Development and application of a reactive plume-in-grid model: evaluation over greater Paris

13th Harmo Conference

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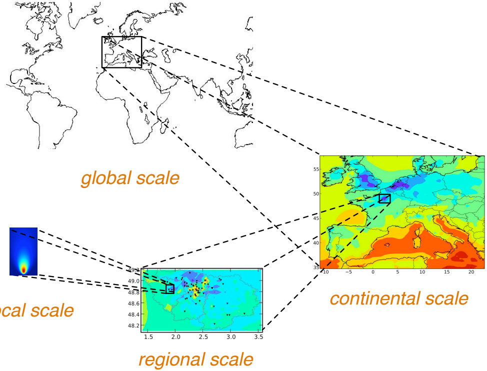
Outline

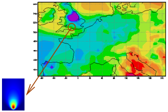
A wide range of scales

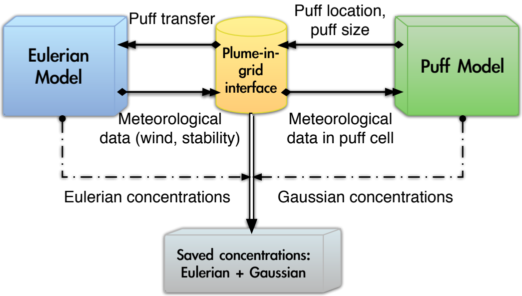
- From μm (particles) to *km* (meteo)
- Gridded representation : usually from 1 to 50 km...
- Subgrid-scale phenomena : emissions, chemistry, clouds, land use, turbulence...



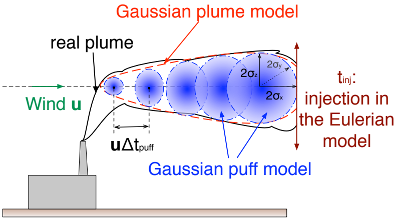
Model coupling within Polyphemus platform

- Using Polyphemus modeling platform : modularity, easy coupling
- Plume-in-grid method : coupling an Eulerian model (Polair3D) and a Gaussian puff model to model point source emissions
- Puffs are “injected” into the Eulerian model after a given time (“injection time”)





Model coupling within Polyphemus platform

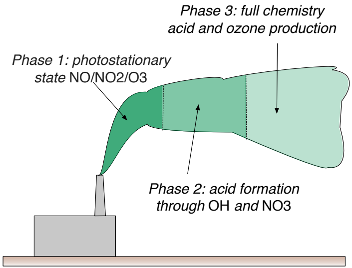


- Puffs size given by standard deviations σ_x, σ_y, σ_z (similarity theory, Briggs)
- $\Delta t_{\rm puff}$ time step between two puffs' emissions
- $t_{\rm inj}$ injection time (puff "lifetime")

$\frac{t_{\rm inj}}{\Delta t_{\rm puff}}$: total number of puffs handled by the model for one continous source

Reference : Korsakissok, I. et Mallet, V. (2010). Subgrid-scale treatment for major point sources in an Eulerian model : A sensitivity study on the European Tracer Experiment (ETEX) and Chernobyl cases. Journal of Geophysical Research. 115 :D03303.

Reactive plume-in-grid model

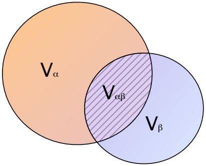


Advantages of subgrid model

- Better representation of local-scale diffusion
- Source height and plume rise
- Near-source chemistry

Chemistry within puffs

- The species in one puff α react with each other
- The species in two overlapping puffs α and β react with each other
- The species in one puff react with the background species (from the Eulerian model)



Chemistry between puffs and background species

$$\mathrm{A} + \mathrm{B} \xrightarrow{k} \mathrm{P}$$

c_A^α, c_B^α puff

c_A^b, c_B^b background

$$\frac{\mathrm{d}(c_A^\alpha + c_A^b)}{\mathrm{d}t} = -k(\underbrace{c_A^\alpha\ c_B^\alpha}_{\text{puff}} + \underbrace{c_A^b\ c_B^b}_{\text{background}} + \underbrace{c_A^\alpha\ c_B^b + c_B^\alpha\ c_A^b}_{\text{interaction}})$$

$$\frac{\mathrm{d}c_A^b}{\mathrm{d}t} = -kc_A^b\ c_B^b \quad \text{background chemistry (Eulerian)}$$

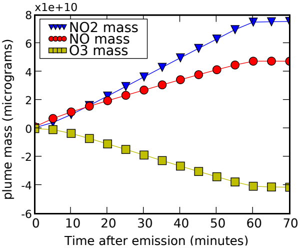
$$\frac{\mathrm{d}c_A^\alpha}{\mathrm{d}t} = \frac{\mathrm{d}\left(c_A^\alpha + c_A^b\right)}{\mathrm{d}t} - \frac{\mathrm{d}c_A^b}{\mathrm{d}t} \quad \text{puff=background perturbation}$$

ozone titration

$$O_3 + NO \xrightarrow{k} NO_2 + O_2$$

- plume of NO_x ($NO+NO_2$)
- uniform background of O_3

→ Decrease of in-plume O_3 concentration



Evolution of in-plume mass for several species (µg) in a continuous plume of NO_x emitted within a background of O_3.

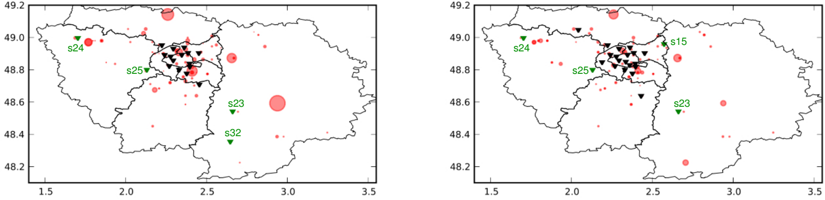
Outline

Issues

1. What is the impact of a subgrid-scale modeling of point emissions on regional photochemistry ?
2. Impact on primary vs secondary species ?
3. Impact on results over six months vs particular days ?
4. Sensitivity to local-scale modeling ?

Reference : Korsakissok, I. et Mallet, V. (2010). Development and application of a reactive plume-in-grid model : Evaluation over Greater Paris. Atmospheric Chemistry and Physics Discussions 10, 5091-5134

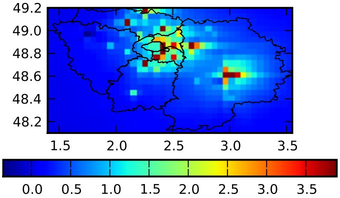
Application over Greater Paris



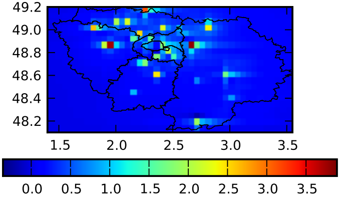
Point sources (●) and measurement stations (rural ▼ and urban ▼). Left : SO_2, right : NO. The circle diameters are proportional to the sources emission rates.

- Ile-de-France (Paris region), summer 2001, six months
- Meteorological fields from ECMWF (0.36° resolution)
- Full gaseous chemistry (RACM mechanism)
- Polair3D (0.05° resolution) with/without subgrid modeling (similarity theory, $t_{\mathrm{inj}} = 20$ min, $\Delta t_{\mathrm{puff}} = 100$ s)
- 89 point sources : $Q_s > 10^6\ \mu\mathrm{g\,s^{-1}}$ for NO_x (20% of total emissions) or SO_2 (55% of total emissions)

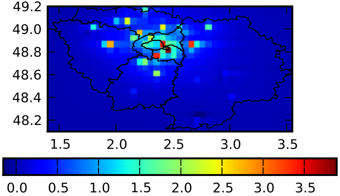
Spatial impact of subgrid-scale modeling



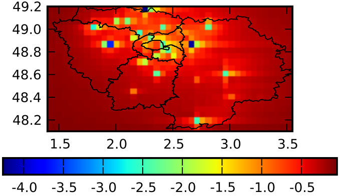
SO_2



NO_2



NO

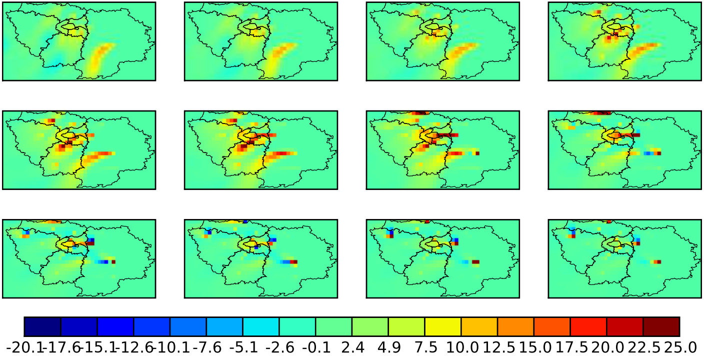


O_3

Differences in mean ground concentrations : Polair3D - plume-in-grid.

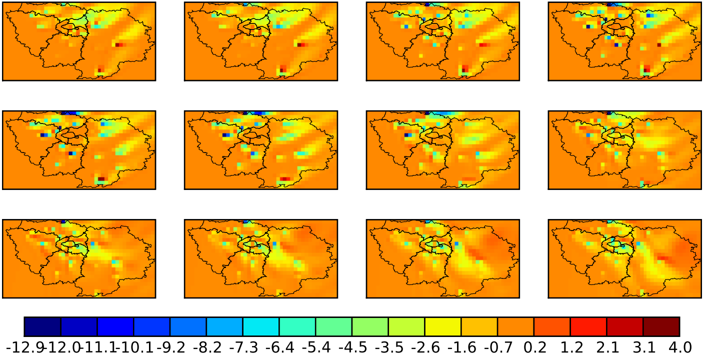
Concentrations averaged over six months ($\mu g\, m^{-3}$).

Spatial impact of subgrid-scale modeling during a low-dispersion day (sulfur dioxide)



Differences in hourly-averaged SO_2 ground concentrations : Polair3D - plume-in-grid ($\mu g\, m^{-3}$), for day 2001-08-24 between 03 and 15h (local hour).

Spatial impact of subgrid-scale modeling during a low-dispersion day (ozone)



Differences in hourly-averaged O_3 ground concentrations : Polair3D - plume-in-grid ($\mu g\, m^{-3}$), for day 2001-08-20 between 03 and 15h (local hour).

Results on stations for SO_2 and NO

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2},$$

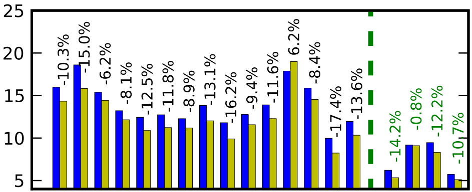
with x_i simulated values,

y_i observed values.

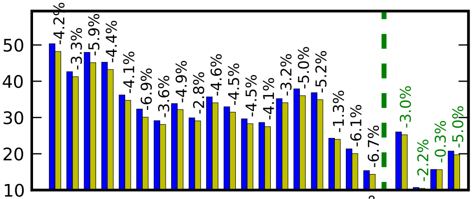
- Blue: Polair3D,
- Yellow: plume-in-grid

Black % : urban stations

Green % : periurban and rural stations.



SO_2 – Mean observed values : 6.2 $\mu g\, m^{-3}$



NO – Mean observed values : 10.42 $\mu g\, m^{-3}$

Comparison to observations on measurement stations, over six months. Mean and RMSE in $\mu g\, m^{-3}$.

Results on stations for SO_2 and NO

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2},$$

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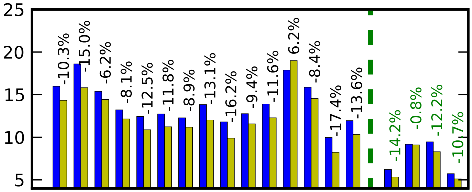
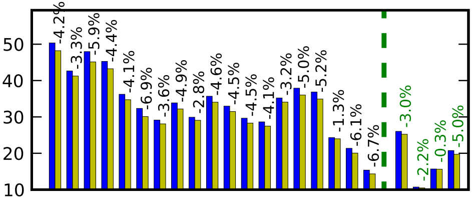


SO_2 – Point sources : 55% of total emissions



NO – Point sources : 20% of total emissions

Polair3D,
plume-in-grid

Black % : urban stations

Green % : periurban and rural stations.

SO_2 more impacted (more point sources) than NO,
urban/rural stations equally impacted

Results on stations for NO_2 and O_3

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2},$$

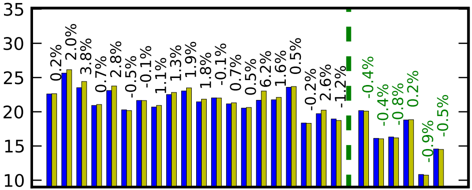
with x_i simulated values,

y_i observed values.

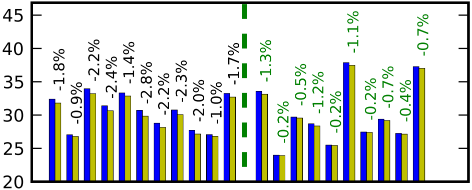
Polair3D,
plume-in-grid

Black % : urban stations

Green % : periurban and rural stations.



NO_2 – Mean observed values : 34.64 $\mu g\, m^{-3}$



O_3 – Mean observed values : 56.87 $\mu g\, m^{-3}$

Comparison to observations on measurement stations, over six months. Mean and RMSE in $\mu g\, m^{-3}$.

Results on stations for NO_2 and O_3

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_i - y_i)^2},$$

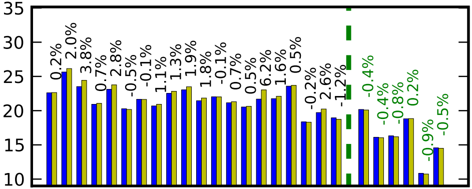
with x_i simulated values,

y_i observed values.

Polair3D, plume-in-grid

Black % : urban stations

Green % : periurban and rural stations.



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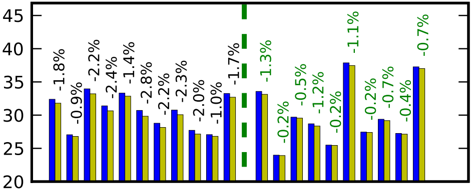
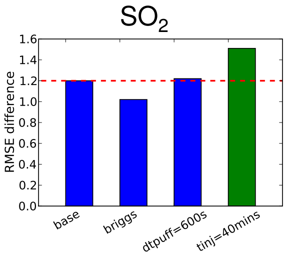


O_3 – Mean observed values : 56.87 $\mu g\, m^{-3}$

Primary species (NO, SO_2) more impacted than secondary species (NO_2, O_3)

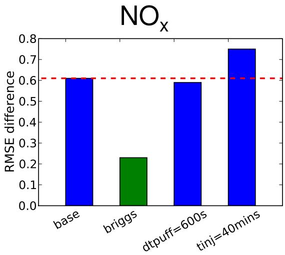
Sensitivity study

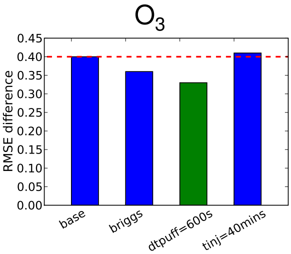
Base case : similarity theory,
$t_{inj} = 20$ min and $\Delta t_{puff} = 100$ s



Alternative cases

- sigma parameterization : Briggs
- $\Delta t_{puff} = 600$ s
- $t_{inj} = 40$ min





Differences (Polair3D - plume-in-grid) in RMSE ($\mu g\, m^{-3}$), computed on all stations and six months for SO_2, NO_x and O_3.

Outline

Summary and conclusions

1. Full non-linear gaseous chemistry implemented in plume-in-grid model
2. Spatial impact, especially during low-dispersion days
3. Impact of plume-in-grid model on averaged statistics is limited by :
    - limited amount of emissions from point sources compared to traffic (except for SO_2)
    - averaging effect (smoothing spatial variability)
    - stations locations (background stations)
4. However, significant improvement is shown for primary species
5. O_3 sensitive to time step between two puffs, primary/less-reactive species (SO_2, NO_x) sensitive to injection time

Future work

1. Handling chemistry for particulate matter
2. Extension to line sources and application to road emissions

Thank you for your attention