Development of local-scale and subgrid-scale models in Polyphemus

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1 Introduction

We present Gaussian plume and puff models implemented in Polyphemus platform [Mallet et al., 2007] with an evaluation against Prairie Grass experimental data. These local-scale models were used as a basis to develop a plume-in-grid model in order to better represent major point source emissions at regional or continental scale. For this purpose, the Gaussian puff model is coupled with the main Eulerian model in Polyphemus, Polair3D. This plume-in-grid model is currently used to deal with passive tracers, and its evaluation against ETEX (European Tracer Experiment) data is presented. The aim of this study is:

1. to investigate whether a plume-in-grid model can be useful in a passive case,
2. to evaluate Polyphemus plume-in-grid model in order to extend it to reactive cases.

2 Local scale

The Gaussian plume model

The Gaussian plume model is used to model continuous emissions from point sources, where steady-state flow and constant meteorological conditions can be assumed (see [Arya, 1999]). The concentration C at a given point is computed by the formula:

$$C(x,y,z) = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}}\exp\left(-\frac{(y-y_s)^2}{2\sigma_y^2}\right)\times \left[\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right)+\exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right]. \quad (1)$$

Q is the source emission rate, $\bar{u}$ is the mean wind velocity, and σ_y and σ_z are the Gaussian plume standard deviations. The coordinate y refers to horizontal direction "crosswind". The coordinate z refers to the vertical coordinate, and H is the plume centerline height above ground.

Plume reflections

Reflections on the ground and inversion layer are taken into account by introducing a fictive image source (z_i is the inversion height):

- Ground reflection occurs when $\sigma_z > H$
- Inversion layer reflection occurs when $H + \sigma_z > z_i$

Far field model

When the plume fills the boundary layer, it is supposed to be vertically homogeneous. The concentration is then:

$$C(x,y,z) = \frac{Q}{2\pi\sigma_y z_i\bar{u}}\exp\left(-\frac{(y-y_s)^2}{2\sigma_y^2}\right). \quad (2)$$

Transition to the far field model is made when $\sigma_z > 1.5\ z_i$.

Standard deviations

Polyphemus Gaussian models hold several parameterizations for standard deviations:

1. **Briggs** formulae for rural and urban land (based on Pasquill stability classes),
2. **Doury** formulae (developed for radionuclides dispersion),
3. **Similarity theory** (based on wind velocity fluctuations – formulae from [Irwin, 1979] and [Hanna, 1984]). For vertical wind velocity fluctuation σ_w an alternative parameterization from [Weil, 1988] is proposed.

All formulae and parameterizations are used for both plume and puff models. Only similarity theory gives specific formulae for σ_x (standard deviation downwind, used only in puff model). Otherwise, $\sigma_x = \sigma_y$.

Prairie Grass experiments

- Short-range experiment, flat terrain, continuous source near the ground. No plume rise. Measurements taken on five arcs at 50, 100, 200, 400 and 800m from the source.
- Used to compare results of Polyphemus plume and puff models with several parameterizations, and other models: ADMS, AERMOD and ISCST3 from [McHugh et al., 2001].

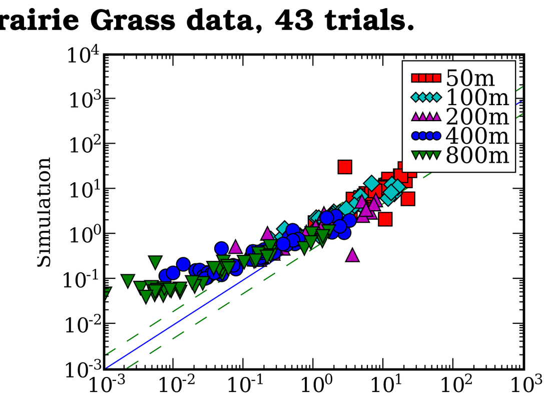
Statistical comparison with Prairie Grass data for several Gaussian models: Polyphemus models compare well with others.

Model	FB	NMSE	MG	Corr	FAC2
Obs	0.00	0.00	1.00	1.00	1.00
ADMS	0.56	3.62	–	0.64	0.46
AERMOD	0.00	1.87	–	0.75	0.76
ISCST3	0.06	1.76	–	0.72	0.62
Briggs	0.0	1.83	1.23	0.78	0.74
Doury	0.46	4.47	1.05	0.42	0.27
Similarity	-0.08	1.25	0.72	0.82	0.61

1. Evaluation of maximum arc concentration – 43 trials in PG Experiment: fractional bias (FB), geometric mean bias (MG), normalized mean square error (NMSE), geometric variance (VG), fraction of predictions within a factor two of observations (FAC2) and correlation coefficient (Corr).

All models give very good results, except Polyphemus with Doury and ADMS. Polyphemus with Briggs formulae, AERMOD and ICSCT3 use formulations directly fitted on PG results. Polyphemus with similarity theory has the highest correlation (82%).

Scatter plot for Polyphemus plume model with similarity theory: Prairie Grass data, 43 trials.



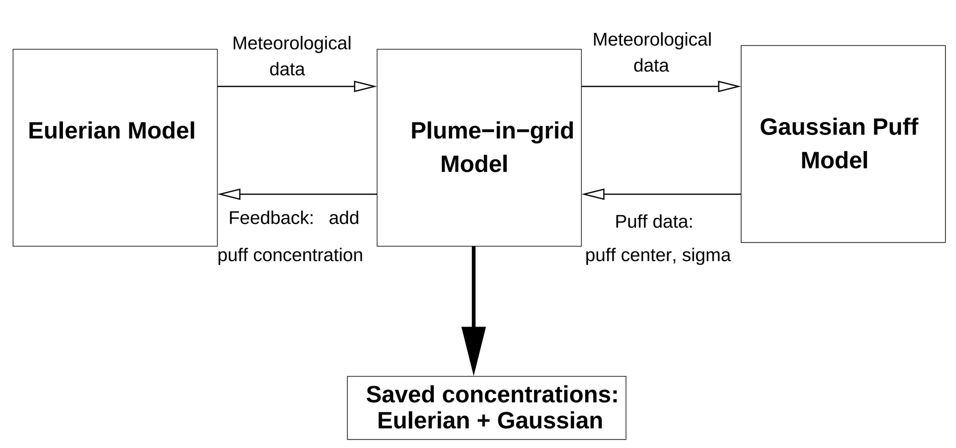
2. Scatter plot of maximum arc concentrations for Polyphemus with similarity theory. Concentrations normalized by source rate Q (unit is $\mathrm{mg \cdot s^{-1}/g \cdot s^{-1}}$).

3 Plume in Grid

Plume-in-grid models are generally used to deal with chemically reactive plumes, and have been proved useful to model ozone chemistry in particular (e.g. [Viyaraghavan et al., 2006]). This study is dedicated to the mecanisms of a passive plume-in-grid model, especially to compare parameterizations and injection methods.

Model description

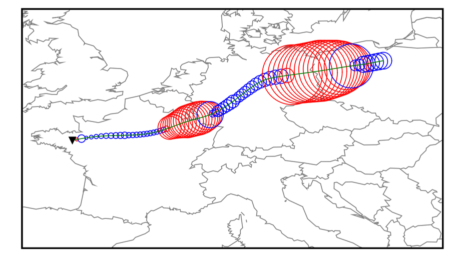
The plume-in-grid model couples an Eulerian and a Gaussian puff model. It exchanges information with both, and saves concentrations (sum of both contributions).



Increasing sigma method

To compute standard deviation, meteorological data are supposed to be stationary. Hence, switching from an unstable case at time t_1 to a stable situation (e.g. if night falls) at time $t_2 = t_1 + \Delta t$ leads to an unrealistic puff size decrease.

Evolution of the puff size: without the increasing sigma method, the puff size decreases during nighttime.

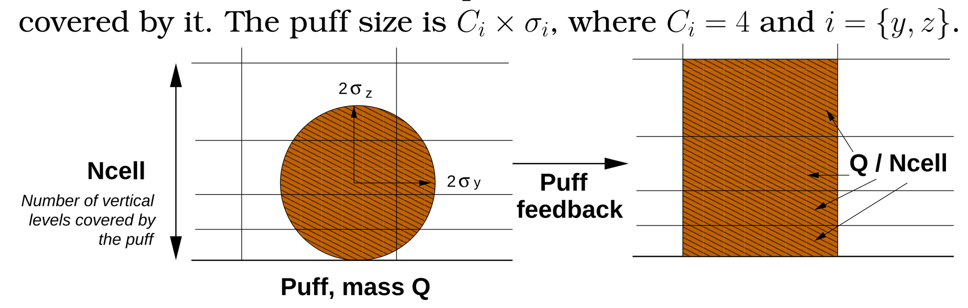


3. Puff size evolution. The puff is represented at each time step at its present location (in latitude/longitude), and the circle radius is proportional to σ_y. Red is daytime, blue is nighttime. Triangle is ETEX source location.

To deal with this problem, at time t_2, we compute the virtual time t_1' corresponding to the time when the puff would have reached the size σ_1 if the meteorological conditions had been stationary and equal to those at time t_2. The new puff size σ_2 is then computed at time $t_2' = t_1' + \Delta t$ and corresponds to a realistic puff growth during Δt.

Puff feedback

When the feedback criterion has been reached, puff is injected into the Eulerian model. Part of the puff mass is added to each cell vertically covered by it. The puff size is $C_i \times \sigma_i$, where $C_i = 4$ and $i = \{y, z\}$.



There are two possible criteria:

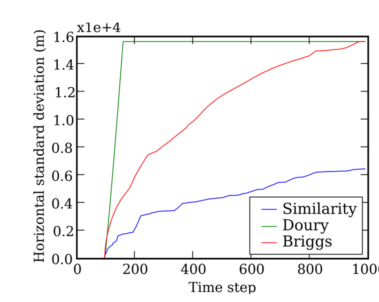
- If the puff horizontal size has reached the cell size,
- If the time after puff emission exceeds a chosen value.

Model results with size criterion

We carried out comparisons between results for plume-in-grid with several parameterizations and the Eulerian model Polair3D alone, thanks to ETEX data. (passive tracer experiment over Europe, seven days of measures).

Results for plume-in-grid with size criterion strongly depend on the parameterization. Evolution of σ_y illustrates these differences.

Model	Mean	FB	NMSE	Corr	FAC2
Obs	0.21	0.00	0.00	1.00	1.00
Polair3D	0.44	0.72	24.87	0.61	0.19
1	0.18	-0.15	64	0.31	0.02
2	0.18	-0.13	61.7	0.35	0.02
3	0.20	-0.05	6.86	0.66	0.19
4	0.11	-0.57	20.14	0.51	0.02
5	0.08	-0.81	26.3	0.37	0.02



4. Left: (1) similarity theory with Weil parameterization, (2) similarity theory with Hanna parameterization, (3) Doury, (4) Briggs with rural formulae, (5) Briggs with urban formulae. Right: Evolution of σ_y in time for one puff for the different parameterizations. Time step is 600 s. When the puff has been injected into the Eulerian model, σ_y becomes constant.

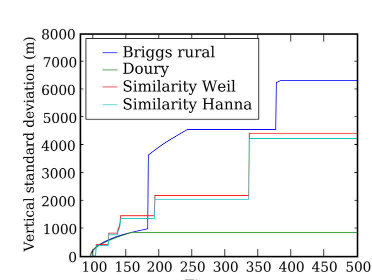
- Use of plume-in-grid improves the bias
- Global results are higher without plume-in-grid for all parameterizations except Doury: in most plume-in-grid models, injection criterion is met very late or not at all.

Model results with time criterion

We present the same comparison with simulations imposing the reinjection of a puff twelve hours after its emission.

Results for injection criterion based on time are better. Evolution of σ_z shows differences in puff vertical extent at injection time.

Model	Mean	FB	NMSE	Corr	FAC2
Obs	0.21	0.00	0.00	1.00	1.00
Polair3D	0.44	0.72	24.87	0.61	0.19
1	0.42	0.67	48.38	0.36	0.15
2	0.42	0.67	48.38	0.36	0.15
3	0.20	-0.05	6.86	0.66	0.19
4	0.21	-0.001	7.32	0.63	0.18
5	0.17	-0.22	8.917	0.51	0.17



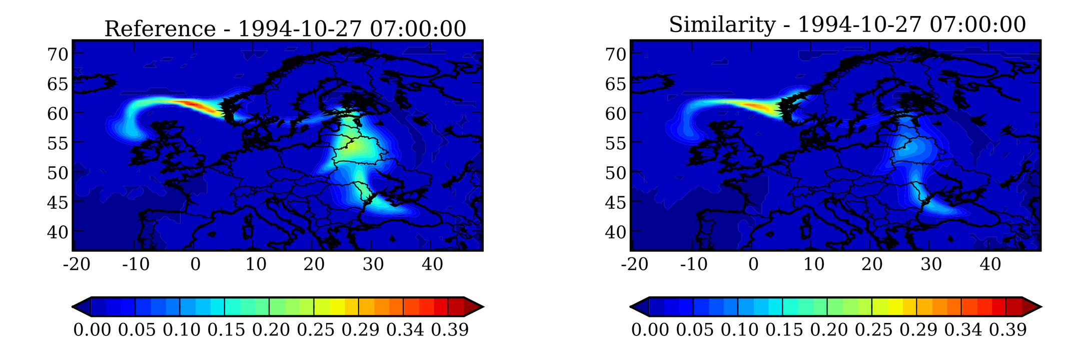
5. Left: ETEX experiment statistics for the five plume-in-grid configurations. Reinjection time is 12 hours after puff release (time step 168). Right: Evolution of σ_z in time for the different parameterizations, for one puff. The evolution has been plotted without imposing the injection time.

- Results are better than with size criterion
- Global results with similarity theory are still lower than results for Polair3D alone: σ_z is too high, puff is injected on 11 vertical levels instead of 8 for Doury.

Results analysis

We present an analysis for different stages of the simulation, and several stations, since local improvements can be overlooked in global statistical results.

Three days after emission, the plume is split in two parts. Plume-in-grid gives substantially lower concentrations than Polair3D in the smaller part of the plume (eastern Europe).

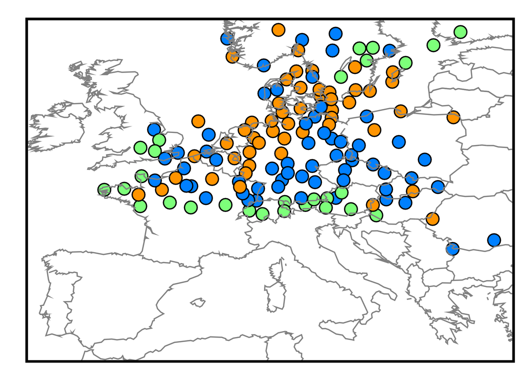


6. Concentration on the domain, three days and a half after beginning (release beginning: 1994-10-23 at 4 pm, release duration is twelve hours). Unit is $\mathrm{ng \cdot m^{-3}}$. The plume has been split in two parts. Left: simulation without plume-in-grid – Right: plume-in-grid with similarity theory.

We can distinguish three different zones in the domain:

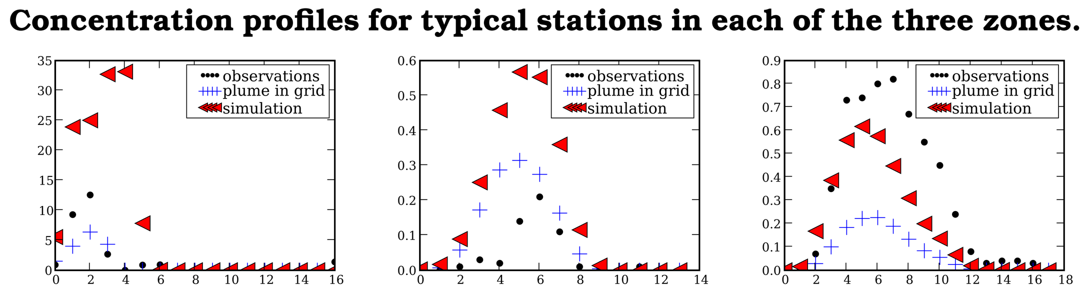
1. Near the source: north of France. The puffs have not been injected yet (nearest injection occurs in north-east of France). The splitting occurs shortly after injection.
2. North-west of Europe, where the greater concentrations are observed. Plume-in-grid models improve results at stations in this zone.
3. East of Europe. Concentrations are smaller. Polair3D tends to underestimate concentrations, and plume-in-grid model gives even lower concentrations. When puff injection is late in the simulation (with size criterion), there are no concentrations modeled in this part.

Difference of FMT for all stations between plume-in-grid model (with similarity theory) and Polair3D alone.



7. Difference of fmt (figure of merit in time) between simulation with plume-in-grid (similarity theory) and with Polair3D alone, for all stations. Red: fmt for plume-in-grid is greater. Blue: fmt for plume-in-grid is lower. Green: no difference (stations where no significant concentrations are modeled).

Concentration profiles for typical stations in each of the three zones.



8. Left: Concentrations in Rennes (near source) – Middle: concentrations in south of Sweden (main plume) – Right: concentrations in west of Hungary (smaller plume in eastern Europe). Observations, Polair3D results and plume-in-grid results with similarity theory are shown.

The Eulerian model tends to overestimate concentrations near the source, since diffusion is too important. For these stations, plume-in-grid results are generally better for all parameterizations.

4 Conclusions

- Evaluation of Polyphemus Gaussian models against Prairie Grass data is satisfactory.
- The plume-in-grid model for passive tracers gives a wide range of results, depending on parameterization and feedback method.
- Plume-in-grid results with feedback time criterion are more robust. Even if global performances can be lower, it always improves results near the source and in the main plume trajectory.
- Other feedback methods will be developed to improve results. The plume-in-grid model will be extended to the reactive case.

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