Local scale and subgrid-scale models in Polyphemus

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Why use Gaussian models ?

Main advantages

- Analytical formulae for concentrations
- Computationally cheap, few input data
- Good results in local-scale simulations (a few km)

Limitations

- Necessity to compute the standard deviations with empirical parameterizations
- The plume can be non-Gaussian in convective cases
- Heterogeneities are not taken into account (wind shear...)

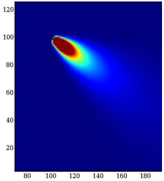
Principle

Modeling a continuous source with a Gaussian plume :

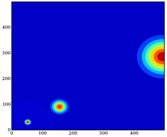
$$C(y,z) = \frac{Q}{2\pi\sigma_y\sigma_z\bar{u}} \exp\left(-\frac{(y-y_s)^2}{2\sigma_y^2}\right)\left[\exp\left(-\frac{(z-z_s)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+z_s)^2}{2\sigma_z^2}\right)\right]. \qquad (1)$$

Here, 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. z_s is the source height above ground.

Plume model



Puff model



Existing parameterizations in Polyphemus

Two generations of Gaussian models

- **Old generation** : Discretized representation of the atmosphere, purely Gaussian (AERMOD, ISC)
- **New generation** : better representation of the boundary layer (LMO), skewed Gaussian in convective cases (ADMS)

Standard deviations (σ_y, σ_z)

- **Briggs** (rural or urban) - Pasquill stability classes
- **Doury** (radionuclides) - 2 stability classes
- **Similarity theory** (based on wind standard deviations)

Existing parameterizations in Polyphemus

Plume reflections and far field

- Reflections on the ground and inversion layer z_i.
- Far field model (homogeneous plume on the vertical when $\sigma_z > 1.5\ z_i$).

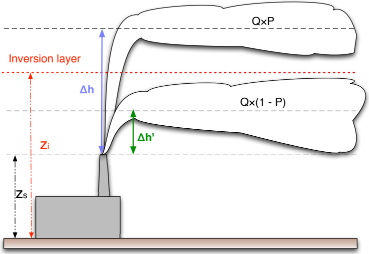
Loss processes

- Scavenging (constant, Belot) for gaseous and aerosol species
- Dry deposition (constant deposition velocity), taking into account the aerosol diameter for gravitationnal settling
- Radioactive and biological decay
- Chemistry (RACM mechanism) for gasous species, in puff model

Existing parameterizations in Polyphemus

Plume rise Δh

- The final plume height is computed as $z_s + \Delta h$
- Briggs-HPDM, Concawe and Holland formulae
- Initial plume spread due to plume rise : $\Delta h/2$
- Partial penetration in the inversion layer : a fraction P of the plume is above z_i.



Validation : Prairie Grass

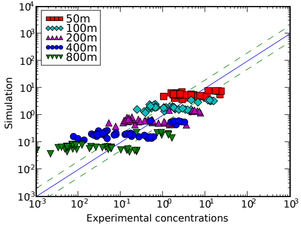
Experiment

- Point source, ground level, flat terrain
- 43 experiments
- Widely used for models calibration

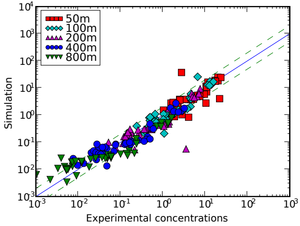
Model	Mean	FB	NMSE	Corr	FAC2
Observations	2.23	0.00	0.00	1.00	1.00
ADMS 4	1.56	0.36	3.01	0.63	0.66
AERMOD	2.14	0.04	1.83	0.75	0.73
ISCST3	2.01	0.11	1.78	0.72	0.61
Observations	2.32	0.00	0.00	1.00	1.00
Polyphemus - Briggs	2.33	0.00	1.83	0.78	0.74
Polyphemus -Doury	1.74	0.29	2.58	0.67	0.29
Polyphemus -Similarity	2.34	-0.01	0.91	0.85	0.62

TAB.: Statistics for several Gaussian models : comparison of maximum arc concentration for simulation

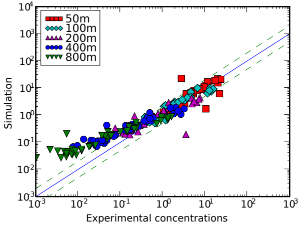
Validation : Prairie Grass



(a) Doury parameterization



(b) Briggs parameterization

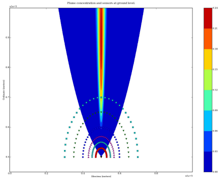


(c) Similarity theory

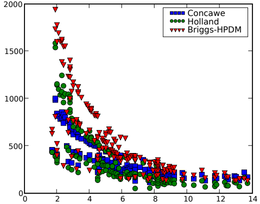
Validation : Kincaid

Experiment

- Elevated point source, high temperature
- 171 experiments
- Very convective case



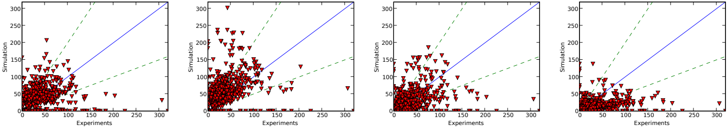
Plume rise (m) as a function of the wind speed (m/s), for all Kincaid experiments.



Plume rise comparison

- Very high plume rise
- Plume rise decreases with higher wind speeds
- Briggs overestimates plume rise at low wind speeds

Validation : Kincaid



(a) Similarity theory - Briggs/HPDM (b) Similarity theory - Concawe (c) Briggs - Concawe (d) Doury - Concawe

Model	Mean	std	FB	NMSE	Corr	FAC2
Obs	41.0	39.3	0.00	0.00	1.00	1.00
ADMS3	43.2	33.5	-0.05	0.77	0.49	0.58
AERMOD	20.3	24.1	0.67	2.28	0.34	0.33
ISCST3	23.1	53.3	0.55	3.83	0.26	0.26
Obs	39.89	39.22	0.00	0.00	1.00	1.00
Briggs/Concawe	32.83	32.80	0.19	1.50	0.27	0.47
Doury/Concawe	16.75	17.81	0.82	3.32	0.12	0.30
Sim.th./Concawe	61.70	53.91	-0.43	1.58	0.25	0.43
Sim.th/HPDM	41.99	34.76	-0.05	1.33	0.19	0.44

TAB.: Statistics for several Gaussian models : comparison of centerline values C/Q for simulation and observation - Kincaid data of quality 2 and 3. Unit is $ng.m^{-3}/(g.s^{-1})$.

Gaussian model validation : conclusions

Prairie Grass

- Very good results, especially similarity theory
- Compares well with the new generation model results

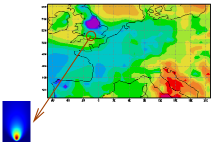
Kincaid

- The Concawe plume rise gives the best results
- Briggs/Concawe and similarity/HPDM are the best combinations
- Results are between AERMOD/ISC and ADMS
- Possible improvements : skewed formulae for convective cases, better representation of the penetration of the inversion layer

Plume-in-grid model

Principle

- Coupling between an Eulerian and a Gaussian puff model, in order to better represent major point source emissions
- Puffs are injected after some time into the Eulerian model



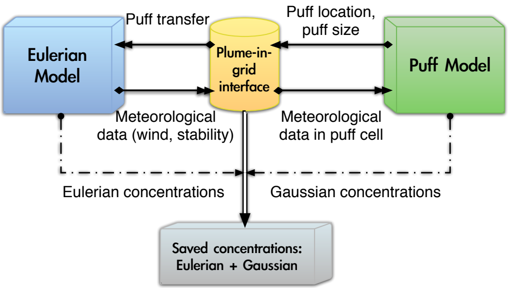
Questions

- What is the impact of plume-in-grid, compared to an Eulerian model ?
- What is the model sensitivity to the Gaussian parameterizations ?
- What are the appropriate time and spatial scales to use the puff model ?

Model coupling

The plume-in-grid model couples Polair3D with the Gaussian puff model. It exchanges information, and saves the concentrations :

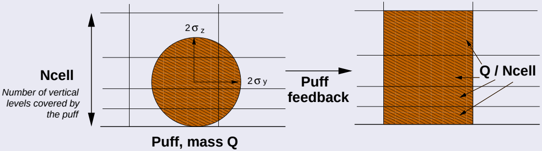
1. **On the whole domain** : the Gaussian contribution for each cell is computed with the puff injection method,
2. **On stations** : the Gaussian contribution is directly computed at each point.



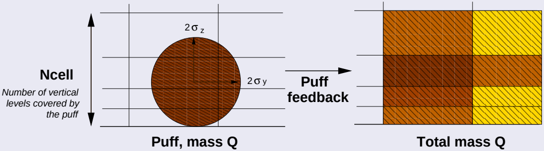
Puff injection methods

When the puff has reached a given criterion (a given time or puff size), it is injected in the Eulerian model. There are two methods :

1. **Column injection** : part of the puff mass is added to each cell vertically covered by it.



2. **Integrated injection** : part of the puff mass is added to each cell within the puff horizontal or vertical size.



ETEX results

Experiment and modeling set-up

- ETEX case : passive tracer release, seven days of measurements over Europe
- Comparison of results with Polair3D and plume-in-grid, for the three Gaussian parameterizations
- Table : statistics for Polair3d and plume-in-grid, for all concentrations and 168 stations. Injection time : 80 minutes. Saving method 1 (whole domain). Column injection.

Model	Mean	FB	NMSE	Corr	FAC2
Obs	0.21	0.00	0.00	1.00	1.00
Polair3D	0.68	1.07	183.5	0.60	0.19
Sim.th.	0.48	0.80	36.13	0.68	0.19
Doury	0.41	0.64	17.70	0.71	0.19
Briggs	0.43	0.69	29.99	0.60	0.19

Plume-in-grid impact

Spatial impact of plume-in-grid : simulation with similarity theory, injection time of one hour, column injection. Unit is μg m^{-3}.

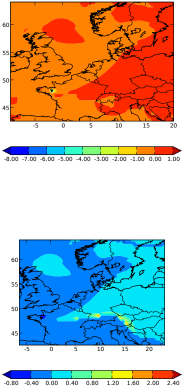


FIG.: Horizontal impact : absolute (top) and relative (bottom) differences in mean ground concentration between plume-in-grid and Polair3D simulations.

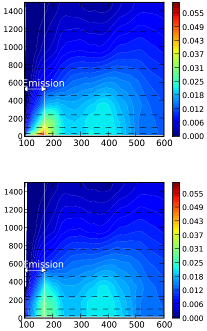


FIG.: Vertical impact : Concentration profile averaged on the domain, against the simulation time step. Top : Polair3D – Bottom : plume-in-grid.

Sensitivity to the parameterization and injection method

Impact on vertical diffusion

- The Gaussian formulation gives more vertical diffusion than the Eulerian model, around the source.
- More vertical diffusion for Doury and Briggs than similarity theory
- More vertical diffusion for column injection than integrated injection

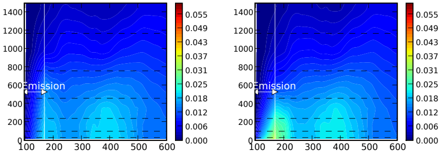


FIG.: Vertical impact : Concentration profile averaged on the domain, against the simulation time step. Left : Doury, column injection – Right : Doury, integrated injection.

Conclusions

- More vertical diffusion around the source gives better results (less bias) : Doury parameterizations and column injection give better results.
- For passive tracers, the plume-in-grid model acts as a subgrid parameterization of the dispersion, that adapt to the puff location and distance from source.

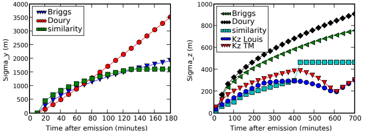


FIG.: Evolution of σ_y and σ_z during 3 hours for the three parameterizations (daytime). Comparison with the vertical diffusion of the Eulerian model for 2 parameterizations, Louis (used here) and Troen Mahrt : the relationship is given by $\sigma_z = \sqrt{2\, K_z\, t}$.

What is the appropriate time scale ?

(Sensitivity to the puff injection time)

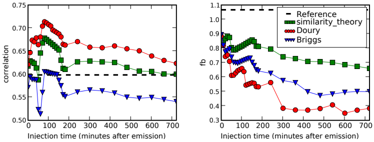


FIG.: Evolution of the correlation and fractional bias against the puff injection time (0 to 12 hours). Statistics on all concentrations. Injection method : column. Saving method : whole domain.

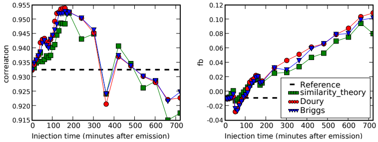


FIG.: Evolution of the correlation and fractional bias against the puff injection time (0 to 12 hours). Statistics on arrival times on stations. Injection method : column. Saving method : whole domain.

Conclusions

- The correlation is more sensitive to the injection time than other indicators.
- The use of plume-in-grid has an impact on global statistics even if puffs are injected only after 10 minutes.
- The best performance is shown for injection times between 80 minutes and 3 hours.
- After 3 hours, the statistics drop for arrival time, and decrease slowlier for all concentrations.

What is the appropriate spatial scale ?

(Sensitivity to the saving method)

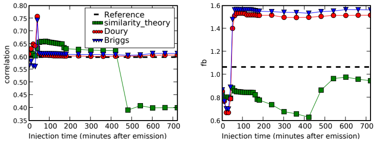


FIG.: Evolution of the correlation and fractional bias against the puff injection time (0 to 12 hours). Statistics on all concentrations. Injection method : column. Saving method : on stations.

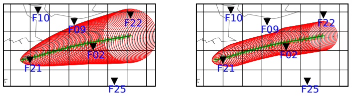


FIG.: Puff trajectory during 12 hours. Green : puff center. Red : puff radius. The circle radius is $2 \times \sigma_y$, and one circle is drawn at each time step (ten minutes). Black triangles are the measurement stations. Left : Briggs parameterization – Right : similarity theory.

Conclusions

- The results are very sensitive to the saving method : it shows the importance of the few stations reached before the puff injection.
- The stations Rennes (F21) and Alençon (F02) are the only directly impacted : they drive the global results. Rennes is reached around 40 minutes, and Alençon 480 minutes after a puff emission.
- With this saving method, similarity theory is the best parameterization, Briggs and Doury considerably overestimate the concentrations.

What is the appropriate spatial scale ?

(Sensitivity to the grid resolution)

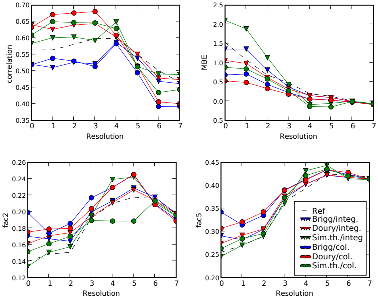


FIG.: Evolution of the correlation, bias, fac2 and fac5 for several grid resolutions. Results are for Polair3D ("Ref") and plume-in-grid with an injection time of 1 hour. Statistics on all concentrations, saving on the whole domain.

Changing the grid resolution

- The impact of plume-in-grid is tested for several resolutions.
- Results are better for large resolution, for all models.
- The models dispersion is greater for low resolution.

What is the appropriate spatial scale ?

(Sensitivity to the grid resolution)

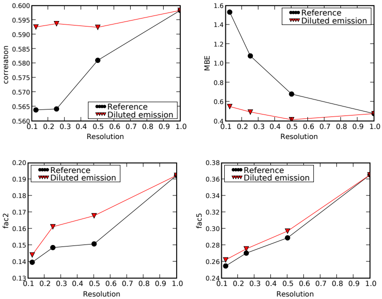


FIG.: Evolution of the correlation, bias, fac2 and fac5 for several grid resolutions, statistics on all concentrations. Results are for Polair3D with emission in one grid cell (black), or diluted in several cells to have the same injection volume with lower resolution (red).

Changing the grid resolution

- The impact of the emission volume explains the lower results for correlation and bias.
- The fac2 and fac5 are still low.

Further work

Applications

- Validation of the reactive plume-in-grid model over Paris (summer 2001), in process
- Use of reactive plume-in-grid at the European scale

Possible developments

- Improving the plume rise model
- Adding other parameterizations (second order standard deviations)
- Better taking into account the wind shear (puff splitting)
- Plume-in-grid with aerosols and heavy metals