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Resolving Neighborhood Scale in Air Toxics Modeling: A Case Study in Wilmington, CA

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ABSTRACT

Air quality modeling is useful for characterizing exposures to air pollutants. Whereas models typically provide results on regional scales, new concerns regarding the potential for differential exposures among racial/ethnic populations and income strata within communities are driving the need for increasingly refined modeling approaches. These approaches need to be capable of resolving concentrations on the scale of tens of meters, across modeling domains 10–100 km^2 in size. One approach for refined air quality modeling is to combine Gaussian and regional photochemical grid models. In this paper, the authors demonstrate this approach on a case study of Wilmington, CA, focused on diesel exhaust particulate matter. Modeling results suggest that pollutant concentrations in the vicinity of emission sources are elevated, and, therefore, an understanding of local emission sources is necessary to generate credible modeling results. A probabilistic evaluation of the Gaussian model application indicated that spatial allocation, emission rates, and meteorological data are important contributors to input and parameter uncertainty in the model results. This uncertainty can be substantially reduced through the collection and integration of site-specific information about the location of emission sources and the activity and emission rates of key sources affecting model concentrations.

IMPLICATIONS

This paper describes a refined approach to resolve fine-scale in air quality modeling applications. Resolving neighborhood scale is critical for evaluating whether differential exposures among ethnically or economically stratified subpopulations in an urban area are occurring. This paper addresses the impact of uncertainty in model inputs and parameters on air quality assessments through a case study of diesel exhaust particulate matter in Wilmington, CA. This uncertainty can be substantially reduced through the collection and integration of site-specific information about the location of emission sources and the activity and emission rates of key sources affecting model concentrations.

INTRODUCTION

Refined air quality modeling approaches are necessary for evaluating whether differential exposures among ethnically or economically stratified subpopulations in an urban area are occurring. These modeling approaches must be capable of resolving air pollutant concentration gradients on 10–100-m spatial scales, such as urban blocks, across large modeling domains. One approach for generating refined modeling results is to combine regional photochemical grid and Gaussian model results.[1] Modeling on refined spatial scales poses special problems, because Gaussian model results are heavily dependent on the spatial allocation and rate of emissions,[2-4] which are often limited in their availability and/or detail. In addition, the air quality model must account for special features of dispersion within the urban canopy. This paper addresses the impact of uncertainty in model inputs and parameters on refined air quality assessments through a case study of diesel exhaust coarse particulate matter (DPM) in Wilmington, CA. This work follows a technical approach similar to that used earlier by Sax and Isakov.[4] However, it goes beyond the earlier work by: (1) addressing a pollutant emitted from both stationary and mobile sources (Sax and Isakov[4] addressed hexavalent chromium, which is emitted primarily from stationary sources), (2) analyzing a larger area (6 km × 4 km vs. 3.5 km × 2.5 km), and (3) investigating various levels of detail in the model inputs. Although new models have been developed to account for urban building effects on dispersion,[5–7] this paper focuses on the uncertainties introduced by errors in model inputs corresponding to Industrial Source Complex Short Term model (ISCST3), which is the model that is most commonly used in air toxics applications.

The community of Wilmington has been the focus of intensive study through several programs of the California Air Resources Board (CARB)[8,9]; as a result, it provides a useful platform to analyze refined modeling techniques. The community of Wilmington contains a diverse array of emissions sources, including petroleum refineries, heavily traveled freeways, distribution centers, and local businesses, all located in close proximity to or interspersed with residential and mixed-use development. DPM was chosen for this analysis, because it is thought to be responsible for the majority of air toxics cancer health risk because of air pollution in Southern California[10] and is ubiquitously emitted from a

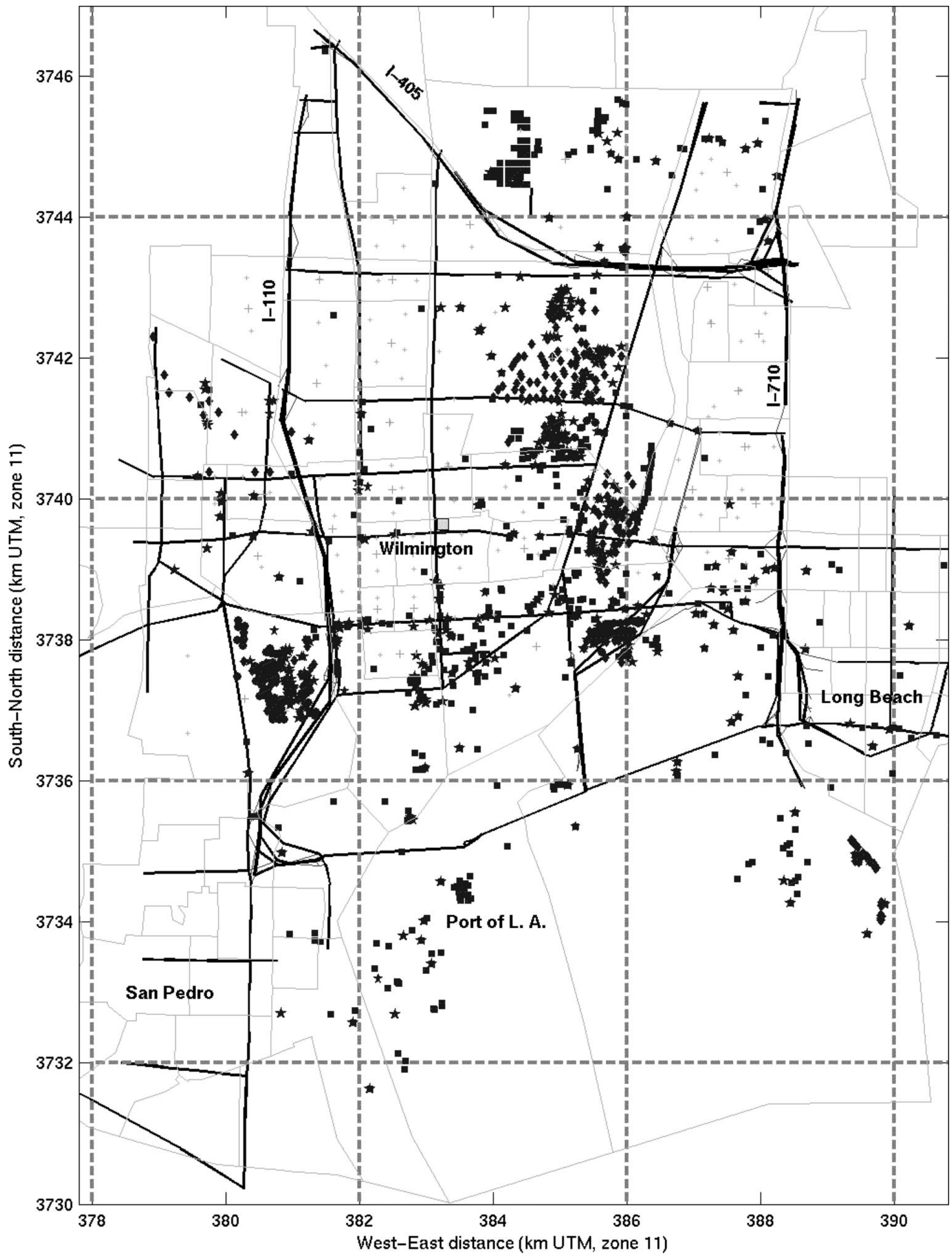

Figure 1. Schematic map of the modeling domain. Mobile sources (road links), black lines; stationary sources, stars (stacks) and squares (volume sources); and census tracts, gray polygons; regional modeling 4-km × 4-km grid, dashed lines.

wide variety of stationary and mobile sources that were assessed through CARB studies. The Wilmington modeling domain is shown in Figure 1. In this figure, mobile sources (road links) are shown as black lines, and stationary sources are shown as symbols. Census tracts are also shown in the figure as gray polygons.

MODELING CONCENTRATIONS AT THE NEIGHBORHOOD SCALE

Air quality in a neighborhood of a large city is governed by local emissions, as well as by transport and transformation of air pollutants into the region from the surrounding areas. This analysis uses a combination of microscale and regional-scale models to estimate air pollutant concentrations on refined spatial scales. The ISCST3 dispersion model was used to simulate ambient average concentrations on a local scale. CALGRID, a regional scale photochemical regional model,[11] was used to estimate the impact of the surrounding area. A 4-km × 4-km model grid, shown in Figure 1 (indicated as gray dashed lines), was used in the CALGRID simulations. The entire grid covers the area of 230,000 km^2 in Southern California, including Los Angeles and San Diego.

To obtain an estimate of the impact of the surroundings areas on Wilmington for DPM concentrations, two annual simulations with CALGRID have been conducted.[12] First, all of the emissions, including the Wilmington area, were created for the 4-km × 4-km grid. The second

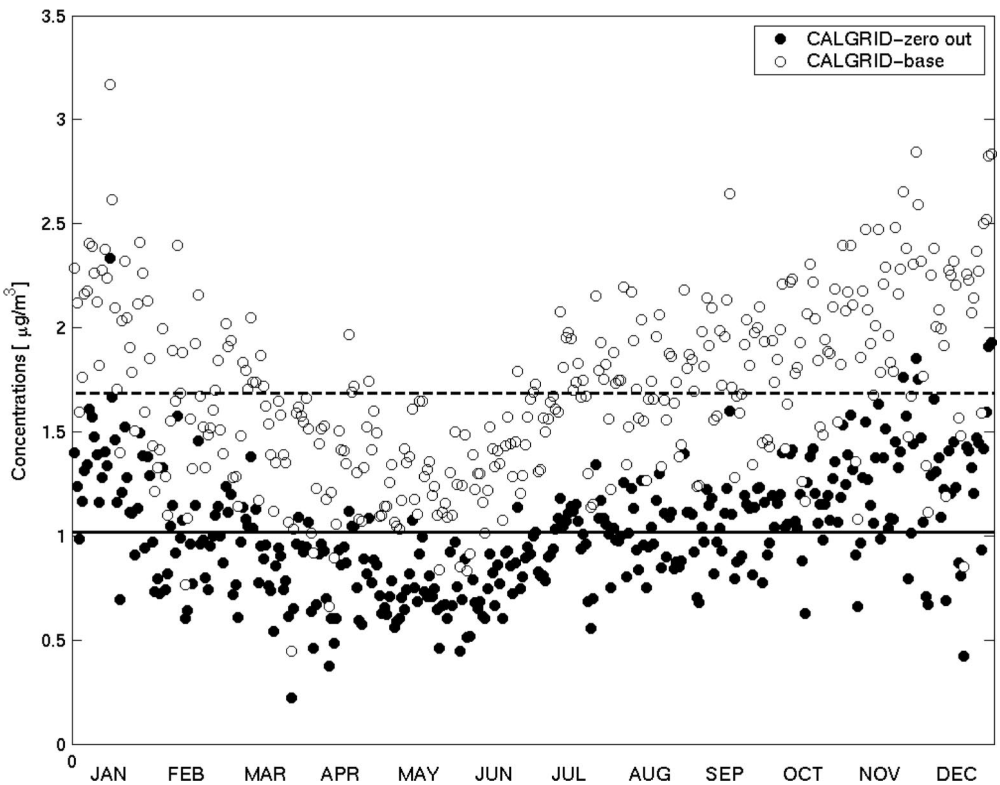

Figure 2. Time series of 24-hr modeled concentrations (μg/m^3) from CALGRID representing a regional background of DPM in Wilmington. Results from two annual simulations are presented: (1) "base," using all the emissions, including the Wilmington area; (2) "zero out" excluded emissions from those grid cells in the modeling domain that defined the communities of interest. Dashed lines and solid lines represent annual averages of hourly modeled concentrations.

simulation excluded emissions from those grid cells in the modeling domain that defined the communities of interest. The details of this zero-out modeling approach, a description of the emissions inventory, and specific steps used to generate gridded emissions for CALGRID are given by CARB.[12] The results from the two simulations at the Wilmington grid square, shown in Figure 2, show that the regional background, on an annual average basis, is comparable to the impacts from sources of DPM in Wilmington. This stresses the need to account for regional inflows in estimating the concentrations within a neighborhood. A similar conclusion was obtained with a different modeling approach by Seigneur et al.[13]

The authors next examined the impact of local DPM sources at the neighborhood scale. Several different input databases are modeled to analyze how the level of detail in model inputs could affect model results. They used ISCST3 to model three scenarios: scenario A used readily available statewide emission inventory and meteorological databases; scenario B used the best available information based on local data; and scenario C was the same as scenario B but enhanced by the best available information on mobile sources. Scenario A includes emissions from point sources available from a statewide emission inventory.[14] The database contains information on stationary sources that are required to routinely report criteria and toxic emissions inventories to regulatory authorities. Meteorological data were obtained from the nearest National Weather Service (NWS) site to the modeling domain, located in Long Beach, CA. The model results are shown in Figure 3. The figure reveals high gradients of ground-level DPM concentrations close to emissions sources.

For scenario B, ISCST3 model inputs were refined by using several on-site data sources developed specifically for the Wilmington Air Quality Study.[15] DPM emissions were included representing stationary, on-road, and off-road sources at industrial and commercial facilities that were developed by CARB using on-site surveys.[16] For this scenario, on-site surface meteorological data collected by CARB in 2001 were also used. Regional background concentration estimates from CALGRID were added to concentration estimates corresponding to scenarios A and B.

The differences in modeled concentrations using locally derived emissions and the base case (scenario A) are shown in Figure 4. Figure 4a shows the difference between results from the two scenarios A and B. The spatial pattern of concentrations from scenario B is very different from that of scenario A, with many more hotspots appearing in the simulation with refined emissions estimates. This suggests that modeling with well-developed and spatially resolved emissions estimates is critical for ensuring that pollutant gradients on a refined scale are credible.

A critical issue for refined scale air quality modeling is mobile sources. A number of studies have identified elevated concentrations[17-19] near freeways and traffic. Unfortunately, emissions inventories for mobile sources are most often calculated on coarse spatial scales that were not included for Gaussian modeling applications. In this study, DPM was allocated to individual roadway locations (roadway links) using the Southern California Association

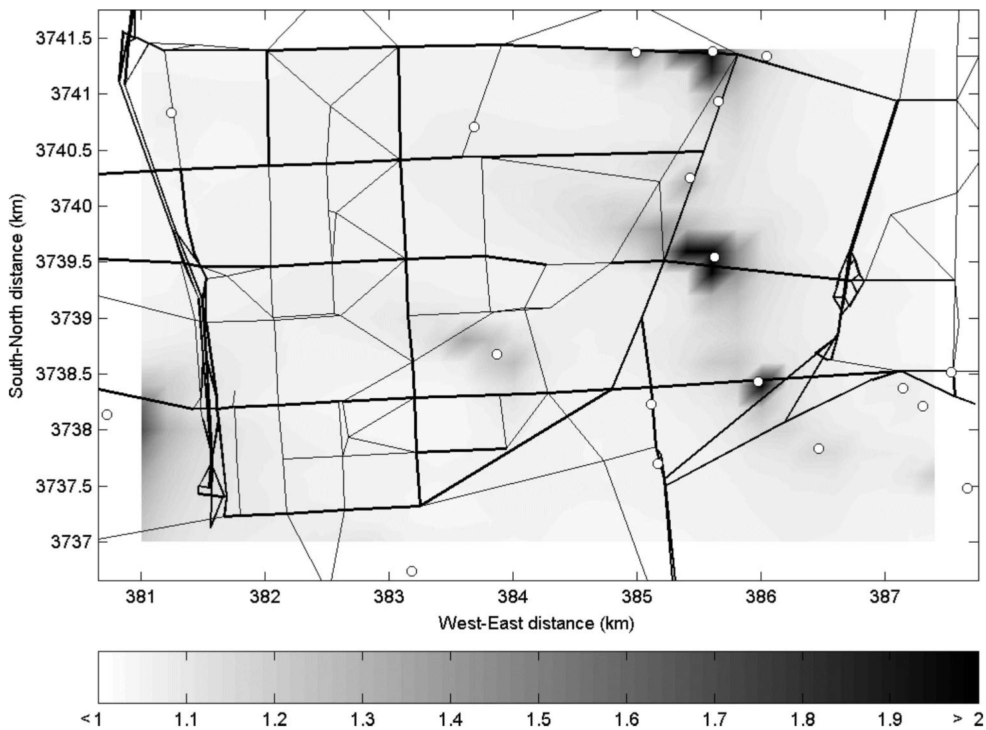

Figure 3. Modeled concentrations (μg/m^3) of DPM in Wilmington based on readily available emissions from a statewide inventory (scenario A). Roads, black lines; stationary sources, white circles.

of Governments (SCAG) travel demand model (TDM) and default fleet average emission factors developed using the EMFAC2002 model.[20] Emissions from on-road mobile sources were modeled using ISCST3 by treating individual links as area sources.[21] Figure 4b displays the difference between results generated using local stationary and mobile sources (scenario C) and those from scenario A. Again, the spatial pattern of concentrations from scenario C is very different from that of scenario A. A map of modeled concentrations corresponding to scenario C is shown in Figure 5. The figure displays the stationary sources as dots and roadway sources as lines in the modeling domain. Results demonstrate steep gradients of concentrations near major roads and significant stationary sources. Concentrations exceed 1.5 μg/m^3 close to sources and decrease close to a regional background of 1 μg/m^3 at nonimpacted receptors. Results suggest that the regional background and local sources are both significant factors impacting a community.

UNCERTAINTY ANALYSIS

The significance of the differences among the three scenarios can be understood by conducting an uncertainty analysis. To conduct this analysis the authors followed a methodology developed previously.[4] This analysis consists of conducting simulations in which the model inputs are varied through ranges that are indicative of their uncertainty. This analysis generates an ensemble of possible model estimates; each receptor is associated with a distribution of concentrations rather than a single value. Model estimates from the three scenarios considered earlier can be placed within these distributions to determine the probability that they will be exceeded by other equally plausible model estimates. If it is assumed that the distribution of model estimates is similar to that of observed concentrations, one can estimate the probability that the model estimate will be exceeded by observed values at the receptor of interest.

The uncertainty analysis was conducted by classifying the model inputs into categories: emission rates, spatial allocation of emissions, temporal allocation of emissions, emissions release parameters, and meteorology.[4] Uncertainty in each component was assessed and expressed as a percentage relative to a base case, which is defined as the emissions from a statewide inventory, temporal allocation, spatial location, and release parameters, as well as on-site meteorology.[4] The uncertainty in each component was propagated using an additive Monte Carlo statistical metamodel,[22] and the results were summarized for each receptor of interest. Eight receptors were chosen for the uncertainty analysis. Each of the receptors is represented in Figure 5 as a box and numbered from 1 to 8. The receptors represent main characteristic locations in the community, they were chosen based on their proximity to stationary and mobile sources, and several represent schools in the community. Receptor 1 represents the area impacted by industrial sources and a major highway; receptor 2, major highway; receptor 3, residential area impacted by industry; receptor 4, residential area; receptor 5, industrial area close to stationary source; and receptors 6–8 are sensitive receptors (schools).

Input Data Uncertainty: Emissions From Industrial and Commercial Facilities

There are >400 toxics emitting facilities in the Wilmington Air Quality Study modeling domain. A detailed emissions inventory has been developed in Wilmington using multiple local, state, and federal inventory databases, plus

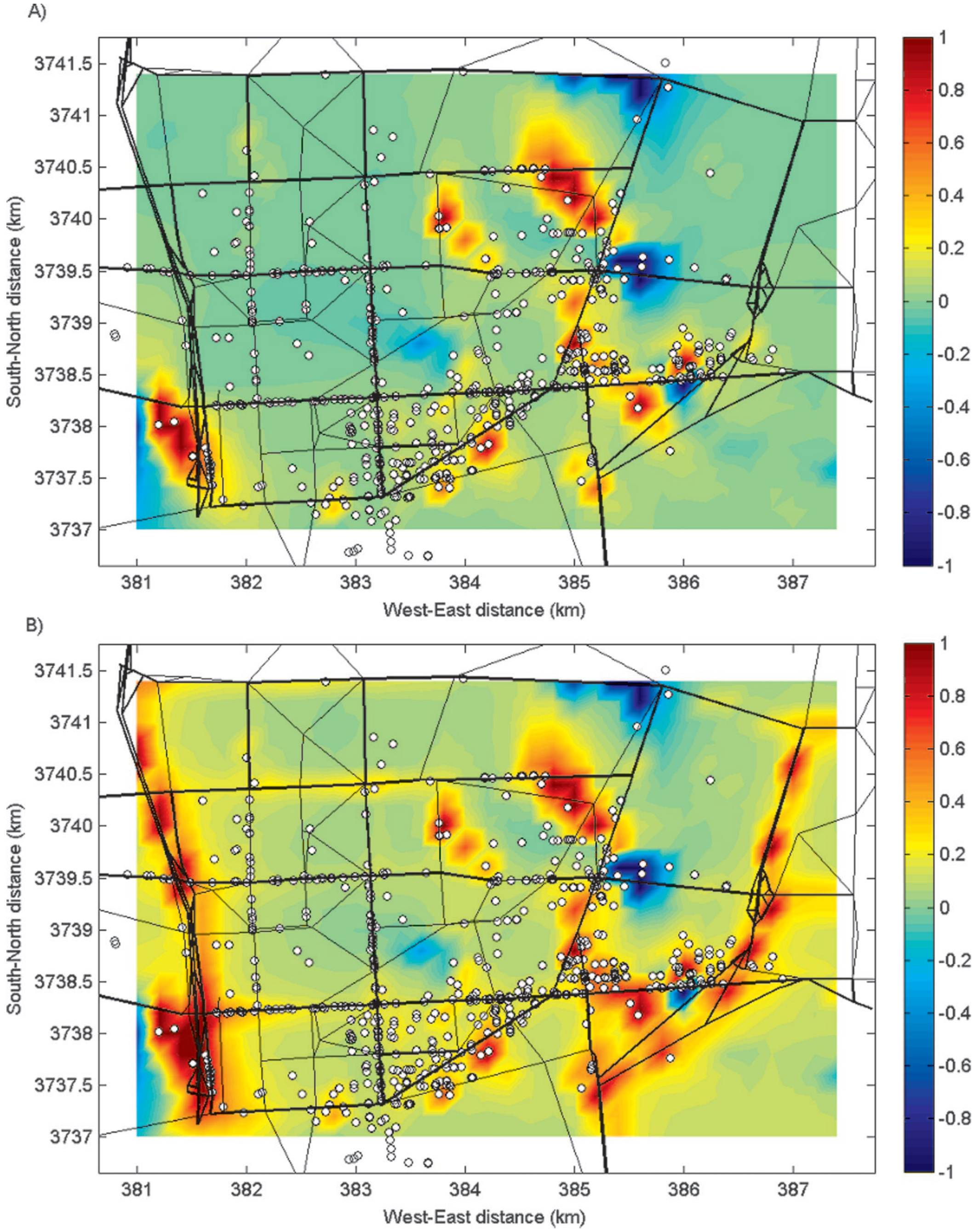

Figure 4. Differences of modeled concentrations ($\mu g/m^3$) using locally derived data and the base case: for stationary sources (a) and for stationary and mobile sources (b). Roads, black lines; stationary sources, white circles.

on-site surveys.[16] The industrial and commercial facility inventory contains stationary source emissions representing all of the facilities and on-site mobile source emissions at 170 surveyed facilities.[16] Ultimately, 6.5 t/yr of DPM emissions generated by stationary sources and surveyed on-site mobile sources were identified in Wilmington, and an additional 5.5 t/yr (2–16 t/yr) were estimated to be generated by the operation of mobile sources at nonsurveyed facilities in Wilmington.[16] More than 90% of these emissions were generated by on-site operation of mobile sources at surveyed and nonsurveyed facilities.[16] To assess uncertainty in diesel exhaust particulate emissions at industrial-commercial facilities, emissions at four surveyed case study facilities were analyzed using methods demonstrated in previous studies.[23-25] A range of total emissions at each facility was calculated using Monte Carlo techniques and applied to total emissions at each release location at surveyed and nonsurveyed industrial-commercial facilities.

Input Data Uncertainty: On-Road Emissions

A simple random-sampling Monte Carlo technique was applied to assess the uncertainty in on-road emissions calculations. As demonstrated by Pollack et al.,[26] a comprehensive uncertainty analysis of on-road emissions estimates is not feasible. Instead, the authors focused on three factors thought to have a substantial influence on

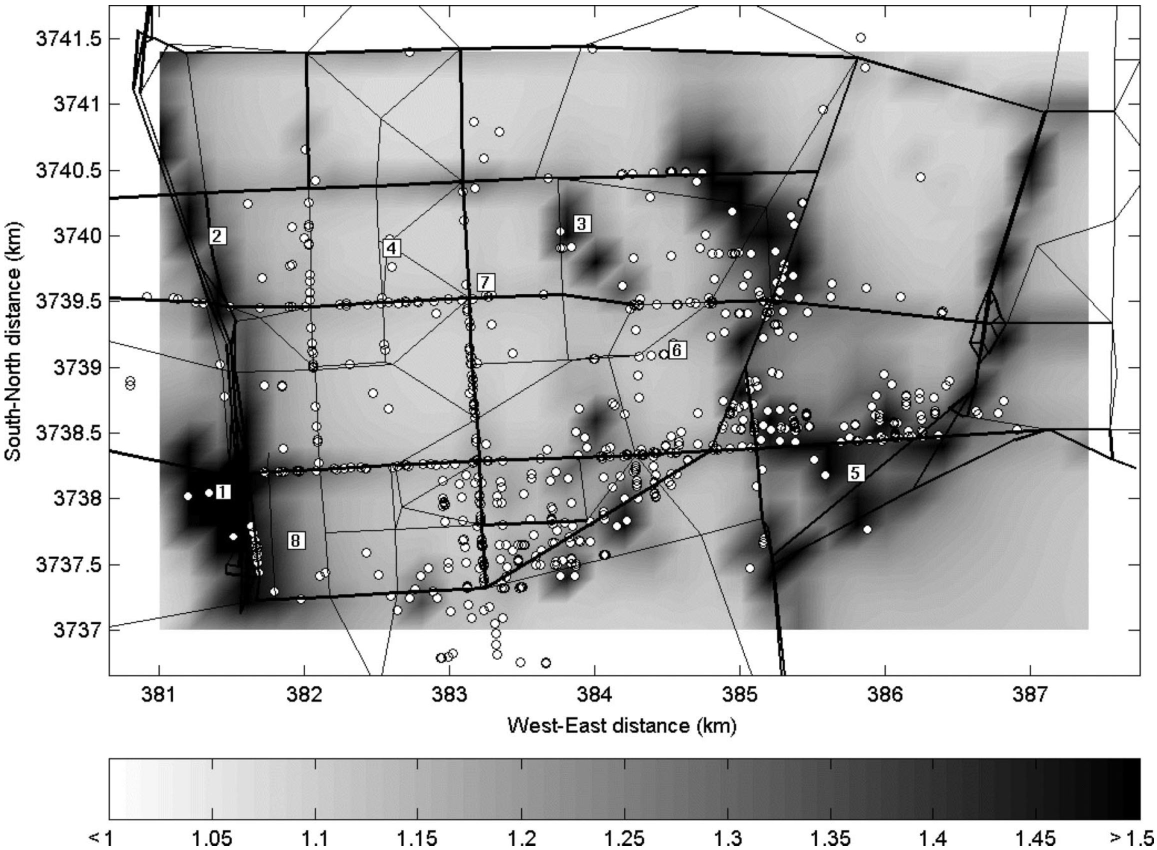

Figure 5. Modeled concentrations ($\mu g/m^3$) of DPM using locally derived emissions from stationary and mobile sources in Wilmington (scenario C). Roads, black lines; stationary sources, white circles; eight selected receptors for the uncertainty analysis, squares with numbers.

emissions uncertainty: the number of vehicles on each link, the possible age distribution of vehicles on each link, and emission factors. Details of this analysis are given in Sax and Isakov.[2] The analysis suggested that the truck fleet in Wilmington may be substantially older than the Los Angeles County fleet as a whole and that the number of vehicles on each link is uncertain, with a higher probability of underestimating than overestimating truck counts on any given link. Together, these factors suggest that a uniform county level emissions inventory, distributed uniformly by number of vehicles per link to each link, may substantially underestimate mobile source DPM in Wilmington. They also suggest the potential for underestimating both the number of vehicles on any link, the average fleet vehicle age, and the associated emission factors in Wilmington.

Uncertainty in the Spatial Allocation of Emissions

The locations of facilities and emissions releases have been assigned using emissions inventory databases, on-site surveys, and geocoding using a geographic information system (GIS). Nonsurveyed facilities were geocoded based on their reported address in the facility list compiled for this study. To assess uncertainty in locating emissions releases, the authors made assumptions based on on-site survey results and their best judgment of the accuracy of GIS-based geocoding in Wilmington. Locations of major roadways (freeways, ramps, and major arterials) in the SCAG TDM have been compared with a GIS street layer, which was verified using several data sources to be reasonably accurate in the Wilmington area.[27] Major roadways followed GIS street layers accurately and, as a result, it is assumed there is no uncertainty in the location of major roadways. In a few cases, the TDM contained simplifications for the location of curved roads. Minor roadways (minor arterials, collectors, and connectors) in the SCAG TDM were found to provide a simplified and inaccurate depiction of the actual location of smaller roadways in the modeling domain.

To assess uncertainty in the spatial allocation of sources, ISCST3 model simulations were conducted five times for each source, moving each source relative to its assigned location to the north, south, east, and west by the appropriate distance to reflect inaccuracies in identifying the location of facilities using GIS. All verified industrial-commercial inventory sources were assumed to be accurate to within 25 m of their assigned location, all nonsurveyed facilities within 200 m of their assigned locations, and the uncertainty in the spatial location of minor roadways within 500 m. Then, the resulting differences in source contribution from each source to each receptor were analyzed.

Uncertainty in the Temporal Allocation of Emissions

Information regarding the temporal allocation of emissions was limited, both for industrial-commercial facilities and roadways. For the industrial-commercial facilities, temporal emissions profiles were assigned based on data collected during on-site surveys and information reported in inventory reports. To assess uncertainty in temporal profiles representing industrial-commercial facilities, the sensitivity of the contribution of each facility to each receptor was tested by using 8-, 10-, 12-, 16-, and 24-hr temporal profiles. To assign an initial temporal profile for roadways, the authors used a profile developed by University of California at Davis representing the South Coast Air Basin.[28] To estimate uncertainty in this temporal allocation, the sensitivity of the contribution of each roadway to each receptor was tested by offsetting the University of California at Davis profile by −2, − 1, +1, and +2 hr. Because the ports, which generate a large portion of truck traffic in the modeling domain, may in the future operate on a 24-hr schedule, a 24-hr temporal profile was also tested. Weekday-weekend activity profiles were not examined for this assessment, but emissions were calculated based on annual activity accounting for weekend shutdowns where applicable.

Uncertainty in the Emissions Release Parameters

Emission release parameters (such as source configuration, stack temperature, and exist velocity) were determined using information collected from emissions inventory reports, health risk assessments, and on-site surveys. Where release characteristics were not available, defaults from the Emission Modeling System for Hazardous Air Pollutants (EMA-HAP) emissions model were applied.[29] A default value of 5×5 m volume source has been assigned to geocoded locations of every nonsurveyed facility. To assess uncertainty in release parameters, alternate release parameters for stationary and mobile sources were developed within the acceptable range of values. For roadway sources, release parameters for ISCST3 area sources were assigned consistent with Kinnee et al.[21]

Uncertainty in the Meteorological Inputs

On-site meteorological observations obtained during 2001–2002 at a temporary monitoring station in Wilmington were used in the ISCST3 simulations. Surface observations were enhanced with cloud data obtained from the Long Beach NWS monitoring station (located within several kilometers of the temporary monitoring station) to develop a meteorological data set suitable for modeling. The data set includes wind speed, wind direction, temperature, stability class, and mixing height. To assess the uncertainty caused by year-to-year variability in meteorology, meteorological data sets were collected representing the Long Beach NWS site for the years 1984–1990 and 2001. The variability in concentrations generated using these data were assumed to be representative of actual meteorological variability in the community. Model simulations were conducted for each meteorological year, and the results were scaled by the 2001 Long Beach data set. Then, a distribution of relative uncertainty in model results generated by year-to-year variability in meteorological conditions was derived.

Propagating Uncertainty Using the Monte Carlo Metamodel

To propagate uncertainty across model components, a Monte Carlo–based metamodel was constructed[22] using the methodology demonstrated in Sax and Isakov.[4] An additive model, assuming independence between model components, was used to propagate uncertainty. ISCST3 was applied using unit emission rates and scaled to emissions estimates for multiple metamodel iterations. To test the assumption of independence in the Monte Carlo metamodel ISCST3 was run for all sources contributing >1% of the total pollutant concentration at receptor 5. More than 200 model runs were performed, combining different combinations of spatial allocation, emissions release characteristics, and meteorology. It was found that the metamodel agreed with ISCST3 results from the 200 model runs to within 5%.

RESULTS AND DISCUSSION

Results of the uncertainty analysis for two cases were compared: the base case (scenario A), when readily available emissions data were used, and the advanced modeling case, when locally derived data were used (scenario C). Figure 6 displays model results as cumulative distributions of concentration estimates from the uncertainty analysis at two receptors. The first receptor is impacted by industry and a major highway, and the second receptor represents a clean residential area. Concentration estimates from scenario A (dashed lines) fall in the low end of the distribution, which means that most of the plausible estimates of concentrations will exceed the value corresponding to scenario A. This is the result of the uncertainty in spatial allocation of emissions sources and a bias toward underestimation in the base case.

The results of the uncertainty analysis for all eight of the receptors in the modeling domain are summarized in Table 1. The table provides probabilities of exceeding the model estimates for the three scenarios at each of the receptors. These probabilities indicate the "risk" associated with using the model estimate in making decisions on emission control. Notice that at most receptors, this risk is close to 100% for all three scenarios.

The probability distribution shown in Table 1 can be used to minimize the risk associated with using uncertain model inputs. For example, if one can accept a risk of 25% of model estimates being larger than that used in this analysis, the forth row of concentrations corresponding to the 75% percentile of the distribution of concentrations would be accepted. The risk can be lowered by using the first row corresponding to a percentile of 2.5%. The choice of the appropriate percentile to use has to be decided through the consensus of concerned parties.

Figure 7 displays the contributions of the sources of uncertainty: emissions, temporal allocation, spatial allocation, model release parameters, and meteorology. The uncertainty in emission rates makes the largest contribution of the variance of the model estimated concentrations. The uncertainty associated with temporal allocation of emissions and release parameters had relatively little impact on uncertainty. The uncertainty because of spatial allocation is very important; it can be large when lacking local data but still significant even when locally derived data are used. The variability in meteorology caused significant uncertainty for annual average concentrations, but this might be much higher for shorter time averaging periods (daily or hourly).

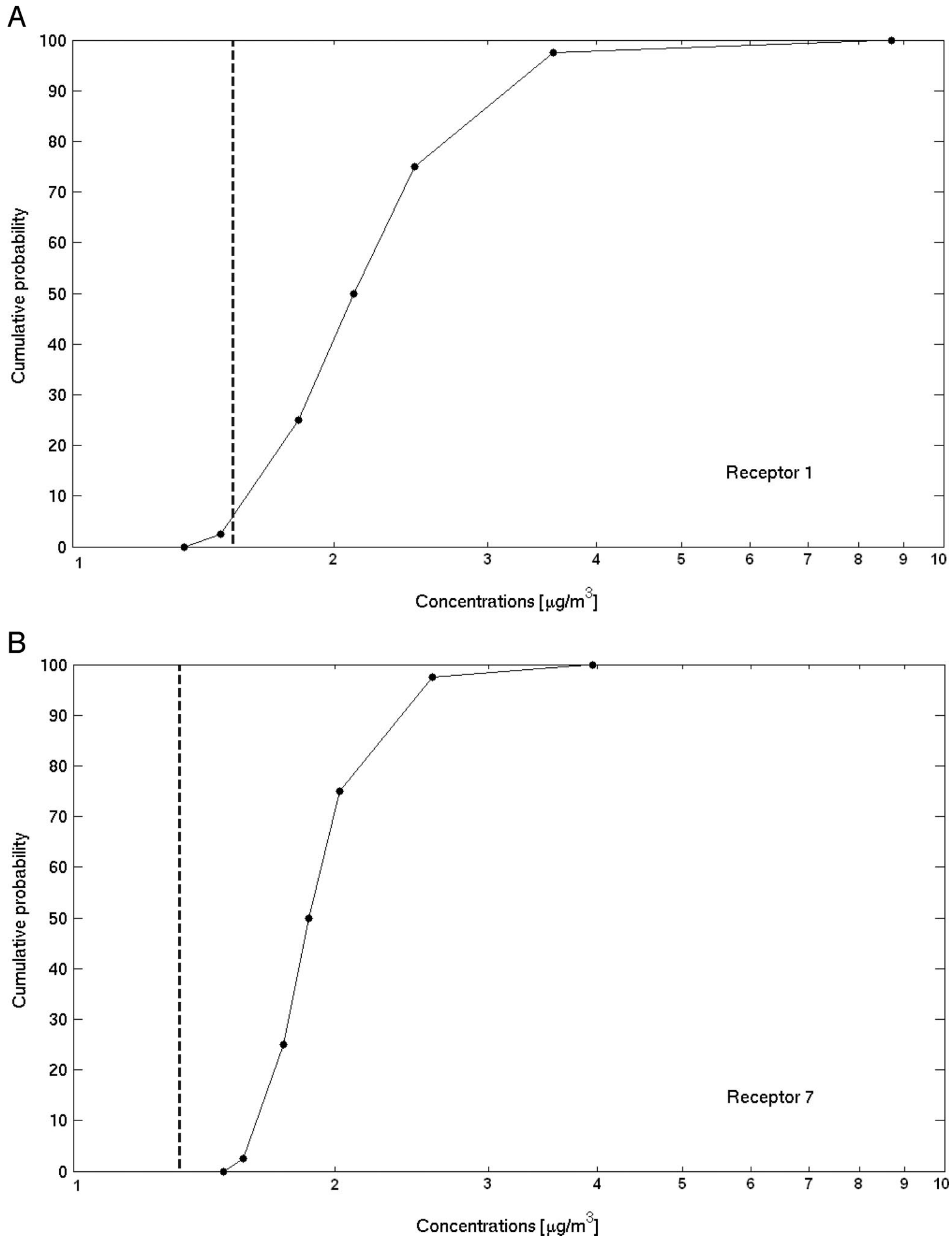

Figure 6. Cumulative probability of concentrations based on the uncertainty analysis for two receptors in the modeling domain: receptor 1, impacted by highway and industry; receptor 7, residential clean. Concentration estimates from the base case (scenario A), dashed lines.

Uncertainty in on-road emissions in this case study is significant (see Figure 4b) and arises from the lack of locally derived on-site vehicle activity data specific to individual links in the modeling domain. Uncertainty is also caused by application of driving-cycle–based emission factors where the driving cycle on any link is not known. Obtaining site-specific vehicle activity data and improving emission factors to account for link-specific conditions would help reduce uncertainty.

CONCLUSIONS

Resolving pollutant concentrations on refined spatial scales of 10–100 m presents a challenge in air quality modeling. This study demonstrates an approach to achieving this spatial resolution and evaluates the level of detail in data necessary to generate credible modeling results. Results demonstrate that both near-field contributions from local sources and regional background contributions from distant sources are important to consider in refined modeling applications.

This case study demonstrates the importance of site-specific, refined emissions data for developing local-scale assessments using Gaussian models. In this case, refined data, when modeled, provided a much more refined picture of the magnitude and distribution of possible community "hot spots" than more traditional, regionally refined data. In particular, this analysis demonstrated the importance of key inputs to locally derived mobile source

Table 1. Comparison of modeled concentrations from a base case, locally derived inventory, and uncertainty analysis.

Concentration	Rec.1	Rec.2	Rec.3	Rec.4	Rec.5	Rec.6	Rec.7	Rec.8
Scenario A—stationary sources from statewide inventory								
Concentrations (μg/m^3)	1.18	1.03	1.07	1.04	1.23	1.05	1.04	1.08
Probability of exceedance (%)	99	99	99	99	99	99	99	99
Scenario B—stationary sources from locally derived inventory								
Concentrations (μg/m^3)	2.09	1.03	2.77	1.02	3.95	1.09	1.04	1.25
Probability of exceedance (%)	50	99	25	99	15	99	99	99
Scenario C—stationary and mobile sources from locally derived inventory								
Concentrations (μg/m^3)	2.17	1.9	2.8	1.07	4.04	1.13	1.13	1.4
Probability of exceedance (%)	50	95	25	99	15	99	99	99
Distributions of concentrations (μg/m^3) obtained by including all components of uncertainty in model input								
2.5th percentile	1.46	2.11	1.66	1.52	1.84	1.42	1.55	1.70
25th percentile	1.8	2.7	1.93	1.66	2.32	1.54	1.72	2.0
50th percentile	2.09	3.32	2.12	1.79	2.72	1.65	1.84	2.27
75th percentile	2.45	4.29	2.5	2.03	3.26	1.8	2.0	2.6
97.5th percentile	3.54	7.04	5.11	6.82	4.99	2.34	2.56	3.69

Notes: Rec. indicates receptor.

emissions data, including fleet and activity distribution on specific links in the community. Models are typically applied using the best available input data representing the modeling domain to generate a single concentration estimate at each receptor. For neighborhood assessment, incorporating site-specific data can lead to improvement in modeled concentrations estimates, especially where site-specific data are lacking in regulatory databases.

This study also demonstrates that using models to generate a single concentration estimate at each receptor may be misleading if the full range of conditions in the modeling domain is not assessed. In this case study, uncertainty analysis suggests that point estimates at case study receptors may be substantially biased because of the potential for bias in on-road emissions estimates. In addition, concentration estimates at case study receptors were uncertain. This uncertainty was caused by uncertain emission rates in all of the sources and, specifically, by the limited data available on roadway-specific activity and emission factors.

Finally, this study indicates the need to use a comprehensive assessment approach in communities that

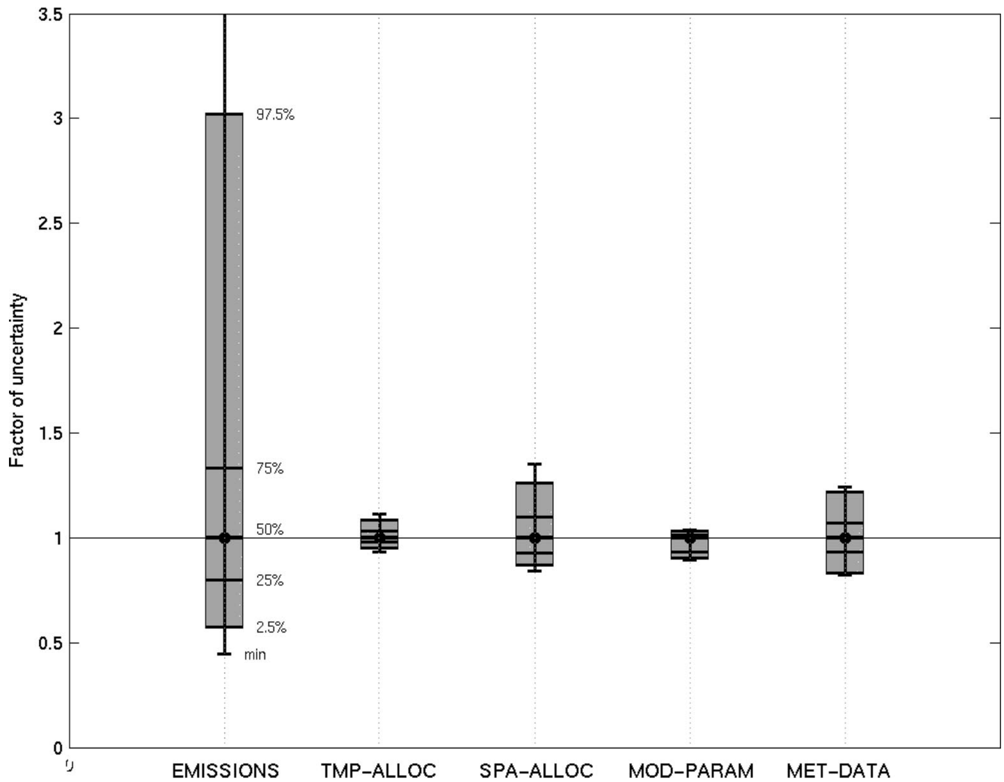

Figure 7. Uncertainty factors for different modeling components: emissions (EMISSIONS), temporal allocation (TMP-ALLOC), spatial allocation (SPA-ALLOC), model release parameters (MOD-PARAM), and meteorology (MET-DATA).

combines both monitoring and modeling data. Especially on refined spatial scales, modeling by itself or observations by themselves can only provide a limited and possibly incomplete and inaccurate picture of the air quality problem.

DISCLAIMER

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