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Assessment of SHEDS model for air sample placement based on population exposure estimates following a *Bacillus anthracis* outdoor release

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by

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This document has been reviewed by the U.S. Environmental Protection Agency, Office of Research and Development, and approved for publication.

Abstract

As part of EPA/ORD's Homeland Security research program, there is a need to improve strategies for emergency response following a wide-area release of a biological agent. Modeling tools that simulate the dispersion of biological agents for a wide-area release may be used to prioritize air sample placement based on estimated concentrations. However, dispersion models don't account for people's behaviors and activities which could result in some populations having greater risk of exposure. Human exposure models that account for variability in population demographics, human activity patterns, and the factors influencing infiltration of outdoor air indoors have previously been developed, and could be used to better guide decontamination efforts by incorporating potential risk of exposure in air sampling strategies.

To explore this, a case study application was performed to assess the utility of the Stochastic Human Exposure and Dose Simulation for Particulate Matter (SHEDS-PM) model that provides estimates of human exposures by simulating representative individuals for a specific geographic location. The individuals time series of exposure and dose are estimated using human activity pattern data matched to each individual and the concentrations for each location they spend time in such as outdoors, indoors, and in vehicles. Results from the case study highlighted the impact that demographics and other factors such as day of week have on model estimates of exposure and dose due to their influence on activity patterns, as well as the importance of accounting for population mobility. Key advantages of the SHEDS model and its output identified through this case study are summarized, as well as current limitations and options for addressing them.

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Acronyms and Abbreviations

Ba	Bacillus anthracis
CHAD	Consolidated Human Activity Database
GUI	Graphical user interface
LANL	Los Alamos National Laboratory
MMD	Mass median diameter
PM	Particulate matter
QUIC	Quick Urban and Industrial Complex
SHEDS	Stochastic Human Exposure and Dose Simulation
Yp	Yersinia pestis

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1. Introduction

As part of EPA/ORD's Homeland Security research program, there is a need to improve strategies for emergency response following a wide-area release of a biological agent. Estimating the potential risk of human exposures to biological agents for this type of scenario could provide useful information to support these strategies, given that human behavior and activities can impact the level of exposures. For example, people typically spend much of their time indoors (>80%), and the amount of outdoor air that gets indoors depends on several factors including building characteristics, meteorological conditions, and occupant behaviors. Population mobility within an area such as for work and school commuting, will also impact exposures if levels at those locations differ from the home location. Human exposure models that account for variability in population demographics, human activity patterns, and the factors influencing infiltration indoors have previously been developed to predict exposures to air pollutants for exposure and risk assessments. This type of modeling may also be useful for informing emergency response and planning for wide-area releases of airborne biological agents.

To explore this, research was initiated to assess the utility of a specific model, the Stochastic Human Exposure and Dose Simulation for Particulate Matter (SHEDS-PM), for estimating population distributions of exposure and dose for biological agents such as *Bacillus anthracis* following an outdoor release within an urban area.

The SHEDS-PM model is a physically-based probabilistic model for estimating population exposures and dose for particulate matter (PM) air pollution that was previously developed by EPA/ORD's National Exposure Research Laboratory (NERL). The SHEDS-PM model estimates population distributions of exposure and dose by simulating the time series of exposure for individuals that demographically represent a population of interest. US Census demographic data are used to randomly select individuals from the population, and human activity pattern data from EPA's Consolidated Human Activity Pattern Database (CHAD) are randomly assigned to each simulated individual to account for the time people spend in different locations (i.e. indoors, outdoors, in vehicles). Time varying exposures are calculated for each simulated individual based on PM concentrations and exposure factors provided as input to the model. The model algorithms also calculate inhaled PM dose by estimated breathing rates that vary with physical activity over the time series of exposures, as well as deposited PM dose based on particle-size specific deposition to three regions of the lung. Statistical methods for incorporating both variability and uncertainty in the model inputs are used to obtain the predicted distribution of exposure and dose that characterizes the variability across the population, and the uncertainty associated with those predicted distributions.

SHEDS-PM has previously been applied for estimating population distributions of exposures to PM_{2.5}, particles less than 2.5 µm in diameter (Berrocal et al., 2011; Cao and Frey, 2011; Isakov et al., 2009). However, the model is not specific to PM_{2.5} as the model algorithms have the flexibility to simulate particles of different sizes and density. The SHEDS-PM model can therefore be applied to airborne biological agents, and the output can provide the range in exposure and dose across a population (variability), as well as the likelihood of exposures above a certain level. Additional relevant features of the SHEDS-PM model include:

- Simulates individuals representing the population of a specific geographic location in the U.S.
- Particle size distribution can be specified as an input
- Uses a microenvironmental approach to estimate concentrations for each location an individual spends time in (indoors/outdoors/in-vehicles)

- Calculates inhalation exposure and dose (inhaled dose, deposited dose) for airborne particles
- Accounts for movement of commuters away from home location
- Has user interface for selecting model inputs and visualizing results

In addition, this approach has previously been used as the human exposure modeling component of a source-to-dose-to-effect modeling framework for emergency events that was applied to assess the impact of hypothetical releases of *Bacillus anthracis* spores (Isukapalli et al., 2008).

Therefore, the overall goal of this research was to assess the utility of the SHEDS-PM model for supporting EPA's emergency response research needs for a wide-area release of a biological agent. Program partners had identified air sample placement as a high-priority research need, and the SHEDS model could provide population exposure estimates to inform air sample placement. The approach used for the assessment focused on development of a demonstration case study application of the model. The case study approach identified requirements for application of the model to outdoor releases of biological agents, including input data for the model and model code refinements needed.

This report summarizes the research conducted to date for the three main aspects of this assessment: (a) perform test runs of the SHEDS-PM model using outdoor concentrations of a biological agent in order to identify and prioritize required changes to the model code, (b) obtain air concentrations from an outdoor release scenario for a biological agent to use as input for application of the model, and (c) apply the model using the air concentrations from the outdoor release scenario to demonstrate the potential utility of the model output.

2. Methods

2.1. Overview of SHEDS-PM

SHEDS-PM was developed using MATLAB® software (The Mathworks Inc., Natick, MA) and compiled as a stand-alone executable that runs on Windows operating systems without any specific software required. The model has a graphical user interface (GUI) for selecting input data files, specifying model run parameters, and analysis of model results (Figure 1). To apply SHEDS-PM, the user must provide an input file of outdoor concentrations for the population of interest. The input concentration data should ideally be at the census tract level in terms of spatial resolution but can be from multiple monitoring locations or a single domain-wide concentration, and the temporal resolution can be hourly concentration values or 24-hour average concentrations. The particle size distribution for the input concentration data must also be specified, and includes options for defining mass median diameter (MMD) and standard deviation for up to two size modes. Other required inputs such as population demographic data from the US Census and human activity pattern data are included as databases with the model.

Options for a model run scenario are also selected through the GUI, and include the range of dates and specific census tracts for the run, as well as the number of individuals or percent of population to simulate for each census tract. Human activity diaries are matched to the simulated individuals by age, gender and day type (weekday, Saturday, Sunday) with optional diary matching by employment status and housing type. Additional required inputs include parameters of equations used to estimate concentrations in various locations that people spend time based on the outdoor concentrations supplied as input to the model. Different options for these equations can be selected for each location (e.g. indoors at home, school or store) depending on the amount of data available for the indoor/outdoor

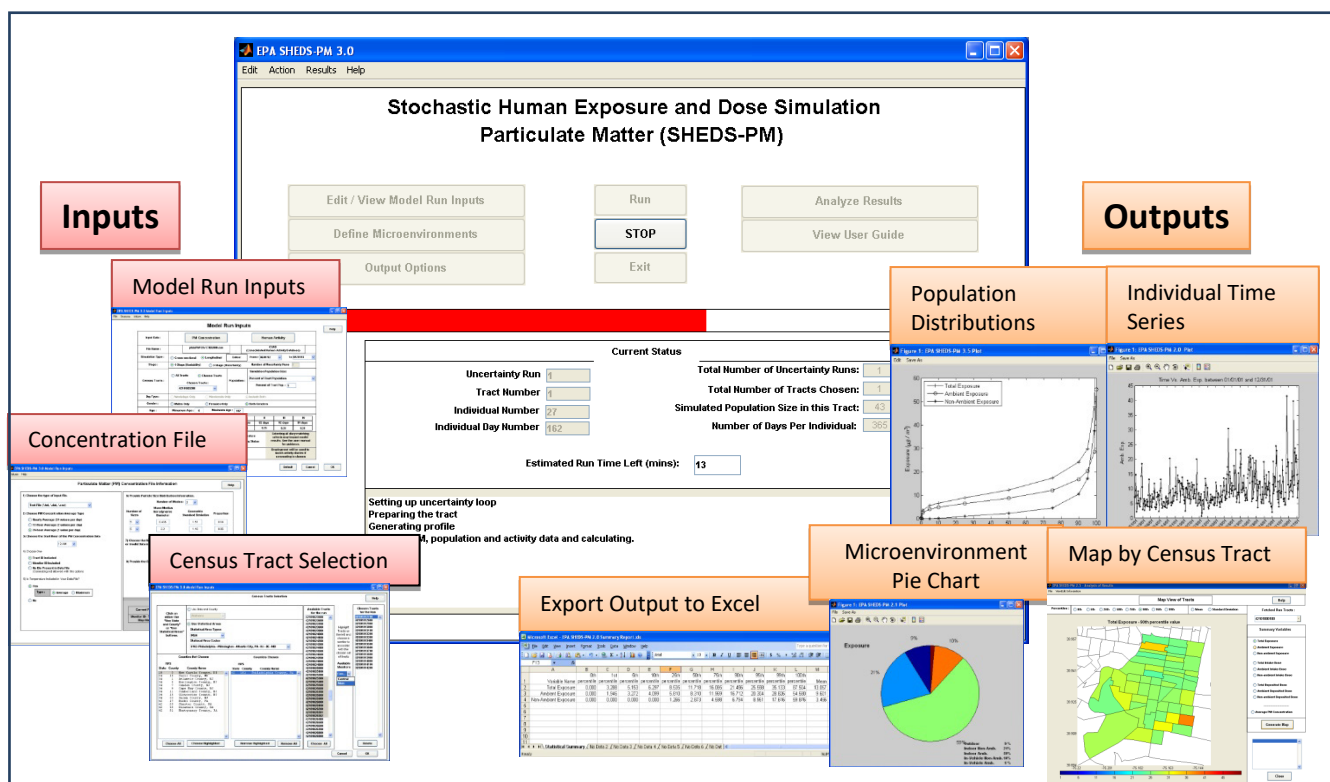


Figure 1. EPA SHEDS-PM 3.7 user interface showing screens for selection of inputs and analysis of model outputs.

concentration relationship. The options include a simple scaling factor, a linear regression equation (with slope and intercept parameters), and a mass balance equation that requires several parameters for calculating indoor concentrations such as penetration, deposition, and air exchange rates.

2.1. Initial test runs of the SHEDS-PM model

Initial test runs were conducted with EPA SHEDS-PM 3.7, the latest version of the stand-alone executable (ver. 12/9/2011), to identify modifications to the model code needed for application to biological agents. Input databases provided in EPA SHEDS-PM 3.7 were used for these test runs, and included census tract population, employment, housing and commuting data from the 2000 U.S. Census, as well as human activity data from CHAD (version 2010 update). Default values for PM_{2.5} particle size distribution and microenvironmental equation parameters were used (Burke and Vedantham, 2009), as these initial test runs were exploratory and focused on the functionality of the model.

Input concentrations for a hypothetical release of a biological agent within an urban area were needed to conduct the model test runs. Options for obtaining concentration data were investigated, and included a search of published measurement studies and model applications. Criteria used to assess available data included relevance to the objectives of this case study application (i.e. data for an outdoor release of *Bacillus anthracis* or similar biological agent), and appropriateness for use as input concentrations to the model (i.e. includes data for multiple census tracts within an urban area and over multiple time periods).

The QUIC (Quick Urban & Industrial Complex) model (<http://www.lanl.gov/projects/quic/>) was identified as an appropriate source of input concentration data from the literature review based on these criteria. The QUIC dispersion modeling system was developed at Los Alamos National Laboratory (LANL) to resolve the three-dimensional flow and plume transport and dispersion of airborne contaminants around buildings at neighborhood scales with fast runtimes (Brown, 2014). The developer of the model at LANL agreed to provide modeled concentration data from a previous application of QUIC with permission from the application sponsor. However, LANL's prior applications of the QUIC model for an outdoor release of *Bacillus anthracis* (*Ba*) were classified, and could not be provided for this project. LANL was able to provide QUIC model output from a simulated release of *Yersinia pestis* (*Yp*) at a single location in Los Angeles, CA since these results were in the public domain and could serve as example concentration output from QUIC for a biological agent in the exploratory initial testing (Inglesby et al., 2000; Inglesby et al, 2002).

LANL provided gridded hourly *Yp* concentrations (in g/m³) across downtown Los Angeles over a 4-hour period from the QUIC model (Figure 2). The release scenario was 100 g of *Yp* released as a line source along a roadway at 10 am on 05/08/2015, and a particle size of 5 microns MMD was used for *Yp* in this simulation. The downtown Los Angeles domain was 3.5 km by 3.5 km in size with a grid resolution of 20 m by 20 m, a higher resolution than a typical census tract. The gridded output was modified to the census tract format required for input to SHEDS-PM using ArcGIS (Esri, Redlands, CA). Spatial Analyst tools in ArcGIS were used to calculate the mean of all grid points within the borders of each census tract, and mean concentration converted to units of µg/m³. The resulting hourly mean census tract concentrations were used to conduct initial test runs of SHEDS-PM.

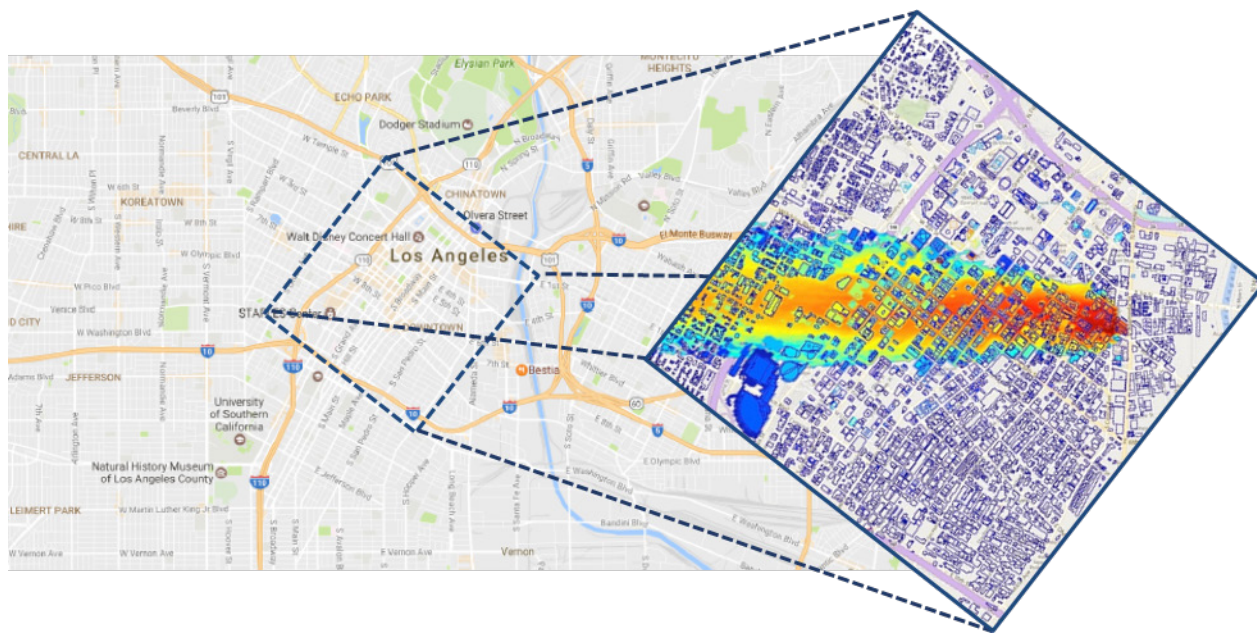


Figure 2. QUIC model domain for Los Angeles simulation showing concentration plume for *Yp* release scenario provided by LANL

2.2. SHEDS-PM refinements

The goal of the initial test runs of the EPA SHEDS-PM 3.7 executable was to identify code modifications required for application of the model to an outdoor release of a biological agent. However, the Windows computing environment had improved substantially since the model code was last changed. Consequently, the SHEDS-PM source code had to be updated first to run within MATLAB on the Windows 10 (64-bit) operating system before any modifications could be made.

A major update to the SHEDS-PM source code was a structural change to the input databases. Open Database Connectivity (ODBC) between MATLAB version R2016b and Microsoft Access 2016 was implemented for the databases used as input to the model. Also, primary keys and other indices were added to the Access input databases to increase data throughput. MATLAB code for connecting to the Access databases was also streamlined using object-oriented classes in MATLAB along with member functions that are called. Additionally, some MATLAB functions were no longer supported and had to be replaced with current functionality, and minor changes in syntax for many MATLAB functions throughout the source code required updating.

In addition to updates required by the current software platform, parts of the code that were identified as hardcoded rather than defined by the inputs needed to be modified. One example is in the code for particle size distribution which is an important input that differs for biological agents. This code was revised to make all variables used in the particle size distribution calculation be defined by the user input specified through the GUI.

The open source repository GitHub was used to manage code changes and archive source code. As incremental changes to the SHEDS-PM source code were made, branches off the main trunk were created to provide inline documentation of all changes. Unit testing was performed to evaluate if the incremental updates worked as expected. All source code and database changes have been committed to a Git repository.

2.3. QUIC model application

Initial test runs of the SHEDS-PM model using QUIC input concentration data for an outdoor release in downtown Los Angeles demonstrated that a combined application of the models could accomplish the goals for the case study. However, the input concentration data provided by LANL from QUIC were not ideal for assessment of the SHEDS model for several reasons. First, the location of the bioagent release for the QUIC simulation was near ‘Skid Row’, a homeless area covering several city blocks to the east of downtown Los Angeles. As a result, the area with highest concentrations was not a typical residential or commercial area, and the most highly exposed population had limited demographic and housing variability. Second, the bioagent simulated was *Yp*, which differs from *Ba* in physical properties that influence concentrations. The 5-micron MMD and decay rate of 10% per minute used for the *Yp* simulation resulted in near zero concentrations after just 30 minutes. The MMD for *Ba* is likely smaller and the decay rate is considered negligible, 1% per minute (Stuart and Wilkening, 2005), so concentrations of *Ba* would be higher over the same simulated time period. Also, the predominant wind direction for Los Angeles is generally from the west, whereas winds from the east were used for the *Yp* simulation.

To create input concentrations specifically for the SHEDS assessment, LANL provided EPA/ORD with a license for the QUIC model along with the set of inputs used for the Los Angeles *Yp* application. A

hypothetical *Ba* release scenario for Los Angeles was developed for the QUIC model simulation with the goal of producing higher concentrations in more populated areas over a longer time.

2.3.1. Development of *Bacillus anthracis* release scenario

Meteorological conditions conducive to higher concentrations were identified using data from the Los Angeles Intl Airport (LAX). Five-minute wind direction and wind speed data for 2017 (obtained from <https://mesonet.agron.iastate.edu/ASOS/>) showed both a diurnal and seasonal trend of alternating between land and sea breeze conditions. The diurnal trend for all of 2017 is shown in Figure 3. Overnight and in the morning, winds tended to be from the east at lower wind speeds (land breeze), which transitions after sunrise to winds from the west with higher wind speeds (sea breeze). Sea breeze conditions dominate throughout the daytime and continue until late evening with a transition back to land breeze after sunset. Changing wind direction and wind speed during these transitions between land and sea breeze conditions should result in a release being dispersed across a larger area compared to the more consistent winds midday, for example, and were further investigated for this scenario. The time of day for the transition between wind patterns changed with season, with April and May 2017 having the transition from land to sea breeze occur around 9 am. Several dates in April and May were identified as having similar transitions between land and sea breeze conditions that could be used for this scenario.

Pershing Square was selected for the release because of its central location within the QUIC domain and proximity to the downtown area with tall buildings (Figure 4). Public events are often held in Pershing Square, such as lunchtime concerts and Friday night movies. A large public event occurred at Pershing Square on Saturday April 22, 2017 starting at 9 AM. Conditions on this date had the potential for higher concentrations over a broad area with calm winds at 10 am changing to winds from the southeast and then from the west with higher wind speeds by 11 am, and so was selected for the QUIC model scenario. This outdoor release scenario was used to examine exposures for the population residing at their home location on a Saturday morning (not those attending the event in Pershing Square).

2.3.2. Model inputs

QUIC version 6.26 (02/03/2017) was applied for a release of *Ba* (100 g) as a line source along the road adjacent to the east side of the park for approximately 100 m over 5 minutes beginning at 10 am on April 22, 2017. Particle size distribution was specified as 3.5 μm MMD and geometric standard deviation of 1.05, to represent the relatively uniform size distribution of *Ba* spores assumed for weapons-grade quality anthrax (Nicogossian et al., 2011). Wind speed and wind direction inputs for the 2-hour simulation are shown in Table 1. QUIC output concentrations (in g/m^3) were saved every 15 minutes, and output to text files.

2.4. SHEDS-PM model application

EPA SHEDS-PM 3.7a, the updated version of the source code running within MATLAB R2016b (Windows 10), was applied with *Ba* input concentrations produced by the QUIC model for the *Ba* release scenario described above. Figure 5 shows the 27 census tracts for Los Angeles that were at least partially within the QUIC model domain. To create census tract concentration input files for the SHEDS-PM application, the Spatial Analyst tools in ArcGIS (Esri, Redlands, CA) were used to calculate the mean of all grid points from QUIC within the borders of each census tract for each 15-minute output file from QUIC. The 15-minute census tract concentrations were averaged over each hour to provide hourly averaged input concentrations for each census tract and converted to units of $\mu\text{g}/\text{m}^3$. The particle size distribution was set to the same as specified for the QUIC simulation: 3.5 μm MMD and geometric standard deviation of 1.05.

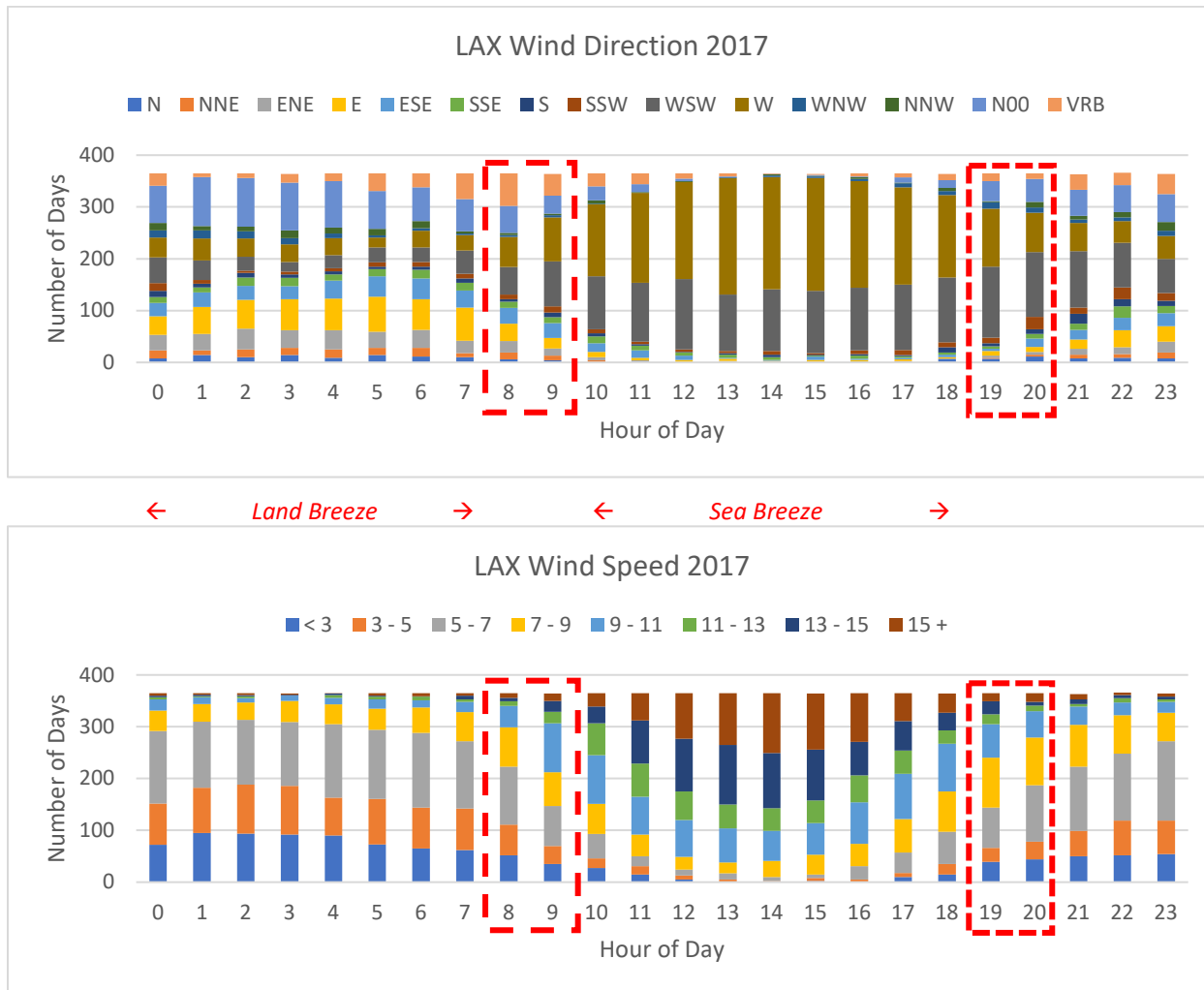


Figure 3. Meteorological data (wind direction, wind speed) from Los Angeles Intl Airport (LAX) for 2017 by hour of the day illustrating pattern of nighttime land breeze (easterly winds with lower wind speeds) and daytime sea breeze (westerly winds with higher wind speeds), with transition periods noted by red dash boxes. Wind direction divided into 12 categories of 30 degrees each, with additional categories for no wind (N00) and variable wind (VRB). Wind speed units=miles per hour.

Input databases for the 2000 U.S. Census, as well as human activity data from CHAD (version 2010 update) currently available in the SHEDS-PM model were used. The number of individuals simulated per tract was 100, a minimum representative sample for characterizing variability in population demographics for a census tract. Time-activity diaries were matched to each simulated individual based on the default criteria of age, gender and day of week. Microenvironments specified for the simulation included outdoors, indoors at home, school, office, store or other indoor locations, as well as in vehicles. Default values for microenvironmental equation parameters available for $PM_{2.5}$ were used (Table 2), since the particle size distribution for the *Ba* input concentrations was similar ($3.5 \mu m$). Daily inhalation exposure ($\mu g/m^3$), inhaled dose (μg), and deposited dose (μg) for each simulated individual were output from the model.

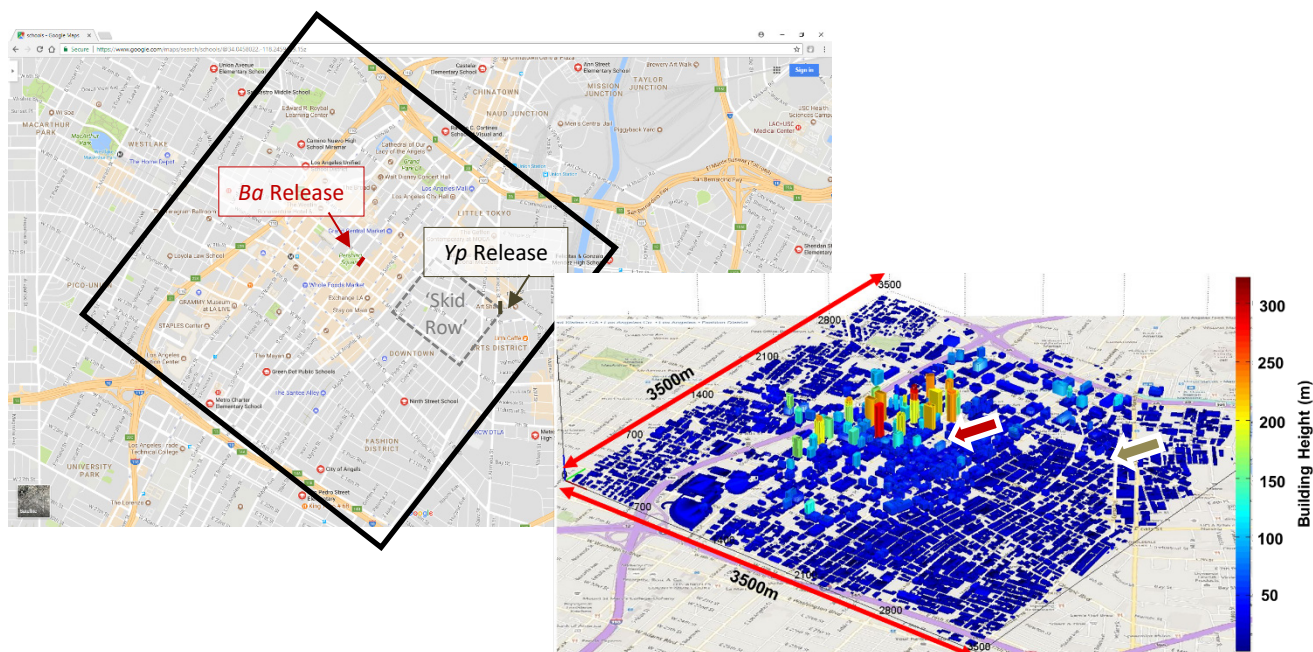


Figure 4. Location of hypothetical releases of biological agents used in QUIC model application scenarios (*Ba* release at Pershing Square and *Yp* release near Skid Row) (left); and 3D view of buildings within Los Angeles domain (color indicates building height) (right).

Table 1. Wind direction and wind speed inputs used in application of QUIC model for Pershing Square *Ba* release scenario April 22, 2017.

Time	Wind Direction (degrees)	Wind Speed (m s^{-1})
10:00	30	0.5
10:15	170	2.1
10:30	160	2.1
10:45	270	4.1
11:00	270	4.1
11:15	280	4.1
11:30	270	4.1
11:45	280	5.1
12:00	270	5.7

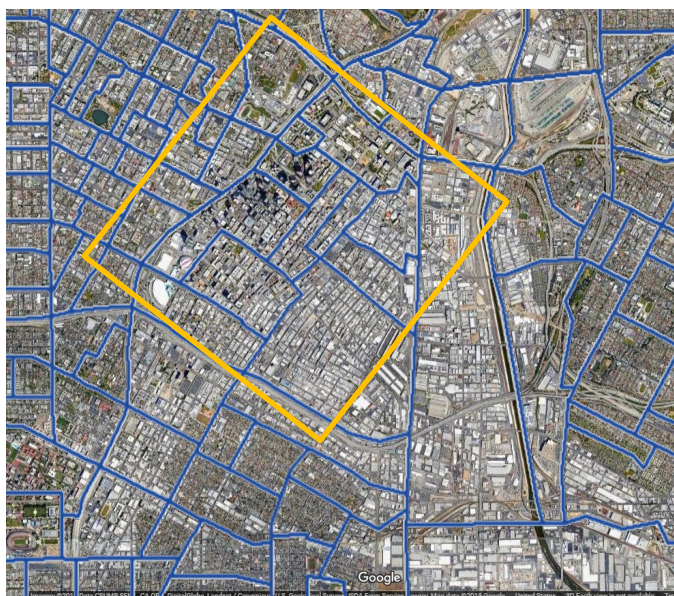


Figure 5. Satellite view of Los Angeles with census tract boundaries (blue) and QUIC model domain (yellow).

Table 2. Input parameters for SHEDS-PM microenvironment concentration equations.

Microenvironment		Equation Type	Parameter	Parameter Value*
Indoors	All Outdoors	Scaling factor		1.0
	Home	Mass balance	Penetration	$N(0.97, 0.02)$
			Deposition	$N(0.3, 0.095)$
			Air exchange rate: - Spring	$\log N(0.449, 2.226)$
			Volume: - Single family detached - Single family attached - Apartment - Other	$\log N(411.6, 1.649)$ $\log N(327.0, 1.649)$ $\log N(219.2, 1.553)$ $\log N(208.5, 1.433)$
	Office	Scaling factor		0.3
	School	Scaling factor		0.6
	Store	Scaling factor		0.75
	Other Indoor	Scaling factor		0.5
	In vehicle	Scaling factor		0.8

* $N(x,y)$ = Normal distribution with mean x and standard deviation y ; $\log N(x,y)$ = Lognormal distribution with geometric mean x and geometric standard deviation y .

To compare estimates of *Ba* exposure and dose when work commuting is considered, an additional SHEDS-PM model run was conducted with the commuting algorithm applied. This algorithm uses data from the US Census on where the population from each tract commutes to for work. If a simulated individual is employed, and the activity diary assigned to that individual includes the work activity, then the individual is randomly assigned to a work tract. The concentration for the work tract is used to calculate exposure and dose for that individual during the work activity instead of the home tract concentration. However, the work tract could be the home tract depending on the commuting proportions for each tract. All the same SHEDS-PM model run specifications were used, along with the same input concentration data from the QUIC simulation except that the date in the input concentration file was changed to a weekday (April 24, 2017) and diary matching by employment status required for simulation of commuting.

Since *Ba* concentrations for only 27 census tracts were able to be obtained from the QUIC model domain for this scenario, the commuting algorithm in SHEDS-PM was only able to move individuals between this limited set of census tracts. An additional SHEDS-PM simulation was performed to address that individuals living outside the QUIC domain commute to the area of Los Angeles for work. This third simulation was performed using a total of 326 census tracts with *Ba* concentrations of zero added to the input file for all the other census tracts and the same SHEDS-PM model run specifications as above.

3. Results

3.1. QUIC modeled concentrations

Application of QUIC for the *Ba* release scenario described above provided a time series of input concentrations needed for the assessment of SHEDS-PM. The QUIC modeled concentrations are displayed in Figure 6, which shows the progression of the concentration plume at 15-minute intervals from the simulation of a *Ba* release near Pershing Square on April 22, 2017. The plume remains centered over the release location initially (10:15 am), then is gradually dispersed across the downtown area with high-rise buildings (10:30 am). The plume continues to expand over more residential areas to the north (10:45 am) until the wind direction shifts to from the west (11:00 am). The higher wind speeds with winds from the west, further disperses the concentration plume to the east over additional areas north and east of Pershing Square (11:15 am). This hypothetical *Ba* release scenario resulted in higher concentrations in more populated areas over a longer time period for the SHEDS-PM case study when compared to the previous *Yp* release scenario.

As described above, hourly mean *Ba* concentrations for each of the 27 census tracts within the QUIC modeling domain were calculated from the gridded concentration output from QUIC to create the input concentration file for SHEDS-PM. Figure 7 shows the variation in *Ba* concentrations in $\mu\text{g}/\text{m}^3$ by hour of the day for 17 of the census tracts that had above zero concentrations for at least one hour (i.e. 10 census tracts had zero concentration for all hours). Census tract mean concentrations were zero until the release at 10 am. Census tracts with red and orange bars had the highest mean concentrations over the first hour of the simulation (hour 10), and lower concentrations for the second hour (hour 11), with concentrations dropping to very low or to zero by the third hour (hour 12). Census tracts with yellow bars had mean concentrations in the middle of the range, with some tracts increasing in concentration from the first hour to the second hour. Census tracts with blue bars had lower mean concentrations and typically only above zero for one hour (11 am). Figure 8 (right) displays the location of the census tracts within the QUIC model domain (yellow) and relative to the release.

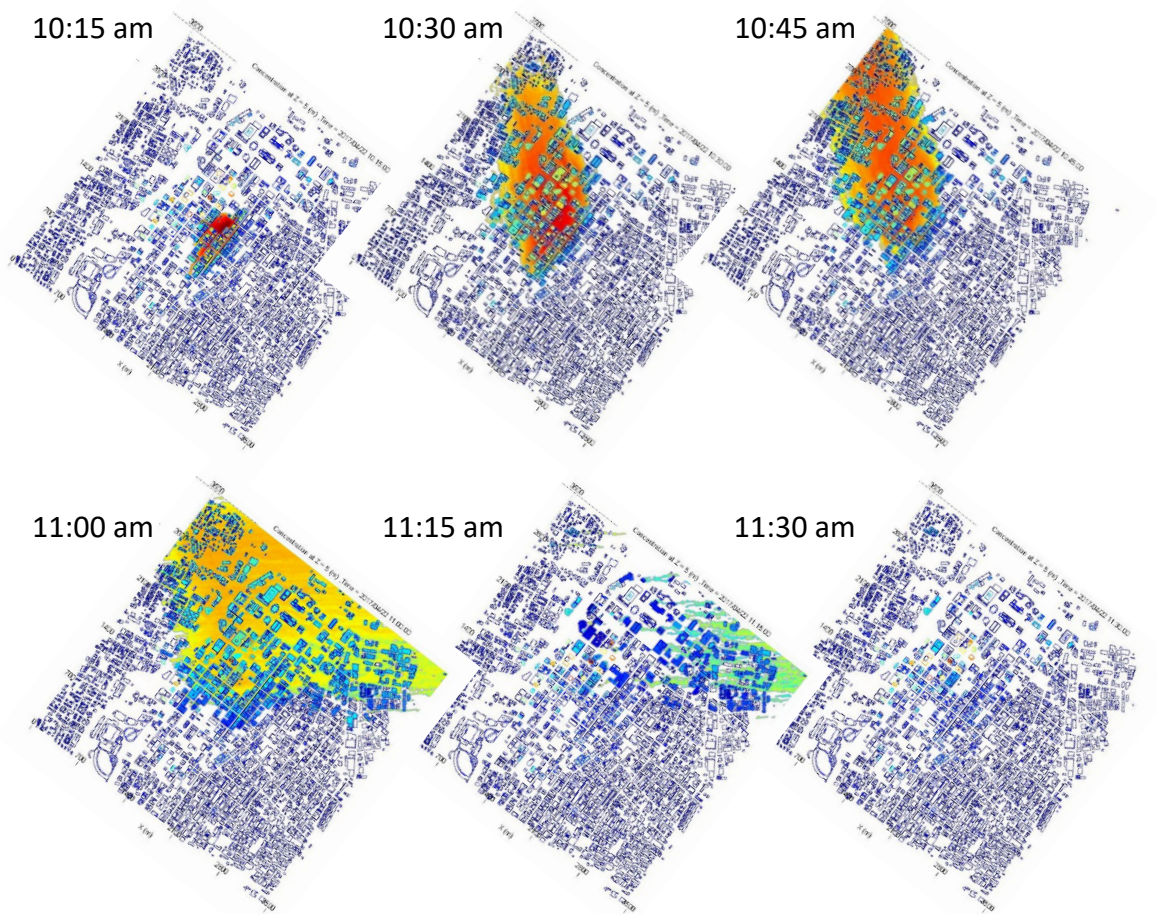


Figure 6. QUIC model results for Pershing Square *Ba* release scenario April 22, 2017.

The table in Figure 8 shows that total population also varied among the census tracts. Several census tracts with higher concentrations also had larger populations (approx. 4000 people or more for 207300, 207500, 208000, 208300), while other tracts with higher concentrations had fewer people (207710, 209200). The type of housing also varied by census tract, with similar numbers of single family homes and apartments for a few tracts, whereas housing for most tracts was dominated by apartments. Most census tracts had similar levels of employed versus unemployed people, except for 206020. Tract 206020 had unusual demographics (high total population with none employed and few housing units) due to it containing a large prison and railyard, so it was excluded from the SHEDS-PM simulation.

3.2. SHEDS-PM modeled exposure and dose

The SHEDS-PM model was applied using the hourly mean *Ba* concentrations for April 22, 2017 from the QUIC model, and the results are displayed in Figures 9 through 13. Figure 9 shows the distribution of the daily mean exposure ($\mu\text{g}/\text{m}^3$) and deposited dose (μg) across all simulated individuals, overall and by the different locations they spent time in. In all cases, the median value is zero due to the hours prior to and following the release where concentrations were zero for individuals in the tracts impacted by the

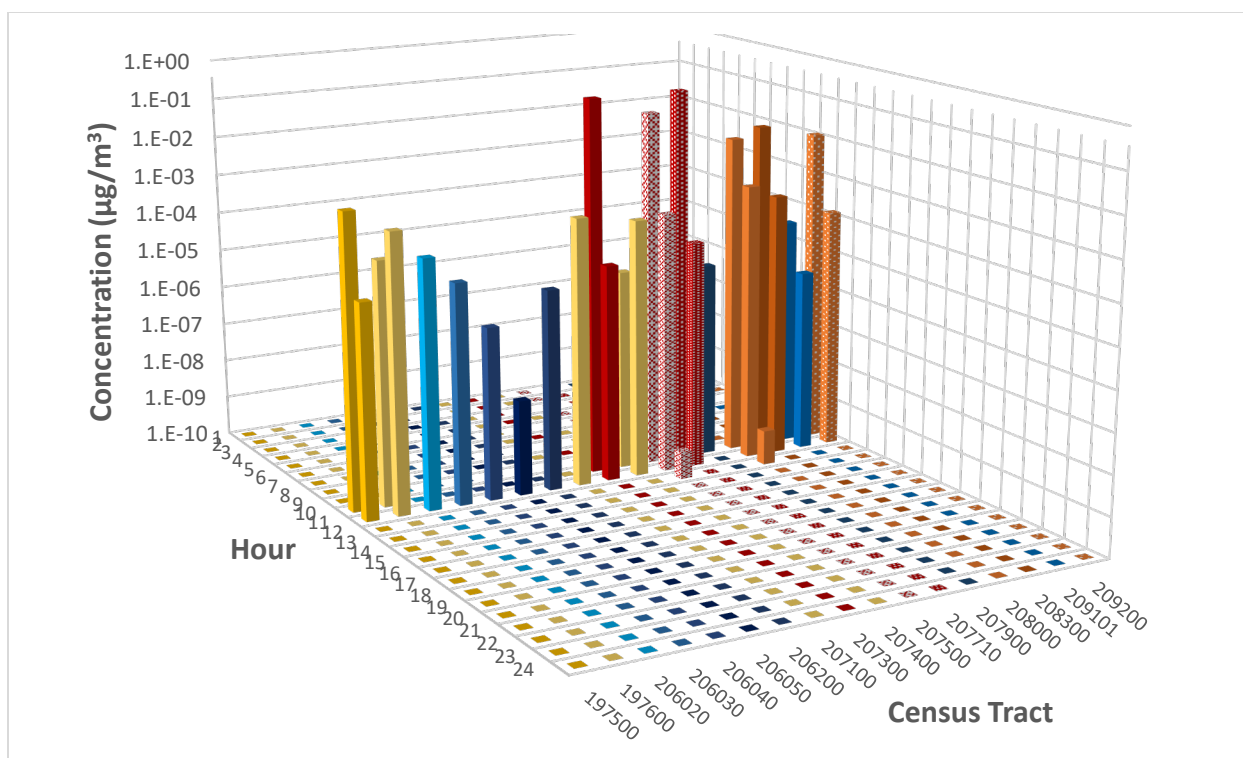


Figure 7. Hourly Ba concentrations ($\mu\text{g}/\text{m}^3$) for census tracts with concentrations above zero.

release, as well as the individuals for tracts not impacted by the plume having concentrations of zero for the entire 24 hours. Daily exposure and dose were much higher for the home location compared to any other location due to individuals spending most of their time at home as shown in Figure 10(a). Since April 22, 2017 was a Saturday, and this simulation matched activity patterns by day of week and did not include any mobility between census tracts such as for commuting, the exposure concentrations for each location differed only by the fraction of the outdoor *Ba* concentration assigned to that location. For example, when a simulated individual spent time outdoors the exposure concentration would be equivalent to the input *Ba* concentration for that hour, whereas for time spent in an office building the exposure concentration would be calculated as 30% of the input *Ba* concentration for that hour (see Table 2).

For the home location, one of the important drivers of indoor concentrations is the air exchange rate which represents the relative volume of air indoors that is exchanged with outdoor air per hour. Many factors influence the air exchange rate in homes such as the size and age of the home, as well as meteorological conditions (temperature, wind speed). Distributions of air exchange rates for different regions based on housing stock and seasons are used as input to the SHEDS-PM model. Figure 11 displays the variability in residential air exchange rates for this simulation, overall and between census tracts. While most homes were assigned air exchange rates of $0.4 - 0.6 \text{ hr}^{-1}$, others had air exchange rates of 1.0 hr^{-1} or higher, which would contribute to greater infiltration of outdoor *Ba* indoors for these homes. Variation between census tracts was also evident, with mean values ranging from $0.52 - 0.76 \text{ hr}^{-1}$, indicating that exposures while indoors at home can also vary due to factors such as air exchange rates.

Census Tract	Total Population	Housing		Employment	
		Total Single Family/ Duplex	Total Apartments	Total Employed	Total Unemployed
197500	5263	758	996	2264	1619
197600	2984	467	477	1182	1049
206020	10852	15	0	18	10868
206030	955	60	250	306	315
206040	3445	322	952	1296	1197
206050	2488	126	489	1038	1032
206200	3477	45	289	765	2547
206300	4995	72	466	1062	3576
207100	5753	332	1239	1632	3212
207300	3739	66	235	847	2788
207400	1237	7	0	0	1094
207500	4098	71	344	1880	2079
207710	1229	15	270	287	921
207900	1993	58	138	835	858
208000	4253	384	731	1211	1534
208300	6893	398	1390	2342	2510
209101	6800	161	1141	2376	2428
209102	4677	54	1007	1756	1785
209200	1467	5	399	563	477
209300	3100	75	909	1189	1244
209520	2772	58	768	1168	948
209820	2708	194	798	919	960
210010	3607	129	715	1187	1403
224010	2529	53	354	886	1095
224200	3067	234	700	1004	1202
224320	3293	198	847	1133	1161
226000	4232	495	514	1337	1897

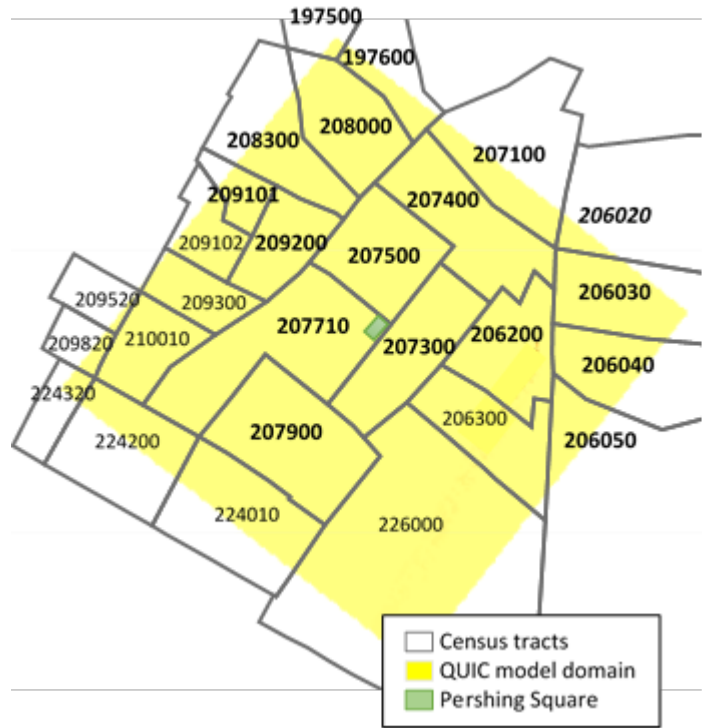


Figure 8. Table of population, housing and employment data for census tracts within the QUIC model domain for Los Angeles, CA with map showing census tract locations (**bold** tracts had *Ba* concentrations above zero following release).

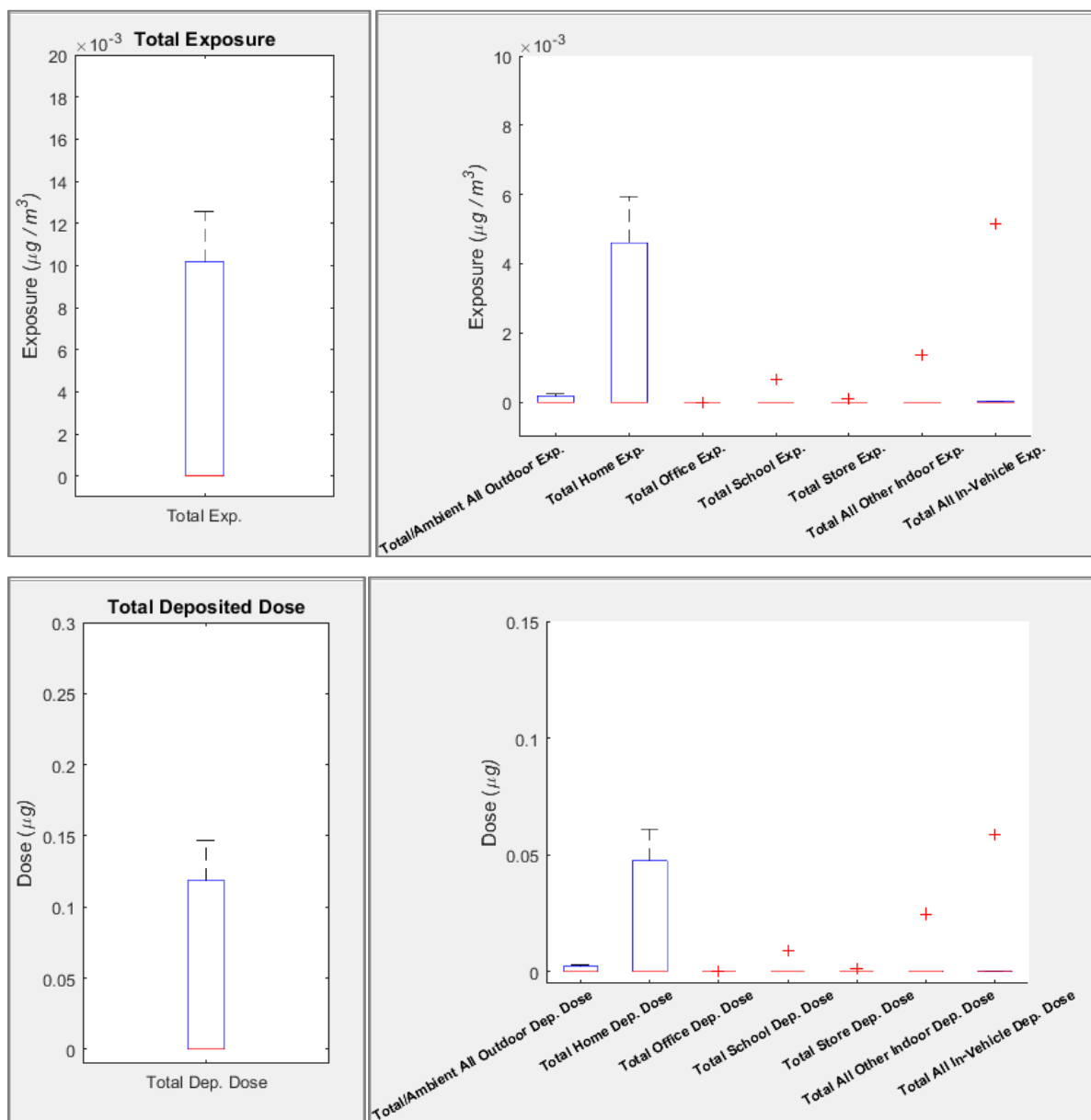


Figure 9. Distribution of daily mean exposure ($\mu\text{g}/\text{m}^3$) and deposited dose (μg) across all SHEDS-PM simulated individuals based on QUIC modeled concentrations for *Ba* release at Pershing Square on Saturday April 22, 2017, overall (left) and by different locations (right). [Note axis scale for total exposure is $\times 10^{-3}$]

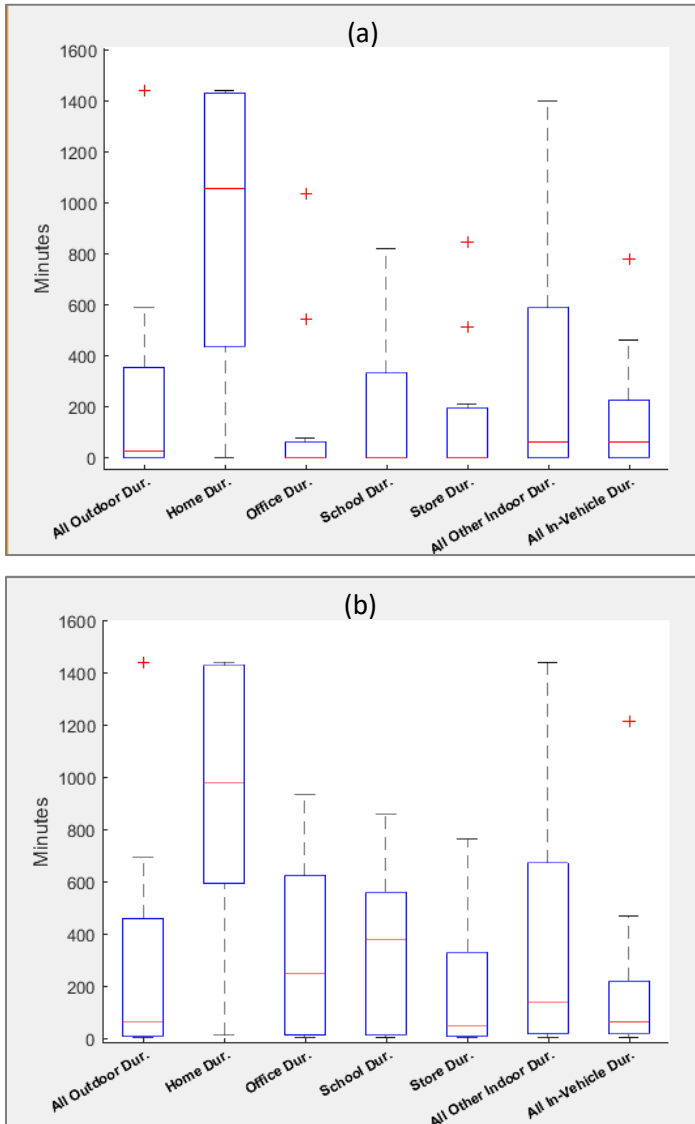


Figure 10. Distribution of time spent in different locations (minutes) across all simulated individuals for (a) weekend (Saturday, no commuting) and (b) weekday with commuting included.

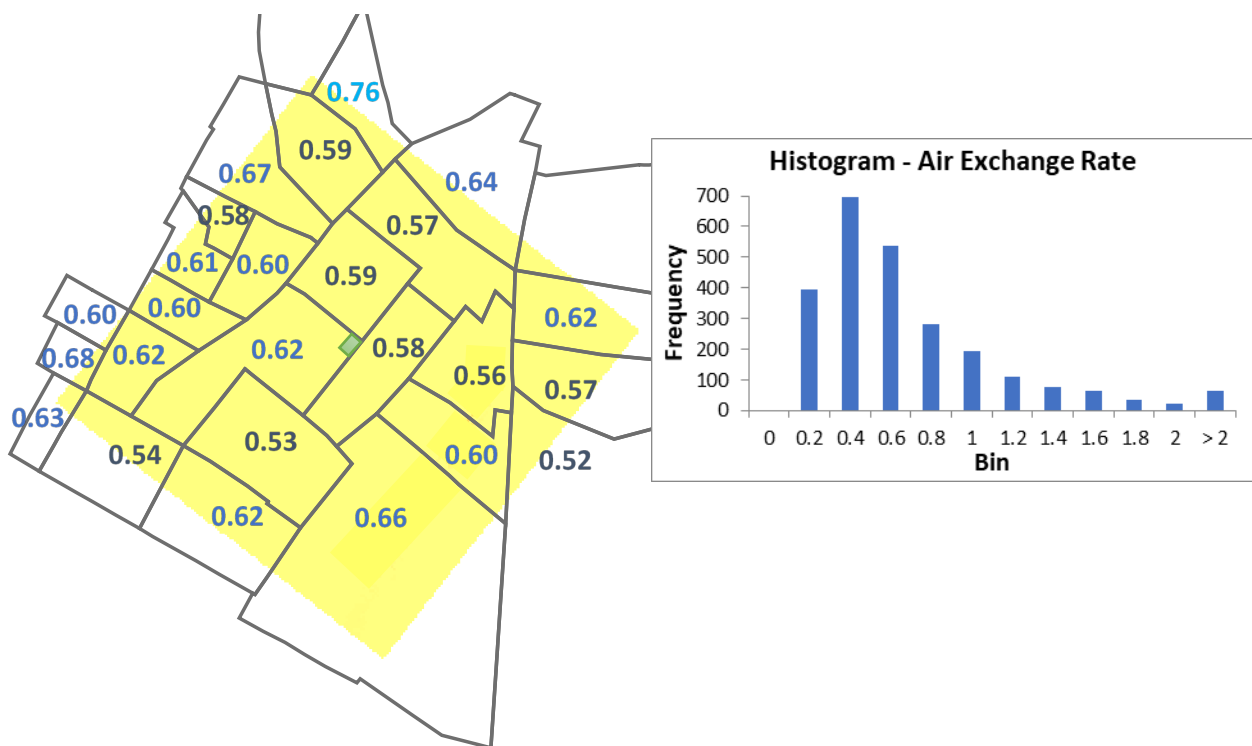


Figure 11. Variability in residential air exchange rates (hr^{-1}) for SHEDS-PM simulation. Census tract mean air exchange rate for 100 simulated individuals in each tract (left) and frequency distribution of air exchange rate for all simulated individuals (n=2500) (right).

Figure 12 shows that the distributions of the daily mean exposure ($\mu\text{g}/\text{m}^3$) and deposited dose (μg) for the three census tracts surrounding the *Ba* release at Pershing Square were different than for all census tracts combined. For these three census tracts (207300, 207710 and 207500), all simulated individuals had daily mean exposures and deposited dose values above zero. Tract 207500 had exposure and deposited dose values similar to the range for all tracts combined, while the other two tracts (207300 and 207710) had exposures 2 to 4 times higher, and deposited dose values as much as an order of magnitude higher. These differences in exposures and deposited dose between census tracts are also shown in the maps of the mean and 99th percentiles for each tract in Figure 13. Only the three census tracts surrounding the *Ba* release at Pershing Square had mean exposure and deposited dose above zero, and individuals living in census tract 207300 had higher exposure and dose.

The potential impact of commuting on exposure and dose for this release scenario was also investigated. As described above, the SHEDS-PM model was applied using the same concentration input file of modeled *Ba* concentrations for the census tracts within the QUIC domain, only the date was modified to a weekday (April 24, 2017) and the commuting option selected for the model run. Although the input concentrations were the same, the activity patterns assigned to the simulated individuals were different since they were selected from weekday diaries, and concentrations from census tracts other than the home tract may have been assigned for individuals when at work. Results for this SHEDS-PM simulation that included commuting are displayed in Figures 14 through 17.

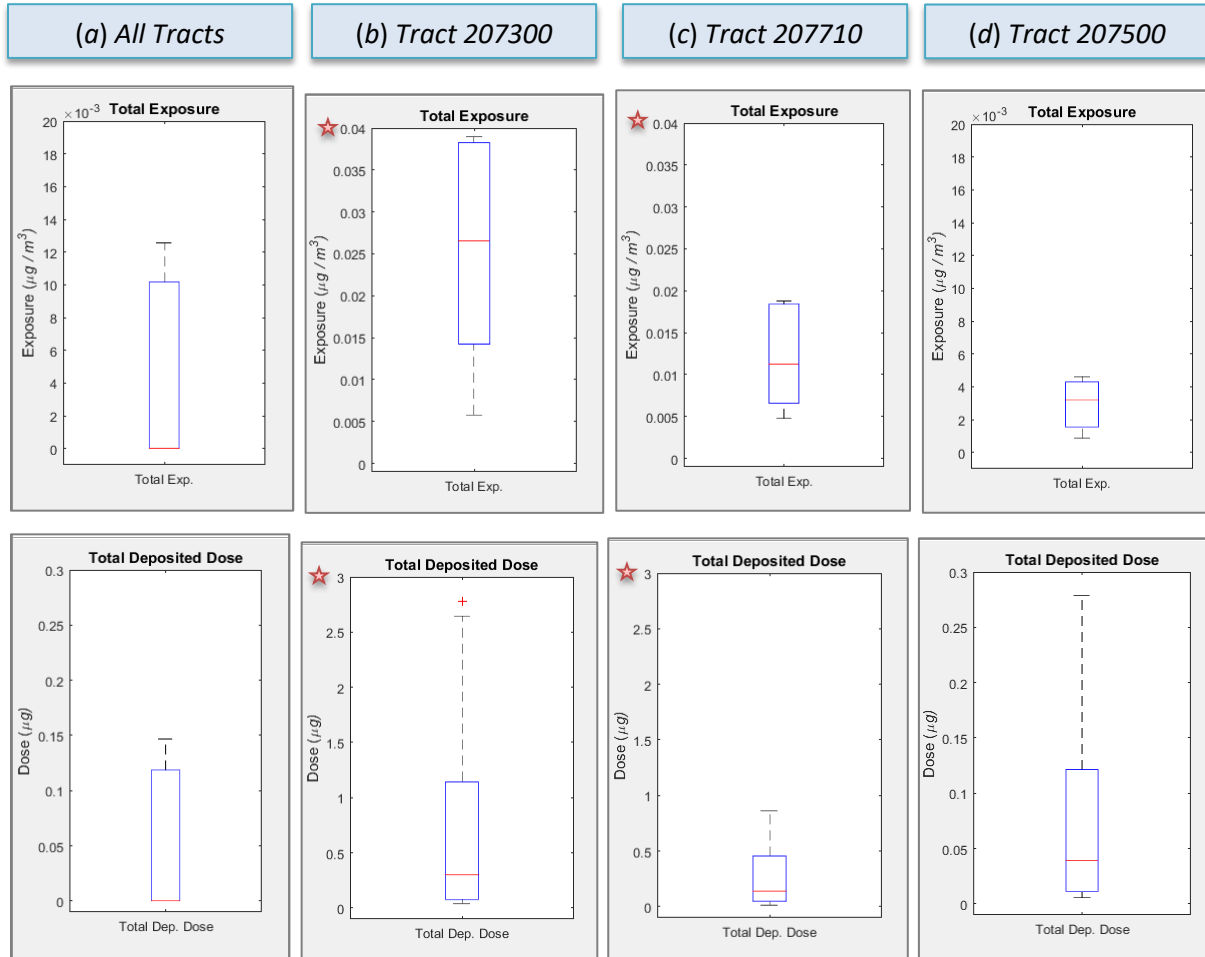


Figure 12. Distribution of daily mean exposure ($\mu\text{g}/\text{m}^3$) (upper) and deposited dose (μg) (lower) for all SHEDS-PM simulated individuals (a), and for individuals in the three census tracts surrounding the *Ba* release at Pershing Square (b, c, d) on Saturday April 22, 2017. Orange star indicates different range for axis.

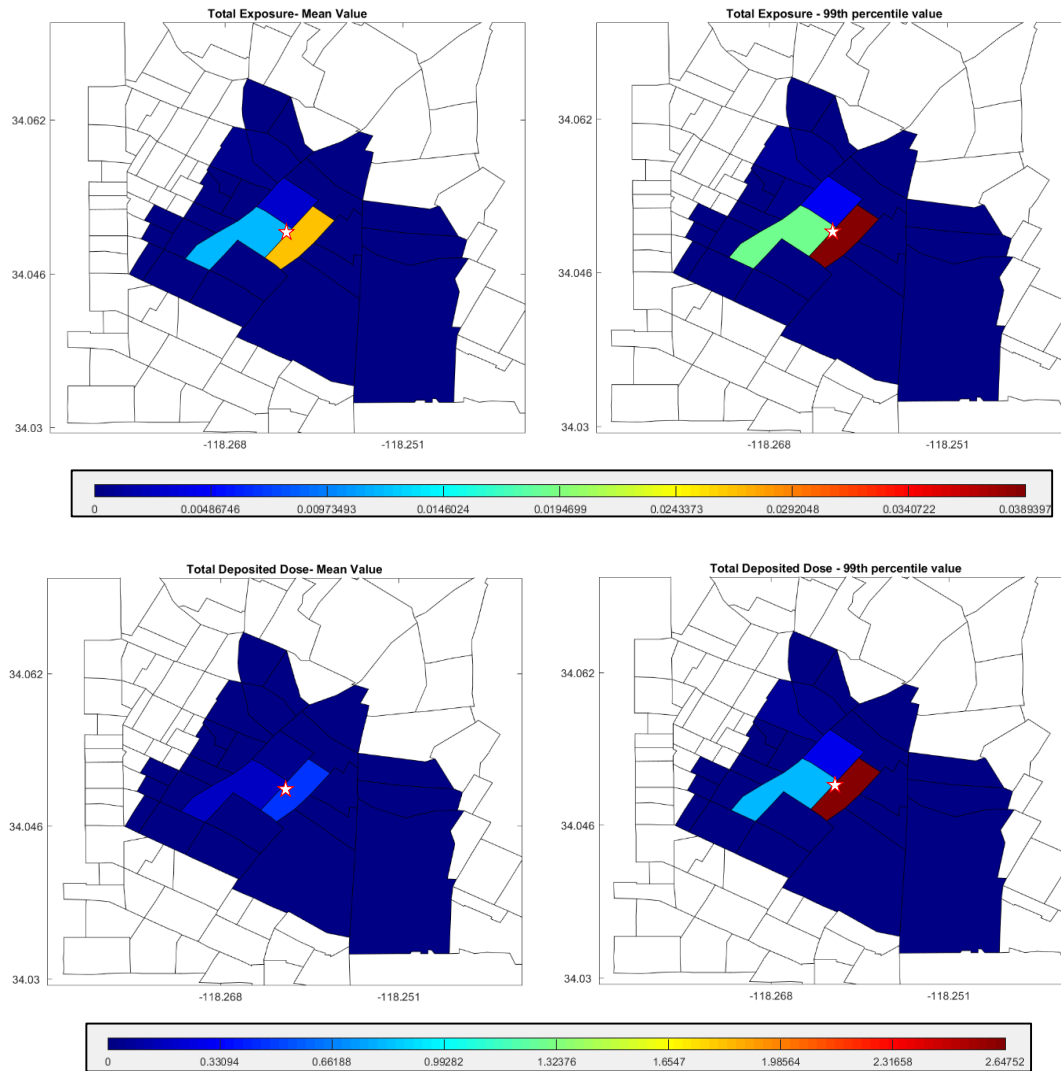


Figure 13. Census tract mean and 99th percentile exposures ($\mu\text{g}/\text{m}^3$) (upper) and deposited dose (μg) (lower) predicted by SHEDS-PM based on QUIC modeled concentrations for *Ba* release at Pershing Square (star) on Saturday April 22, 2017.

Figure 14 shows that the overall distribution of exposure was slightly lower, while deposited dose was somewhat higher overall, compared to the simulation for a Saturday without commuting (Figure 9). Higher deposited dose with similar exposure levels could be due to the weekday activity diaries having greater physical activity levels (higher breathing rates resulting in greater dose) than the Saturday diaries. Although exposure and dose were also highest for the home location for this weekday simulation with commuting, the time spent in other locations was significantly higher as shown in Figure 10(b). This is further highlighted in Figure 15 which compares exposure and dose for individuals that were employed (31% of the population) to the rest of the population. Because employed individuals could be assigned to census tracts different than their home tract while working, exposure and dose were highest for the office location for employed individuals. For individuals not employed (children, elderly and non-working adults), the home location dominated their exposure and dose.

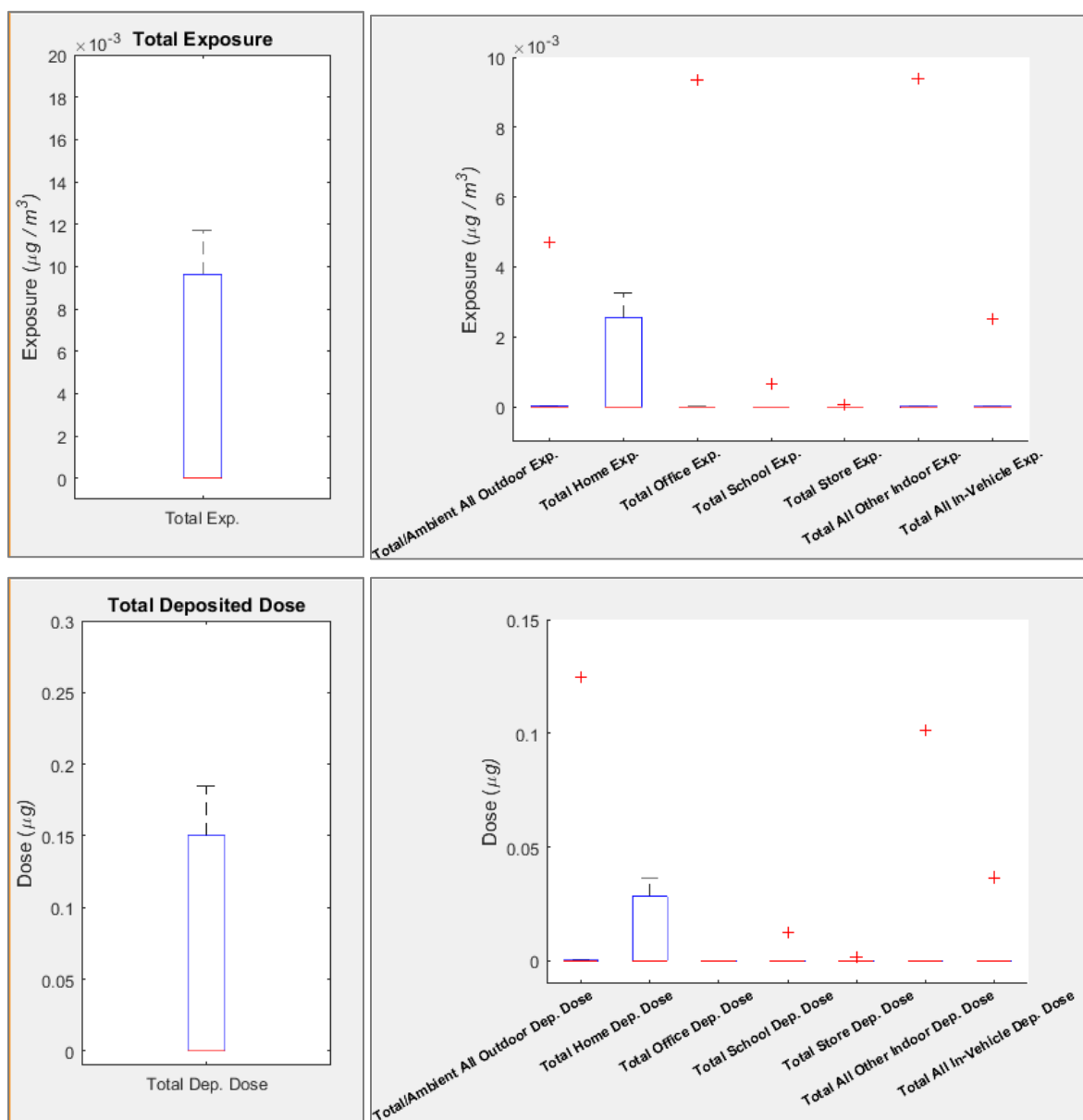


Figure 14. Distribution of daily mean exposure ($\mu\text{g}/\text{m}^3$) and deposited dose (μg) across all SHEDS-PM simulated individuals based on QUIC modeled concentrations for *Ba* release at Pershing Square on a weekday with commuting included, overall (left) and by different locations (right). [Note axis scale for total exposure is $\times 10^{-3}$]

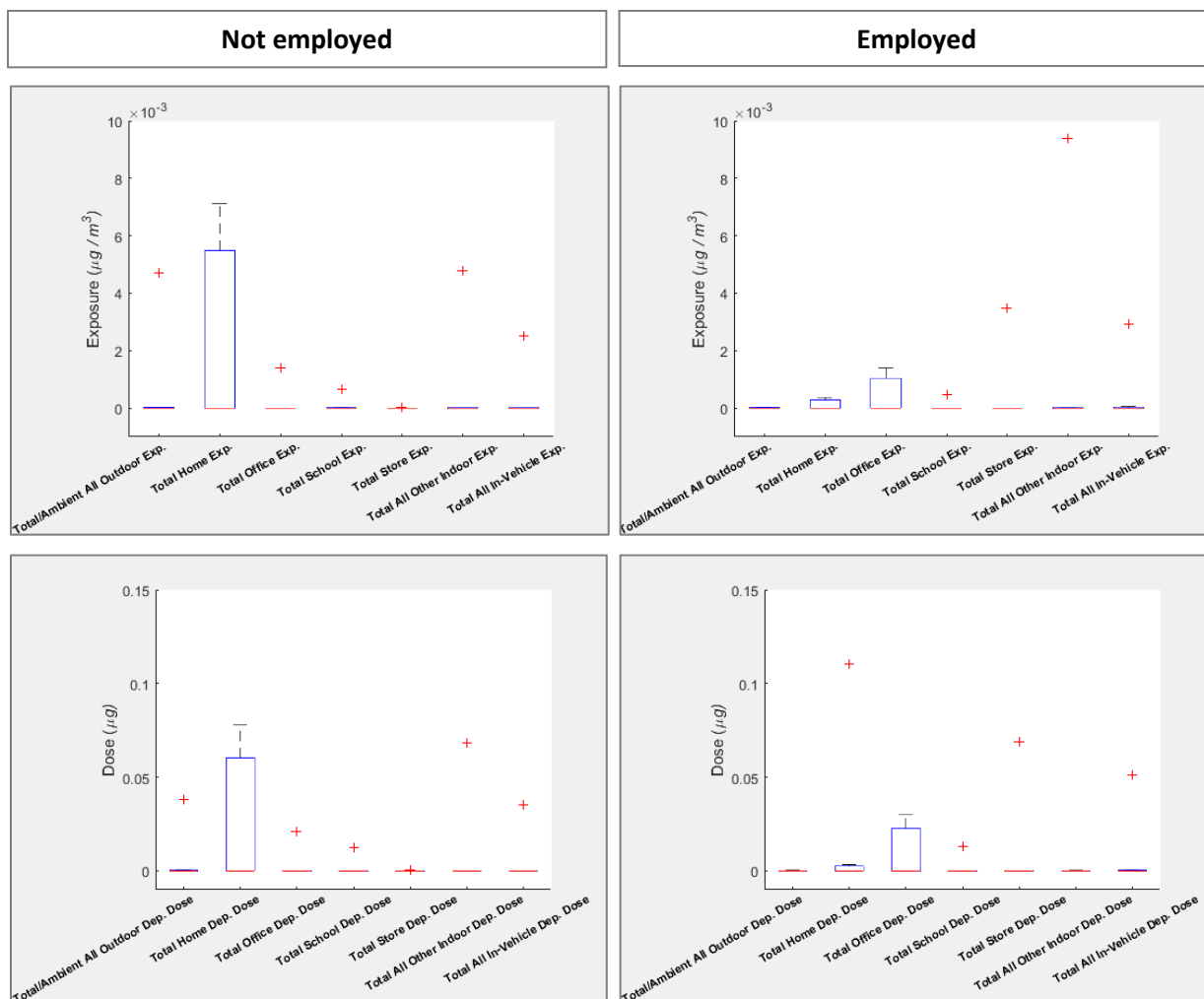


Figure 15. Distribution of daily mean exposure ($\mu\text{g}/\text{m}^3$) and deposited dose (μg) by different locations for employed (right) and not employed (left) simulated individuals based on QUIC modeled concentrations for *Ba* release at Pershing Square on a weekday with commuting included. [Note axis scale for total exposure is $\times 10^{-3}$]

Maps of the mean and 99th percentile exposures and deposited dose for each census tract in Figure 16 show that accounting for worker commuting patterns in the SHEDS-PM simulation affected the results in multiple ways. Overall, less than a third of the population for these tracts were employed so the mean exposures and deposited dose were generally similar between the simulations with and without commuting. But for some individuals, commuting to census tracts near the *Ba* release resulted in daily exposures and dose as high as the individuals residing in those tracts near the release location. This is evident in the higher 99th percentiles for census tracts farther from the release. In addition, one census tract near the release location (207500) had higher levels of exposure and dose with commuting, indicating individuals commuted to the other census tracts near the release that had even higher *Ba* concentrations. In contrast, both the mean and 99th percentile maps show lower values for one census tract near the release (207710), indicating that some individuals commuted away from this high concentration tract to census tracts with lower concentrations.

Results for the third SHEDS-PM simulation that included census tracts from outside the QUIC model domain to examine the impact of worker commuting across the broader Los Angeles area are shown in Figure 17. These maps show that for the more than 300 census tracts with *Ba* concentrations of zero for all hours, some individuals who commuted spent enough time in the tracts impacted by the *Ba* release to result in elevated daily exposure and dose.

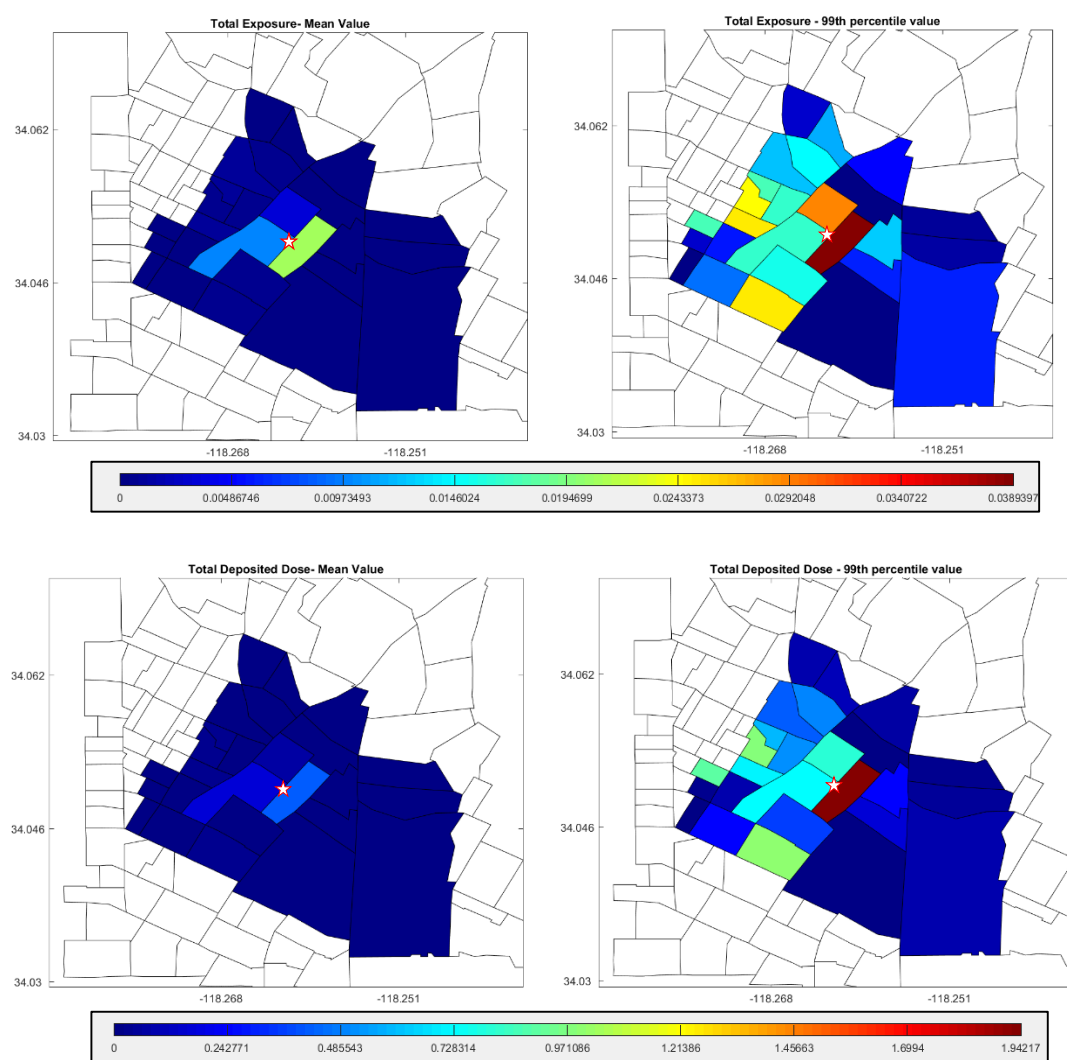


Figure 16. Census tract mean and 99th percentile exposures ($\mu\text{g}/\text{m}^3$) (upper) and deposited dose (μg) (lower) predicted by SHEDS-PM based on QUIC modeled concentrations for *Ba* release at Pershing Square (star) on a weekday with commuting.

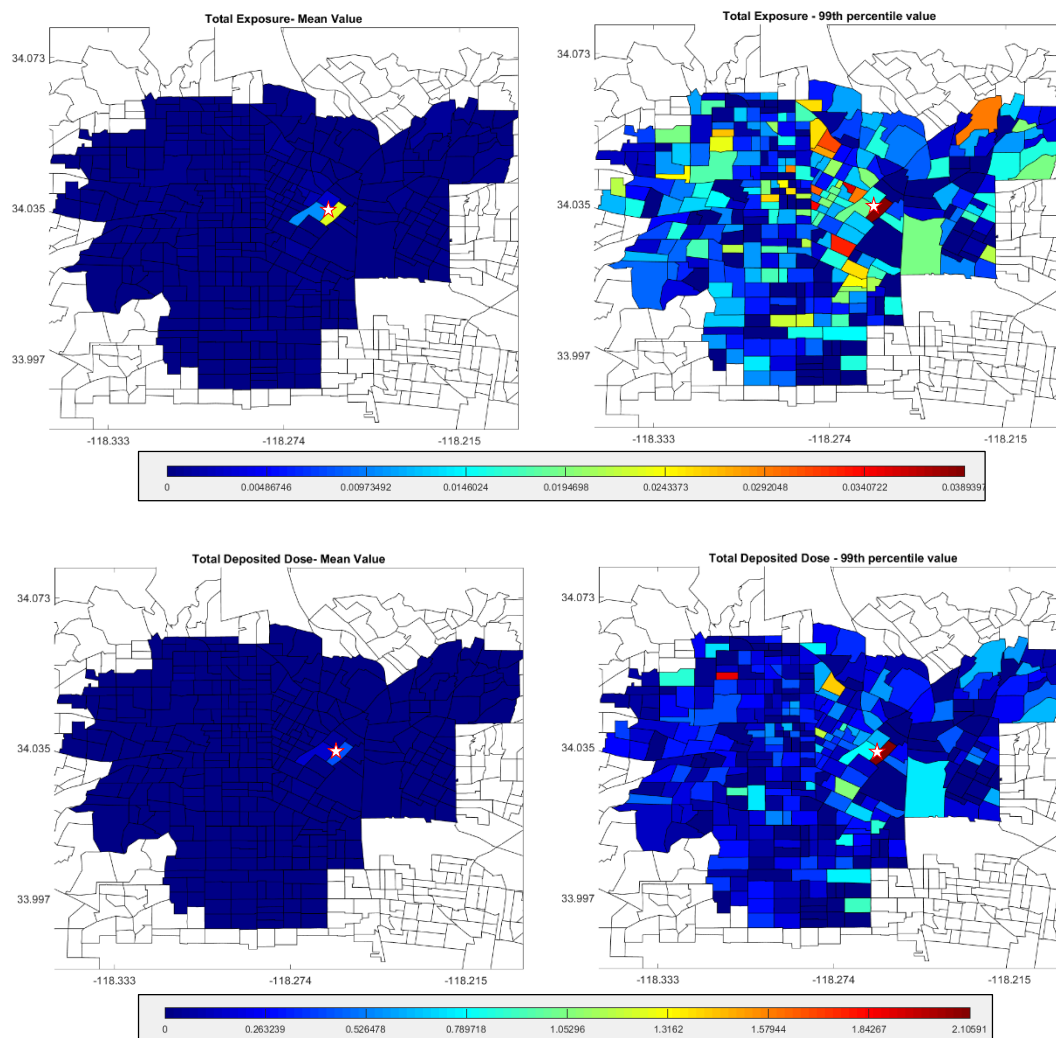


Figure 17. Census tract mean and 99th percentile exposures ($\mu\text{g}/\text{m}^3$) (upper) and deposited dose (μg) (lower) predicted by SHEDS-PM based on QUIC modeled concentrations for *Ba* release at Pershing Square (star) on a weekday with commuting.

4. Discussion

EPA's SHEDS-PM model provides estimates of human exposures by simulating representative individuals for a specific geographic location. The individuals time series of exposure and dose are estimated using human activity pattern data matched to each individual by factors that influence activity patterns (e.g., demographics and day of week), and the air concentrations for each location they spend time in (e.g., outdoors, indoors, in vehicle). This assessment of the SHEDS model was initiated because these features of the model had potential to provide useful information on human exposures following an outdoor release of a biological agent for emergency response and planning, such as for guiding air sample placement.

Overall, the results of this initial assessment demonstrate the potential utility of the SHEDS model for this purpose. However, the SHEDS model in its current form is likely too complex for application during the response immediately following a wide-area release of a biological agent. The SHEDS modeling approach may be more appropriate for emergency response planning when another model such as QUIC is also applied, and various scenarios are investigated, such as for future high-profile security events or locations. Alternatively, the combination of the underlying data sources included in the SHEDS model (i.e. population demographics, housing types, and commuting patterns from US Census data along with human activity pattern data) may provide the most important information for prioritizing decontamination to reduce potential risk of exposure, and could be incorporated in other tools or approaches for guiding air sample placement in emergency response.

Key advantages of the SHEDS model and its output identified through this case study are summarized below, as well as current limitations and options for addressing them. In addition, the exposure and dose modeling capabilities within the QUIC model are discussed.

4.1. Advantages of SHEDS model

The main advantages of the SHEDS modeling approach are that the inputs are referenced to a specific geographic location, that the relationships between population demographics and human activity patterns are accounted for, and that the mobility of the population in space and time for worker commuting can be included.

Population simulated for a geographic location. Use of census data in the SHEDS model provides the reference to the geographic location for the inputs to each simulation. Currently, census tracts are the spatial unit of the input data for population demographics and housing type data. A simulation population is generated that demographically represents the population of each census tract in terms of age and gender, as well as for employment status and types of housing units if selected. When the concentration data used as input to the model have similar spatial resolution, the model provides the ability to link concentration variability with population variability for that geographic location. This aspect of the model provides refined estimates of human exposures that could be important for application to biological agents for emergency response planning given the potential for large spatial gradients in concentrations following an outdoor release and the need to identify the population at risk and locate samplers to appropriately assess their risk.

Population demographics, housing factors and activity patterns. The case study results highlighted the impact that demographics and other factors such as day of week have on model estimates of exposure and dose due to their influence on activity patterns. The census tracts near the release location differed in concentrations as well as population characteristics, housing types and employment status. The age and gender proportions differed by census tract and the activity patterns assigned contributed to the variation in exposure and dose in addition to the concentration differences. Age and gender differences in time spent outdoors, indoors and in vehicles can influence the risk of exposure, and age and gender specific factors are also used in the calculation of dose.

Comparison of the SHEDS simulations for a weekday versus a weekend day showed that overall the time spent at home contributed the most to exposure and dose for both, although the amount was lower for the weekday simulation. More time was spent in locations other than the home for the weekday simulation, with median time spent in offices and schools increasing to approximately 4 and 6 hours respectively. Although the same concentrations were used as input for both simulations, the estimates of

exposure and dose were not the same due to the time spent in locations other than home and the different indoor-outdoor factors for those locations. However, since time spent at home typically contributed the most to exposure and dose, an important feature of the SHEDS model is the ability to specify different types of housing and the factors that contribute to residential indoor exposure estimates such as air exchange rates.

These relationships between demographics, activity patterns and housing factors were incorporated in the SHEDS model design for air pollutant exposure assessment, but may be equally relevant for estimating exposures and dose following an outdoor release of a biological agent.

Population mobility for worker commuting. Mobility of the population in space and time such as for worker commuting may also be a critical component of exposure assessment for biological agents. In this case study, accounting for worker commuting patterns affected the SHEDS results in both directions depending on location and population. Some census tracts far from the release and outside the QUIC model domain had high 99th percentile exposures and deposited dose despite no direct impact from the release on those census tracts. The population simulated for these tracts had individuals that commuted to census tracts near the release location which had higher concentrations than their home census tract, thus elevating their exposure and dose. On the other hand, some individuals whose home census tract was near the release location commuted to census tracts with lower or zero concentrations (not impacted by plume) which lowered their exposure and dose. Using the worker commuting capability in the SHEDS model, this case study highlighted the importance of accounting for population mobility due to the impact that may have on exposures to biological agents following an outdoor release.

4.2. Limitations of SHEDS model

Since SHEDS-PM was developed for application to particulate matter air pollution and to estimate the overall variability in exposure and dose across a population, the demonstration case study also identified limitations for application of the model to outdoor releases of biological agents. These limitations include the relevant spatial and temporal scales, options for map display of outputs, the concentration units used, population mobility factors simulated, and lung deposition calculations for bioaerosols.

Spatial and temporal scale. Clearly, one major limitation for application of the SHEDS model for emergency response is the scale, with the current model limited to census tracts for the spatial scale and hourly concentrations inputs for the temporal scale. Simulation of releases of biological agents (or other airborne releases relevant to emergency response) require higher spatial and temporal resolution due to the potential for short duration extreme concentrations over a localized area that may be the most relevant exposures to capture.

However, the structure of the SHEDS model code allows for more flexibility in scale if the input data for different scales could be developed and a consistent set of inputs provided for an application. For example, a database of US Census demographic, housing, and commuting data could be compiled with data for all spatial levels of census units available, including census tracts, block groups, and blocks. Figure 18 displays the boundaries of US Census tracts, block groups, and blocks for the Los Angeles domain for comparison. The appropriate spatial scale of input data could then be selected by the user for the application. Modification of the model code to support this flexibility in spatial scale would require relatively straightforward changes to the code. Development of the database from census data would also be relatively straightforward, but would also require routine updating as new US Census data are released.

For temporal resolution, the SHEDS model currently has code that is flexible in the input data, from hourly to 24-hour data. Human activity pattern data in the CHAD database is also available at a finer temporal resolution, with 1 hour being the maximum length for an activity record. Modification of the model code to support time resolution less than 1 hour would also be relatively straightforward.

Map display of model outputs. One of the key features of the SHEDS model that could be directly useful for guiding air sample placement based on human exposure estimates for biological agents is the capability to display model outputs on a map of the census tracts included in the simulation. However, the options currently available for mapping of outputs are limited to the display of distribution statistics for exposure, intake dose, and deposited dose, as well as the input concentrations. Mapping of the model results could be modified to include more relevant information for emergency response such as population demographics, housing characteristics, indoor concentrations or infiltration. An additional map feature that could display the impact of commuting on exposures could also make the output more useful. Model code for the mapping feature would also have to be modified to support the different census unit options if the model was made more flexible in spatial resolution as described above.

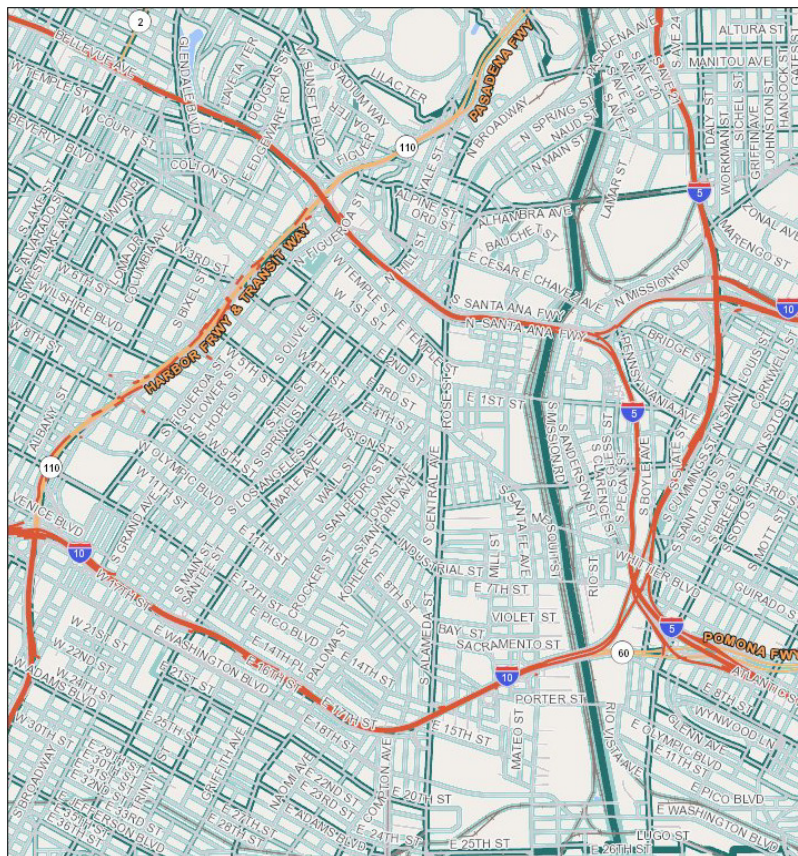


Figure 18. Map of US Census unit boundaries for Los Angeles with tracts (dark green), block groups (light green) and blocks (gray) which could be implemented into SHEDS for simulation at finer spatial resolutions. [Source: https://tigerweb.geo.census.gov/tigerwebmain/TIGERweb_apps.html]

Concentration units. Currently, the SHEDS model assumes input concentrations in units of $\mu\text{g}/\text{m}^3$. For biological agents such as *Ba* the units may need to be modifiable to allow for the metric of interest for infection or detection to be simulated (e.g. the number of spores). Options for addressing the units issue could include revising the code to allow complete flexibility in the model for user defined units so the model would perform exposure and dose calculations and provide output in the units specified, or continue to require input concentrations in mass units but allow conversion of the model output to different units based on a conversion factor (default or user provided).

Population mobility factors. The SHEDS model currently captures population mobility within the model domain related to worker commuting. However, other types of mobility may be important for some segments of the population such as children commuting to school or for activities such as shopping, especially for suburban areas with large retail locations. Incorporating these aspects of population mobility within the SHEDS model has been constrained by the lack of a single source for available data (e.g., US Census) and differences between urban areas such as for school commuting (Xue et al., 2009). The availability of population mobility data may improve as approaches for utilizing different data sources advances. For example, Landscan USA provides high-resolution population distribution data over space and time (Bhaduri et al, 2007), but the data are limited to static daytime and nighttime population counts that do not include demographic data (e.g. age, gender). Agent-based modeling approaches are also being used to create synthetic populations that accounting for movement in space and time (Pires et al, 2018). This type of data could be of value for guiding air sample placement as an indicator of potential exposure by providing estimates of the location of the population in space and time with the demographic characteristics needed for human exposure estimates (Aubrecht et al, 2013).

Lung deposition for bioaerosols. The SHEDS model includes the standard ICRP model for calculating the deposition of particles to three regions of the lung (Burke and Vedantham, 2009). The ICRP model assumes particles are spherical shaped, but bioaerosols tend to be non-spherical or elongated in shape. Guha et al. (2014) modified the ICRP model to address this limitation and the Matlab code is publicly available for download. The SHEDS model could be updated with this new ICRP model code to account for the specific nature of bioaerosol deposition to the lung.

4.3. Other modeling approaches

The QUIC model was applied to generate *Ba* input concentrations for this assessment of the SHEDS model. However, QUIC also has capabilities for estimating population exposures and dose. For example, using the building data required as input to the model, infiltration can be calculated based on typical parameters for each type of building (e.g. office building) or specified for each individual building, to estimate indoor concentrations. The QUIC model also has a population exposure calculator that uses either daytime or nighttime population counts provided with the model to assign counts to the buildings, outdoors, or in vehicles, and uses a fixed ‘protection’ factor for indoors and vehicles. The QUIC model approach to estimating exposures takes advantage of the individual building data required as input to the model to allocate the population to different locations spatially and the concentrations for those locations. In contrast, the focus of the SHEDS model is on simulating individuals in the population using population demographics and housing type proportions that vary spatially. The individuals are assigned to different locations (indoors, outdoors, in vehicles) over time with different concentrations, but these are not fixed locations such as the individual buildings defined for QUIC simulations.

Inhalation of aerosols can also be simulated by QUIC based on a single breathing rate and fixed lung deposition fractions. This differs from the SHEDS modeling approach that incorporates variability in

breathing rates by age and gender as well as for different activities (e.g., sleeping vs. exercise), and particle-size specific deposition to the lung. However, the QUIC model goes beyond inhalation and dose to estimate response using lethal concentration thresholds provided as input. Estimates of the total affected population, the affected population by location (indoor, outdoor and vehicle), and the total area affected, can be generated and output from the QUIC model.

Additional features of the QUIC model were identified that could also be further explored for improving estimates of exposure and dose for biological agents following an outdoor release. One example is the resuspension feature which uses the deposition output from a release simulation as input to a second model run for incorporating resuspension.

Finally, although there would be an advantage to having one modeling tool that integrates simulation of dispersion, concentrations, exposures and dose, as well as response, it is important to also consider other sources of concentration data that could be used as input to SHEDS and whether further development of SHEDS for biological agents should be oriented toward application with other data or models. One possibility is application of SHEDS together with screening level models used for emergency response such as HPAC (DTRA, 2015) which do not have the extensive input data requirements of the QUIC model.

5. Conclusions

Current research supports the need for models for emergency preparedness that not only include dispersion modeling but also estimate doses based on exposure duration, breathing rate, lung volume, and particle size distribution, as well as dose-response models to estimate infection probabilities (Van Leuken et al, 2016). The SHEDS model provides many features that could be useful when applied to wide-area releases of biological agents to address this research need. The SHEDS model could be refined to provide output that informs air sample placement based on population exposure estimates to help prioritize areas for decontamination when applied with other models such as QUIC. Other potential uses of the SHEDS model could include estimating residual risk for populations outside the primary contaminated zone following an event, estimating the risk of exposure to resuspended biological agents that remain after the release, or reconstruction of exposures in a post-event analysis. Future research should focus on maximizing the utility the exposure modeling approach either through modification of the current SHEDS model or enhancing the exposure and dose estimation methods within other modeling tools.

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