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

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Outline

1. Subgrid-scale modeling of emissions
   - Why use a subgrid model?
   - Model coupling
   - Non-linear chemistry

2. Application over Greater Paris

3. Conclusions
A wide range of scales

- From $\mu m$ (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 $\sigma_x$, $\sigma_y$, $\sigma_z$ (similarity theory, Briggs)
- $\Delta t_{puff}$ time step between two puffs’ emissions
- $t_{inj}$ injection time (puff “lifetime”)

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

Reactive plume-in-grid model

Phase 1: photostationary state NO/NO2/O3
Phase 2: acid formation through OH and NO3
Phase 3: full chemistry acid and ozone production

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 $\alpha$ react with each other
- The species in two overlapping puffs $\alpha$ and $\beta$ react with each other
- The species in one puff react with the background species (from the Eulerian model)
Chemistry between puffs and background species

\[ A + B \xrightarrow{k} P \]

\[ \frac{d(c_A^\alpha + c_B^\alpha)}{dt} = -k(c_A^\alpha c_B^\alpha + c_A^b c_B^b + c_A^\alpha c_B^b + c_B^\alpha c_A^b) \]

\[ \frac{dc_A^b}{dt} = -kc_A^b c_B^b \] background chemistry (Eulerian)

\[ \frac{dc_A^\alpha}{dt} = \frac{d(c_A^\alpha + c_A^b)}{dt} - \frac{dc_A^b}{dt} \] 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

1. Subgrid-scale modeling of emissions

2. Application over Greater Paris
   - Spatial impact of subgrid-scale modeling
   - Results on measurement stations
   - Sensitivity study

3. Conclusions
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?

Application over Greater Paris

- 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, $t_{\text{inj}} = 20 \text{ min}$, $\Delta t_{\text{puff}} = 100 \text{ s}$)
- 89 point sources: $Q_s > 10^6 \mu g s^{-1}$ for NO$_x$ (20% of total emissions) or SO$_2$ (55% of total emissions)

Point sources (●) and measurement stations (rural ▼ and urban ▲). Left: SO$_2$, right: NO. The circle diameters are proportional to the sources emission rates.
Differences in mean ground concentrations: Polair3D - plume-in-grid. Concentrations averaged over six months ($\mu$g m$^{-3}$).

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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 (µg 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 \( \text{SO}_2 \) and \( \text{NO} \)

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

with \( x_i \) simulated values, \( y_i \) observed values.

**Polair3D, plume-in-grid**

**Black % : urban stations**

**Green % : periurban and rural stations.**

**Comparison to observations on measurement stations, over six months.**

**Mean and RMSE in \( \mu g \text{ m}^{-3} \).**
Results on stations for $\text{SO}_2$ and NO

The Root Mean Square Error (RMSE) is given by:

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

with $x_i$ simulated values, $y_i$ observed values.

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,**

- **Blue** : urban stations
- **Green** : periurban and rural stations

Comparison to observations on measurement stations, over six months.

Mean and RMSE in $\mu g m^{-3}$.
Results on stations for NO\textsubscript{2} and O\textsubscript{3}

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

with \(x_i\) simulated values, \(y_i\) observed values.

**Polair3D, plume-in-grid**

Black \%: urban stations  
Green \%: periurban and rural stations.

Primary species (NO, SO\textsubscript{2}) more impacted than secondary species (NO\textsubscript{2}, O\textsubscript{3})
Sensitivity study

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

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

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

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Outline

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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 SO₂)
   ▶ averaging effect (smoothing spatial variability)
   ▶ stations locations (background stations)
4. However, significant improvement is shown for primary species
5. O₃ sensitive to time step between two puffs, primary/less-reactive species (SO₂, NOₓ) 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