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DEVELOPMENT AND APPLICATION OF A REACTIVE PLUME-IN-GRID MODEL: EVALUATION OVER GREATER PARIS

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Abstract: Classical air quality models at regional scale, based on Eulerian gridded approaches, suffer from several limitations when applied to the dispersion of elevated point emissions (e.g. from power plant stacks). In particular, emissions from point sources are assumed to mix immediately within a grid cell, whereas a typical point-source plume does not expand to the size of the grid cell for a substantial time period. In addition, the incorrect representation of concentrations within the plume leads to a poor estimation of the chemical reaction rates, in the case of reactive plumes. The plume-in-grid method is a multiscale modeling technique that couples a Gaussian puff model with an Eulerian model in order to better represent these emissions.
We present the reactive plume-in-grid model developed in the air quality modeling system Polyphemus, and its evaluation for photochemical applications. The chosen application domain is the Ile-de-France region, during six months (summer 2001). There were 89 major point sources selected for the subgrid-scale treatment. Comparisons are made between the results with the Eulerian model alone, and with the plume-in-grid treatment. The analysis is based both on global results for the whole period, and on a few selected days of interest. A sensitivity study is also carried out, especially to point out the influence of the local-scale parameterizations.

Key words: *Reactive plume-in-grid, point sources, Polyphemus, air quality*

INTRODUCTION

Emissions from major point sources are badly represented by classical Eulerian models. Aside from an overestimation of the horizontal plume dilution, the K-theory approach often used in Eulerian models to represent the vertical diffusion does not properly represent the near-source diffusion. In the case of reactive plumes, the incorrect representation of in-plume concentrations also leads to a poor estimation of the chemical reaction rates. As a consequence, subgrid-scale modeling techniques for point sources have been developed and applied over the years (e.g. Seigneur *et al.* (1983), Kumar and Russel (1996), Karamchandani *et al.* (2002)...). These so-called plume-in-grid models consist in embedding a local-scale model (usually a Gaussian plume or puff model) within an Eulerian 3D model, in order to treat the plumes at subgrid scale and eliminate some of the aforementioned errors.

The plume-in-grid model presented here has been developed on the air quality modeling system Polyphemus (Mallet *et al.*, 2007). The aim is to provide an easy-to-use, modular model, fit for applications from regional to continental scales, and for both reactive and non-reactive pollutants. It was described and applied at continental scale for passive tracers on the ETEX-I experiment (Korsakissok and Mallet, 2010a). It was then extended to handle full gaseous chemistry, and is applied in the study presented here to photochemistry over the Paris region (Korsakissok and Mallet, 2010b). This application is somewhat different from previous reactive plume-in-grid studies: instead of handling a small number of point sources with a high emission rate, and focusing on particular ozone episodes, we handle a large number of sources (89), well distributed over the region. Our analysis is carried out on six months, for summer 2001, and based on global results for the whole period as well as particular days of interest. The aim of the study, aside from a model evaluation, is to determine whether the use of plume-in-grid is interesting in the case of a high number of point sources well distributed over an urban area, and to give insights on the sensitivity to various parameters.

MODEL DESCRIPTION

Model coupling

The plume-in-grid model presented here couples, on the Polyphemus platform, the Polyphemus Gaussian puff model (Korsakissok and Mallet, 2009) with the Eulerian model Polair3D (Boutahar *et al.*, 2004). Both models run independently from one another, and exchange some information at each time step: (1) background data (meteorological data, background concentrations, photolysis rates, deposition velocities and scavenging coefficients) are retrieved from the Eulerian model and interpolated at the center of each puff, to be used by the Gaussian puff model, and (2) the puff mass is eventually transferred into the Eulerian grid cells. The transfer consists in distributing the puff mass over the grid cells vertically covered by the puff, and it is done when the puff satisfies a given criterion. In this study, we use a time criterion: the puff is injected into the Eulerian model after a given time.

Chemistry

The chemistry within the puffs is handled with the following assumptions:

- The species in one puff react with each other,
- The species in two overlapping puffs react with each other, within the “overlap volume”,
- The species in one puff react with the background species (species already in the atmosphere, handled by the Eulerian model)

The chemistry within two overlapping puffs, and between puffs and background species, is handled in a similar way as in Karamchandani *et al.* (2000). In particular, the puffs are assumed to carry a “perturbation” to the background concentrations. Thus, if a background species is depleted by reactions within the puffs, they can carry a negative perturbation, which is added

to the background (Eulerian) concentration to model this depletion. This is illustrated by Figure 1, which represents the plume mass evolution over time when a continuous plume of NO_x is released within a uniform background of O_3. The O_3 background is depleted by the NO titration, to form NO_2.

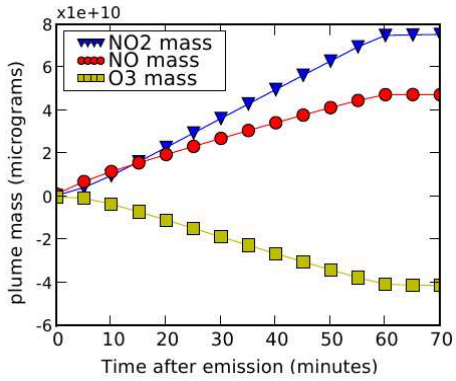

Figure 6. Plume mass evolution with time for NO_2, NO and O_3. Simulations are carried out with the plume-in-grid model, for a continuous point source of NO and NO_2 in a uniform background of O_3.

APPLICATION: AIR QUALITY OVER PARIS REGION

Emissions

The emission inventory comes from Airparif, which is in charge of the local air quality monitoring, for year 2000. Surface and diffuse emissions are interpolated in the simulation grid and used by the Eulerian model. From a total of 295 point sources, we selected, for the subgrid treatment, the 89 sources with an emission rate of NO_x or SO_2 higher than $1 g.s^{-1}$. The selected sources account for 94% of the total NO_x emissions from point sources, and 98% of the SO_2 point emissions. However, it is emphasized that this only represents a small part of the total emissions: point emissions account for only 16% of the NO_x total emissions, which mainly come from traffic, and 60% of the SO_2 emissions. Thus, the impact of the plume-in-grid treatment for point emissions should be higher for SO_2 than for the other species.

Configurations

The simulations are carried out over Paris region, from 2001-04-01 to 2001-09-27. The cells size in longitude and latitude is 0.05°. There are nine vertical levels, and the first layer is 50m high. The time step is 100s, for the Eulerian simulation as well as for the puffs advection and diffusion. Meteorological data are interpolated from ECMWF fields of resolution 0.5°. Only gas-phase chemistry is taken into account. The Regional Atmospheric Chemistry Mechanism (RACM, Stockwell *et al.*, 1997) is used, both in the Eulerian model and for in-plume chemistry. Several simulations are carried out:

- A benchmark simulation with only the gridded model Polair3D, without plume-in-grid treatment (*reference simulation*),
- Three simulations with the plume-in-grid model, using three different Gaussian parameterizations for the standard deviations (Briggs, Doury and similarity theory), and an injection time of 20 minutes,
- A Polair3D simulation excluding the 89 point sources, called *background simulation*.

RESULTS

Impact on mean concentrations

Results are presented here for the mean concentrations over the whole simulation period (six months). For the sake of clarity, we only present here the plume-in-grid results with similarity theory parameterization for the Gaussian standard deviations. Briggs parameterization yields similar results, with slightly worse RSME and higher correlation, while Doury parameterization gave worse results, though still slightly better than the reference. Table 1 shows the models comparison to Airparif measurement stations for the four species of interest (SO_2, NO_x and O_3), in the following order: reference/plume-in-grid. Using plume-in-grid simulations improves the bias and RMSE, although the impact is limited. As explained, this is due to the small overall impact of point sources, compared to traffic emissions. Thus, as expected, SO_2 is the most impacted species. The use of a plume-in-grid treatment seems to impact more primary emitted pollutants (SO_2 and NO) than secondary pollutants (NO_2 and O_3). The plume-in-grid treatment decreases the RMSE by 9% for SO_2 and 4.5% for NO.

Table 1. Comparison to observations over six months: mean value and root mean square error in micrograms per cubic meter, correlation, and mean fractional bias error. The indicators are given for four chemical species (SO_2, NO, NO_2 and O_3). The first value is for Polair3D alone (reference), and the second for the plume-in-grid treatment.

Species	Mean ($\mu g.m^{-3}$)	RMSE ($\mu g.m^{-3}$)	MFBE	Correlation
SO_2	13.76/11.98	13.08/11.88	0.66/0.55	0.35/0.31
NO	20.93/19.64	33.08/31.62	0.41/0.36	0.47/0.46
NO_2	35.84/35.23	20.57/20.81	0.06/0.04	0.58/0.57
O_3	40.24/41.25	30.58/30.18	-0.46/-0.44	0.68/0.68

Figure 2 shows the spatial impact of the plume-in-grid model on mean ground concentrations over six months. The differences are shown (reference concentrations – plume-in-grid concentrations) for the four species. Using a plume-in-grid treatment tends to lower ground concentrations for the emitted species (positive differences), because the plumes are emitted by elevated sources (more than 50 meters high): in the plume-in-grid simulations, the plumes stay longer above the ground. As a consequence, ozone concentrations are higher around the sources, since there is less titration with the plume-in-grid model.

As expected, the impact is larger for SO_2. For secondary species NO_2 and O_3, the differences can be as high as for primary species, but the impact is more localized around point source locations. Thus, it does not show on concentrations taken at the measurement stations locations. When looking at the concentrations during particular days of interest, however, the plume-in-grid impact can be much less localized, since there is a clear downwind direction (which is not the case on the six-month averaged concentration maps). This is particularly true during low-dispersion days when the Eulerian error is higher, and concentrations are larger.

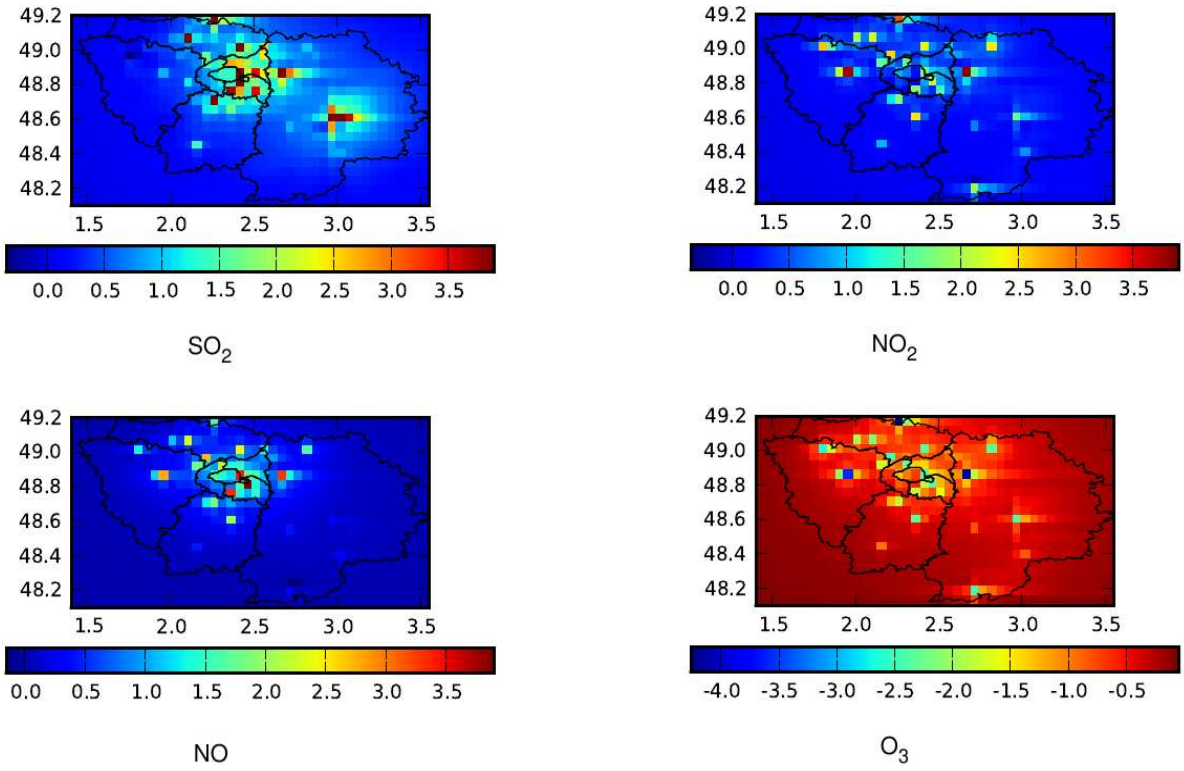

Figure 2. Differences between mean ground concentrations with Polair3D alone, and with plume-in-grid treatment. Mean values over six months, in micrograms per cubic meter.

Impact on stations

We now focus on the plume-in-grid impact station per station, in an attempt to determine whether the impact can be locally higher on particular stations. Results are shown only for primary species, for which there is a significant impact: the RMSE on stations is reduced by up to -17.4% for SO_2, and -6.7% for NO. There is no significant trend to discriminate between urban and rural stations (Figure 3).

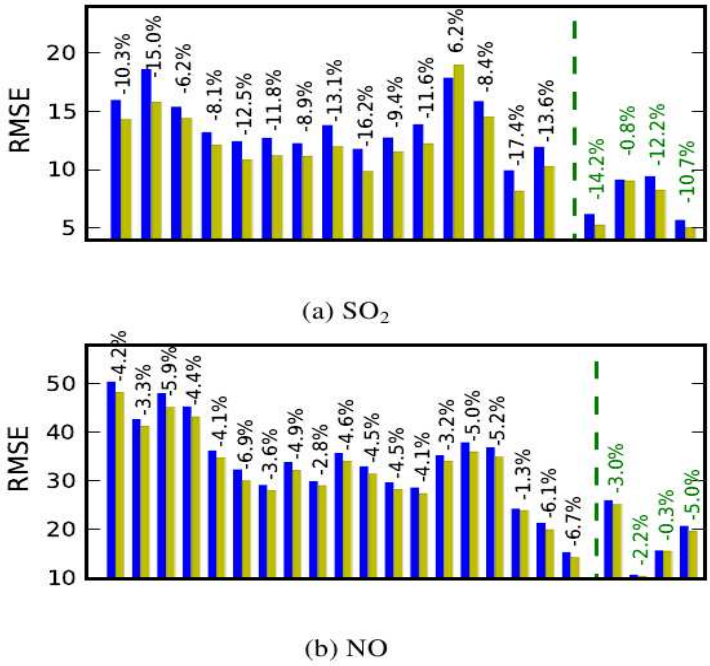

Figure 3. RMSE on stations, over six months, in micrograms per cubic meter. Blue: RMSE with reference simulation. Yellow: RMSE with plume-in-grid simulation, similarity theory. The percent indicated over the bars is the relative difference in RMSE between plume-in-grid and reference. The first group of bars corresponds to urban stations (percent in black), the second to peri-urban and rural stations (percent indicated in green).

SENSITIVITY STUDY

A sensitivity study was also carried out on several parameters. In particular, the sensitivity to "local-scale" parameters, used for the subgrid model configuration, was assessed. Aside from the influence of Gaussian standard deviation parameterizations, we investigated, in particular, two parameters: (1) the injection time, and (2) the time step between two puffs releases. The injection time is the time during which the puffs are treated by the Gaussian puff model, before being released into the Eulerian model. The time step between two puffs determines the puffs overlap during the first time steps: if it is too large, the plume is not realistically represented since two consecutive puffs do not overlap before a substantial time period.

These two parameters are important, since they determine the total number of puffs handled by the model (for a given number of sources), and consequently the computational time. Since we use full gaseous chemistry within the puffs, the computational burden increases dramatically with the number of puffs, in a quadratic manner (because of the interactions between overlapping puffs). Additional simulations using the plume-in-grid model with similarity theory are carried out to evaluate the impact of these two parameters:

- a simulation with a 40-minute injection time (instead of 20 minutes),
- a simulation with a time step between two puffs equal to 600 seconds (instead of 100 seconds).

The injection time has much more influence on SO_2, which is an almost-passive species when considering only gaseous chemistry, than on reactive species. Using a larger injection time leads to an additional decrease in RMSE (compared to the plume-in-grid impact shown Figure 3) which is significant on several stations (up to -8.4% on one station). By comparison, the impact for the other three species is less than 1% for all stations. The plume composition is modified by the chemical reaction and after some time, the plume composition becomes closer to the background composition. After that time, increasing the injection time has a small effect on the results for reactive species.

On the contrary, SO_2 is fairly insensitive to the time step between two puffs. Results for reactive species with a 600-second time step are slightly worse for O_3 and NO_2, and slightly better for NO. If the time step between two puffs is not sufficient, the overlap volume between two consecutive puffs is small during the first simulation time steps. On the other hand, each puff carries a larger mass of each species. As a result, the chemistry within each puff is enhanced. In the case of ozone and nitrogen oxides, this leads to slightly overestimate the titration. The impact of this phenomenon is not very large, but not negligible compared to the global plume-in-grid impact for these species.

CONCLUSIONS

The plume-in-grid model implemented on the Polyphemus platform has been applied to regional photochemistry over the Paris region. Model-to-data comparisons have been performed over six months during summer 2001, and compared to simulations carried out with the Eulerian model without subgrid-scale treatment. The plume-in-grid treatment appears to improve the global results, especially for primary emitted species (SO_2 and NO). SO_2 is the most impacted species, since point sources account for a large part of its total emissions, whereas NO_x and O_3 are mostly influenced by traffic emissions.

As far as the sensitivity study is concerned, the time step between two puff releases mostly influences reactive species, whereas the almost-passive species SO_2 is mostly impacted by a change in the injection time. Since these two parameters determine the number of puffs handled by the model – on which depends the computational burden – they must be carefully chosen according to the target species.

Future developments and applications of this model include an application at continental scale over Europe, and an extension to aerosol dynamics. In addition, the model will be extended to handle line sources in order to use the subgrid-scale treatment with road emissions. This application is expected to show much more striking results, because of the importance of traffic emissions on the pollutants of interest.

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