical gradient.

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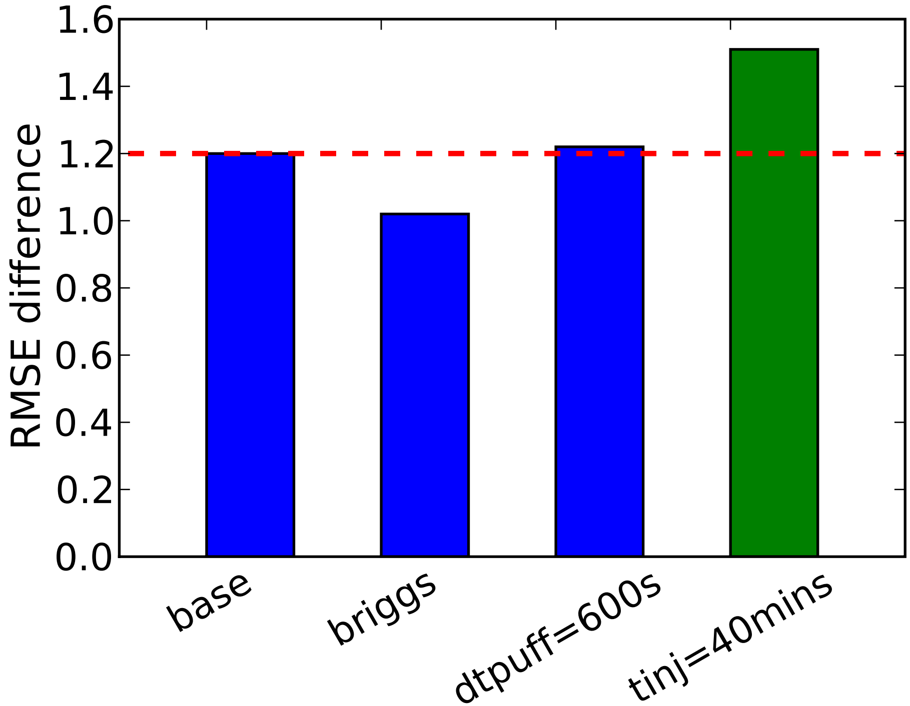

Fig. 1. RMSE difference (Polair3D - plume-in-grid) for SO2: "base" case and three sensitivity tests (changing dispersion parameters, time step between two puffs and injection time).

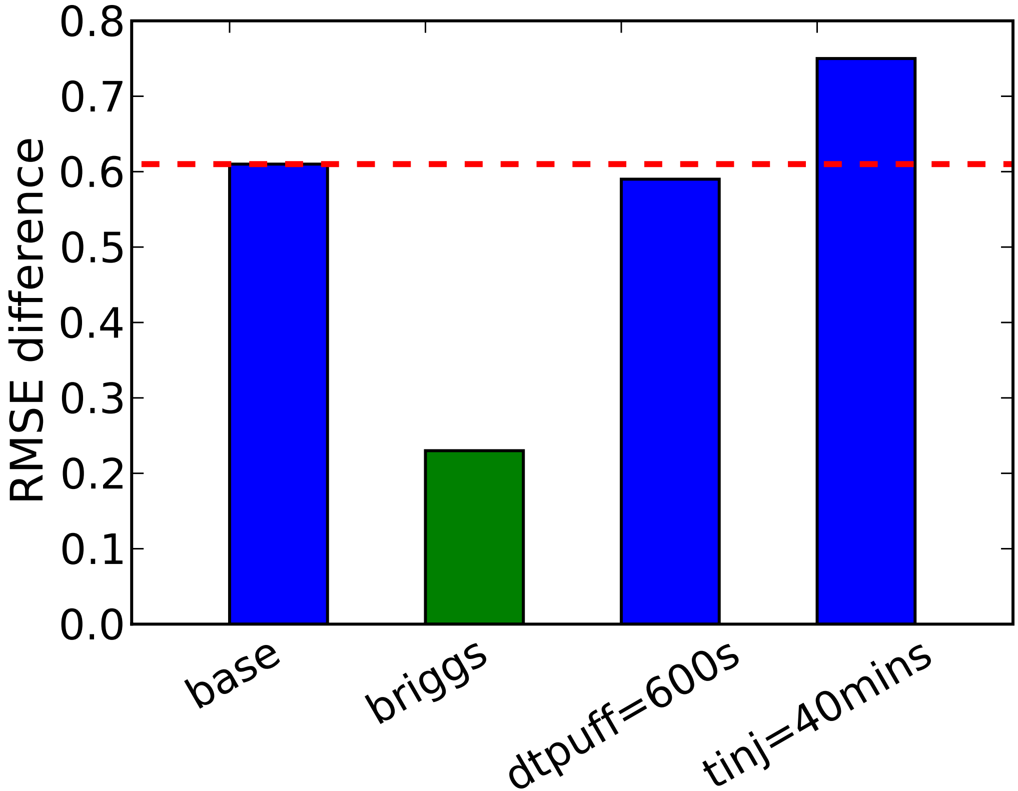

Fig. 2. RMSE difference (Polair3D - plume-in-grid) for NOx : "base" case and three sensitivity tests (changing dispersion parameters, time step between two puffs and injection time).

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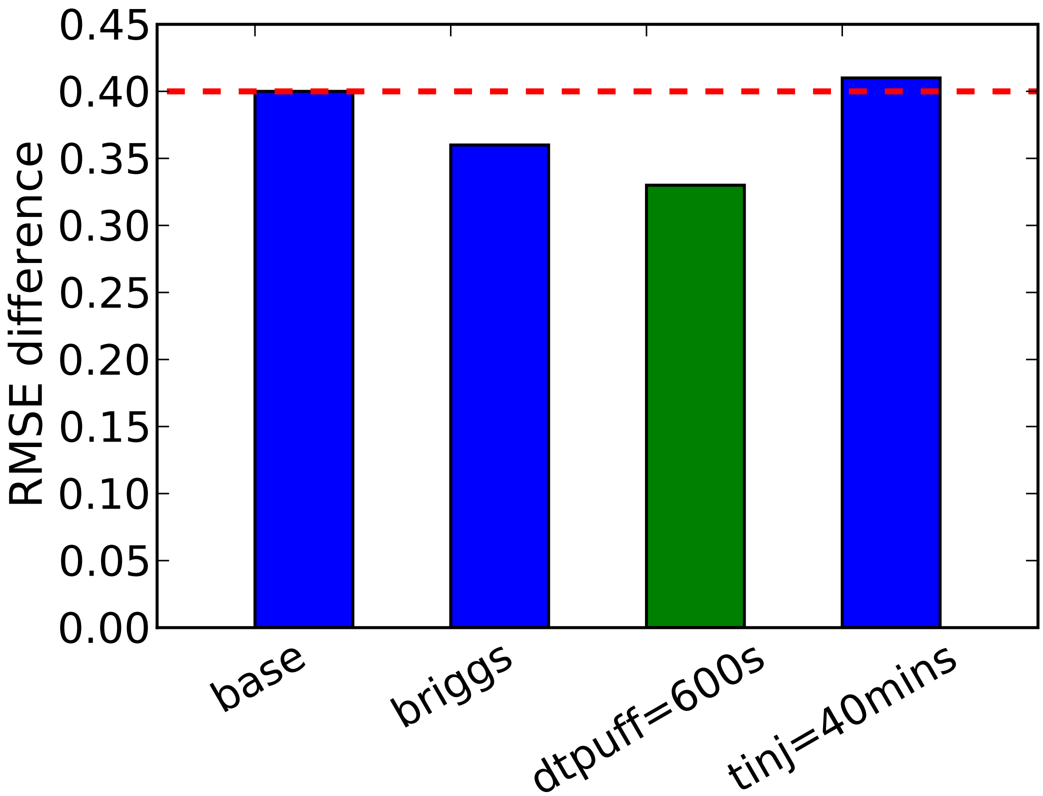

Fig. 3. RMSE difference (Polair3D - plume-in-grid) for O3 : "base" case and three sensitivity tests (changing dispersion parameters, time step between two puffs and injection time).

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