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Combining Regional- and Local-Scale Air Quality Models with Exposure Models for Use in Environmental Health Studies

Vlad Isakov, Jawad S. Touma, and Janet Burke
Office of Research and Development, National Exposure Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC

Danelle T. Lobdell
Office of Research and Development, National Health and Environmental Effects Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC

Ted Palma
Office of Air Quality, Planning and Standards, U.S. Environmental Protection Agency, Research Triangle Park, NC

Arlene Rosenbaum
ICF International, San Francisco, CA

Halûk Özkaynak
Office of Research and Development, National Exposure Research Laboratory, U.S. Environmental Protection Agency, Research Triangle Park, NC

ABSTRACT

Population-based human exposure models predict the distribution of personal exposures to pollutants of outdoor origin using a variety of inputs, including air pollution concentrations; human activity patterns, such as the amount of time spent outdoors versus indoors, commuting, walking, and indoors at home; microenvironmental infiltration rates; and pollutant removal rates in indoor environments. Typically, exposure models rely upon ambient air concentration inputs from a sparse network of monitoring stations. Here we present a unique methodology for combining multiple types of air quality models (the Community Multi-Scale Air Quality [CMAQ] chemical transport model added to the AERMOD dispersion model) and linking the resulting hourly concentrations to population exposure models (the Hazardous Air Pollutant Exposure Model [HAPEM] or the Stochastic Human Exposure and Dose Simulation [SHEDS] model) to enhance estimates of air pollution exposures that vary temporally (annual and seasonal) and spatially (at census-block-group resolution) in an urban area. The results indicate that there is a strong spatial gradient in the predicted mean exposure concentrations near roadways and industrial facilities that can vary by almost a factor of 2 across the urban area studied. At the high end of the exposure distribution (95th percentile), exposures are higher in the central district than in the suburbs. This is mostly due to the importance of personal mobility factors whereby individuals living in the central area often move between microenvironments with high concentrations, as opposed to individuals residing at the outskirts of the city. Also, our results indicate 20–30% differences due to commuting patterns and almost a factor of 2 difference because of near-roadway effects. These differences are smaller for the median exposures, indicating the highly variable nature of the reflected ambient concentrations. In conjunction with local data on emission sources, microenvironmental factors, and behavioral and socioeconomic characteristics, the combined source-to-exposure modeling methodology presented in this paper can improve the assessment of exposures in future community air pollution health studies.

IMPLICATIONS

This paper presents a new methodology to demonstrate the linkage of regional- and local-scale air quality models with human exposure models for improving community-level environmental health studies involving near-source exposures to multiple ambient air pollutants. The extent of variability in spatial and temporal concentration gradients associated with large point sources and roadways shown in this research is especially important given the growing body of literature on the potential adverse health effects associated with elevated concentrations near such sources.

INTRODUCTION

Many epidemiological studies have documented poor air quality as a risk factor for a variety of human health outcomes. For example, the cardiac and respiratory effects of air pollution range from decreased lung function[1,2] to exacerbation of symptoms of asthma[3,4] and chronic bronchitis[3] to more serious cardiopulmonary events, such as increased hospitalizations[4,5] or mortality.[6,7]

Understanding the magnitude and nature of human exposure is clearly the first step in assessing the likelihood of adverse health effects that could result from contact with environmental pollutants. Undertaking this type of research requires identification of the key sources and constituents of indoor and outdoor air pollutants of health concern, such as particulate matter (PM), ozone, and determination of personal exposures to these pollutants.[8,9] However, necessary information on personal exposures is often not readily available, and therefore, various surrogates of personal exposure are typically used instead.

For criteria pollutants, available ambient monitoring data from a central outdoor monitoring station has been historically used in air pollution epidemiology studies.[10,11] The direct use of such data inherently assumes that these ambient measurements are representative of the air quality over a broad area. Also, these studies assume that a single monitor, or an average of only a few monitors, is representative of complex patterns of exposures within a large urban area. Moreover, for toxic pollutants, monitoring data are often nonexistent or limited because regulatory compliance monitoring stations do not always measure air toxic pollutants. Also, many toxic pollutants can have large concentration gradients, especially near large emitters such as major roadways, and require the use of many closely spaced monitors to approximate community impacts.[12,13] These and other limitations may hamper the use of ambient air quality data alone as a reliable proxy of personal or population exposures when investigating health effects due to either the short- or long-term exposures to air toxic pollutants.

Recently, more refined approaches have been used in epidemiological studies to enhance the spatial resolution of monitoring data by applying geographic information systems (GIS)-based interpolation methods to approximate outdoor concentrations near communities.[14] Some researchers have used Land Use Regression (LUR) models in the analysis of cohort study health data. These LUR models incorporate landscape characteristics such as proximity to roadways and other outdoor sources of air pollution.[15–19] Other researchers have used air quality models and microenvironmental personal exposure modeling tools to support air pollution exposure and health studies.[11,20–24] A few studies have also used results from atmospheric dispersion models in the analysis of health data.[25–27]

These approaches may improve the spatial resolution of ambient outdoor concentrations; however, they do not address the fact that people spend the majority of their time indoors.[28] Individuals spend time in different microenvironments during the day (e.g., indoors and outdoors at residences, commuting, at school or workplace, etc.) and may experience varying levels of exposure to air pollutants of outdoor origin in these microenvironments. Thus, to accurately characterize the exposure, it is important to determine the relative contributions of air pollutants in microenvironments of concern to human exposures.[29,30] Although air quality modeling is a preferred approach to improve spatial/temporal resolution of air pollutant concentrations, exposure models are designed to utilize modeled air concentrations, combined with human activity data and indoor/outdoor relationships for pollutants, to estimate distributions of exposures for populations of interest. Thus, linking air quality with exposure models can better account for human mobility and indoor exposure issues.

In this paper, we present a new methodology for using a hybrid air quality modeling approach[31] that combines results from a grid-based chemical transport model with a local plume dispersion model to provide spatially and temporally resolved air quality concentration estimates at the census-block-group level and link these air quality estimates with human exposure models also at census-block-group resolution. Thus, instead of assuming uniform distribution of exposures over a large urban area if central site monitoring data are solely used, we use here two different exposure models developed by the U.S. Environmental Protection Agency (EPA) (the Hazardous Air Pollutant Exposure Model [HAPEM][32] and the Stochastic Human Exposure and Dose Simulation [SHEDS] model[20,23]) to produce spatially and temporally resolved exposure estimates. Both of these models require input information on time activity and commuting patterns; microenvironmental concentrations; air exchange rates; heating, ventilation, air conditioning, and housing characteristics; and pollutant penetration and removal rates.

We demonstrate how this linked air quality/exposure modeling approach may be used in future community health studies by providing exposure estimates that reflect residences in proximity to large industrial facilities or major roadways. We present the results from this approach for two pollutants: benzene, an example of an important urban air toxics pollutant; and fine PM ($PM_{2.5}$), an example of a major local- and regional-scale criteria pollutant of concern. This research is an important component of an EPA feasibility study being conducted in New Haven, CT, that examines the cumulative impact of various air pollution reduction activities (at the local, state, and national level) on changes in air quality concentrations, human exposures, and potential health outcomes in the community. In conjunction with local data on emission sources, demographic and socioeconomic characteristics, and indicators of exposure and health, the methodology presented in this paper can serve as a prototype for providing high-resolution exposure data in future community air pollution health studies. For example, these methodologies can be used to provide the baseline air quality assessments of impacts due to regional- or local-scale air pollution control measures and to estimate the likely impact of future projected air pollution control measures on human exposures and health in the community that are dependent on air pollution reduction activities or are due to the addition of new sources in a community.

AIR QUALITY MODELING

Detailed information on air quality is a key concern for air-pollution-related environmental health studies. To provide the best estimates of air concentrations, air quality modeling estimates should include local-scale features, long-range transport, and photochemical transformations. There are several available modeling approaches capable of assessing pollutant concentration gradients at a fine resolution[33] and these can be categorized into two major types of air quality models: source-based dispersion models and Eulerian grid-based chemical transport models. Grid-based chemical transport models such as the Community Multi-scale Air Quality (CMAQ)[34] model are used to simulate the transport and formation of ozone, acid rain, $PM_{2.5}$, and other pollutants formed by chemical reactions among precursor species that are emitted from hundreds or thousands of sources. CMAQ provides average hourly concentration values for each grid cell in the modeling domain. Such models may be set up to be applied to a wide range of spatial scales ranging from national to urban. However, these models cannot address the local-scale processes affecting pollutant gradients such as those occurring close to roadways.

Local plume dispersion models such as AERMOD[35] are designed to capture local pollutant concentration gradients (e.g., within a few kilometers from the source) and can provide detailed resolution of the spatial variations in hourly average concentrations. However, they do not take into account atmospheric chemical reactions, except for highly simplified representations such as first-order pollutant decay. Although it is desirable to combine the capabilities of grid-based models and dispersion models into one model, this an evolving area of research. Currently, a hybrid approach[31,36] is the most computationally efficient way to combine regional-scale photochemical grid and local-scale plume dispersion models to provide the total ambient air pollutant concentrations from nearby and distant sources. Because dispersion models are less resource intensive than regional models, a hybrid methodology can be used to study the sensitivity of local concentration to changes in model parameters. This constitutes a clear advantage of the hybrid approach, because the estimation of local concentration variability using a photochemical grid model at higher resolution would be a computationally resource-intensive task, especially when annual concentrations over larger urban areas are needed.

In the hybrid modeling approach, concentrations from a grid-based chemical transport model and a local plume dispersion model are added to provide contributions from photochemical interactions, long-range (regional) transport, and details attributable to local-scale dispersion.[31] However, combining the results from such models is not straightforward because the same emission sources may be included in both types of models and adding the modeled concentrations could result in double-counting the impact of these sources. To avoid this double-counting problem, a "zero-out" approach can be used.[33,36] In this approach, two regional model simulations are conducted: one for the base case in which local emission sources are included, and another simulation (zero-out) in which the local emissions are excluded. The difference in concentrations between these two simulations provides an indication of the magnitude of the impacts from local emission sources. This approach was not used in this paper because of various constraints; however, the difference between the results based on this approach and the hybrid approach that was used here needs to be further investigated. However, in one study, Stein et al.[36] compared the zero-out approach with the hybrid approach for benzene concentrations in Houston, TX, and also compared the zero-out approach with a simple combination of a local- and regional-scale modeling. The comparison showed that this difference was less than 10%, and therefore, we believe that the double-counting effects have no noticeable impacts in our example.

EXPOSURE MODELING

Rather than assuming ambient air concentrations are equivalent to exposure concentrations, exposure models are designed to better represent human contact with pollutants and to some degree account for human behavior and physiology. Population-based exposure models provide estimates of the range of exposures for a population of interest and the fraction of population above a level of concern. Two physically based probabilistic population exposure models were used in this study, HAPEM and SHEDS. Both models use census demographic data to simulate a representative population and combine air pollutant concentrations with human activity pattern data to estimate actual human exposures. These exposure models produce population distributions of exposures at the spatial resolution defined by the census data used (e.g., census tract, block group, or block), and can utilize modeled air pollutant concentrations at the same resolution. The main difference between the models is in the temporal resolution and how input concentration data are used to predict microenvironmental and personal exposures. Some of the key features of these models are described in the following sections.

HAPEM Model

HAPEM is a screening-level stochastic exposure model appropriate for assessing average long-term inhalation exposures of the general population, or a specific subpopulation, and over spatial scales ranging from local to national. The simulated population is first stratified according to demographic variables, such as age and gender. HAPEM uses the general approach of tracking representatives of the demographic groups as they move among indoor and outdoor microenvironments (MEs; i.e., a location in which human contact with an ambient pollutant may take place) according to human time-activity data (i.e., sequences of activities for an individual), corresponding durations, and ME locations (e.g., at home for 45 min, followed by driving in a car for 20 min). The estimated pollutant concentrations in each ME visited are combined with the fraction of time spent in that ME to calculate a time-weighted average exposure concentration for a representative individual assigned to a particular demographic group.[37]

HAPEM uses four primary sources of information: population data from the U.S. Census, population activity data, air quality data, and microenvironmental data. Four standard databases are used in HAPEM: the 2000 U.S. Census provides population demographics[38]; statistical distributions of ME factors derived from various literature sources are used in a Monte Carlo sampling framework to estimate ME concentrations; EPA's Consolidated Human Activity Database (CHAD) provides daily human time-location-activity patterns[39]; and air quality data for each specified demographic group. To simulate activity sequences over long periods of time, HAPEM combines CHAD-analyzed daily time-activity patterns with an algorithm that reflects day-to-day correlations for a simulated individual with a combination of cluster analysis and a Markov selection process. HAPEM also includes commute and near-roadway databases.[11]

The HAPEM model requires annual-averaged, diurnally distributed air quality levels at eight 3-hr intervals (e.g., 0–3, 3–6, etc.). In addition, HAPEM can also evaluate the contributions of subsets of the air quality data (e.g., air concentration values for specific source sectors such as point, area, and mobile sources). Although the air concentration data input to HAPEM must be in a specific format (e.g., annual average and diurnally distributed), the source of the data could be either from an air dispersion model or an ambient monitor.

HAPEM was originally designed to estimate annual average concentrations at the spatial resolution of U.S. Census tracts. For this study, HAPEM6 was modified to operate at finer temporal resolution (i.e., seasonal and monthly averages) and finer spatial resolution (i.e., U.S. Census block groups and blocks). In this application, modeled annual average ambient air concentrations estimated for each U.S. Census block group in New Haven, CT, was input in HAPEM6.

Another modification made to HAPEM6 for this study was the capability of considering correlations in exposure concentrations from multiple pollutants for a simulated individual. For example, an individual who spends more time on the roadways than average would be expected to have relatively high exposure concentrations for all on-road-related pollutants. Some exposure models accomplish this by estimating exposure concentrations to multiple pollutants in a single simulation (e.g., APEX[40]).

Although HAPEM is typically used to predict exposures to a single pollutant at a time, it can be configured to estimate exposures to multiple pollutants. Probabilistic models such as HAPEM randomly select activity patterns and other variables for simulated individuals. If a model can ensure that the random elements are selected in the same sequence for each simulation, then the simulated individuals and their associated exposure concentrations can be matched from one simulation to the next. Thus, by tracking the random seed used in each of the exposure simulations, it is possible to ensure that the same set of time-activity patterns, ME factors, and other randomly selected attributes are assigned to the same individual while predicting exposures to multiple pollutants. In essence, this approach has been used in the application of HAPEM to predict exposures to multiple air toxics. For this study, ME factor distributions developed for the recent National Air Toxics Assessment[37] were incorporated into both HAPEM and SHEDS. Both models were then applied to the ambient air concentration predictions from the air modeling portion of the study to estimate exposure concentrations across the population of the modeling domain.

SHEDS Model

SHEDS is a stochastic exposure model appropriate for more detailed assessments of short- or long-term inhalation exposures and intake dose at the local to regional scale. The SHEDS model randomly generates a population of individuals to be simulated on the basis of census demographic data (gender/age proportions) that statistically represent a defined percentage of the population for the study area (i.e., 10% of the total population), rather than particular demographic groups as done in HAPEM. A time series of locations and activities is randomly assigned to each simulated individual through the use of time-location-activity diaries appropriately matched to each simulated individual by demographics and other characteristics such as employment status.[39] In addition, gender- and age-appropriate physical attributes (e.g., body weight) are randomly assigned to each individual for estimating intake dose. Similar to HAPEM, an individual's time-location-activity data are combined with the microenvironmental concentration estimates to calculate each individual's time-weighted average exposure concentration. However, SHEDS has flexibility in the time resolution of the microenvironmental and exposure concentration calculations on the basis of the type of input concentrations provided (i.e., hourly average, daily average, etc.) and in the complexity of the algorithms used for estimating concentrations in the various MEs (i.e., how indoor sources are handled). In addition, SHEDS includes algorithms for estimating intake dose on the basis of activity-specific breathing rates.

In this study, SHEDS was applied to the 318 census block groups in New Haven, CT, using the same time series of ambient concentrations for each census block group as for the HAPEM6 simulations. SHEDS estimated simultaneous exposures to multiple pollutants for each simulated individual.

RESULTS AND DISCUSSION

To illustrate an application of the hybrid air quality modeling approach to provide resolved local-scale pollutant concentrations, this study was part of a feasibility study to assess public health impacts of cumulative air pollution reduction activities in New Haven, CT. The city of New Haven, with an estimated 2006 population of approximately 127,000, is small compared with other urban centers in the United States, but it includes many stationary sources such power plants, large ports and marine terminals, and several major roadways such as Interstates 91 and 95 (Figure 1). Here we focus on a 20- by 20-km area that covers most of these emission sources. This city was selected because it was a recipient of one of EPA's nationally funded Community Air Toxics projects. Through this project, New Haven has implemented a comprehensive Clean Air Initiative, which includes several voluntary air pollution reduction measures to reduce both criteria and toxic air pollutants.[41] The city of New Haven has begun implementing some of the air pollution control programs, and others will begin in the next several years. Along with some of the local and state efforts that are ongoing in New Haven, there are also several federal regulations that have recently been or soon will be implemented. This project also sought to develop collaborations and partnerships with state and local agencies including government, academia, and the New Haven

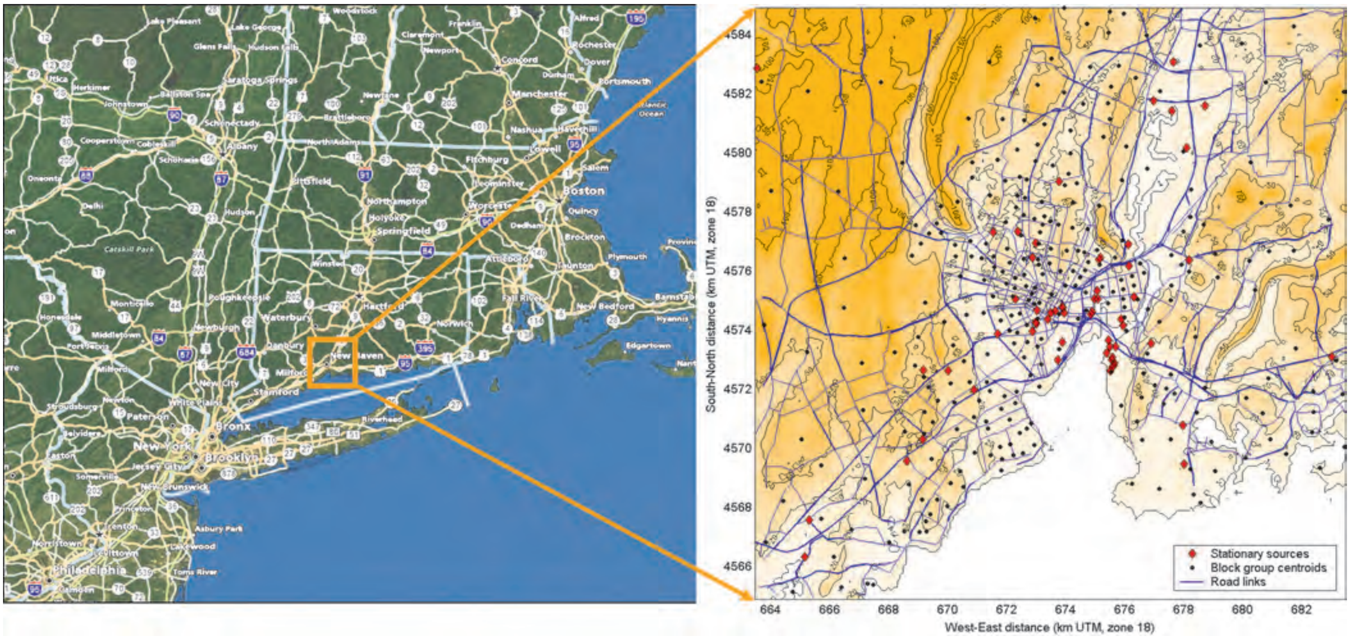

Figure 1. New Haven, CT, modeling domain.

community. The New Haven modeling effort reported here is part of a broader feasibility study to evaluate impacts of regulatory and voluntary actions to reduce air toxic emissions on human exposures and health.

In the New Haven modeling study, we used a hybrid approach as described in Isakov et al.,[31] in which we combined the concentration from two air quality models that were run independently. Average hourly concentrations in the modeling domain encompassing the central part of New Haven were extracted from the CMAQ model and were added to the hourly concentrations calculated by the AERMOD local plume model at 318 census-block-group receptors in the same geographic domain. To provide local-scale variability, we calculated differences between an average value from a dispersion model for all receptors within a grid cell and actual modeled concentrations at every receptor in a grid cell. Then, we added CMAQ concentrations and dispersion model concentrations. A schematic of the hybrid approach is shown in Figure 2.

The CMAQ modeling system was run for an annual period in a nested mode at 36- and 12-km horizontal grid

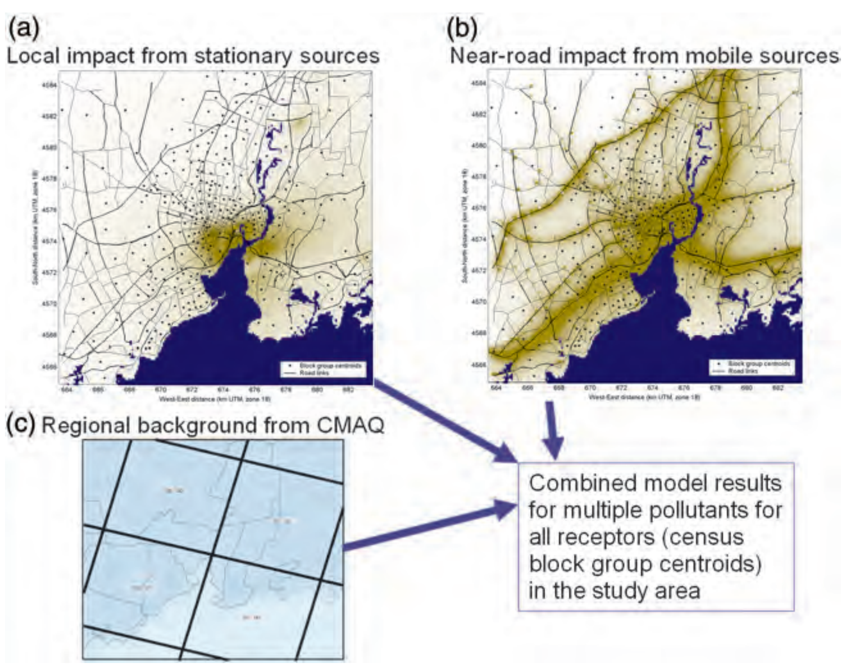

Figure 2. Schematics of the hybrid modeling approach showing (a) local impact from stationary sources, (b) near-road impact from mobile sources, and (c) regional background from CMAQ.

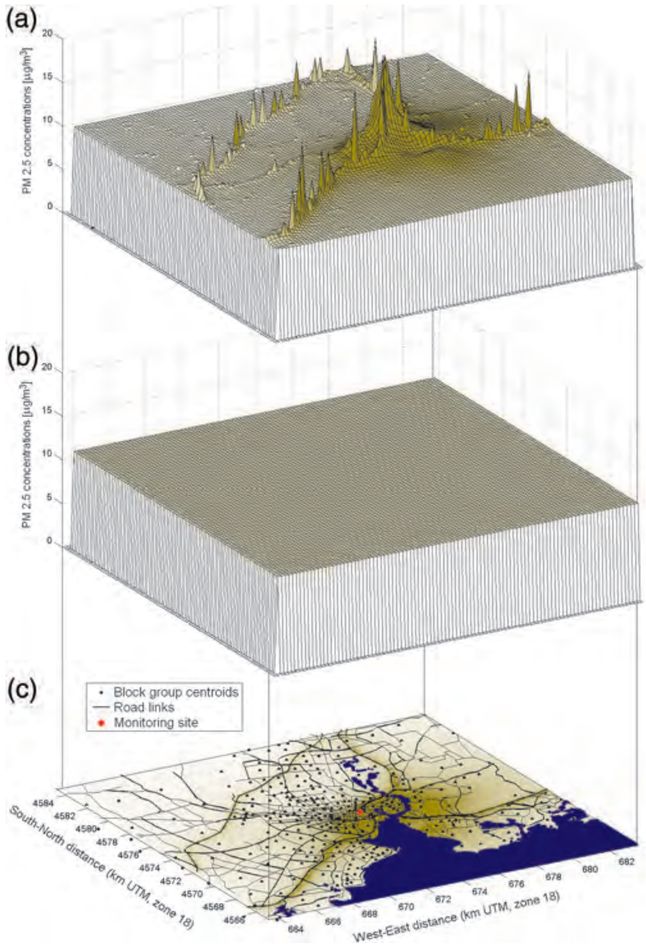

Figure 3. Application of the hybrid modeling approach in New Haven, CT: (a) combined results, (b) regional background from CMAQ, and (c) local gradients from AERMOD.

dimensions using the 1999 National Emission Inventory and meteorological outputs from 2001 using the MM5 meteorological model.[42,43] The CMAQ model concentration reflects modeled regional background values and concentrations due to any photochemical interactions in the atmosphere. The AERMOD model uses detailed site-specific information from the "bottom-up" emissions inventory for highway vehicle exhaust and evaporative running emissions on roads,[44] as well as local point source, marine port, and airport emissions data, to provide this resolution. Emissions of area sources and nonroad sources not associated with ports and airports were assumed to be uniformly distributed across the modeling domain and were represented in CMAQ regional model simulations. The AERMOD model estimated concentrations for several toxics and criteria pollutants, but results presented here are an illustration of this methodology for two representative pollutants, benzene and $PM_{2.5}$. Benzene is representative of mobile-source-driven air toxic pollutants and $PM_{2.5}$ is representative of pollutants that can undergo photochemical transformations.

A graphical illustration of the application of this hybrid approach using $PM_{2.5}$-modeled concentrations in New Haven is shown in Figure 3. Figure 3c shows the geographic domain and the locations of the major highways. The gray colors show areas of high concentrations as predicted by the AERMOD dispersion model. As expected, higher predicted concentrations are near high-emission sources such as marine terminals, interstate highways, and large industrial sources. Lower concentrations are predicted in the surrounding suburban areas. Figure 3b shows predicted concentrations from the CMAQ model at 12- by 12-km grid-cell resolution. In this panel, CMAQ provides a uniform distribution across the modeling domain. Figure 3a shows total concentration, in which AERMOD concentrations are added with CMAQ modeled concentrations. Figure 3a shows greater "texture" in the concentration field when AERMOD concentrations are added. This combined estimate also clearly shows high concentrations at locations of major $PM_{2.5}$ emitters.

The total concentrations predicted by the hybrid air quality model were then used by the HAPEM and the SHEDS models to predict exposures to benzene and $PM_{2.5}$, respectively. Spatial distributions of modeled benzene and $PM_{2.5}$ exposures are shown in Figure 4, b, c, e, and f. For comparison purposes, spatial distributions of concentrations are also presented (Figure 4, a and d). Figure 4, a–c, shows the spatial distribution of the annual average concentrations and exposures (median and 95th percentiles) for benzene, and Figure 4, d–f, shows 6-month summertime average (from April to September) concentrations and exposures for $PM_{2.5}$. This 6-month averaging period was selected based on the CMAQ model evaluation[45] to exclude wintertime biases in the model results. As can be observed from the figure, there is a strong spatial gradient in pollutant concentrations and exposures; as expected, higher values are observed close to major highways. There are also large gradients near major industrial facilities (ports) where there are high benzene emissions from fuel storage tanks and marine vessels. At the high end of the distribution (95th percentile), exposures are generally higher than ambient concentrations. They are also much higher in the central district than in the suburbs, showing the importance of accounting for commuting while modeling exposures. We also found that the individuals living in the central area are typically moving between MEs with high concentrations, whereas the individuals residing at the edge of the city are not.

Figure 5 presents a comparison between annual average benzene exposures from the HAPEM model with modeled annual average concentrations at census-block-group centroids obtained using the hybrid modeling approach. Figure 6 shows a similar comparison using the summertime exposure concentrations from the SHEDS model for $PM_{2.5}$. Two metrics of distributions are shown—median and 95th percentiles of total inhalation exposure for all population groups. For benzene, median values of the exposure distributions are close to ambient concentrations, but the tail of the distribution (95th percentile) shows higher values (exposures are almost twice higher than modeled ambient concentrations). In general, both Figures 5 and 6 show that the exposure patterns are different than the predicted concentration patterns. Because benzene can readily infiltrate indoors, median benzene exposures are similar to ambient concentrations. However, exposure estimates from HAPEM are higher than the

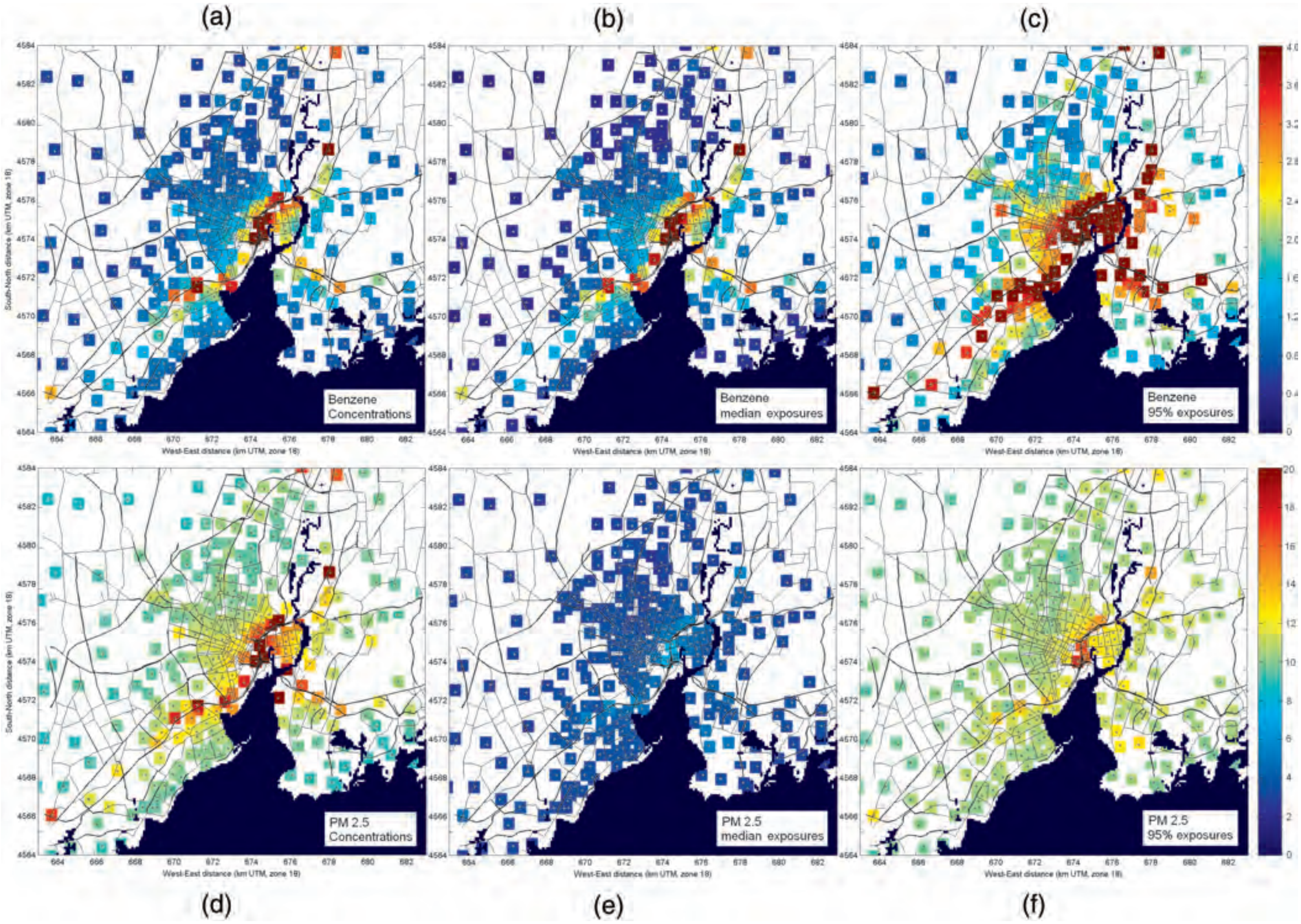

Figure 4. Maps of modeled (a) annual average concentrations, (b) median, and (c) 95th-percentile exposures for benzene. (d) Six-month average concentrations, (e) median, and (f) and 95th-percentile exposures for $PM_{2.5}$.

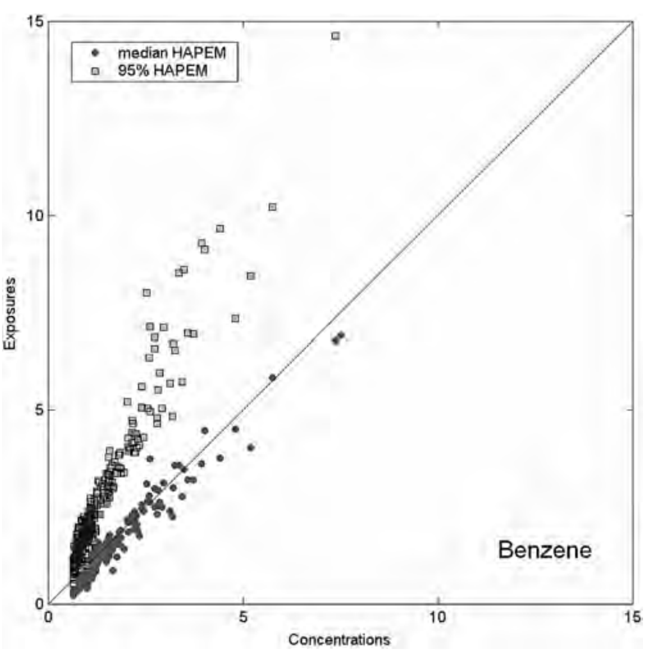

Figure 5. Comparison of benzene exposures from HAPEM model with modeled ambient concentrations.

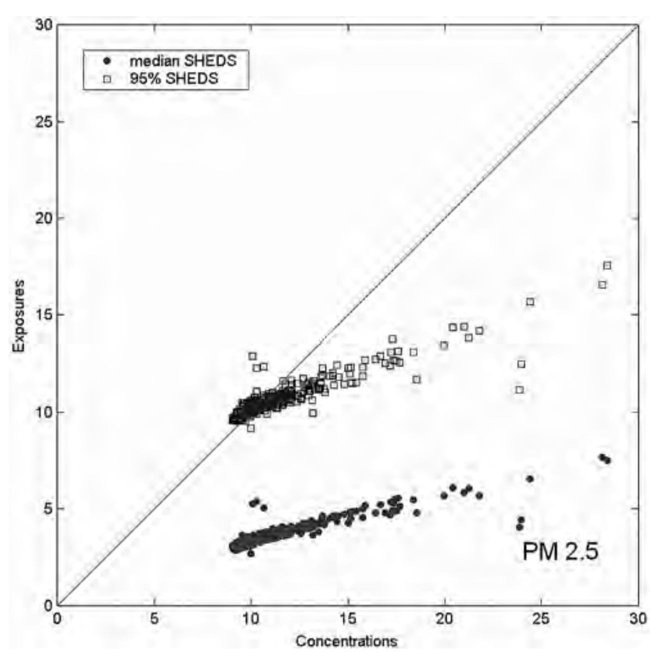

Figure 6. Comparison of $PM_{2.5}$ exposures from SHEDS model with modeled ambient concentrations.

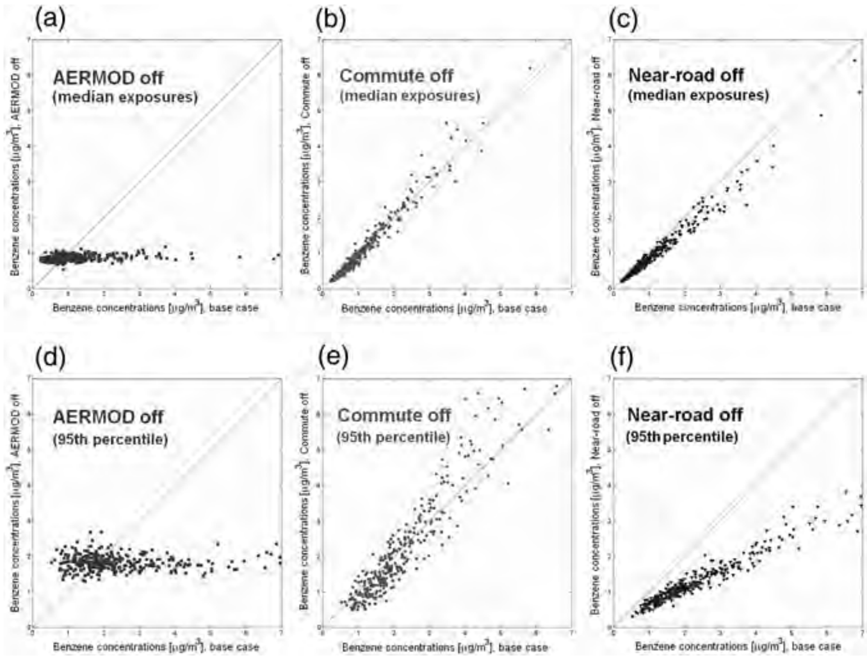

Figure 7. Impact of key model components on exposure concentrations: (a–c) median and (d–f) 95th percentile of exposure distribution.

predicted ambient benzene concentrations at census block groups, with greater influence of roadways because of adjustments made to account for elevated residential outdoor benzene levels for homes near roadways. In contrast, the relationship between modeled exposure and predicted ambient $PM_{2.5}$ concentrations are much different. $PM_{2.5}$ penetrates less efficiently indoors, thus exposures to $PM_{2.5}$ are typically found to range between 30 and 100% of ambient $PM_{2.5}$ concentrations, depending on the exposure percentile selected and the impact of commuting.

To investigate the relative importance of several exposure modeling features such as commuting and near-road factors, we conducted a series of sensitivity tests in which we ran the model with and without these features. We also investigated the impact of using refined spatial resolution in air quality and exposure concentrations. The results for these sensitivity analyses for benzene are presented in Figure 7. Figure 7, a–c, shows the median values of the entire exposure distribution, and Figure 7, d–f, shows the 95th percentile. The median values are representative of exposures to typical populations, whereas the 95th percentile is representative of higher exposed subgroups. The first sensitivity analysis (Figure 7, a and d) was conducted to evaluate exposure concentrations from HAPEM with two types of inputs: (1) using only a regional grid model (CMAQ) to estimate air quality, and (2) using air quality concentrations from the hybrid approach (e.g., CMAQ combined with AERMOD). The figure shows that modeled exposures are much higher and have a wider range when based on the hybrid approach than when only based on the CMAQ results. This is observed for both median and 95th percentiles of the exposure distribution. This clearly indicates that providing spatially resolved concentrations in air quality modeling can be quite important for exposure modeling.

The second sensitivity analysis was conducted to evaluate the relative importance of the commute algorithm in the exposure model. The need for incorporating the effects of commute patterns is well recognized.[23] As can be seen from Figure 7, b and e, the modeled exposures differ by approximately 10% for median percentile values of the exposure distribution and 20–30% for the 95th percentile of the distribution.; however, there is no clear bias in either case. These results point out the importance of the commuting algorithms in the modeled benzene exposure concentrations. Ignoring the contribution of commuting would result in as much as a 30% difference in the benzene exposure estimates for certain population subgroups.

The third sensitivity analysis (Figure 7, c and f) was conducted to evaluate the relative importance of the near-road algorithm in HAPEM. Many people live in the vicinity of large transportation corridors in large urban areas and this additional mechanism was included in HAPEM because of recent interest in near-roadway exposures. As shown in Figure 7, c and f, the near-roadway algorithm is responsible for an approximate 20% difference in median exposure distribution and almost a factor of 2 difference for the 95th percentile of the exposure distribution. These results clearly show the importance of including near-road adjustment factors in HAPEM for populations residing near roadways. Results from all three sensitivity analyses underscore the importance of developing a hybrid air quality model along with exposure modeling that incorporates commuting and near-roadway factors as considered by HAPEM6. However, further evaluation of these methods with new or additional observations is still warranted.

Typically, exposure modeling has been conducted on a census-tract level.[37] To investigate the importance of providing higher resolution in air quality concentrations for use in exposure modeling, we conducted a sensitivity

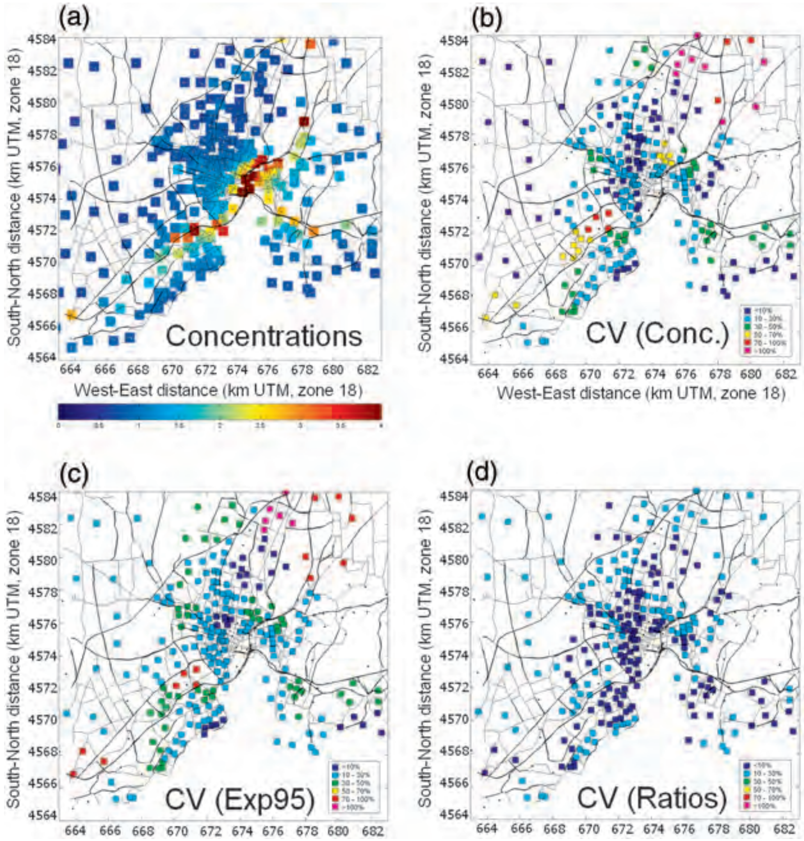

Figure 8. (a) Spatial map of annual average benzene concentrations at census-block-group centroids, (b) CVs for concentrations, (c) CVs for the 95th percentile of the exposure distribution, and (d) range of variability in the E/C ratios for benzene. (CV = SD/mean × 100%).

analysis for benzene and $PM_{2.5}$ at two levels of spatial resolution—census tract and census block group. We used the coefficient of variation (CV), defined as standard deviation divided by the mean multiplied by 100%, to estimate the magnitude of spatial variability within each census tract. CVs for each of the census tracts (for concentrations and exposures) were estimated at the census-block-group level. Figure 8a provides a spatial map of benzene concentrations at census-block-group centroids. The map shows a wide range of concentrations in the study area and high values near major highways. The CVs for concentrations (Figure 8b) show values ranging from less than 10% to up to 100% in different parts of the modeling domain. A similar feature is observed for the CVs for the 95th percentile of the exposure distribution (Figure 8c). These results indicate that in urban areas there are locations where there are high ambient and exposure concentrations attributable to the presence of large emitting sources that create hot spots, and that a higher spatial resolution than census-tract level (e.g., census block group) is informative and desirable for assessing the impacts at the community or intraurban level.

Finally, we investigated whether the predicted exposure-to-concentration ratios (E/C) were consistent across the study area (as assumed by most ambient monitoring-based time-series epidemiological studies), so that ambient concentrations could be used as a reliable surrogate of personal exposures in air pollution health effect studies. However, our analysis indicated that the range of variability in the E/C ratios for benzene (Figure 8d) were spatially variable and went up to 30% across the modeling domain. In particular, we found that spatial variability within census tracts for benzene was significant. The key factors influencing this variability were determined to be the relative size and geometry of the census tract and proximity to (mobile or point) emission sources. The spatial variability in the summertime average concentrations and exposures of $PM_{2.5}$ are shown in Figure 9. Similar to benzene, this map shows a wide range of concentrations in the study area and high values near major highways. However, spatial variability within census tracts for $PM_{2.5}$ is smaller than for benzene. The CVs for $PM_{2.5}$ concentrations range from less than 10% to up to 70% in different parts of the study area. The CV for 95th-percentile exposures are typically smaller but could be as high as 50% depending on size of the census tract and nearby influences from roadway or point sources. The CVs for the E/C ratios are also small (<30%) and similar in spatial distribution of the exposure coefficients. Overall, these results indicate that the hybrid modeling analysis linked with exposure modeling tools yields more detailed information on exposures than can be obtained by using central site monitoring data alone in conducting cohort or community-level air pollution epidemiological studies.

SUMMARY

The extent of variability in spatial and temporal concentration gradients associated with large point sources and roadways presented here is especially important given the growing body of literature on the potential adverse health

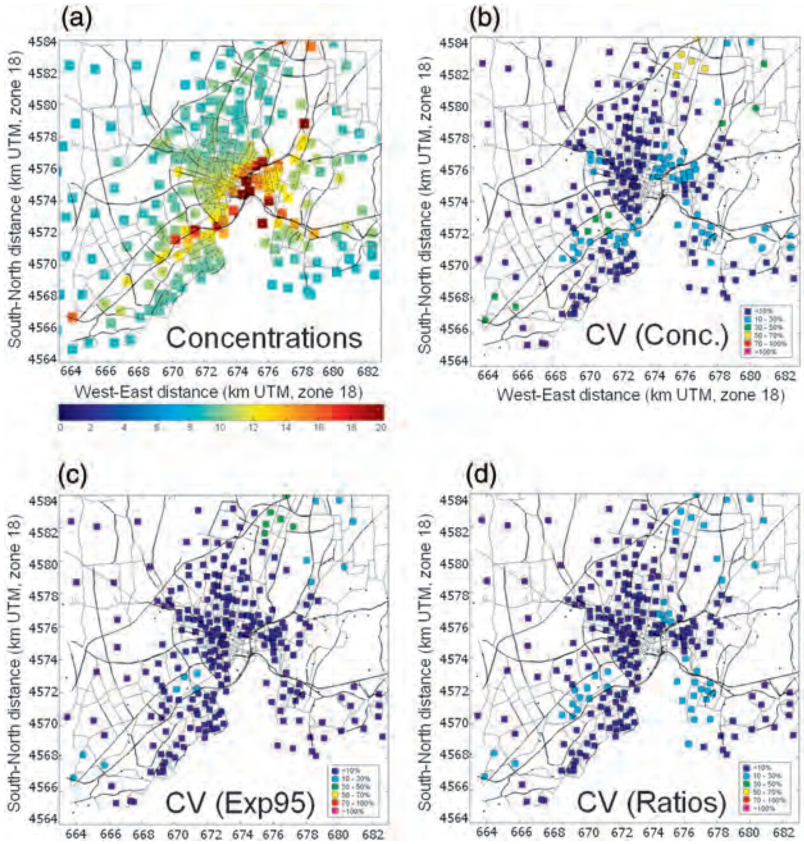

Figure 9. (a) Spatial map of 6-month average $PM_{2.5}$ concentrations, (b) CVs for concentrations, (c) CVs for the 95th percentile of the exposure distribution, and (d) range of variability in the E/C ratios for $PM_{2.5}$ (CV = SD/mean × 100%).

effects associated with elevated concentrations that can occur near these sources. In this analysis, we presented a methodology for using a hybrid modeling approach whereby ambient air quality estimates from the CMAQ photochemical grid model are combined with the AERMOD dispersion model to provide hourly air quality estimates for multiple pollutants at the census-tract and census-block-group levels. This hybrid air quality modeling approach combines the advantages of both air quality models to provide higher spatial resolution than can obtained from either model alone. These hybrid modeled concentrations were then used in driving the two different EPA exposure models, HAPEM and SHEDS. We determined that the local detail provided by this hybrid modeling approach can enhance the analysis of spatially and temporally resolved exposures within a community.

In this study, several assumptions were made that should be re-examined in future applications. For example, the emissions inventory must be consistent when the results from the AERMOD model are added to the CMAQ model. In particular, meteorological data periods must be consistent between AERMOD and the CMAQ models and any monitoring data periods needed for model evaluation purposes. Because model evaluation is a critical part in any modeling study, the air quality models used here have been previously evaluated in various settings.[43–45] In contrast, however, evaluation of exposure models have been limited because of the paucity of studies that collect indoor, outdoor, and personal exposure measurements, along with air exchange information.[46] Clearly there is a need for more evaluation of the key exposure model components (e.g., microenvironmental and roadway proximity factors) in future research.

In addition, estimating uncertainties is an integral part of the health risk assessment process. It is, therefore, desirable to incorporate some treatment of uncertainties in the entire modeling process, including emissions and meteorological inputs, model formulation, monitoring data, and exposure and risk. In this study, a major contribution to the uncertainty in the model simulation results originated from the model inputs rather than from the model formulation. Therefore, to reduce uncertainty in the high-resolution concentration fields, it is important to improve spatial allocation of emissions. For mobile sources, we have developed a practical, readily adaptable methodology to create a spatially resolved, link-based highway vehicle emission inventory. This methodology takes advantage of GIS software to improve the spatial accuracy of the activity information obtained from a Travel Demand Model. An example of application of this methodology in New Haven, CT, is shown in Cook et al.[44] Therefore, it is desirable to incorporate some treatment of uncertainty in the entire modeling process, including emissions, meteorological inputs, model formulation, and exposure.

The models provided in this paper can serve as prototypes for air quality and exposure assessments in future community air pollution health studies. The air quality models can be used to provide the baseline air quality for future assessments of impacts because of regional- or local-scale air pollution control measures. These same models can also be used to estimate the projected air quality and exposures for future years that are dependent on air pollution reduction activities or are due to the addition of new sources in a community. Projected future air quality and exposure model results can then be used to estimate the likely impact of air pollution control measures on human exposures and health in the community, as carried out in the New Haven air accountability feasibility project.

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REFERENCES

1. Dockery, D.W.; Cunningham, J.; Damokosh, A.I.; Neas, L.M.; Spengler, J.D.; Koutrakis, P.; Ware, J.H.; Raizenne, M.; Speizer, F.E. Health Effects of Acid Aerosols on North American Children: Respiratory Symptoms; *Environ. Health Perspect.* **1996**, *104,* 500-505.
2. Gauderman, W.J.; McConnell, R.; Gilliland, F.; London, S.; Thomas, D.; Avol, E.; Vora, H.; Berhane, K.; Rappaport, E.B.; Lurmann, F.; Margolis, H.G.; Peters, J. Association between Air Pollution and Lung Function Growth in Southern California Children; *Am. J. Respir. Crit. Care Med.* **2000**, *162,* 1383-1390.
3. Dockery, D.W.; Speizer, F.E.; Stram, D.O.; Ware, J.H.; Spengler, J.D.; Ferris, B.G., Jr. Effects of Inhalable Particles on Respiratory Health of Children; *Am. Rev. Respir. Dis.* **1989**, *139,* 587-594.
4. Sheppard, L.; Levy, D.; Norris, G.; Larson, T.V.; Koenig, J.Q. Effects of Ambient Air Pollution on Nonelderly Asthma Hospital Admissions in Seattle, Washington, 1987–1994; *Epidemiol.* **1999**, *10,* 23-30.
5. Dominici, F.; Peng, R.D.; Bell, M.L.; Pham, L.; McDermott, A.; Zeger, S.L.; Samet, J.M. Fine Particulate Air Pollution and Hospital Admission for Cardiovascular and Respiratory Diseases; *JAMA* **2006**, *295,* 1127-1134.
6. Burnett, R.T.; Brook, J.; Dann, T.; Delocla, C.; Philips, O.; Cakmak, S.; Vincent, R. Association between Particulate- and Gas-Phase Components of Urban Air Pollution and Daily Mortality in Eight Canadian Cities; *Inhal. Toxicol.* **2000**, *12,* 15-39.
7. Pope, C.A., III, Burnett, R.T.; Thun, M.J.; Calle, E.E.; Krewski, D.; Ito, K.; Thurston, G.D. Lung Cancer, Cardiopulmonary Mortality, and Long-Term Exposure to Fine Particulate Air Pollution; *JAMA* **2002**, *287,* 1132-1141.
8. Adgate, J.L.; Ramachandran, G.; Pratt, G.C.; Waller, L.A.; Sexton, K. Spatial and Temporal Variability in Outdoor, Indoor, and Personal $PM_{2.5}$ Exposure; *Atmos. Environ.* **2002**, *36,* 3255-3265.
9. Adgate, J.L.; Mongin, S.J.; Pratt, G.C.; Zhang, J.; Field, M.P.; Ramachandran, G.; Sexton, K. Relationships between Personal, Indoor, and Outdoor Exposures to Trace Elements in $PM_{2.5}$; *Sci. Total Environ.* **2007**, *386,* 21-32.
10. Ito, K.; Thurston, G.D.; Nadas, A.; Lippmann, M. Monitor-to-Monitor Temporal Correlation of Air Pollution and Weather Variables in the North-Central U.S. *J. Expo. Anal. Environ. Epidemiol.* **2001**, *11,* 21-32.
11. Özkaynak, H.; Palma, T.; Touma, J.; Thurman, J. Modeling Population Exposures to Outdoor Sources of Hazardous Air Pollutants; *J. Expo. Sci. Environ. Epidemiol.* **2008**, *18,* 45-58.
12. Touma, J.S.; Cox, W.M.; Tikvart, J.A. Spatial and Temporal Variability of Ambient Air Toxics Data; *J. Air & Waste Manage. Assoc.* **2006**, *56,* 1716-1725.
13. Westerdahl, D.; Fruin, S.; Sax, T.; Fine, P.; Sioutas, C. Mobile Platform Measurements of Ultrafine Particles and Associated Pollutant Concentrations on Freeways and Residential Streets in Los Angeles; *Atmos. Environ.* **2005**, *39,* 3597-3610.
14. Jerrett, M.; Arain, A.; Kanaroglou, P.; Beckerman, B.; Potoglou, D.; Sahsuvaroglu, T.; Morrison, J.; Giovis, C. A Review and Evaluation of Intraurban Air Pollution Exposure Models; *J. Expo. Anal. Environ. Epidemiol.* **2005**, *15,* 185-204.
15. English, P.; Neutra, R.; Scalf, R.; Sullivan, M.; Waller, L.; Zhu, L. Examining Associations between Childhood Asthma and Traffic Flow Using a Geographic Information System; *Environ. Health Perspect.* **1999**, *107,* 761-767.
16. Jerrett, M.; Burnett, R.T.; Ma, R.; Pope, C.A., III; Krewski, D.; Newbold, K.B.; Thurston, G.; Shi, Y.; Finkelstein, N.; Calle, E.E.; Thun, M.J. Spatial Analysis of Air Pollution and Mortality in Los Angeles; *Epidemiol.* **2005**, *16,* 727-736.
17. Smith, L.; Mukerjee, S.; Gonzales, M.; Stallings, C.; Neas, L.; Norris, G.; Özkaynak, H. Use of GIS and Ancillary Variables to Predict Volatile Organic Compound and Nitrogen Dioxide Levels at Unmonitored Locations; *Atmos. Environ.* **2006**, *40,* 3773-3787.
18. Arain, M.A.; Blair, R.; Finkelstein, N.; Brook, J.R.; Sahsuvaroglu, T.; Beckerman, B.; Zhang, L.; Jerrett, M. The Use of Wind Fields in a Land Use Regression Model to Predict Air Pollution Concentrations for Health Exposure Studies; *Atmos. Environ.* **2007**, *41,* 3453-3464.
19. Marshall, J.D.; Nethery, E.; Brauer, M. Within-Urban Variability in Ambient Air Pollution: Comparison of Estimation Methods; *Atmos. Environ.* **2008**, *42,* 1359-1369.
20. Burke, J.; Zufall, M.; Özkaynak, H. A Population Exposure Model for Particulate Matter: Case Study Results for $PM_{2.5}$ in Philadelphia, PA; *J. Expos. Anal. Environ. Epidemiol.* **2001**, *11,* 470-489.
21. Isakov, V.; Özkaynak, H. In *Air Pollution Modeling and its Applications XIX*; Borrego, C., Ed.; Springer Science & Business Media: Dordrecht, The Netherlands, 2008; pp 616-624.
22. Isakov, V.; Graham, S.; Burke, J.; Özkaynak, H. Linking Air Quality and Exposure Modeling; *EM* **2006**, *September,* 26-29.
23. Georgopoulos, P.; Wang, S.; Vyas, V.; Sun, Q.; Burke, J.; Vedantham, R.; McCurdy, T.; Özkaynak, H. A Source-to-Dose Assessment of Population Exposures to Fine PM and Ozone in Philadelphia, PA, during a Summer 1999 Episode; *J. Expo. Anal. Environ. Epidemiol.* **2005**, *15,* 439-457.
24. Jimenez-Guerrero, P.; Jorba, O.; Baldasano, J.M.; Casso, S. The Use of a Modeling System as a Tool for Air Quality Management: Annual High-Resolution Simulations and Evaluation; *Sci. Total Environ.* **2007**, *390,* 323-340.
25. Levy, J.I.; Greco, S.L.; Spengler, J.D. The Importance of Population Susceptibility for Air Pollution Risk Assessment: a Case Study of Power Plants near Washington, DC; *Environ. Health Perspect.* **2002**, *110*, 1253-1260.
26. Hoffmann, B.; Moebus, S.; Mohlenkamp, S.; Stang, A.; Lehmann, N.; Dragano, N.; Schmermund, A.; Memmesheimer, M.; Mann, K.; Erbel, R.; Jockel, K.H. Residential Exposure to Traffic is Associated with Coronary Atherosclerosis; *Circulation* **2007**, *116,* 489-496.
27. Zambon, P.; Ricci, P.; Bovo, E.; Casula, A.; Gattolin, M.; Fiore, A.R.; Chiosi, F.; Guzzinati, S. Sarcoma Risk and Dioxin Emissions from Incinerators and Industrial Plants: a Population-Based Case-Control Study (Italy); *Environ. Health* **2007**, *6,* 19.
28. Klepeis, N.E.; Nelson, W.C.; Ott, W.R.; Robinson, J.P.; Tsang, A.M.; Switzer, P.; Behar, J.V.; Hern, S.C.; Engelmann, W.H. The National Human Activity Pattern Survey (NHAPS): a Resource for Assessing Exposure to Environmental Pollutants; *J. Expo. Anal. Environ. Epidemiol.* **2001**, *11,* 231-252.
29. Ozkaynak, H.; Xue, J.; Spengler, J.; Wallace, L.; Pellizzari, E.; Jenkins, P. Personal Exposure to Airborne Particles and Metals: Results from the Particle TEAM Study in Riverside, California; *J. Expo. Anal. Environ. Epidemiol.* **1996**, *6,* 57-78.
30. Kinney, P.L.; Chillrud, S.N.; Ramstrom, S.; Ross, J.; Spengler, J.D. Exposures to Multiple Air Toxics in New York City; *Environ. Health Perspect.* **2002**, *110(Suppl 4),* 539-546.
31. Isakov, V.; Irwin, J.; Ching, J. Using CMAQ for Exposure Modeling and Characterizing the Sub-Grid Variability for Exposure Estimates; *J. Appl. Meteorol. Climatol.* **2007**, *46,* 1354-1371.
32. Rosenbaum, A.S.; Axelrad, T.J.; Woodruff, Y.H.; Wei, M.P.; Ligocki, M.; Cohen, J.P. National Estimates of Outdoor Air Toxics Concentrations; *J. Air & Waste Manage. Assoc.* **1999**, *49,* 1138-1152.
33. Touma, J.S.; Isakov, V.; Ching, J.; Seigneur, C. Air Quality Modeling of Hazardous Pollutants: Current Status and Future Directions; *J. Air & Waste Manage. Assoc.* **2006**, *56,* 547-558.
34. Byun, D.W.; Schere, K. Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System; *Appl. Mechanics Rev.* **2006**, *59,* 51-77.

35. Cimorelli, A.J.; Perry, S.G.; Venkatram, A.; Weil, J.C.; Paine, R.J.; Wilson, R.B.; Lee, R.F.; Peters, W.D.; Brode, R.W. AERMOD. A Dispersion Model for Industrial Source Applications. Part I: General Model Formulation and Boundary Layer Characterization; *J. Appl. Meteorol.* **2005**, *44,* 682-693.
36. Stein, A.F.; Isakov, V.; Godowitch, J.; Draxler, R.R. A Hybrid Approach to Resolve Pollutant Concentrations in an Urban Area; *Atmos. Environ.* **2007**, *41,* 9410-9426.
37. *1999 National-Scale Air Toxics Assessment*; U.S. Environmental Protection Agency; Office of Air Quality Planning and Standards: Research Triangle Park, NC, 2004; available at *http://www.epa.gov/ttn/atw/nata1999/* (accessed November 7, 2007).
38. *Census 2000 Data*; U.S. Census Bureau; Systems Support Division: Washington, DC, 2002; available at *http://www.census.gov/main/www/cen2000.html* (accessed April 26, 2008).
39. McCurdy, T.; Geln, G.; Smith, L.; Lakkadi, Y. The National Exposure Research 615 Laboratory's Consolidated Human Activity Database; *J. Expo. Anal. Environ. Epidemiol.* **2000**, *10,* 566-578.
40. Efroymson, R.E.; Murphy, D.L. Ecological Risk Assessment of Multimedia Hazardous Air Pollutants: Estimating Exposure and Effects; *Sci. Total Environ.* **2001**, *27,* 219-230.
41. *New Haven Community Clean Air Initiative*; U.S. Environmental Protection Agency; Office of Air and Radiation: Research Triangle Park, NC, 2008; available at *http://www.epa.gov/air/toxicair/community/newhaven.html* (accessed April 14, 2008).
42. Gilliland, A.B.; Appel, K.W.; Pinder, R.W.; Dennis, R.L. Seasonal NH_3 Emissions for the Continental United States: Inverse Model Estimation and Evaluation; *Atmos. Environ.* **2006**, *40,* 4986-4998.
43. Luecken, D.J.; Hutzell, W.T.; Gipson, G.L. Development and Analysis of Air Quality Modeling Simulations for Hazardous Air Pollutants; *Atmos. Environ.* **2006**, *40,* 5087-5096.
44. Cook, R.; Isakov, V.; Touma, J.; Benjey, W.; Thurman, J.; Kinnee, E.; Ensley, D. Resolving Local Scale Emissions for Modeling Air Quality near Roadways; *J. Air & Waste Manage. Assoc.* **2008**, *58,* 451-461.
45. Appel, K.W.; Bhave, P.V.; Gilliland, A.B.; Sarwar, G.; Roselle, S.J. Evaluation of the Community Multiscale Air Quality (CMAQ) Model Version 4.5: Sensitivities Impacting Model Performance. Part II: Particulate Matter; *Atmos. Environ.* **2008**, *42,* 6057-6066.
46. Burke J.; Rea, A.; Suggs, J.; Williams, R.; Xue, J.; Özkaynak, H. Ambient Particulate Matter Exposures: a Comparison of SHEDS-PM Exposure Model Predictions and Estimates Derived from Measurements Collected during NERL's RTP PM Panel Study. In *ISEA Conference Proceedings*; International Society of Exposure Analysis: Durham, NC, 2002.

About the Authors

Vlad Isakov, Jawad S. Touma, and Janet Burke are physical scientists, and Halûk Özkaynak is a senior research scientist with the EPA Office of Research and Development (ORD) National Exposure Research Laboratory in Research Triangle Park, NC. Danelle T. Lobdell is an epidemiologist with the EPA ORD National Health and Environmental Effects Research Laboratory in Research Triangle Park, NC. Ted Palma is a physical scientist with the EPA Office of Air Quality, Planning, and Standards in Research Triangle Park, NC. Arlene Rosenbaum is a senior scientist with ICF International in San Francisco, CA. Please address correspondence to: Vlad Isakov, Ph.D., U.S. Environmental Protection Agency, Mail Drop E243-04, 109 T.W. Alexander Drive, Research Triangle Park, NC 27711; phone: +1-919-541-2494; fax: +1-919-541-1379; e-mail: Isakov.Vlad@epa.gov.