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DEVELOPMENT AND APPLICATION OF METHODS TO ESTIMATE THE AIR QUALITY IMPACT OF URBAN EMISSIONS OVER MULTIPLE LENGTH SCALES

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Abstract: We formulate a model to estimate concentrations of NO_2, NO_x, and O_3averaged over a spatial scale of the order of a kilometer in a domain extending over tens of kilometers. The model can be used to estimate hourly concentrations of these species over time periods of years. It achieves the required computational efficiency by separating transport and chemistry using the concept of species age. The model computes concentrations by tracing the history of an air parcel reaching a receptor.This history is traced through back trajectories driven by surface winds. The pollutant is well mixed through the boundary layer, which varies with time and location.Chemical reactions within the parcelaremodeled through the Carbon Bond IV mechanism, which distributes the volatile organic compounds among 8 surrogate species. Evaluation with data measured at 21 stations distributed over the Los Angeles air basin indicates that the model provides an adequate description of the spatial and temporal variation of the concentrations of NO_2, NO_x. Estimates ofmaximum hourly O_3 concentrations show little bias compared to observations, but the scatter is not small.

Key words: *Urban background concentrations, Species age, Los Angles Air basin, Trajectory model, Photochemistry*

INTRODUCTION

The air quality in an urban area is affected by a large number of sources, such as vehicles, distributed over the urban area. Thus, the contribution of sources within meters from an urban receptor might be comparable to that of sources outside the local area of interest. In principle, an air quality model can be used to estimate the contributions of all the urban sources to concentrations at a receptor. However, the large number and variety of sources in an urban area necessitates computational resources that can become impractical even with current computers, especially when it is necessary to conduct sensitivity studies over long averaging times. The current approach to this problem is to use models applicable to several scales so that sources at different distances from the area of interest can be treated with different levels of source aggregation. The concentration at a receptor has three components: a regional contribution computed from a long-range transport model with a grid spacing of the order of tens of kilometers, an urban "background" contribution from sources aggregated over kilometer sized grids, and a local contribution from models that estimate concentrations at meters from a receptor (See Brandt et al., 2003 for an example).

This paper focuses on a model that estimates urban "background" concentrations of NO_x, NO_2, and O_3, averaged over a scale of the order of kilometers. These species can be estimated from photochemical models such as CMAQ (Byun and Schere, 2006) and UCI-CIT model (Carreras et al., 2004), but their application becomes a computational burden if concentrations are required over a year. The simple urban background model (UBM) developed by Berkowicz (2000) addresses this problem through two simplifications: a straight line steady dispersion model, and chemistry based on photostationarity neglecting the role of hydrocarbons. The model presented here is intermediate between comprehensive photochemical models and the simple UBM.It treats unsteady meteorological conditions with trajectories that reflect space and time varying winds, and it reduces the computational requirements of photochemical models by separating transport and chemistry using a method described in Venkatram et al. (1998). The model is evaluated with data from measurements made in Los Angeles.

THE LAGRANGIAN MODEL

The model, based on that proposed by Venkatram and Cimorelli (2007), computes the concentrations at a receptor by following the history of an air parcel that reaches a receptor of interest every hour. The history of the air parcel is traced back 24 hours through back trajectories calculated using surface winds measured at meteorological stations. To facilitate the use of the model, the meteorological inputs are taken directly from the surface input files used by AERMOD (Cimorelli et al., 2005).

The air parcel has horizontal dimensions of 5 km by 5 km, and a height that depends on the local mixed layer height. Emissions are injected into the box and mixed through its volume as the box moves over the urban area, which is described with a gridded emission inventory of NO_x and VOC.The concentrations are stepped from the *(i-1)*th to the i^{th} time step through

$$C_i = C_{i-1} \min\left(\frac{z_{i-1}}{z_i}, 1\right) + \frac{\Delta m_i}{z_i}, \quad (1)$$

where z_i is the mixed layer height. The term within the parenthesis on the right hand side of the equation ensures that the concentration does not increase when the mixed layer decreases during a time step.

The mass of pollutant injected per unit surface area of the air parcel is$\Delta m_i = q_i(\vec{r})\Delta t$,where$q_i(\vec{r})$ is the emission density at the location of the parcel, $\vec{r}$, and Δt is the time step of the trajectory calculation. The incremental concentration during the last hour of the air parcel's path is computed with a steady state dispersion model that accounts for incomplete vertical mixing,

$$\Delta C_i = \sqrt{\frac{2}{\pi}}\frac{q}{\sigma_w}\ln\left(1 + \frac{\sigma_w \Delta t}{h}\right), \quad (2)$$

where$\sigma_w$is the standard deviation of the vertical velocity fluctuations, and *h* is the initial vertical spread of surface emissions. The equation is modified (Venkatram and Cimorelli, 2007) if the pollutant is well mixed through the boundary layer during the last time step before the parcel reaches the receptor.

In addition to concentrations, the model also calculates the effective age of each species in the box (Venkatram et al. 1994, 1998).The effective age of a molecule is the time taken for the molecule to travel from source to receptor. We can build upon this simple idea to formulate a conservation equation for species age that accounts for complex flows and emissions in an Eulerian grid model. This equation allows the calculation of age in addition to concentration of a species at every receptor.
In this simple Lagrangian model, the formulation for the species age, A_i, reduces to

$$A_i = A_{i-1}\left(1 - \frac{\Delta m_i}{m_i}\right) + \Delta t\left(1 - \frac{1}{2}\frac{\Delta m_i}{m_i}\right). \quad (3)$$

In the absence of fresh emissions, that is $\Delta m_i = 0$, we obtain the expected result: $A_i = A_{i-1} + \Delta t$. Note that fresh emissions always decrease the effective age of the species within the parcel.

Then, the chemical transformation of this species is estimated by reacting it with other species in a box with initial concentrations corresponding to those in the absence of chemistry. The time period for chemical calculations is specified by the end time corresponding to the time of interest and a start time, which is the end time minus the species age.The chemical calculation is performed over the maximum of the ages of the species in the air parcel. The chemistry accounts for the variation of photolysis rates with time of day.

The chemistry uses the Carbon Bond IV mechanism in which the volatile organic compounds (VOC) are assumed to be a mixture typical of ambient measurements made in Los Angeles; the VOC is distributed among 8 surrogate species and one inert species.

EVALUATIONOF BACKGROUND MODEL

The model is applied to estimating NO_x, NO_2, and O_3 concentrations in the South Coast Air Basin (SoCAB) of Los Angeles, depicted in Figure 1. The left panel of the figure shows the NO_xemissions developed by Samuelsen et al. (2005) for the SoCAB. The right panel shows the assumed diurnal variation of NO_x emissions, which roughly corresponds to traffic volume. The background ozone is taken to be 20 ppb. In view of the uncertainty in VOC emissions, we do not calculate VOC concentrations in the air parcel, but assume that the VOC concentrations are a constant multiple of thecomputed NO_xconcentrations, which is taken to be 6 in our case. We then add a background VOC concentration of 20ppbC. Such empirical adjustments to the VOC concentrations are not unusual even in comprehensive grid based modeling.
Model estimates are compared with NO_x concentrations measured at 20 monitoring stations operated by CARB, which are numbered in the left panel of Figure 1.

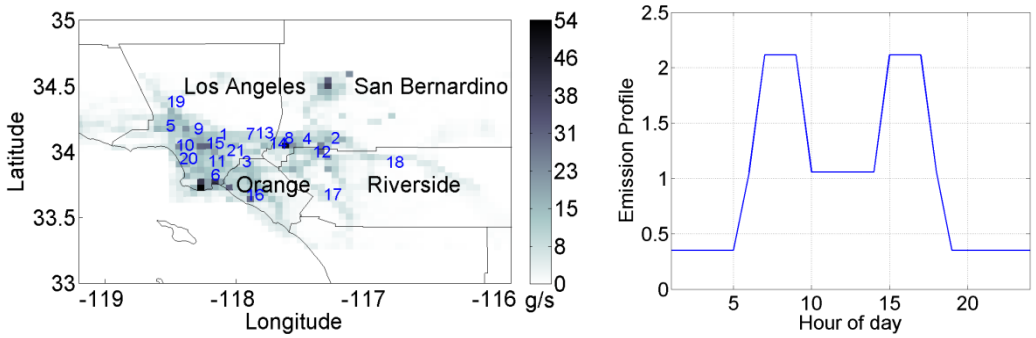

Figure 1.Gridded NO_x emissions and monitoring stations located in the South Coast Air Basin, Los Angeles. The right panel shows the assumed temporal profile of NO_x emissions.

The model was run withsurface meteorological data corresponding to 2007, measured at 26 meteorological stations operated by the South Coast Air Quality Management District. Model performance is described in terms of the geometric mean and standard deviation, m_g, $s_g$of the ratio of the estimated to the observed concentrations(Venkatram et al. 2005). FAC2 refers to the fraction of the model estimates within a factor of two of the corresponding observations.

The performance of the model is illustrated by considering two sites, one on the west and the other located in the east of the Los Angeles basin. The top two panels ofFigure 2 show that the modeled NO_2 and NO_xconcentrations, averaged over a month, are well correlated with the corresponding observations. However, the model overestimates the NO_2 and NO_x during the winter and fall months at the San Bernardino site as seen in Figure 2. The bottom panels compare the modeled and observed maximum daily ozone concentrations at these stations.Although the scatter is not small, the model shows little bias as indicated by$m_g$values close to unity.

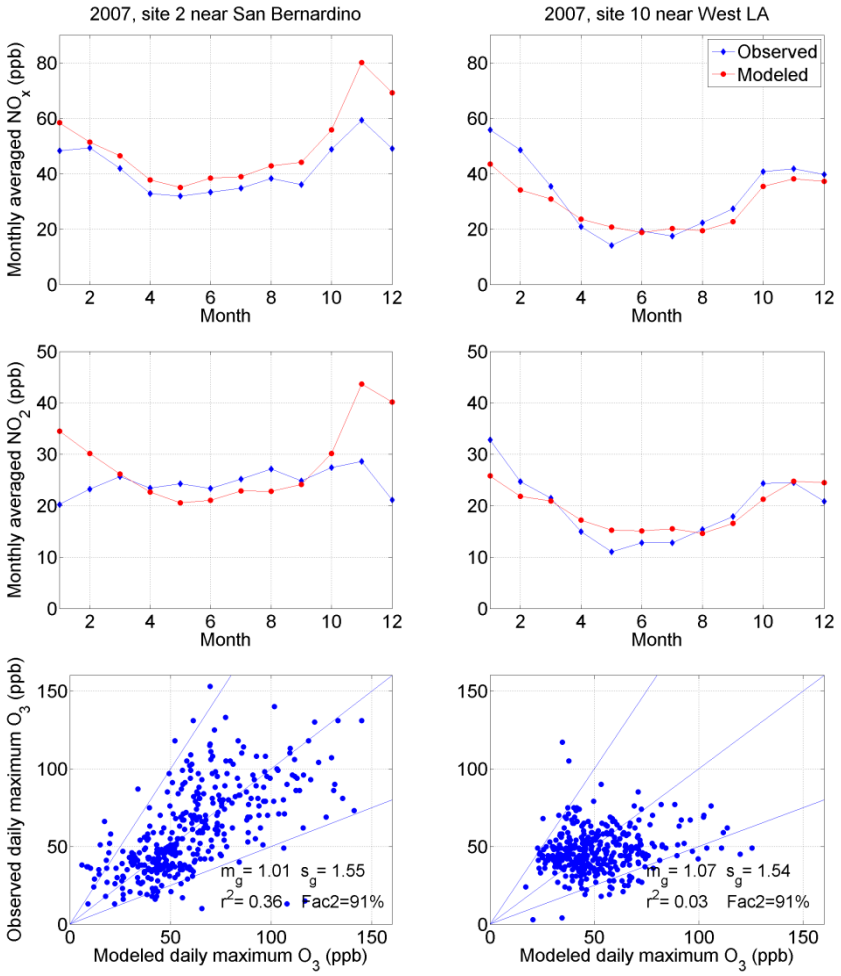

Figure 2. Monthly averaged NO_x, NO_2, and daily maximum ozone concentrations compared with observations at two sites in the SoCAB

Figure 3 shows that the model overestimates NO_2 and NO_x concentrations in the early morning hours at the San Bernardino site. This might be related to the uncertainty in estimating the mixed layer height during these hours. It could also be associated with the assumed temporal profile of NO_x emissions.

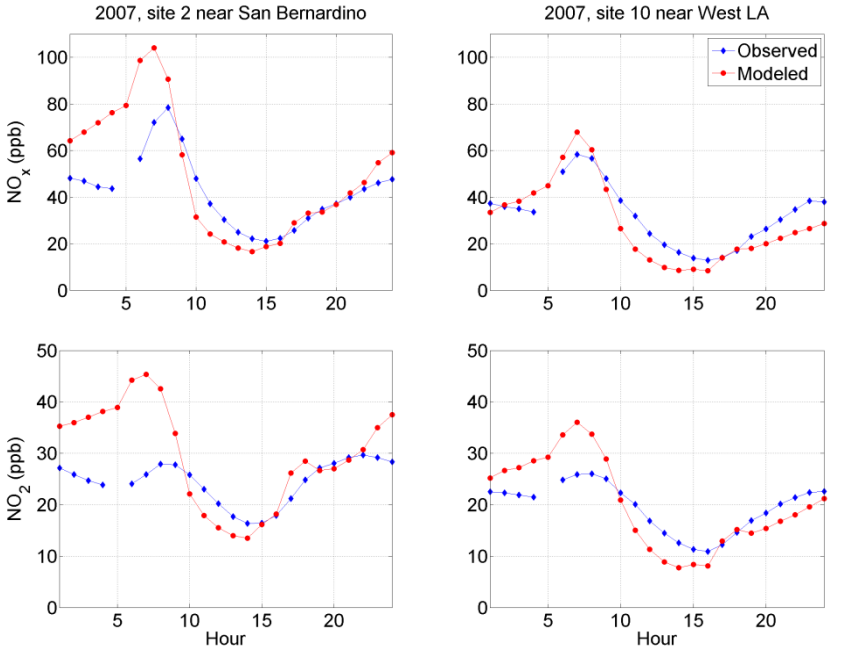

Figure 3. Averaged daily variation of NO_x and NO_2 compared with observations at two sites in the SoCAB.

Figure 4 indicates that the model provides a satisfactory description of the spatial variation of the concentrations of these species across the 21 stations in the SoCAB.

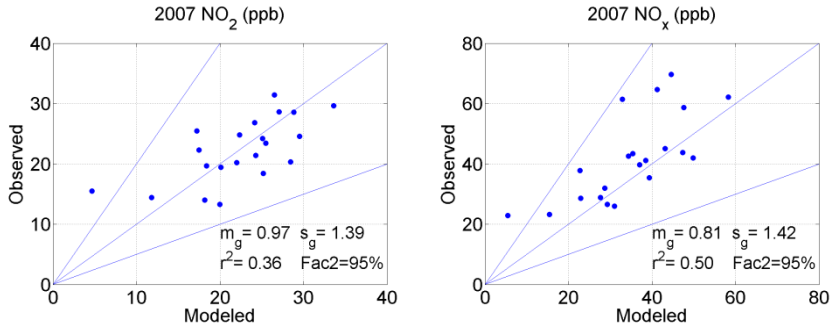

Figure 4. Comparison of modeled and measured annually averaged NO_2 and NO_x concentrations at 21 sites in the SoCAB.

SUMMARY AND CONCLUSIONS

We have formulated a simple Lagrangian model that can be used to estimate background concentrations of NO, NO_2, and O_3 in an urban area. The model can provide hourly concentrations of these species over time periods of a year, which is required in exposure studies. The model achieves its computational efficiency by separating transport and chemistry using the concept of species age.Evaluation with measurements made in SoCAB during 2007, indicates that the model can provides adequate descriptions of the spatial and temporal behavior of NO_x and NO_2.Model estimates of maximum hourly ozone concentrations are unbiased relative to observations but the 95% confidence interval($\approx s_g^2$) of the ratios of observed to estimated concentrations is over a factor of two.

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