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Multi-scale modeling of roadway air quality impacts: Development and evaluation of a Plume-in-Grid model

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HIGHLIGHTS

► Development of a PinG model for roadway.
► Evaluation of the model.
► Sensitivity study.

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ABSTRACT

Eulerian three-dimensional (3D) grid-based models are widely used in air quality modeling. In such models, emissions are instantaneously diluted within the grid cells and, therefore, the near-source impacts of large point and line sources cannot be properly resolved. Plume-in-Grid models (PinG) use a subgrid-scale treatment to better represent local source contributions in an Eulerian grid-based simulation. PinG models already exist for point sources. However, modeling emissions from roadway traffic with point sources implies a very large computational burden. We present here a new PinG model that uses a Gaussian line source model, better suited than point sources to model roadway traffic emissions, embedded within an Eulerian model. The model is evaluated with a large dataset of nitrogen dioxide (NO_2) concentrations over a 800 km road network. The PinG model leads to greater NO_2 concentrations and shows better performance than the Eulerian model.

1. Introduction

Eulerian three-dimensional (3D) grid-based models are widely used in air quality modeling at urban, regional, and global scales. In such models, emissions are instantaneously diluted within the grid cells and, therefore, the near-source impacts of large point and line sources cannot be properly resolved. Furthermore, in regional-scale simulations, the approximation made by a grid-based model on the emissions from point and line sources of precursors of secondary pollutants can have a significant impact on the concentrations of those secondary pollutants, in particular with large grid cells. On the other hand, Gaussian plume and puff models are designed to model pollutant dispersion at local scales. Puff models can be applied to simulate pollutant concentrations with complex chemistry at long distances from their sources but can treat only a limited number of sources. Analytical Gaussian plume models are computationally efficient but cannot be applied far from sources and cannot treat complex chemistry. It is, therefore, of interest to combine a "local" plume or puff model with an Eulerian grid-based model in order to treat jointly the local and regional air quality impacts of major sources. Such a combination of local and regional models is typically called Plume-in-Grid (PinG) model, because a subgrid-scale treatment (local model) is used to better represent local source contributions in an Eulerian simulation. In a standard PinG model, Gaussian puffs 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 from the plume to the Eulerian model, which can then compute the dispersion and transformation of pollutants at the regional scale. The PinG model is thus able to combine local precision from the puff/plume model with the background information from the Eulerian grid-based model at a regional scale.

This PinG modeling approach was initially developed for point sources (Seigneur et al., 1983) and it has been used for point sources

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in different forms in a large array of Eulerian models since then (Karamchandani et al., 2011, and references therein). The current formulation of PinG models for point sources in standard Eulerian air quality models (e.g., CMAQ, AMSTERDAM, Polyphemus) uses Gaussian puffs for subgrid-scale modeling (Karamchandani et al., 2006, 2010; Korsakissok and Mallet, 2010a). 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 (e.g., Karamchandani et al., 2009). It is, therefore, desirable to develop efficient modeling techniques for subgrid-scale modeling of mobile sources.

Jacobson et al. (2011) developed a parameterization based on large-eddy simulations to represent contrails from aircraft in a global model. Simpler box-model parameterizations have typically been used to treat ship emissions in global or regional Eulerian models (e.g., Franke et al., 2008; Huszar et al., 2010). To date, the characterization of the local impacts of roadway emissions in air quality modeling have mostly been based on a parameterization of the subgrid-scale variability of the concentrations of the pollutants of interest obtained from a local-scale dispersion model (e.g., Touma et al., 2006; Isakov et al., 2007; Cook et al., 2010) or land-use information (e.g., Valari and Menut, 2010). However, such approaches consist in a postprocessing of the Eulerian model output and cannot account explicitly for chemical interactions between the emission plumes and the background, including the influence of local plume chemistry on background concentrations. To account for such chemical interactions, a PinG modeling approach is needed. We present here a new PinG model that uses Gaussian line source models, better suited than point sources to model emissions from roadway traffic, embedded within an Eulerian model.

The Gaussian line source model has been presented by Briant et al. (2011). It has been evaluated against near-roadway data available for a large case study and gave satisfactory performance (Briant et al., 2012). Emissions are released from the line sources and dispersed as steady-state plumes. The host Eulerian model is Polair3D (Boutahar et al., 2004; Sartelet et al., 2007) of the Polyphemus air quality modeling platform (Mallet et al., 2007). A challenging aspect of PinG modeling is to simulate the transfer of pollutants from the subgrid-scale model to the host model, here from the Gaussian model to the Eulerian model; this transfer differs significantly from that of a puff model because of the steady-state nature of the Gaussian model. Several additional features are also implemented: a parallelization of the model, a temporal profile for roadway traffic emissions, and a chemistry scheme in the Gaussian model to simulate near-roadway chemical transformations.

The model was developed as part of the Polyphemus modeling platform (Mallet et al., 2007). In Section 2, we present the Gaussian and Eulerian models and we describe in detail the implementation of the coupling between those two models. The parallelization of the new PinG model, the temporal profile option and the Gaussian chemistry scheme for traffic air pollutants are also discussed in Section 2. In Section 3, we evaluate this new model with a real-world case study. Results of sensitivities studies, that were conducted in order to validate choices made during the implementation process, are presented in the Section 3 of Supplementary Material.

2. Model description

The Polyphemus modeling platform (Mallet et al., 2007) includes both the Eulerian Polair3D model and the Gaussian model for line sources. These models are described in Sections 2.1 and 2.2, respectively. The coupling of those two models as a PinG model is described in Section 2.3.

2.1. Eulerian model

Polair3D is a 3D Eulerian model that can be applied from the urban scale up to the continental scale (Boutahar et al., 2004). There are several versions of Polair3D: a passive version, a version with gas-phase chemistry and a version with gas-phase chemistry and aerosols. Polair3D performance has been evaluated extensively (e.g., Quélo et al., 2007; Sartelet et al., 2007; Mallet and Sportisse, 2004; Sartelet et al., 2012). In this work, the gas-phase chemistry version is used with the CB05 chemical kinetic mechanism (Yarwood et al., 2005; Kim et al., 2009).

2.2. Gaussian plume model

The Gaussian plume model for line sources has been presented by Briant et al. (2011) and evaluated with passive diffusion tube measurements of nitrogen dioxide (NO_2) concentrations near roadways on a large case study by Briant et al. (2012).

Its formulation of the concentration field for a pollutant emitted from a line source is based on 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 (Yamartino, 2008). Venkatram and Horst (2006) have presented a formulation, 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 Host-Venkatram (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 improve 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.

The evaluation of the model gives satisfactory results (see Section 4 of supplementary material for the definition of the performance metrics): more than 92% of the predictions are within a factor of two of the observations, the relative mean bias is within $\pm$32%, the relative scatter is less than 1.2 and the Polyphemus modeled values are on average within $\pm$32% of the observed concentrations for the case study considered (Briant et al., 2012).

2.3. Coupling of Polair3D and the Gaussian plume model

2.3.1. Overview

As depicted in Fig. 1, a PinG model uses the local model to disperse pollutants from selected sources. When a criterion is reached (criterion based on the elapsed time since the emission or on the size of the plume, for instance), the plume pollutants are transferred to the Eulerian host model, which is running concurrently. Output concentrations at a given location and at a given time t are then the sum of the concentration in the corresponding grid