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Assessment of Air Quality Impact Associated With Improving Atmospheric Emission Inventories of Mobile and Biogenic Sources

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Photochemical air quality models are essential tools in predicting future air quality and assessing air pollution control strategies. To evaluate air quality using a photochemical air quality model, emission inventories are important inputs to these models. Since most emission inventories are provided at a county-level, these emission inventories need to be geographically allocated to the computational grid cells of the model prior to running the model. The conventional method for the spatial allocation of these emissions uses "spatial surrogate indicators", such as population for mobile source emissions and county area for biogenic source emissions. In order to examine the applicability of such approximations, more detailed spatial surrogate indicators were developed using Geographic Information System(GIS) tools to improve the spatial allocation of mobile and biogenic source emissions. The proposed spatial surrogate indicators appear to be more appropriate than conventional spatial surrogate indicators in allocating mobile and biogenic source emissions. However, they did not provide a substantial improvement in predicting ground-level ozone(O_3) concentrations. As for the carbon monoxide(CO) concentration predictions, certain differences between the conventional and new spatial allocation methods were found, yet a detailed model performance evaluation was prevented due to a lack of sufficient observed data. The use of the developed spatial surrogate indicators led to higher O_3 and CO concentration estimates in the biogenic source emission allocation than in the mobile source emission allocation.

Key words : air pollution control strategies, GIS, photochemical, spatial surrogate

1. Introduction

1.1. Photochemical Air Quality Simulation Models(PAQSMs)

PAQSMs are three-dimensional Eulerian grid-based models considered appropriate in a regulatory context. These models are applied in simulating hourly atmospheric air pollutant concentrations of O_3 and CO in urban or regional areas. The Urban Airshed Model Version IV(UAM-IV)[1] has been utilized in simulating photochemical air pollution dynamics extending from 50x50 to 300x300 km^2 with a grid resolution of 2x2 to 8x8 km^2 horizontally and 50 to 500 m vertically. Along with the UAM-IV, the Regional Oxidant Model Version 2.2 (ROM-2.2)[2] has been applied to regional scale ozone modeling over areas of 1,000x1,000 km^2 or larger with a horizontal grid resolution of approximately 18.5x18.5 km^2. The gross information calculated by the ROM-2.2 has been used to provide boundary and initial conditions for UAM-IV modeling. These models mathematically solve a mass balance through "the species continuity equation" or "atmospheric diffusion equation". The models consider the temporal and spatial variation of pollutants in terms of advection, diffusion, chemical reaction, emissions, and removal processes in the atmosphere. The relationship is expressed in the following equation[3] :

$$\frac{\partial c_i}{\partial t} + \frac{\partial uc_i}{\partial x} + \frac{\partial vc_i}{\partial y} + \frac{\partial wc_i}{\partial z}$$

$$= -\frac{\partial}{\partial x}\left(K_H \frac{\partial c_i}{\partial x} \right) + \frac{\partial}{\partial y}\left(K_H \frac{\partial c_i}{\partial y} \right) + \frac{\partial}{\partial z}\left(K_V \frac{\partial c_i}{\partial z} \right) + R_i + S + L_i$$

Where,

C_i = the concentration of pollutant i that is a function of location(x, y, z) and time (t),

u, v, w = horizontal and vertical wind speed components in x, y, z directions, respectively,

K_H, K_V = horizontal and vertical turbulent diffusion coefficients,

R_i = the net rate of production of pollutant i by chemical reactions,

S = the emission rates of all precursors, P_1, P_2,..., P_p,

L_i = the net rate of removal of pollutant i by surface uptake processes.

PAQSMs employing the above equation require the following five categories of input data :

1. Initial and boundary conditions,
2. Meteorological parameters(mixing height, wind speed and direction, temperature, and solar radiation),
3. Emission inventories(point, area, mobile, and biogenic source emissions),
4. Atmospheric chemical kinetic mechanisms, Carbon Bond Mechanism Version IV(CBM-IV)[4],
5. Topography and surface data(boundary conditions, surface roughness, and deposition factors).

When a PAQSM is applied to the attainment demonstration for air quality standards, a historical ozone or carbon monoxide episode is compared with a base-case simulation. Once the base-case simulation results are evaluated and a prescribed level of accuracy is satisfied, control strategies or future air quality conditions can be simulated using the same meteorological conditions as for the base-case and a projected emission inventory that reflects future changes in emissions.

1.2. Emissions Preprocessing

Most emission inventories are provided in the form of yearly or daily county-level VOC, Nox, and CO emissions. To simulate the hourly photochemistry occurring in grid cells using a PAQSM, the spatial, temporal, and chemical resolutions of the emission inventories have to conform to the resolution of the model. As a result, the emission inventories must be disaggregated into the same temporal and spatial resolutions of the model prior to running the model. In addition, the VOC and NOx in the emission inventories must be chemically speciated according to the chemical mechanism employed by the model.

The chemical mechanism employed in a PAQSM, representing thousands of chemical reactions of organic species in the atmosphere, is a lumped or reduced approach. Because of computer capability limitations, these lumped approaches employ a reduced number of model species to an acceptable degree of accuracy. These approaches include molecular and structural lumping methods. The molecular lumping approach is one in which organic species are grouped into three groups(i.e., alkane, alkene, and aromatics) according to their functional group. Whereas the structural lumping method classifies organic species according to their carbon bond type : carbon single and double, or carbonyl bonds. The Carbon Bond Mechanism Version IV(CBM-IV) utilizes the structural lumping method, including 33 chemical species and 82 chemical reactions. The performances of these chemical mechanisms have already been evaluated through hundreds of environmental chamber experiments.

In order to accurately predict an hourly ozone concentration, PAQSMs require hourly estimates of emissions for each grid cell in the modeling domain. The existing inventory generally contains the annual average or, for the peak ozone season, the daily emission rate. The most accurate approach for the temporal distribution of emissions involves determining emission rates(or activity) for specific sources for each hour of a typical day in the time period being modeled. This approach is sometimes employed for point sources, yet often proves impractical for all but the major sources in the region. More commonly, point source emissions are allocated by hour using the operating schedule information provided in the existing base-year inventory. For area and mobile sources, the emissions modeler usually develops a typical hourly pattern of activity levels for each source category. Ideally, locale-specific temporal information should be collected for all sources that

contribute significantly to the inventory. Regional weekday/weekend activity levels and diurnal variations by source category can be determined through special surveys or estimated using engineering judgement.

To obtain grid-level emissions for photochemical modeling, there are two approaches. One is to directly estimate the emissions in each grid cell. The other uses the grid-level magnitude of a spatial surrogate indicator(e.g., population or land use/land cover). The first approach is mainly applied to point source emissions because the relevant data provide sub-grid level emissions and specific locations. As a result, point source emissions can be simply assigned to the appropriate grid cells, which is the most accurate method for obtaining grid-level emissions. However, the second method is more commonly employed in obtaining grid-level area, mobile, and biogenic source emissions. In this method, the emissions in the grid cells are calculated by multiplying the county-level emissions by the grid fractions of a spatial surrogate indicator. When sub-grid level emissions, like point source emissions, are not available, the use of a spatial surrogate indicator is inevitable. The use of a spatial surrogate indicator assumes that the quantitative spatial distributions of the emissions are similar to those of the selected spatial surrogate indicator. To assure the accuracy of the gridded emissions it is important to choose or develop spatial surrogate indicators that properly represent the emission levels under consideration. The Emissions Preprocessor System Version 2.0 (EPS2.0)[5] and Emission Modeling Systems 1995 version(EMS-95)[6] are the most popular emission preprocessors in use with a PAQSM.

2. Methodology

2.1. Spatial Surrogate Indicators

Population and county-area fractions have been used as the standard spatial surrogate indicators in gridding mobile and biogenic source emissions. The population fraction is defined as the ratio of the population in a grid cell to the county population. The county-area fraction is defined as the ratio of the county-area of the grid cell to the county-area. To obtain computational grid-level emissions for PAQSM modeling, the population or county-area fractions of the grid cells are multiplied by the county-level mobile or biogenic source emissions. However, spatial allocation methodologies employing population and county-area fractions may not be accurate, especially for highway and vegetation emissions. Highways are not necessarily collocated with the residential population concentration and even highway emissions in urban and rural areas tend to have significantly different emission levels. The area of a county does not properly represent the different levels of biogenic emissions from various plant species : Forest and agricultural plants emit distinctively different levels and types of chemicals. Therefore, to estimate a more accurate grid-level emission, more detailed spatial surrogate indicators were developed. For highway emissions, two spatial surrogate indicators were developed, urban and rural highway fractions. For biogenic source emission allocation, six different spatial surrogate indicators were developed corresponding to various categories of emissions, that is, forest, deciduous forest, coniferous, agricultural, grass, and other fractions.

2.2. Geographic Information Systems(GIS) Tools

The development of the new spatial surrogate indicators involved the use of Geographic Information System(GIS) tools. A GIS is a set of computer programs that can produce, store, manipulate, retrieve, and display geographic maps and data[7,8,9]. ArcView and Arc/Info(ESRI, Inc.), from among the commercial GIS software packages, were used to measure, calculate, and display highway distances and areas of land use/land cover. Digital road network data, obtained from the New Jersey Department of Transportation (NJDOT), provided the necessary information for developing the highway spatial surrogate indicators. In addition, New Jersey Integrated Terrain Unit Maps(NJITUM)[10], acquired from the New Jersey Department of Environmental Protection (NJDEP), were used for land use/land cover data. The data were utilized to classify urban and rural areas and obtain necessary land use/land cover information for the development of spatial surro-

gate indicators for biogenic source emissions.

2.3. Modeling Domain

The modeling domain considered in this study included the entire area of New Jersey and parts of its neighboring states(Delaware, Maryland, Pennsylvania and New York). This area covered a 260km by 290km quadrangular area with a 5km by 5km horizontal grid cell size. The Universal Transverse Mercator(UTM) coordinates of this domain were 350km and 4,285km at the southwest and 610km and 4,575 km at the northeast. As suggested in the US EPA's modeling guidelines[11], the modeling domain was set as large as possible as it is much easier to subsequently reduce the size of a modeled area than to increase it. It was also assured that the emissions occurring on the day of interest for each selected episode remained within that domain until 8:00 P.M. on the same day. Plus, the upwind boundaries were located at a sufficient distance to minimize their effects on the model predictions.

2.4. Episode Selection

Since most ozone episodes in the area of concern are associated with predominance of southwesterly flows, i.e. a single meterological regime[12], the following two episodes were selected for this study: (1) July 6 through 8, 1998 and (2) July 18 through 20, 1991. The model simulations typically began at least one day prior to the day of primary interest, in order to minimize the effects of the assumed initial conditions on the predicted concentrations for the primary days. Therefore, the first day of each episode was not considered for the analysis since it was used as an initialization day for modeling purposes.

2.5. Modeling Input Data

The initial and boundary conditions were obtained from the corresponding Regional Oxidant Model(ROM) simulations performed by the US Environmental Protection Agency(EPA). A ROM-UAM interface[2] was implemented to transfer the ROM information at a grid resolution of 18.5km by 18.5km to a UAM-IV grid resolution of 5km by 5km. The wind field inputs to the UAM-IV were obtained through "Diagnostic Wind Model(DWM)[13]" simulations. Spatially varied mixing heights from "the MIXing-height Estimation Methodology for UAM Purpose(MIXEMUP)[14]" algorithm were used in the modeling application. The state emission inventories that were used as the input emissions(point, area, and mobile) were acquired from the relevant state agencies of New Jersey, Maryland, New York, Delaware and Pennsylvania. Since the mobile source emissions from Hunterdon and Cape May counties for 1987 and 1991 episodes were missing from the state inventories, the EPA 1987 and 1991 mobile source emissions for these two counties were extracted by backcasting and projecting the 1990 base emission inventories. The biogenic source emissions for the modeling domain were obtained by using the "Biogenic Emissions Inventory System Version 2 for UAM application(UAM-BEIS2.0)[15]".

3. Results and Discussion

A comparison between the conventional and the newly developed spatial surrogate indicators for gridding volatile organic compounds(VOC) and nitrogen monoxide(NO) emissions was made in Figure 1. The highway VOC emissions gridded with the conventional spatial surrogate indicators are shown in (a) of Figure 1. The highway VOC emissions gridded with the newly developed spatial surrogate indicators are given in (b) of Figure 1. Figure 1 (c) is a plot of the gridded biogenic source NO emission using the conventional spatial allocation method, whereas Figure 1 (d) is a plot of gridded biogenic source NO emission using the newly developed spatial allocation method. When the conventional spatial allocation method was used, a considerable amount of highway emissions was allocated to grid cells with no highways, and the county-level biogenic emissions were evenly assigned to the grid cells within the counties. The highway emissions were more appropriately allocated to grid cells along highways when the newly developed spatial allocation method was used. Accordingly, the newly developed spatial allocation method for biogenic source emissions would appear to be better than the conventional method. The newly developed spatial allocation

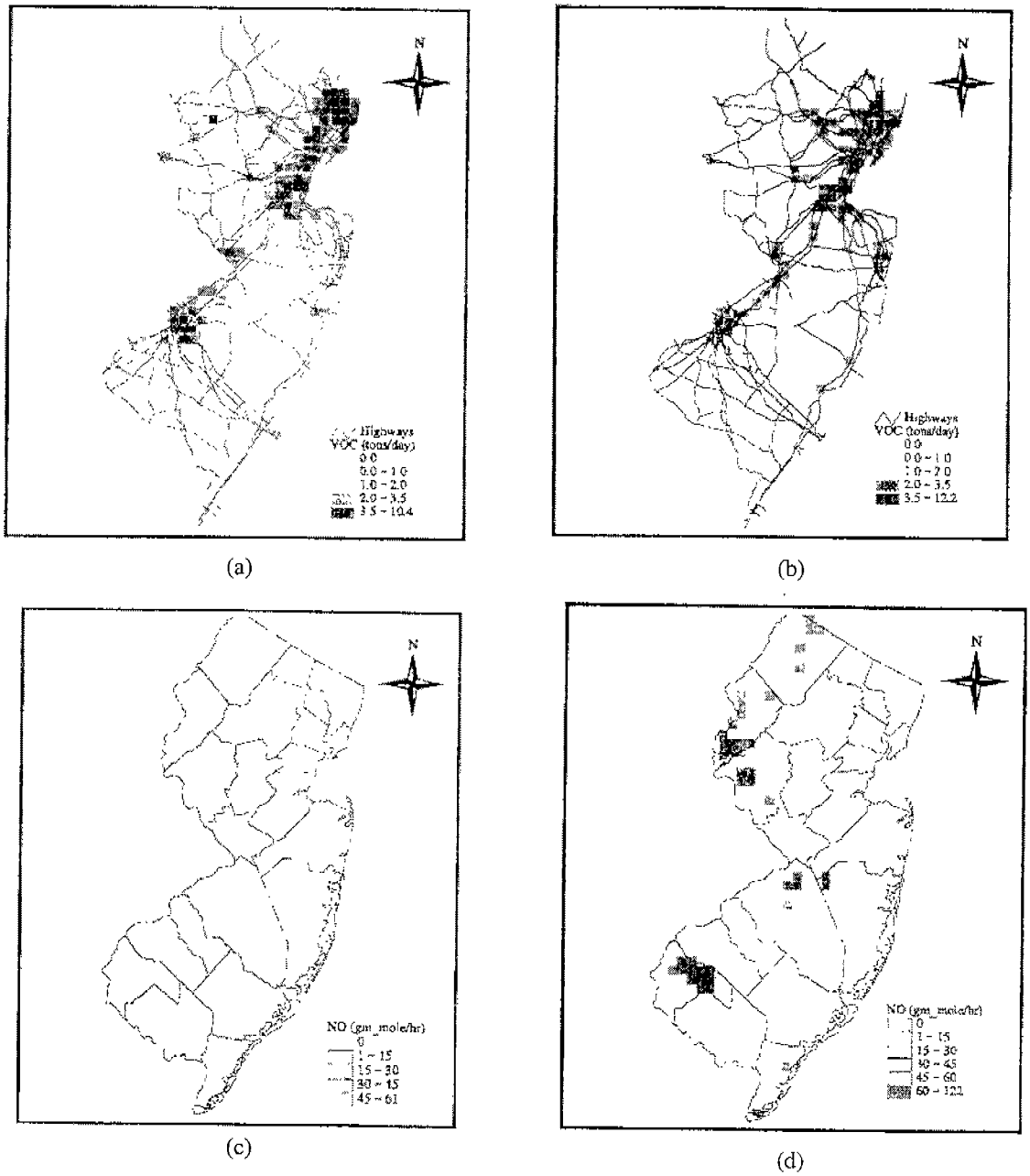
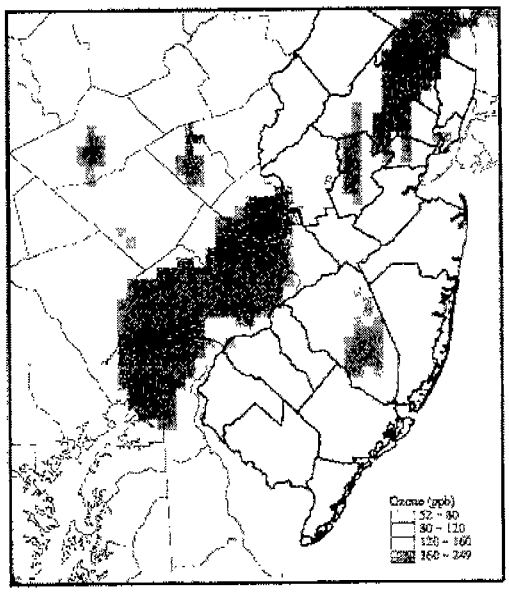


Fig. 1. Comparison of gridded emissions between conventional and newly developed spatial allocation methods : (a) gridded VOC emission of mobile source using conventional method, (b) gridded VOC emission of mobile source with newly developed method, (c) gridded NO emission of biogenic source with conventional method, (d) gridded NO emission of biogenic source newly developed method.

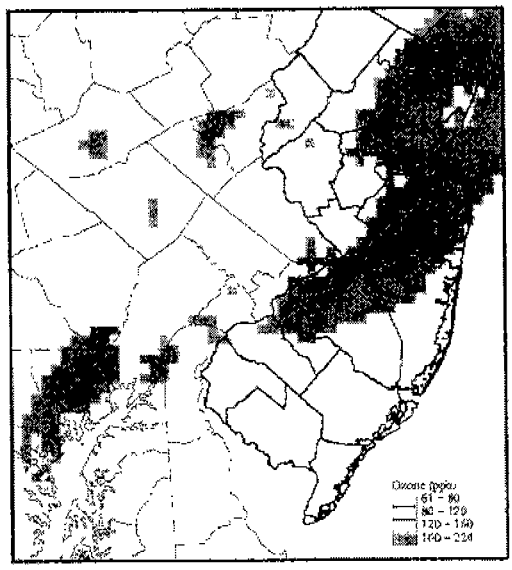
method assigned proportionally higher NO emissions to agricultural areas, which is plausible when considering that agricultural plants emit more NO than any other organisms.

UAM-IV simulations were conducted to obtain base-case ozone and CO concentrations. For the base-case simulations, population fractions were used as the spatial surrogate indicators for the

mobile source emissions and county-area fractions for the biogenic source emissions. Figure 2 shows the estimated daily maximum ozone concentrations for the selected 1988 and 1991 episodes as base-case simulations. Figure 2 indicates that most areas of New Jersey were in non-attainment of the 1-hour averaged ozone standard(120 ppb on July 7 and 8, 1988, and July 19 and 20, 1991). The daily maximum ozone concentrations were predicted at 249 ppb on July 7, 1998, 224 ppb



(a)



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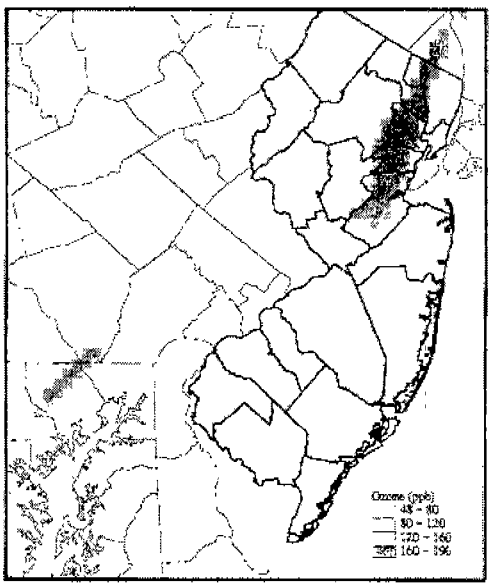

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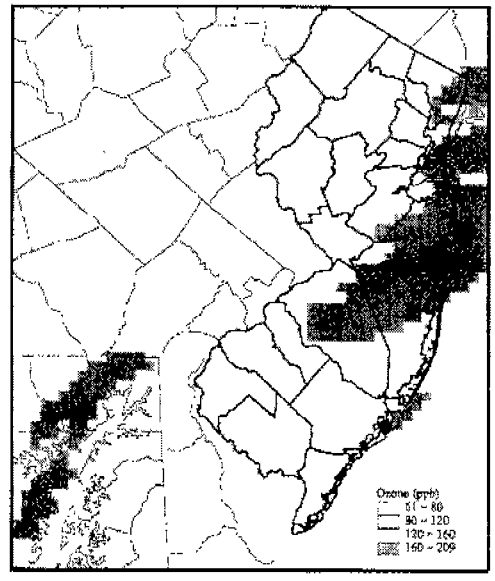


(d)

Fig. 2. UAM-IV daily maximum ozone estimates simulated with conventional spatial allocation method on July 7, 1988 (a), July 8, 1988 (b), July 19, 1991 (c) and July 20, 1991 (d).

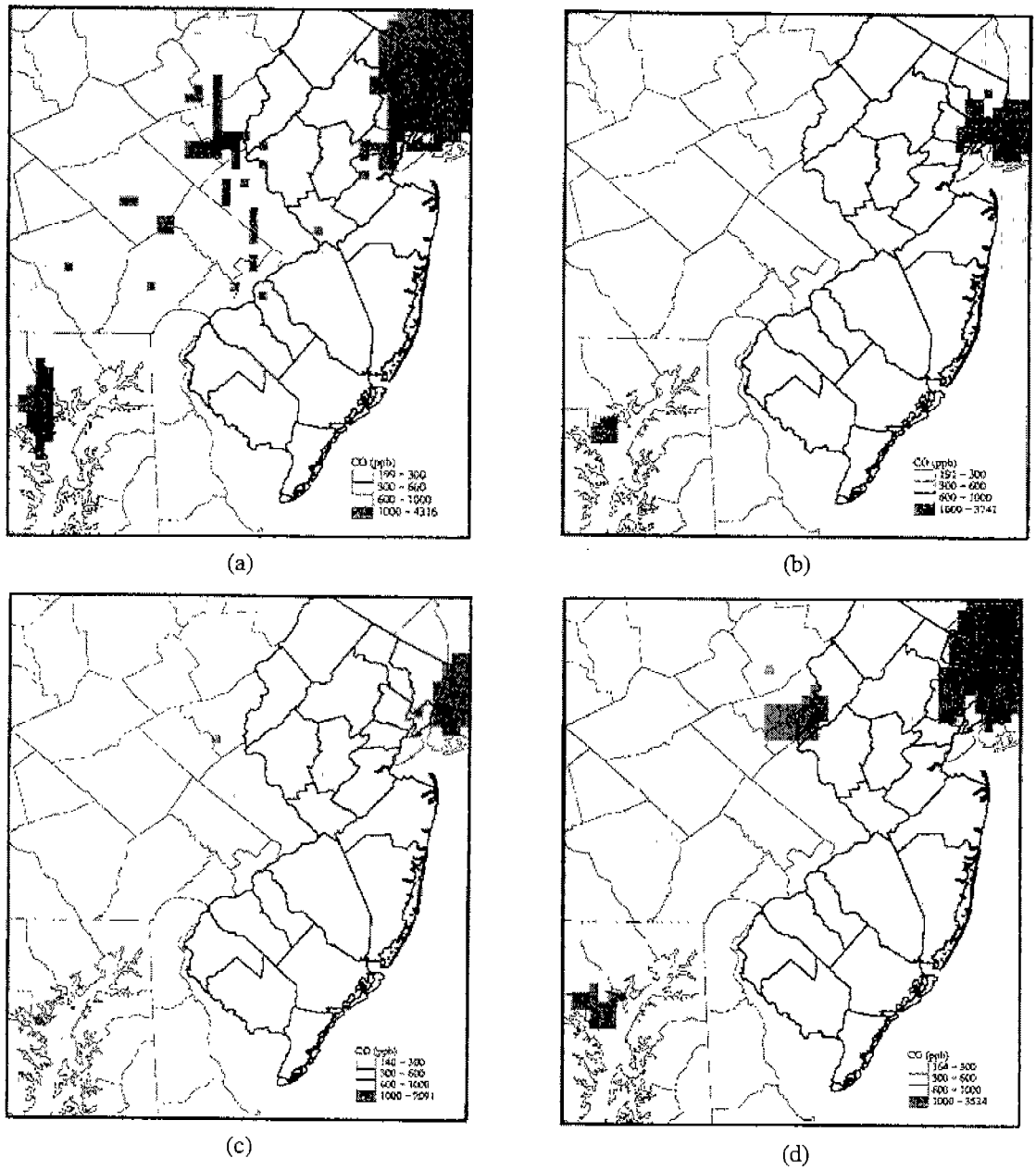


Fig. 3. UAM-IV daily maximum carbon monoxide estimates simulated with conventional spatial allocation method on July 7, 1988 (a), July 8, 1988 (b), July 19, 1991 (c) and July 20, 1991 (d).

on July 8, 1998, 190 ppb on July 19, 1991, and 209 ppb on July 20, 1991, thereby indicating that ozone the concentrations in this modeling domain were somewhat relieved since the implementation of the 1990 Clean Air Act. Figure 3 presents the predicted daily maximum carbon monoxide concentrations for the two selected episodes. As shown in Figure 3, the predicted carbon monoxide concentrations for the selected episodes for the modeling domain were in attainment of the 1-hour NAAQS carbon monoxide standard of 35 ppm(i.e., 35,000 ppb) : the daily maximum CO predictions

were estimated at 4,316 ppb on July 7, 1988, 3,534 ppb on July 8, 1988, 2,091 ppb on July 19, 1991, and 3,741 ppb on July 20, 1991.

Following the base-case simulations, additional UAM-IV simulations for ozone and CO were performed using the newly developed new spatial allocation methods for highway and biogenic emissions. In order to produce a visual estimate of the ozone and CO differences resulting from the use of the conventional and the new spatial

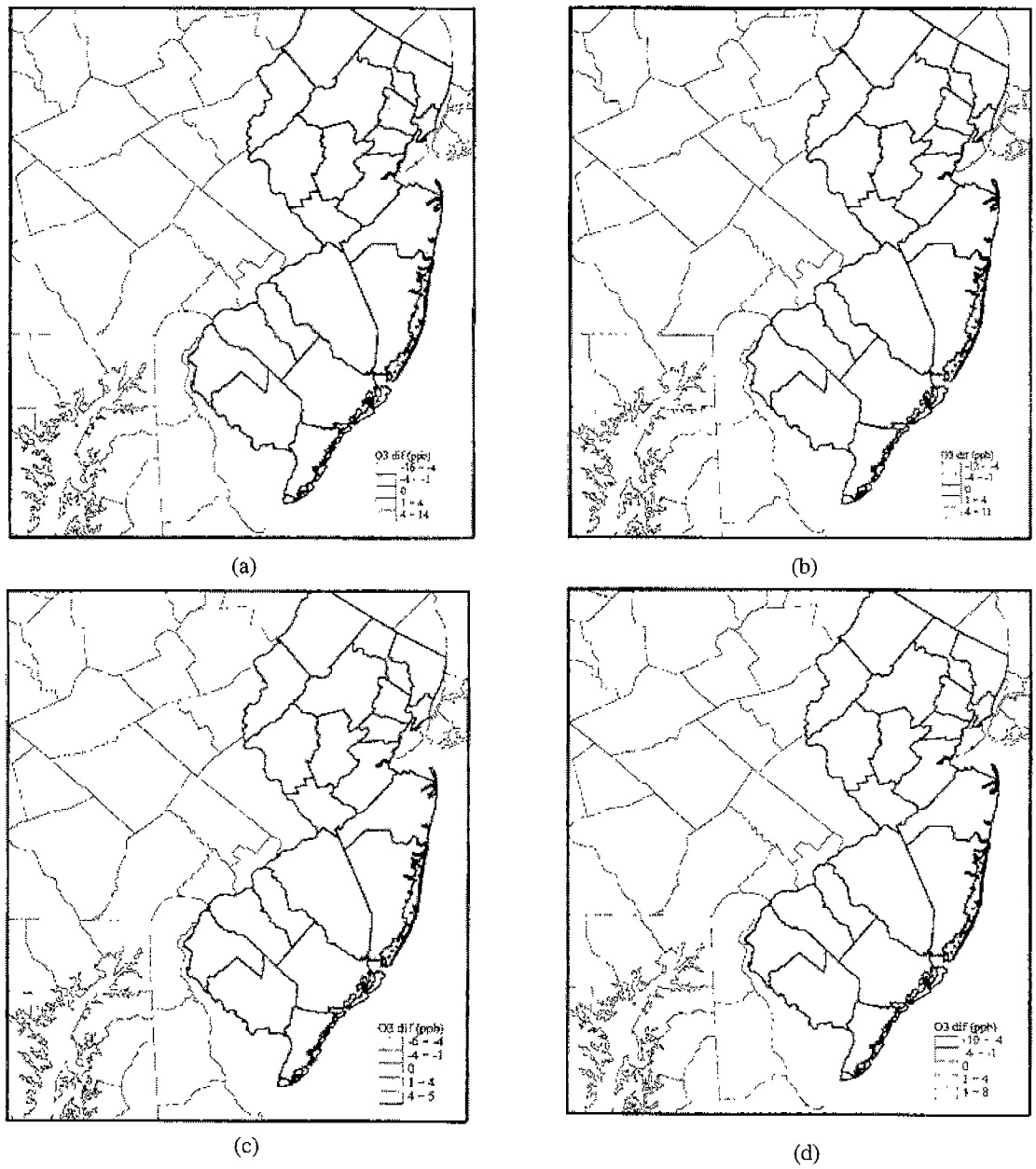


Fig. 4. UAM-IV daily maximum ozone estimate differences between conventional and newly developed spatial allocation methods for mobile source emissions on July 7, 1988 (a), July 8, 1988 (b), July 19, 1991 (c) and July 20, 1991(d).

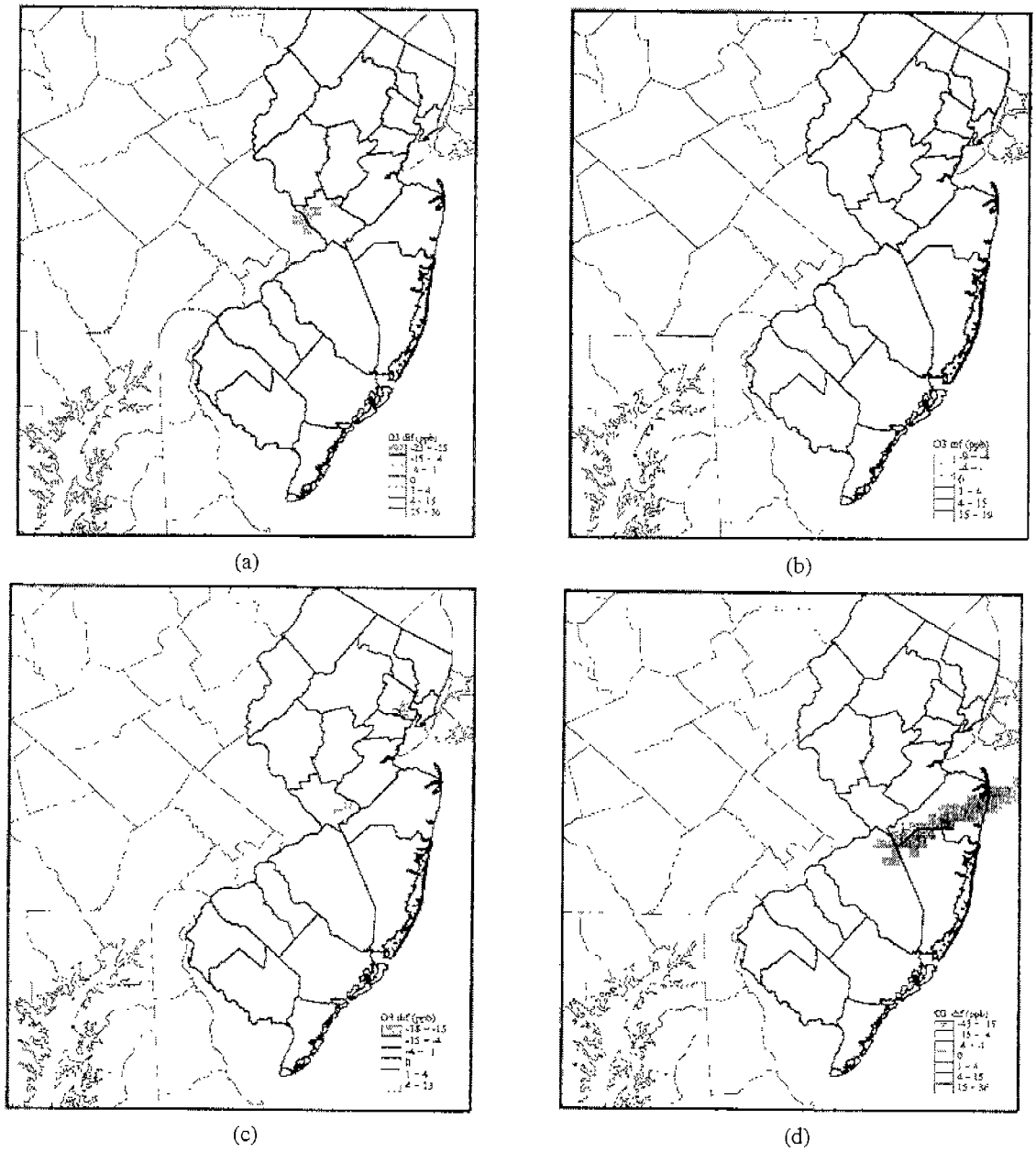
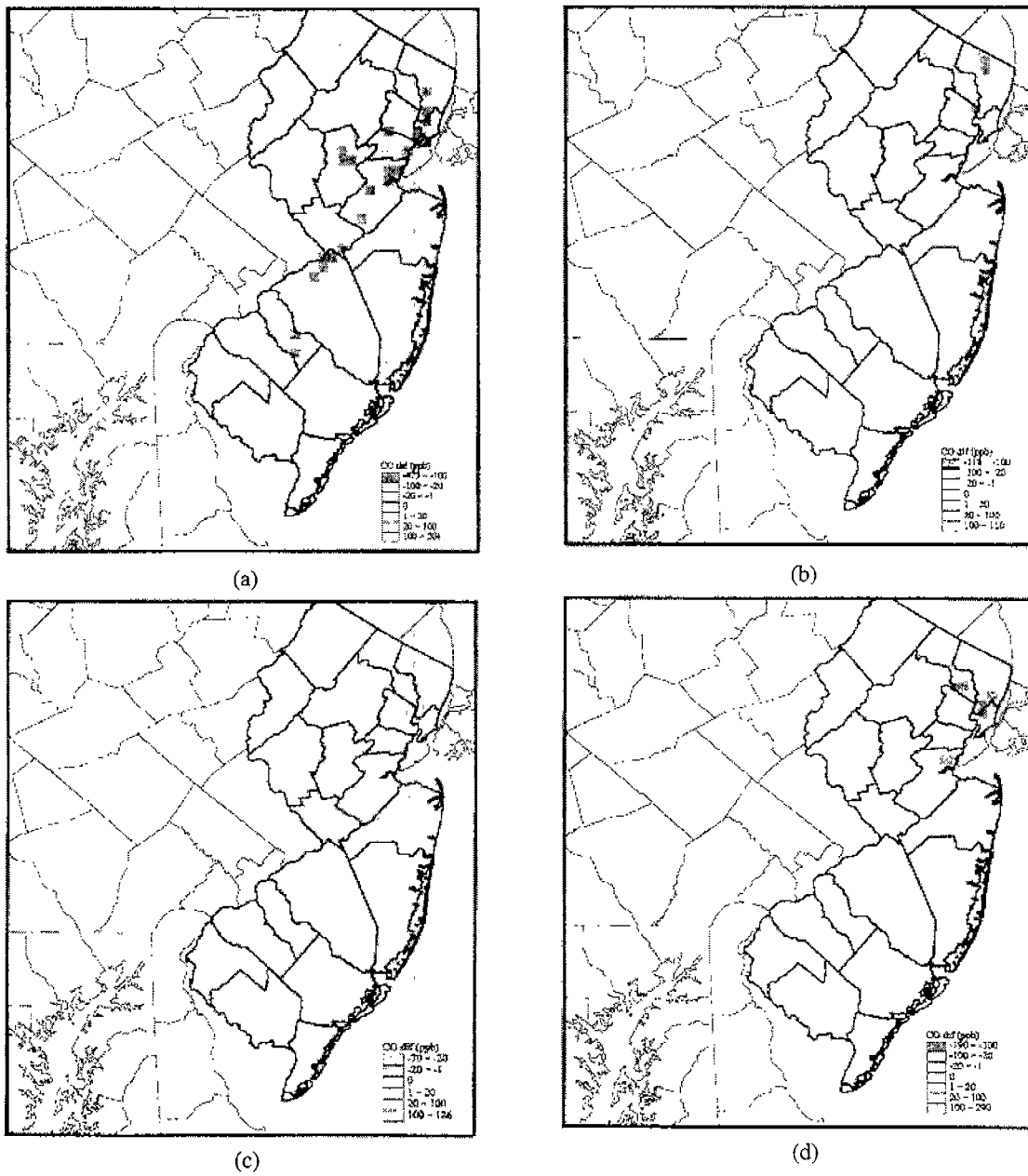


Fig. 5. UAM-IV daily maximum ozone estimate differences between conventional and newly developed spatial allocation methods for biogenic source emissions on July 7, 1988 (a), July 8, 1988 (b), July 19, 1991 (c) and July 20, 1991 (d).

allocation methods, the ozone and CO estimates derived using the new spatial allocation method were subtracted from those derived using the conventional method, that is, the base-case simulation, and then plotted in tile-maps.

The calculated daily maximum ozone differences between the simulations using the conventional and the newly developed spatial allocation methods for highway emissions for July 8, 1988 (a), July 9, 1988 (b), July 19, 1991 (c), and July 20, 1991

(d) are shown in Figure 4. Plus, the daily maximum ozone differences resulting from using the two spatial allocation methods for biogenic emissions for July 8, 1988 (a), July 9, 1988 (b), July 19, 1991 (c), and July 20, 1991 (d) are presented in Figure 5. The purpose of these simulations was to determine how the ozone estimates derived using the new spatial allocation method differed from those of the base-case simulation for both mobile and biogenic emissions.



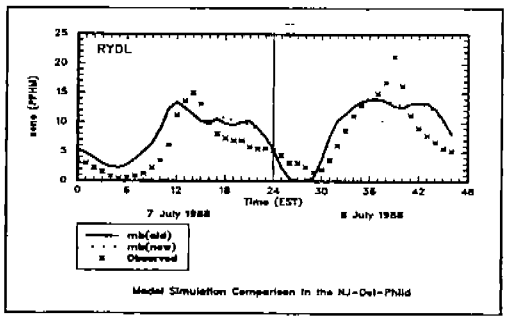
(a) (b) (c) (d)

Fig. 6. UAM-IV daily maximum carbon monoxide estimate differences between conventional and newly developed spatial allocation methods for mobile source emissions on July 7, 1988 (a), July 8, 1988 (b), July 19, 1991 (c) and July 20, 1991 (d).

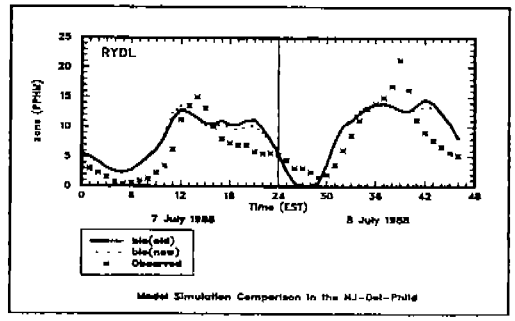
When the effects of the spatial allocation methods on the ozone estimates were examined, it appeared that the results from the simulations using the new spatial allocation method for highway emissions did not differ substantially from those calculated using the conventional allocation method. In contrast, the use of the new spatial allocation method for biogenic emissions caused higher differences in the ozone estimates.

The ambient daily maximum CO concentrations estimated for the modeling domain using the two spatial allocation methods are presented in Figure 6. This figure shows differences between the conventional and newly developed spatial allocation methods in the UAM-IV estimated daily maximum CO in the mobile source emissions on July 9, 1988 (a), July 9, 1988 (b), July 19, 1991 (c), and July 20, 1991 (d). Accordingly, the use of the newly developed spatial allocation method for highway emissions resulted in higher differences from the base-case for CO concentration estimates than for ozone. The maximum absolute differences for ozone were 16 ppb for the 1988 episodes and 10 ppb for the 1991 episodes, whereas the maximum absolute differences for CO were 304 ppb for the 1988 episodes and 290 ppb for the 1991 episodes.

Figure 7 presents a time series comparison of the daily maximum ozone concentration estimates based on the conventional and developed spatial allocation methods for (a) the mobile and (b) the biogenic source emissions for the 1988 episodes at the Ryders Land monitoring station. In Figure 7, three ozone estimates were plotted : (1) the ozone estimate based on the conventional spatial allocation method, (2) ozone estimates based on



(a)



(b)

Fig. 7. UAM-IV hourly ozone simulation comparison between conventional and newly developed spatial allocation methods for (a) mobile and (b) biogenic source emissions at the Ryders Lane ozone monitoring station.

the newly developed spatial allocation method, and (3) observed ozone concentrations at the Ryders Lane monitoring station. The result shows that while the newly developed spatial allocation method provided no significant difference when compared with the conventional spatial allocation method for mobile source emissions, for biogenic source emissions, the newly developed spatial allocation method produced ozone estimates that were slightly closer to the observed values.

4. Conclusions

The new spatial allocation method was expected to be more accurate than the conventional method for both mobile and biogenic source emissions. Although, the ozone estimates were not substantially affected by the use of the new method, small changes were produced in model performance for the biogenic source emissions. The CO estimates also appeared relatively insensitive to the spatial allocation method. The findings obtained from this study can be summarized as follows :

1) The use of the new spatial allocation method for highway emissions appears to be more physically plausible than the conventional spatial allocation method,

2) The use of the new spatial allocation method for biogenic emissions also appears to be more physically consistent than the conventional spatial allocation method,

3) The calculated ozone concentrations appeared to be more sensitive to the biogenic emission allocation method than to the highway emission allocation method,

4) The use of the new method for highway and biogenic source emission allocation exhibited considerable localized differences in the assessment of the atmospheric ozone and CO concentrations,

5) The percentage differences in the calculated ozone and CO ground-level concentrations resulting from the use of the two different methods for spatial highway allocation ranged from 1.5 to 6.4% and from 3.7 to 11% for the five summer days of 1988 and 1991 considered in this study, respectively. The corresponding differences resulting from the use of the different spatial allocation methods for biogenic emissions in calculating ozone were within the range of 8.4 to 20.6%,

6) The above results suggest that the spatial allocation method has a relatively small impact on the overall photochemical model results. However, it should be noted that the new, refined, allocation method was only applied to emissions within New Jersey, which, in reality, is just part of a large regional airshed and thus significantly affected by regional transport. It is expected that the refined allocation of emissions over a regional domain would have a far more significant impact on the calculated air quality.

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