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Simulating near-road reactive dispersion of gaseous air pollutants using a three-dimensional Eulerian model

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HIGHLIGHTS

- Near-road gaseous pollutants can be well simulated using a 3D Eulerian approach.
- On-road emissions can be estimated by MOVES using a axles-based scheme.
- Confirms that NO2/NOx in the emission is much higher than the default value of 5%
- A higher NO2/NOx ratio will lead to higher predictions of O3 in regional models.

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ABSTRACT

In this study, the TAMNROM-3D model, a 3D Eulerian near-road air quality model with vehicle induced turbulence parameterization and a MOVES based emission preprocessor, is tested using near-road gaseous pollutants data collected near a rural freeway with 34% heavy duty vehicle traffic. Exhaust emissions of gasses from the vehicles are estimated using a lumped vehicle classification scheme based on the number of vehicle axles and the default county-level MOVES vehicle fleet database. The predicted dilution of CO and NO_x in the downwind direction agrees well with observation, although the total NO_x emission has to be scaled to 85% of its original emission rate estimated by the MOVES model. Using the atmospheric turbulent diffusion coefficient parameterization of Degrazia et al. (2000) with variable horizontal turbulent diffusion coefficient (K_{xx}) leads to slightly better predictions than a traditional non-height-dependent K_{xx} parameterization. The NO_2 concentrations can be better predicted when emission of total NO_x is split into NO and NO_2 using the NO_2 to NO_x ratio of 29% measured near the road. Simulations using the SAPRC99 photochemical mechanism do not show significant changes in the predicted NO and NO_2 concentrations near the road compared to simulations using a simple three-reaction mechanism that involves only NO_x and O_3. A regional air quality simulation in Houston, Texas during a high O_3 episode in August 2000 shows that using the NO_2 to NO_x ratio of 29% instead of the traditional 5% leads to as much as 6 ppb increase in 8-h O_3 predictions.

1. Introduction

Elevated concentrations of carbon monoxide (CO), oxides of nitrogen (NO_x) and air toxics are frequently observed in the vicinity of a roadway compared to their background ambient levels (Parrish, 2006). Health studies have indicated an increase in lung and respiratory related diseases (Gauderman et al., 2007; Kim et al., 2004), premature mortality (Finkelstein et al., 2004), and hypertension and cardiac problems (Hoffmann et al., 2006) due to exposure to traffic emissions. Near-road air quality models are necessary to aid air quality monitoring programs to provide required data for traffic planning, congestion mitigation and epidemiology studies of traffic pollution exposure.

Although significant progress has been made in numerical simulations of near-road air pollution, most of the well-accepted near-road models (e.g. CALINE4) are based on steady-state solutions of the atmospheric turbulent dispersion equation. However, in many studies it is demonstrated that vehicle-induced-turbulence (VIT) significantly affects near-road pollutant dispersion (Eskridge and Hunt, 1979; Kota et al., 2010; Sahlodin et al., 2007). VIT is usually treated empirically, for example, using the mixing zone concept (Held et al., 2003; USEPA, 2010b). To overcome this limitation, Rao (2002) formulated ROADWAY-2, a two-dimensional (2D) Eulerian model that treats VIT more realistically. Wang et al. (2011) incorporated VIT into a computational fluid dynamics (CFD) model and demonstrated that it yields better near-road predictions of NO_x than CALINE4, using data collected near urban and rural freeways in Texas. The CFD approach, however, is complex to implement and is extremely computationally intensive due to millions of grid cells used in the solution

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processes. Another potential problem in the near-road modeling is that current near-road models typically use relatively simple atmospheric chemistry that includes mainly NO, NO_2 and O_3. The effect of organic peroxy radicals (RO_2) on NO to NO_2 conversion is either neglected entirely (as in ROADWAY-2) or accounted for using representative RO_2 species from simple VOCs (Wang et al., 2011). However, these simple approaches have not been evaluated against a more complete atmospheric chemical mechanism.

Kota et al. (2010) developed a 3D Eulerian model, the TAMU Near-Road Model (TAMNROM-3D), to simulate near-road dispersion and chemical transformation of pollutants. The TAMNROM-3D model predicts vehicle induced turbulent kinetic energy in each grid cell to determine the magnitude of VIT using a parameterization scheme suggested by Bäumer et al. (2005). This allows it to include more mechanistic treatments of the chemical and physical processes that affect near-road pollutant concentrations. The capability of this model to predict the dispersion of a non-reactive tracer was already evaluated using the SF_6 dataset collected at the General Motor's testing track (Kota et al., 2010). It has been demonstrated that TAMNROM-3D performs better than CALINE4 and ROADWAY-2 on that dataset. However, the ability of the model to simulate dispersion and transformation of reactive air pollutants has not been evaluated.

Emissions from on-road mobile sources are key input parameters to near-road and regional air quality models. The United States Environmental Protection Agency (US EPA) developed the MOBILE model to estimate on-road vehicle emission factors. Recently, US EPA has suggested the replacement of the MOBILE model with the MOVES (Motor Vehicle Emission Simulator) model (USEPA, 2010c). Although there are studies that directly evaluate MOVES emission factors with observed vehicle emission data, indirect evaluation of the MOVES model through near-road air quality modeling using vehicle traffic count data has not been previously reported.

Thus, the aim of this study is to (i) test the feasibility of using MOVES to generate necessary emissions for near-road air quality modeling based on simple traffic count data and (ii) to further evaluate the TAMNROM-3D performance on predicting averaged concentrations of reactive gaseous pollutants collected in the field.

2. Model description

The detailed formulation and solution procedures of the TAMNROM-3D model can be found in Kota et al. (2010) and are not repeated here. In the following sections, the photochemical mechanism, the microphysics modules, and the MOVES based emission preprocessor are described.

2.1. Photochemical mechanism

Unlike other near-road air quality models that use simplified representations of NO to NO_2 conversion in near-road environments (Kenty et al., 2007; Kukkonen et al., 2001; Rao, 2002), the TAMNROM-3D model includes a relatively complete description of atmospheric gas phase chemistry based on the SAPRC-99 photochemical mechanism, which is one of the most widely used photochemical mechanism families for both regulatory and research applications (Carter, 1994; Czader et al., 2008). This is necessary because in real atmosphere peroxy radicals (RO_2 or HO_2) also convert NO to NO_2. In addition, some radicals can react with NO_2 to form relatively stable products, acting as a sink to NO_x. Neglecting or unrealistically treating these processes may lead to errors in NO and NO_2 predictions. The detailed treatment of the gas phase chemistry can be used as a reference to evaluate other simplified gas phase mechanisms of NO to NO_2 conversion in near-road models. Emission and photochemical degradation of several air toxics can also be simulated in the mechanism. The original SAPRC-99 mechanism already treats formaldehyde as an explicit species. In this study, the SAPRC-99 mechanism is enhanced to explicitly simulate five additional air toxics from mobile sources: benzene, 1,3-butadiene, acetaldehyde, acrolein and methyl tertiary butyl ether (MTBE) using the reaction rate coefficients and products designations from Carter (2000). Using a relatively complete chemical mechanism allows the concentrations of OH to be estimated mechanistically, which is essential to model the photochemical decomposition of air toxics. The production of formaldehyde, acetaldehyde and acrolein from other VOCs are also more realistically represented in the model.

2.2. Emission processing using the MOVES model

Emissions from the on-road vehicular traffic for the TAMNROM-3D model are estimated using an emission preprocessing program based on vehicle count data and the MOVES model (version 2010a). The MOVES model uses detailed vehicle classifications based on vehicle uses and fuel types. Since most automatic traffic counters measure vehicle velocity and the number of axles when vehicle make and model information is not directly available, it is convenient to classify vehicles into lumped classes based on the number of axles only. In this study, three lumped vehicle classes are used: Class A (two axles, light duty vehicles), Class B (more than 2 axles, heavy duty vehicles) and Class C (motorcycles). Class A includes passenger cars (MOVES ID: 21), passenger trucks (ID: 31) and light commercial trucks (ID: 32). Class B comprises of refuse trucks (ID: 51), single unit short haul trucks (ID: 52), single unit long haul trucks (ID: 53), combination short haul trucks (ID: 61), combination long haul trucks (ID: 62), motor homes (ID: 54) and busses (ID: 41–43). Vehicle Class B also contains 2-axle commercial trucks with 6 tires, which should belong to Class A based on the number of axles. However, since they are mixed with other vehicle classes in MOVES, it is impossible to separately group them into Class A in the average EF calculations. The potential bias in the emission calculations due to grouping the 2-axle, 6-tire trucks in Class B will be discussed in Section 3.

The emission factors predicted for each MOVES vehicle type and fuel combinations are vehicle population averaged to generate emission factors (EF, g mile^{-1} for moving vehicles and g h^{-1} for parked or idling vehicles) for an average vehicle in these three lumped classes using Eq. (1):

$$EF_j = \frac{\sum_{m=1}^{M_j}\sum_{f=1}^{2}\sum_{y=1}^{N} g_{m,f,y}p_{m,f,y}}{\sum_{m=1}^{M_j}\sum_{f=1}^{2}\sum_{y=1}^{N} p_{m,f,y}} \quad (1)$$

where j is the lumped vehicle class index (A, B or C), M_j is the number of MOVES vehicle classes in a lumped vehicle class j, f is the fuel type (gasoline and diesel) index, y is the vehicle age index, N is the total number of years in a vehicle fleet, p is the number of vehicles, and g is the emission factor (g mile^{-1} for moving vehicles and g h^{-1} for parked or idling vehicles) for a specific vehicle year, fuel and class. The vehicles can also be electric or CNG driven but their numbers are small (zero in the current modeling domain based on the MOVES default database) and thus are not considered in the current study. County specific g and p values are extracted from the MOVES default database. With the population-averaged EFs, the emission rate (E, g s^{-1}) of species i from a lumped vehicle class j at each model grid cell can be calculated using Eq. (2):

$$E_{i,j} = 1609.3 N_j V_j EF_{i,j}/3600 \quad (2)$$

Where N_j and V_j are vehicle density and velocity (mph) in each grid cell, respectively. The coefficients 1609.3 and 3600 convert emission rate to the designated units. Obviously, Eq. (2) can only be applied to moving vehicles. For emissions of parked or idling vehicles, the population averaged parking or idling EFs (in g h^{-1}) are used along with the number of parked/idling vehicles in the grid cell to calculate the emissions.