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Photochemical grid model performance with varying horizontal grid resolution and sub-grid plume treatment for the Martins Creek near-field SO_2 study

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HIGHLIGHTS

- Novel comparison of photochemical grid model SO_2 with near-source measurements.
- Sub-grid plume treatment consistently keeps emitted mass in the upper boundary layer.
- Surface layer SO_2 estimates generally lower than when using sub-grid plume treatment.
- Standard 1 km simulation performed better than 4 km and runs with sub-grid treatment.

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ABSTRACT

Near source modeling is needed to assess primary and secondary pollutant impacts from single sources and single source complexes. Source–receptor relationships need to be resolved from tens of meters to tens of kilometers. Dispersion models are typically applied for near-source primary pollutant impacts but lack complex photochemistry. Photochemical models provide a realistic chemical environment but are typically applied using grid cell sizes that may be larger than the distance between sources and receptors. It is important to understand the impacts of grid resolution and sub-grid plume treatments on photochemical modeling of near-source primary pollution gradients. Here, the CAMx photochemical grid model is applied using multiple grid resolutions and sub-grid plume treatment for SO_2 and compared with a receptor mesonet largely impacted by nearby sources approximately 3–17 km away in a complex terrain environment. Measurements are compared with model estimates of SO_2 at 4- and 1-km resolution, both with and without sub-grid plume treatment and inclusion of finer two-way grid nests. Annual average estimated SO_2 mixing ratios are highest nearest the sources and decrease as distance from the sources increase. In general, CAMx estimates of SO_2 do not compare well with the near-source observations when paired in space and time. Given the proximity of these sources and receptors, accuracy in wind vector estimation is critical for applications that pair pollutant predictions and observations in time and space. In typical permit applications, predictions and observations are not paired in time and space and the entire distributions of each are directly compared. Using this approach, model estimates using 1-km grid resolution best match the distribution of observations and are most comparable to similar studies that used dispersion and Lagrangian modeling systems. Model-estimated SO_2 increases as grid cell size decreases from 4 km to 250 m. However, it is notable that the 1-km model estimates using 1-km meteorological model input are higher than the 1-km model simulation that used interpolated 4-km meteorology. The inclusion of sub-grid plume treatment did not improve model skill in predicting SO_2 in time and space and generally acts to keep emitted mass aloft.

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1. Introduction

Characterizing near-source impacts of primary and secondary pollutants from specific sources or a source complex (e.g. roadway or fire) is increasingly important for multiple Clean Air Act

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regulatory programs including Prevention of Significant Deterioration, New Source Review (U.S. Environmental Protection Agency, 2013), transportation conformity (U.S. Environmental Protection Agency, 2010), and the National Ambient Air Quality Standards (U.S. Environmental Protection Agency, 2007). Photochemical grid models are routinely used to assess changes in primary and secondary pollutants that result from changing emissions to quantify the impacts of State and Federal emissions control programs on ozone and particulate matter with aerodynamic diameter less than 2.5 μm (PM2.5) (U.S. Environmental Protection Agency, 2011a, b). Typical photochemical grid model simulations use horizontal grid resolution between 4 and 12 km to cover domains ranging from urban to continental in scale (Simon et al., 2012). The characterization of near-source pollutant impacts from emission controls are sometimes desirable in addition to quantifying regional impacts. Photochemical grid models have been used to characterize near-field impacts from specific source sectors (Arunachalam et al., 2011; Briant and Seigneur, 2013; Joe et al., 2013) and local to regional impacts from specific sources on PM2.5 (Baker and Foley, 2011) and ozone (Baker and Kelly, 2014; Bergin et al., 2008; Zhou et al., 2012).

Even though near-source pollutant gradients are typically associated with primarily emitted pollutants (Joe et al., 2013), the integration of near-source features of both primary and secondarily formed pollutants estimated regionally is often desirable (Briant and Seigneur, 2013). Secondary impacts from a single source have been shown to be adequately characterized with a photochemical grid model using 4-km resolution (Baker and Kelly, 2014; Zhou et al., 2012). Photochemical models can be used to better represent the nature of sources and receptors in close proximity through the use of smaller-sized grid cells in the area of interest (Joe et al., 2013) or through the use of sub-grid plume treatment and sampling (Briant and Seigneur, 2013; Karamchandani et al., 2009). However, finer-scale model applications do not always translate to model estimates that more closely match observation data (Simon et al., 2012). Emissions inventory resolution and meteorological model skill in replicating fine-scale wind flows both contribute to complicating model performance when smaller-sized grid cells are used.

Photochemical grid model sub-grid scale plume treatment combined with sub-grid scale plume sampling may provide enhanced representation of source and receptors in close proximity. These sub-grid plume treatments are designed to allow in-plume chemical reactions and growth to happen on a different scale than the host photochemical grid model using Gaussian puffs. Once the puffs reach a user-specified time limit or grow to a user-specified proportion of the host model grid cell size, the puff mass is transferred to the grid model. Some implementations include additional criteria for moving puff mass to the grid based on chemical age of the plume (Briant and Seigneur, 2013; ENVIRON, 2013; Korsakissok and Mallet, 2010a,b). Currently, sub-grid implementations do not allow for input of sub-grid meteorology, terrain, or land use information which means physical features that may exist (e.g. more refined terrain features) within a single grid cell are not realized by the sub-grid model.

Typically, the impact of using sub-grid plume treatments on regional model performance metrics is small (Karamchandani et al., 2006; Kim et al., 2014). Sub-grid plume treatment for an inert tracer experiment showed increased near-source vertical diffusion and systematically lower near-source mixing ratios at the surface as a result compared to grid model estimates (Korsakissok and Mallet, 2010b). Mixing ratios of primarily emitted pollutants such as sulfur dioxide (SO_2) and nitrogen oxides (NO_x) have been shown to be more impacted by grid resolution than secondary pollutants such as ozone (Kim et al., 2014; Korsakissok and Mallet, 2010a) and PM2.5 (Karamchandani et al., 2006; Kim et al., 2014). Sub-grid plume treatment may be more important at finer grid resolution (2 km compared with 10 km in this instance) due to greater comparability in-plume concentration with background concentration (Kim et al., 2014). Near-road sub-grid plume applications show mixing ratio gradients that better matched observation gradients than the host model predictions (Briant and Seigneur, 2013; Karamchandani et al., 2009). The application of a photochemical grid model with large eddy simulation (LES) at 1 km and 250 m showed a maximum concentration increase in surface layer primarily emitted PM2.5 at the finer resolution by a factor of 2 (Joe et al., 2013).

Grid-based modeling systems are rarely assessed for near-field skill in estimating pollutant mixing ratios. The impacts of horizontal grid resolution and sub-grid plume treatment on mixing ratios of primary pollutants from single source emissions have not been compared to nearby measurements in a single comparative study. A year-long measurement study near the Martins Creek power plant in New Jersey has been used to evaluate near-field skill of dispersion models such as AERMOD and CALPUFF (Dresser and Huizer, 2011; Perry et al., 2005) in a complex terrain environment. Here, measurements of SO_2 at eight monitors ranging from 3 to 6 km from the Martins Creek power plant and 13 to 17 km from the Portland power plant provide a basis for assessing photochemical model representation of a primarily emitted pollutant using varying grid resolutions and sub-grid plume treatment approaches where sources and receptors are in close proximity and separated by complex terrain features. Model predictions are compared to measurements in two ways: using metrics typical for urban and regional scale photochemical model application paired in time and space (Simon et al., 2012) and using metrics relevant for regulatory dispersion model applications unpaired in time and space (Hanna and Chang, 2012; Perry et al., 2005).

2. Methods

2.1. Meteorological model application

The WRF model version 3.3 (Skamarock et al., 2008) was applied using the Pleim-Xiu land surface model (Pleim and Xiu, 2003; Xiu and Pleim, 2001) and the asymmetric convective model boundary layer scheme (Pleim, 2007a,b) for the entire years of 1992 and 1993. WRF was initialized using the 3-hourly 36-km resolution North American Regional Reanalysis (http://nomads.ncdc.noaa.gov). The model domain covers the continental United States with 36-km sized grid cells, the eastern United States with 12-km sized grid cells, an area covering eastern Pennsylvania and New Jersey with 4-km sized grid cells, and a finer domain covering the sources and monitors with 1-km sized grid cells (Figs. S1a, S1b, S1c). The atmosphere up to 100 mb is resolved with 35 layers. The height of layer 1 is approximately 19 m (Table S1).

2.2. Photochemical model application

The Comprehensive Air Quality Model with extensions (CAMx) version 6.1 (ENVIRON, 2013) was applied from May 1, 1992, to May 19, 1993, to match the period of the measurement-intensive study near Martins Creek. The CAMx simulations matched the vertical and horizontal grid structure of the WRF simulations. CAMx allows for interpolation of coarse grid model inputs to finer two-way nested domains called “flexinests”. This feature, also commonly referred to as “downscaling,” is used to generate 1- and 2-km-sized grid cell nests in the 4-km domain and 250- and 500-m nests in the 1-km domain. Emissions of SO_2 are treated as chemically inert in these CAMx simulations. A sensitivity simulation was performed