Development of a new plume-in-grid model for roadways combining an Eulerian model with a Gaussian line-source model.

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Introduction

Eulerian models are widely used in air quality modeling. Such models are based on a three dimensional spatial grid in which emissions are released. Thus emissions are instantaneously diluted within the grid cells and the near-source impacts of large point and line sources cannot be properly resolved. Therefore, in regional scale simulations, the approximation made by the model on the emissions from point and line sources can have a significant impact, in particular with large grid cells. Plume-in-grid (PinG) models combine an Eulerian model and a plume or puff model. This coupling offers a better representation of sources within grid cells, because it uses the plume/puff model to compute locally the dispersion and chemistry of pollutants emitted from the sources. In a standard PinG model, Gaussian puffs (or plumes) are released with a certain frequency to model with a time discretization the evolution of a plume. When a predefined criterion is reached, based on the number of time steps, the size of the puff or the ratio of the puff concentration to the background concentration, pollutants are transferred to the Eulerian model, which can then compute the dispersion at a large scale. The main purpose is to be able to combine local precision from the puff / plume model with the background information from the grid-based model at a regional scale. Plume-in-grid models, already exist for point sources (e.g., CMAQ, AMSTERDAM, Polyphemus (Karamchandani et al., 2006, 2010; Korsakissok and Mallet, 2010)). They have been used in many studies and have been proven to be efficient. Modeling roadway traffic with point sources would require to spatially discretize road sections with point sources, which would induce a significant increase of the computational burden. Although point sources are convenient to model dispersion from a chimney, line sources are better suited for roadway traffic pollution modeling because they provide the Gaussian precision with only one source per road section. Here we present a new plume-in-grid model that uses Gaussian line source models embedded within the Eulerian model Polair3D (Boutahar et al., 2004). Emissions are treated as steady-state plumes that are released from the line sources. A challenging part was to adapt a steady-state model, which by definition assumes no change with time, to a time-dependent Eulerian model. The transfer of pollutants from the Gaussian model to the Eulerian model differs significantly from that of a puff model. It occurs in several cells by distributing the pollutant to be transferred into all cells that should be affected by the plume. The model was developed as a part of the modeling platform Polyphemus (Mallet et al., 2007). First we present here both Gaussian and Eulerian models. Then we present the coupling between those two models and finally we present simulation results conducted on a real-world case study.

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1 Model descriptions

Plume-In-Grid (PinG) models aim at improving the contribution of sources in an Eulerian simulation by using a subgrid-scale treatment with, for example, a Gaussian model. In a PinG model pollutants are dispersed with a plume or puff model until it can be considered as background pollutants. The plume / puff pollutants are then transferred to the Eulerian model that is running concurrently. Therefore, a PinG model requires a plume or puff model and an Eulerian model. We used here the Polyphemus modeling platform which provides both of them (Mallet et al., 2007).

1.1 Eulerian model

The Eulerian model is called Polair3D and is relevant up to the continental scale (Boutahar et al., 2004). There are a passive version of Polair3D, a version with gaseous chemistry and a version with aerosols. Their performances have been evaluated in Quélo et al. (2007); Sartelet et al. (2007); and Mallet and Sportisse (2004) respectively.

1.2 Gaussian model

The Gaussian model, which has been developed especially for the PinG application, is briefly described below. The Gaussian formulation of the concentration field for a pollutant emitted from a line source is the result of the integration of the point source solution over the line source. For wind directions other than perpendicular to the line source, the dependency of standard deviations on the integration variable makes the integration impossible without approximations. Various approximations can be made (Yamartino, 2008). Venkatram and Horst (2006) present a formulation (hereafter called HV), which consists in evaluating the integral by an approximation of the integrand and by excluding from the computation parts of the line source that are downwind of a given receptor. This formulation has been shown to give satisfactory results however, when the wind is parallel to the line source, it diverges. In Briant et al. (2011), this error associated with the HV formulation was computed by comparison to an exact solution (obtained by discretizing the line source into a very large number of point sources) and was parameterized using analytical formulas in order to correct the HV formulation. For cases where the wind is parallel to the line source, the use of an analytical / discretized line source combination, allows one to minimize the error induced by the singularity very effectively. Because this combination is only applied for a small range of wind directions, the increase in the overall computational time is not significant. This formulation performs well for all ranges of angles and provides some improvement in terms of accuracy over previous formulations of the Gaussian line source plume model without being too demanding in terms of computational resources. The model used here also includes a Romberg integration to account for the road width. This model was implemented in the Polyphemus modeling platform.

2 Gaussian and Eulerian model coupling

Existing PinG models use puffs to discretize in time the plume emitted from the source. With the Gaussian plume model presented above a steady state is assumed, therefore, making this discretization of the plume unnecessary. In the following part, the model is described. Information about the method that transfers pollutant from the Gaussian model to the Eulerian model is presented. Finally, we present a simple method to parallelize the model.

2.1 Model description

Algorithm 1 and Figure 1 explain how the model has been implemented. After the initialization of both models, the time loop is launched. Note that for 1 iteration of the Eulerian model only 1 iteration of the Gaussian model is done. Indeed, as stated before, the plume emitted from the source does not need to be discretized with puffs. A Gaussian concentration from the previous time step is considered as background concentration for the Eulerian model and,

therefore, it is added to the current Eulerian concentration before the model iteration. Then, the Gaussian model contribution from each source to each grid cell is computed before the chemistry process can be done. Finally, at the end of the time step, output concentrations are computed at each output receptor location and are saved.

Algorithm 1 Algorithm of the Plume-In-Grid model using the line source Gaussian plume model.

```
1: -Initialize Eulerian model
2: -Initialize Gaussian model
3: -Read sources information (coordinates and emission rates)
4: for time step 0 to the end do
5:    -Transfer to the Eulerian model Gaussian concentration from the previous time step
6:    -Iteration of Eulerian model
7:    for each source do
8:       for each grid cell do
9:          -Compute contribution of the source to the grid cell
10:      end for
11:   end for
12:   -Compute Gaussian chemistry process.
13:   -compute Gaussian contribution at receptor location
14:   return Eulerian concentration + Gaussian contribution at receptor location
15: end for
```

2.2 Transfer of pollutants from the Gaussian model to the Eulerian model

The transfer of pollutants from the Gaussian model to the Eulerian model occurs at the beginning of each iteration of the time loop (line 5 of the Algorithm 1). However, pollutants that are to be transferred are computed at the previous iteration during the loop over all sources (lines 7 to 11 of the Algorithm 1), which computes the contribution of each source to each grid cell (note that for the first iteration no pollutant is transferred to the Eulerian model). Considering that the total amount of pollutant emitted from a given source during the current time step is: $Q \times L \times l \times \Delta t$, where Q is the emission rate in $\mathrm{g\,m^{-2}\,s^{-1}}$, L and l are the width and the length of the source, respectively, and Δt is the time step, we spatially discretize the plume to compute the contribution of the source at several locations in order to know the spatial distribution of the plume. Therefore, we are able to know the contribution of each source to each grid cell.

2.3 Parallelization

Computations can rapidly become cumbersome because two models are running concurrently. Polair3D has already been parallelized using the library Message Parsing Interface (MPI `http://www.mcs.anl.gov/research/projects/mpi/`) but not the Gaussian model. Because most of the computations for the Gaussian model are due to the loop over all sources and because the computation of each source is independent, a simple way to parallelize the model was to split the source list and to reallocate sources to each processor before the loop. Right after the loop, results are collected from each processor. This method allows us to use more efficiently resources from each processor available for a given simulation.

3 Results

The model presented above is applied here with a one-day simulation over the Paris region. We used meteorological data computed with the Weather Research and Forecasting model (WRF) and boundary conditions from the LMDzT-INCA global model (Hauglustaine et al., 2004). Emissions were simulated with Polyphemus preprocessing programs using an emission inventory from the Paris air quality agency (Airparif). We added over 5000 constant line sources in the Gaussian model to account for traffic emissions, representing a total of 831 km of linear road length. Those emissions were computed with the European model COPERT 3 and were provided by the French technical study and engineering center CETE Nord Picardie.

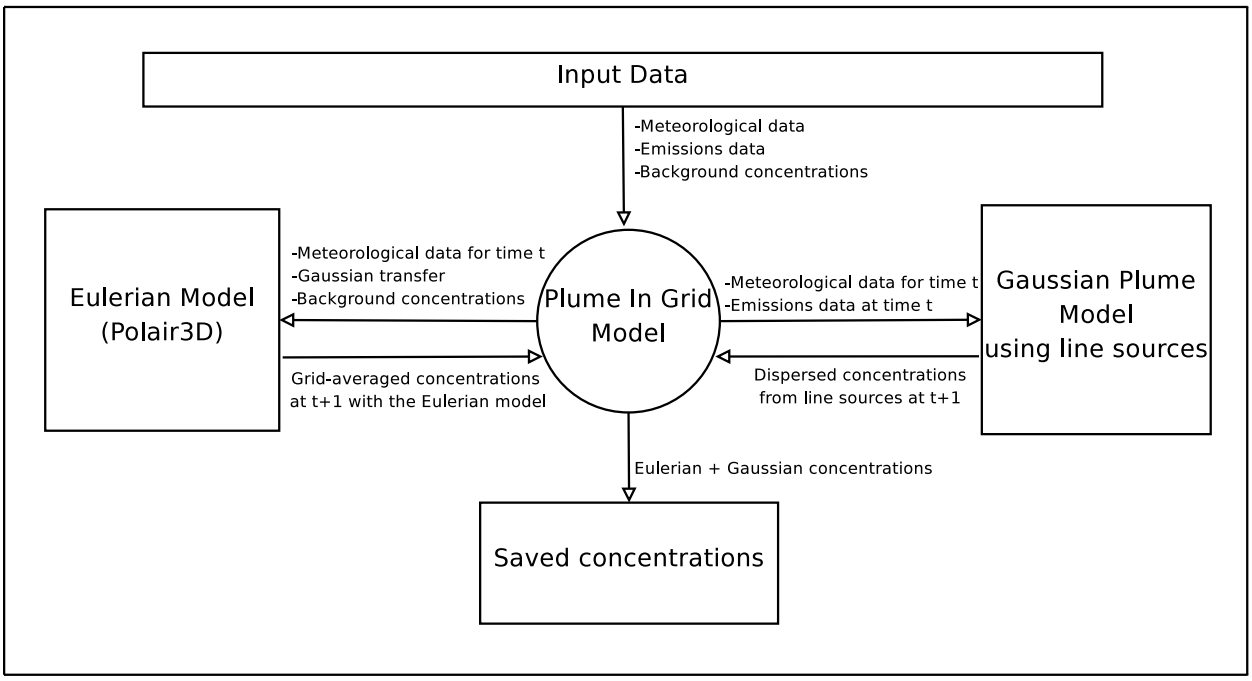
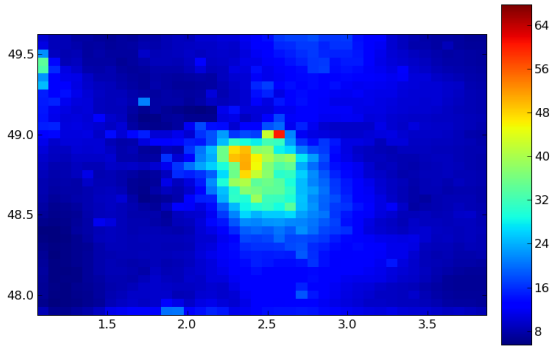
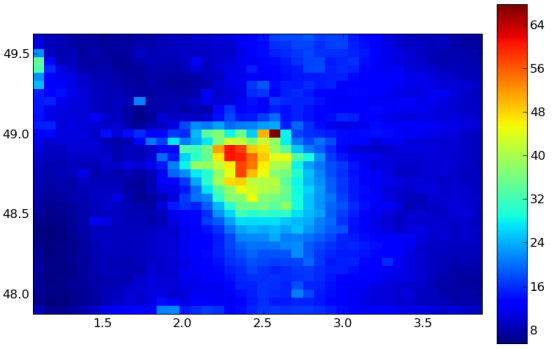


Figure 1: Coupling between the Gaussian model and the Eulerian model (Polair3D).



(a) Polair3D results ($\mu g\,m^{-3}$)



(b) PinG results ($\mu g\,m^{-3}$)

Figure 2: NO_2 concentration over the Paris region simulated with PinG and Polair3D models.

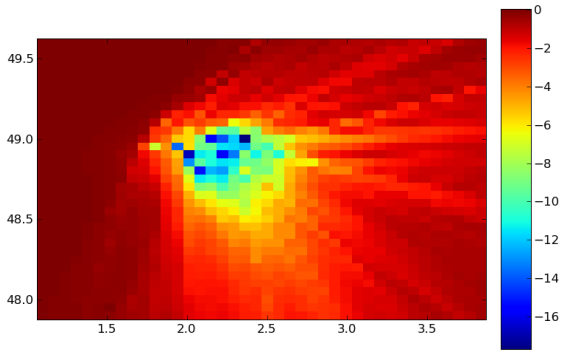


Figure 3: Difference in NO_2 concentration between the model simulations: Polair3D - Polyphemus ($\mu g\,m^{-3}$).

Conclusion

A new Plume-In-Grid model has been developed. It has been tested on a large case study for a one-day simulation. It has shown satisfactory results when compared to the Eulerian model. The next step will be to use this new Plume-In-Grid model for a longer simulation with more complete emission data and to compare results with measurements to evaluate model performance.

We conducted simulations with both the PinG model and the standard Eulerian model (Polair3D). Line source emissions are considered to be constant grid-based emissions in the Eulerian model. Figure 2 shows maps of the NO_2 results obtained with each model and Figure 3 shows the difference map between them. Both models give similar results however, the PinG model gives slightly higher concentrations than Polair3D. This result is due to the use of the Gaussian model in the PinG simulation which computes the contribution of each line source and adds it to background concentration while Polair3D dilutes pollutants immediately in the grid-cell where they are emitted.

Acknowledgments

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