DEVELOPMENT OF LOCAL-SCALE AND SUBGRID-SCALE MODELS IN POLYPHEMUS

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1 THE GAUSSIAN PLUME AND PUFF MODELS

We will briefly present the Gaussian plume and puff models that have been implemented into Polyphemus platform [Mallet et al., 2007]. An evaluation of the models was carried out thanks to comparison with Prairie Grass experiments. It will be presented with an emphasis on comparison between different parameterizations for standard deviations. In the following sections, the Gaussian plume model is described. The Gaussian puff model is based on the same equations and parameterizations, except that it also involves diffusion in the downwind direction.

1.1 Form of the Gaussian plume model

There are many underlying assumptions when using a Gaussian plume model (see Arya [1999]), particularly :

1. Continuous emission from the source so that the material is spread out in the form of a steady plume between the source and the farthest receptor.
2. Steady-state flow and constant meteorological conditions.
3. No wind shear in the vertical direction.
4. Strong enough winds to make turbulent diffusion in the downwind direction negligible in comparison to advection.

In that context, the concentration C at a given point is given by the formula:

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

Here, Q is the source emission rate, given in mass per second, $\bar{u}$ is the mean wind velocity, and σ_y and σ_z are the Gaussian plume parameters. The coordinate y refers to horizontal direction "crosswind", that is, at right angle to the plume axis which is also the wind axis, and y_s is the source coordinate in that direction. The coordinate z refers to the vertical coordinate, and H is the plume centerline height above ground.

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1.2 Plume reflections

The purpose of the last term in equation 1 is to take into account the reflection of the plume on the ground. In the case of inversion, the reflection at the inversion layer can similarly be taken into account. Reflections on the ground and on the inversion layer (noted z_i) are only taken into account when the plume touches them:

- Ground reflection occurs when $\sigma_z > H$
- Reflection on the inversion height occurs when $H + \sigma_z > z_i$

where z_i is the inversion height, which is supposed to be equal to boundary height during daytime and to 0 during nighttime. If inversion height is equal to 0, there is no inversion and hence no reflection on it.

1.3 Far field model

When the plume fills the boundary layer, it is supposed to have been sufficiently mixed to be vertically homogeneous. The concentration formula is then:

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

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

1.4 Dispersion parameterization schemes

For an estimate of the dispersion parameters σ_x, σ_y and σ_z, empirical parameterization schemes are widely used. Many schemes have been proposed, most of them giving the dispersion parameters as functions of the downwind distance and stability class, and based on a few diffusion experiments. In Polyphemus, three parameterizations are proposed. Two of them are based on a discrete description of the atmospheric boundary layer: the Briggs formulae based on Pasquill stability scheme, or, alternatively, the Doury formulae. The third one is based on similarity theory. It uses functions of the wind velocity fluctuation and of other boundary layer parameters like the Monin-Obukhov length, the mixing height and the friction velocity.

1.4.1 Briggs formulae

The Briggs formulae are based on the Pasquill-Turner stability classes and on the Prairie Grass experiment. This parameterization is born from an attempt to synthesize several widely used parameterization schemes by interpolating them for open country and for urban areas. These formulae apply to a distance from the source up to 10 km and may be extended up to 30 km. They are particularly recommended for urban areas.

1.4.2 Doury formulae

An alternative parameterization is the Doury model described in Doury [1976]. It is widely used in French models and recommended by the French Nuclear Energy Agency (CEA). This parameterization has been developed for the specific application of radionuclides dispersion, and fitted on radionuclides measurements. The experimental field was wider than the Prairie Grass field. The formulae use only two stability situations: one for normal dispersion, corresponding to daytime or nighttime with a wind speed greater than 3 meters per second, and one for low dispersion, corresponding to nighttime with low wind speed. The standard deviations are given in both cases in the general form:

$$\sigma_y = (A_h t)^{K_h} \sigma_z = (A_z t)^{K_z} \tag{3}$$

where t is the transfer time since release time. In the case of a steady-state plume $t = x/u$ where x is the distance from the source and u is the wind speed.

1.4.3 Similarity theory

If more accurate meteorological measurements are available, σ_x, σ_y and σ_z can be estimated using the standard deviations of wind velocity fluctuations in downwind direction σ_u, crosswind direction σ_v and in vertical direction σ_w. Whereas in the two other parameterizations, σ_x had to be taken equal to σ_y, it is here specifically computed. Following Irwin [1979] dispersion coefficients are computed in the form:

$$\begin{pmatrix} \sigma_x = \sigma_u \; t \; F_x \\ \sigma_y = \sigma_v \; t \; F_y \\ \sigma_z = \sigma_w \; t \; F_z \end{pmatrix} \tag{4}$$

where t is the time in seconds, and F_y and F_z are functions of a set of parameters that specify the characteristics of the atmospheric boundary layer. Their forms are determined from experimental data. Various expressions of F_y and F_z have been proposed (e.g. Irwin [1979], Weil [1988]). In Polyphemus, wind standard deviations will be computed according to Hanna [1984]. For vertical standard deviation σ_w an alternative parameterization from Weil [1988] is proposed.

1.5 Other processes

Additionnal processes can be taken into account, but will not be developed here since they are not used in the presented work. One can cite:

- Plume rise,
- radioactive and biological decay,
- dry deposition with Chamberlain and Overcamp model (see Arya [1999]),
- wet scavenging,
- dispersion for particulate matter.

2 Evaluation with Prairie Grass Experiment

2.1 Presentation of the Experiment

The Prairie Grass experiment has become a standard database used for many short range models evaluation. The experiment took place in O'Neil, Nebraska, during summer 1956. The site was a flat terrain of short cut grass. A continuous plume of SO_2 was released, without plume rise, near the ground (at 0.46 m). Measurements where taken on five arcs at 50, 100, 200, 400 and 800m from the source. There were nearly 70 trials.

2.2 Comparison with other Gaussian Models

The comparisons are discussed using scatter diagrams as well as the statistical performance measures described below, which include the fractional bias (FB), the geometric mean bias (MG), the normalized mean square error (NMSE), the geometric variance (VG), the fraction of predictions within a factor two of observations (FAC2) and the correlation coefficient (Corr).

Table 1: Statistics for several Gaussian models: comparison of maximum arc concentration for simulation and observation – 43 trials in Prairie Grass Experiment. Results for ADMS, AERMOD and ISCST3 come from McHugh et al. [2001].

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

Table 1 shows that all models compare very well with experimental data, except Polyphemus with Doury parameterization and ADMS. AERMOD, ISCST3 and Polyphemus with Briggs formula show good results, as the Prairie Grass results were used directly in the formulation of their plume spread parameters. Polyphemus with similarity theory shows good results, comparable to those of AERMOD and ISCST3. All indicators are within an acceptable range, and the correlation is the highest of all models presented here (82%). Figure 1 shows the scatter diagram for Polyphemus with similarity theory.

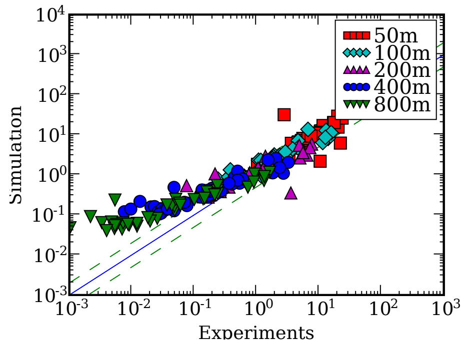


Figure 1: Scatter plot of maximum arc concentrations for observations and simulations with similarity theory parameterization. Concentrations are normalized by source rate Q and the unit is $\mathrm{mg{\cdot}s^{-1}/g{\cdot}s^{-1}}$. Prairie Grass experiment, 43 trials.

Those results provide a first validation of Polyphemus Gaussian models. One should note that the same results were obtained both with the plume model and with the puff model, where the continuous source has been discretized into a series of puffs and the simulation has been made on a period long enough to reach the stationary state. Hence, these models can be taken as a basis for further modeling, such as the plume-in-grid model development.

3 The Plume in Grid model

The principle of a plume-in-grid model is to couple a Gaussian Puff model with an Eulerian model in order to describe the dispersion of a plume emitted by a point source in a more accurate way than the sole Eulerian model. These models are generally used to deal with chemically reactive plumes, and have been proved useful to model ozone chemistry in particular (see Viyaraghavan et al. [2006] for example). However, there is hardly any example of study for this kind of models in passive cases. The plume-in-grid model developed in Polyphemus is currently used to deal with passive tracers, and has been tested on the ETEX experimental data. Hence, the aim of the present study is twofold:

1. To investigate whether or not the use of a plume-in-grid model is relevant in passive cases, and if possible, to issue recommandations concerning its use (which parameterizations to choose, and which criteria for puff feedback) and applications,
2. To validate the method used in coupling the Gaussian and Eulerian models before extending it to the reactive case.

3.1 Model description

The plume-in-grid model developed in Polyphemus is able to couple an Eulerian and a Gaussian puff model, provided that those models have a minimal C++ interface. It is currently tested with Polyphemus Gaussian puff model and with the Eulerian model Polair3D.

The two models run independantly from one another. They only need to exchange some information with the plume-in-grid model:

Meteorological data. They have been computed on the Eulerian grid and can be either interpolated at the puff center or taken as the value of the cell where puff is located. They are then used by the Gaussian model.

Puff data. At each time step, the puff center cell is determined from the puff center coordinates (see section 3.2). A test is made to see whether the puff has to be injected. If it is the case, the puff is erased, and is transfered into the Eulerian model (see section 3.4).

Concentrations are computed as the sum of the Eulerian and Gaussian contributions. Hence, there are three different parts in a simulation that takes into account one point source:

1. When the Eulerian contribution is equal to zero, and concentrations are computed with the Gaussian formula,
2. A period, between the first and last puff injection into the Eulerian model when both Eulerian and Gaussian concentrations are added,
3. After the last puff feedback, there is only the Eulerian contribution.

3.2 Coordinates

Since Polair3D uses longitude and latitude coordinates, and a Gaussian model uses Cartesian coordinates, it is necessary to be able to do the transformation. The Cartesian coordinates are the coordinates in the tangent plane of the point source. If the distance between the source and the puff center becomes too great, the error in assimilating the puff trajectory to that in the plane cannot be neglected anymore. The transformation formulae are:

$$\begin{pmatrix} dx \\ dy \end{pmatrix} = \begin{pmatrix} R\, cos\phi\, d\lambda \\ R\, d\phi \end{pmatrix} \quad (5)$$

Where x, y, z are the point Cartesian coordinates, λ is the longitude and ϕ is the latitude, in radians, and R is the Earth radius in meters.

3.3 The "increasing sigma" method

The parameterizations to compute standard deviations assume that the meteorological data is stationary and homogeneous, which is not the case in the plume-in-grid model. Hence, if at time t_1 the puff has a size σ_1 which has been computed with formulae for unstable cases, and at time $t_2 = t_1 + \Delta t$ meteorological conditions become stable (for example if night has fallen), the new puff size σ_2 will be computed with meteorological data at time t_2, which can lead to the unrealistic situation where $\sigma_2 < \sigma_1$. This is illustrated by Figure 2.

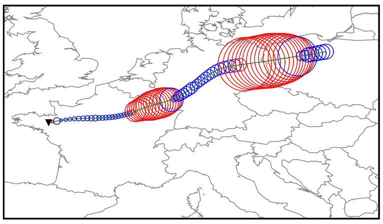


Figure 2: Size evolution of one puff. The puff is represented at each time step at its present location (in latitude/longitude), and the circle radius is proportional to σ_y. Puffs are drawn in red when it is daytime and in blue during nighttime. The green line is the puff center. The black triangle is the 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.

This applies to horizontal standard deviations. For vertical standard deviations, we only insure that the puff size cannot decrease.

3.4 Puff feedback criteria and method

3.4.1 Criteria

There are two possible criteria to feed the puff back to the Eulerian model:

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

The puff size is $C_y \times \sigma_y$, where C_y is a coefficient usually taken equal to 4.

3.4.2 Feedback methods

Since the puff horizontal size is supposed to span at most one cell horizontally at the moment of injection, it is fully injected in the cell where its center is located. However, the puff covers vertically several cells. The puff vertical extent is computed in a similar way than the horizontal size, that is, $C_z \times \sigma_z$ (C_z usually equal to 4). The puff quantity has then to be divided into the number of cells vertically covered, and injected into them, supposing that the concentration is uniform in the puff. Note that the puff will not be reinjected into cells above the boundary layer height.

4 Evaluation with ETEX experiment

4.1 The ETEX case

This experiment has taken place at the European scale on October 1994. A passive tracer, SF_6, was released continuously during twelve hours at a given location in the west of France (location is shown Figure 2). There were about 3000 measurement stations all over Europe. Measurement were made during one week after release.

The simulation was made during seven days with a time step equal to ten minutes. The simulation grid covers all Europe and its cell width is $0.5625°$ in longitude and latitude.

4.2 Model results

Results for several plume-in-grid simulations are presented. Sections 4.2.1 and 4.2.2 are meant to compare the injection criteria. Section 4.2.3 analyses the effect of the plume-in-grid model on results.

4.2.1 Reinjection based on puff size

Table 2 shows the statistical results on all stations for the whole simulation with puff size criterion. The results have been compared for all available parameterizations to compute standard deviations, as well as for Polair3D without plume-in-grid.

Although the use of plume-in-grid seems to better the bias, the correlations are all rather lower than with the Eulerian model alone, except for Doury parameterization. This comes from the fact that puff size meets reinjection criterion very late or never for all parameterizations except Doury. This is illustrated by Figure 3: after a while σ_y becomes constant with Doury parameterization since puff has been injected into the Elerian model, whereas it keeps growing in the other cases.

standard deviations, which has not been attempted yet.

Table 2: ETEX experiment statistics on 168 stations for five plume-in-grid configurations: (1) similarity theory with Weil parameterization, (2) similarity theory with Hanna parameterization, (3) Doury, (4) Briggs with rural formulae, (5) Briggs with urban formulae.

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

Table 3: ETEX experiment statistics on 168 stations for five plume-in-grid configurations. Reinjection time is 12 hours after puff release.

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

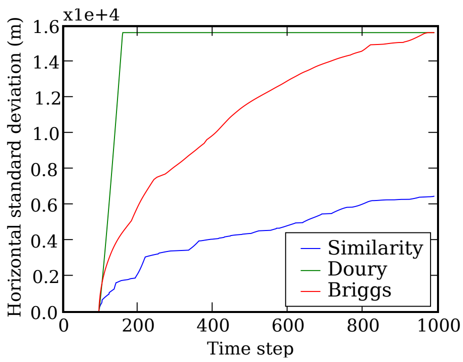


Figure 3: Evolution of σ_y in time for one puff for the different parameterizations. It is computed using the "increasing sigma" method. Time step is 600 s. When the puff has been injected into the Eulerian model, σ_y becomes constant.

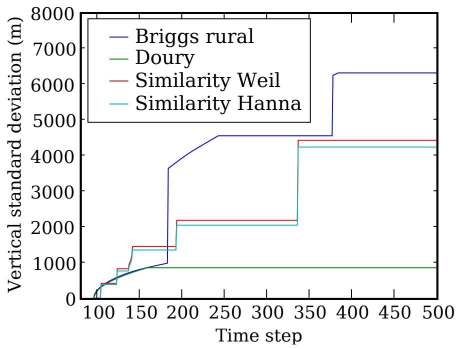


Figure 4: Evolution of σ_z in time for the different parameterizations, for one puff. The evolution has been plotted without imposing the injection time. An injection time of 12 hours after emission corresponds to time step 168.

4.2.2 Reinjection based on time

In Table 3, the same parameterizations are used but the reinjection time is now always set to twelve hours after puff release. When injection time tends toward 0, plume-in-grid results tend toward Polair3D results, so setting a lower injection time should mechanically improve the results for several parameterizations. The results presented here are better than the previous ones, except for Doury parameterization where they do not change. Results for Briggs parameterization with rural formulae are now better than without plume-in-grid. However, the similarity theory parameterizations still give substantially lower correlations. The only difference between parameterizations in that case is the number of vertical levels covered by the puff at reinjection time. As shown Figure 4, the puff vertical extent with similarity theory is about 1.5 times the extent with Doury parameterization at time step 168, which corresponds to the reinjection time. This might be improved by extending the increasing sigma method to vertical

4.2.3 Analysis of the plume-in-grid results

We present an analysis for different stages of the simulation, and several stations, since local improvements can be overlooked in global statistical results. Figure 5 shows that 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).

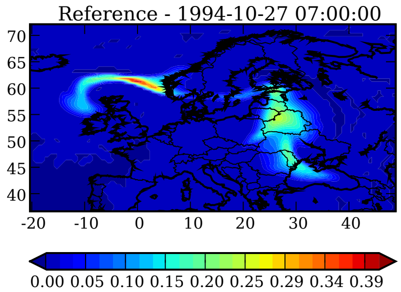
We can distinguish three different zones in the domain:

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.

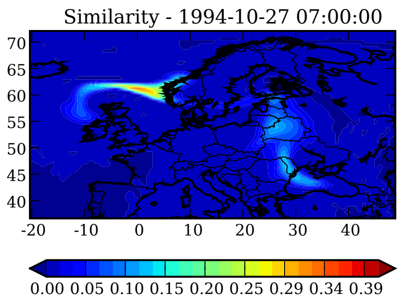
2. North-west of Europe, where the greater concentrations are observed. Plume-in-grid models improve results at stations in this zone.

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.



(a) Polair3D (no plume-in-grid)



(b) Plume-in-grid with similarity theory

Figure 5: ETEX simulation: concentration on the domain, three days and a half after beginning, with and without plume-in-grid. Plume-in-grid simulation was performed with similarity theory. Injection time was set to 12 hours after emission. Unit is $\mathrm{ng{\cdot}m^{-3}}$.

Figure 6 shows the difference of Figure of Merit in Time (FMT) between plume-in-grid and Polair3D. The FMT corresponds to the overlap area at a given station between simulated and observed time series. This figure shows clearly that plume-in-grid is better at stations in the main plume trajectory (north-west of Europe) but is worse than Polair3D alone in the other parts of the plume. The Eulerian model also 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.

4.3 Conclusion

The results presented tend to show that plume-in-grid models should be used very carefully since they can provide a wide range of results, depending on the chosen parameterization and feedback method. However, when computing concentrations on the whole domain and imposing a maximum time for puff feedback, results are promising and can be better than the Eulerian model alone. Also, a finer analysis on stations shows that even if global performances can be lower, the use of plume-in-grid tends to improve the results near the source and in the main plume trajectory.

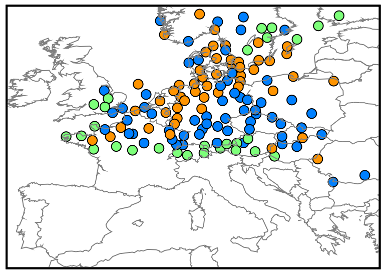


Figure 6: Difference of FMT for all stations between plume-in-grid model (with similarity theory) and Polair3D alone. Red: fmt for plume-in-grid is greater. Blue: fmt for plume-in-grid is lower. Green: no difference (stations where no significant concentrations are modeled).

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