Example Application of Modeling Toxic Air Pollutants in Urban Areas

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1. METHODOLOGY FOR URBAN AIR TOXICS MODELING

1.1 Introduction

This document provides an example application of modeling toxic air pollutants in urban areas. In preparing this document, it was necessary to revise and update techniques described in Dispersion Modeling of Toxics Pollutants in Urban Areas, EPA-454/R-99-021 and incorporate techniques developed in A Simplified Approach for Estimating Secondary Production of Hazardous Air Pollutants (HAPs) Using the OZIPR Model, EPA-454/R-99-054.

The 1990 Clean Air Act Amendments (CAAA) Section 112(k) requires EPA to reduce hazardous air pollutant (HAP) risks in urban areas. The EPA's strategy for reducing these risks is discussed in the Integrated Urban Air Toxics Strategy (U.S. EPA, 1999b). In order to help understand the air toxics problem in an urban area, it is necessary to know the concentrations of air toxics to which people are exposed. Air monitoring data are scarce and limited. Another means for estimating HAP concentrations is through the use of air quality models. Urban areas can vary greatly in terms of the types of emission sources and the legal enforcement options provided by state and local programs to control air toxic emissions and air quality models also allow state and local agencies to test the effectiveness of alternative control measures in reducing ambient concentrations.

The intent of urban wide air toxics modeling applications is to provide data inputs for use in exposure and risk calculation and prioritization, obtain a higher degree of geographic resolution than those obtained from national scale studies, identify data gaps and help allocate resources toward particular issues of interest or concern, and support the planning and implementation of ambient air monitoring programs. Regarding the higher geographic resolution of assessment results, an important benefit of refinement by an urban scale application is illustrated by considering the methods by which emissions data are applied to the models. To achieve the objective of a national scale assessment within a feasible scope of time and resources, assumptions about emissions allocation are typically made to simplify the modeling. An example would be the allocation of unknown emission source locations to the centroid of the census tract. While this approach allows the national scale assessment to broadly identify pollutants of potential concern across large geographical areas, the assigning of source locations or other sensitive parameters in such a manner limits resolution. The urban scale modeling effort is more localized and can compliment the national scale assessment by increase in specificity. However, at this time, the number of assumptions made in urban scale modeling precludes the use in specifying the individual sources that contribute to the total concentrations or the impact of specific sources in specific areas such as a neighborhood. For determining impacts of specific sources, more detailed analysis than is warranted in an urban scale application is needed.

Urban areas contain major sources, numerous smaller, area sources, and mobile source. As a result, modeling analyses for large numbers of air toxics sources possess special challenges. Although most HAPs are emitted directly, some are produced and destroyed through reactions in

the atmosphere. These issues, as well as receptor selection, meteorological data processing, and background concentration selection pose significant technical challenges to the air quality modeler. Although many air quality models can be used for estimating urban wide ambient concentrations, this document deals with the applications of the Industrial Source Complex (ISCST3) model, a model that can estimate close distance impacts from industrial facilities. This model has been extensively used in analyzing impacts from a single or a few facilities and this report should help provide transition to the more complex issues associated with urban-wide applications.

Sections 2 and 3 provides recommendations on specific issues needed for urban-wide air quality modeling of air toxic pollutants. Section 2 focuses on modeling methodology and section 3 focuses on emissions and source characterization issues. Section 4 provides an overview of an application of a Gaussian model to an urban-wide study, i.e., the Houston, Texas urban area. Section 5 provides study summary and conclusions.

2. MODELING METHODOLOGY

The extent to which a specific model is suitable for the evaluation of source impact depends on several factors that include the meteorological and topographic complexities of the area; the level of detail and accuracy of the data base (i.e., emissions inventory), and the resources available.

There are a number of design criteria which need to be satisfied in order to yield an acceptable modeling study of toxic pollutants. For the air dispersion model, for example, these include:

1. readily available/public domain/recommended by EPA
2. represents state-of-modeling practice
3. applicable to urban areas and irregular terrain
4. capable of handling point, area and mobile sources
5. capable of accounting for dry and wet deposition of pollutants
6. capable of treating atmospheric chemical transformations - pollutant chemistry
7. capable of accounting for pollutant emissions that vary by season and hour-of-day
8. ability to group source types for assessing impact
9. capable of providing annual average concentration estimates (as well as shorter time averages)
10. computationally efficient
11. demonstrate good performance with measurements - estimated vs. observed concentrations.

The Gaussian plume model is a widely used technique for estimating the impacts of nonreactive pollutants because of its good performance against field measurements, and because it is computationally efficient relative to other types of models, such as grid and puff models.

The plume dispersion model used in estimating urban-wide concentrations of toxic air pollutants is the ISCST3 model. This section describes some of the most important considerations needed to apply ISCST3 for these types of applications. Other sources of detailed information are listed below:

For general information on air quality modeling, consult Appendix W to CFR Part 51-Guideline on Air Quality Models.

For information on how to use the ISCST3 model, consult the ISC3 model user's guide (U.S. EPA, 1995b).

For information on how to preprocess the meteorological data for input in ISCST3, consult the MPRM User's Guide (U.S. EPA, 1996a) and PCRAMMET User's Guide (U.S. EPA, 1996b).

For information on chemical parameters required for estimating deposition, consult Wesely et al., 2002.

For information on estimating secondary production of hazardous air pollutants, consult U.S. EPA, 1999c.

All of the items listed above can be obtained from EPA's SCRAM web site at http://www.epa.gov/ttn/scram.

Information on the "Integrated Urban Air Toxics Strategy" developed under the authority of Section 112(k) and 112(c) of the Clean Air Act is obtained from EPA's web site at http://www.epa.gov/ttn/atw/index.html.

2.1 Model Features

Key features of the ISCST3 dispersion model that are useful for urban-wide air toxics applications include:
• handles multiple point, area, and mobile sources
• incorporates building downwash effects
• includes an urban dispersion option
• contains considerable flexibility for specifying receptor locations and for grouping of source impacts
• includes algorithms to treat the effects of elevated and/or complex terrain
• treats the effects of deposition of gaseous and particulate emissions
• includes an option to vary emissions by season and hour-of-day
• includes an option to treat atmospheric transformations by exponential decay.

2.2 Model Options

The regulatory default model option in ISCST3 should be selected for urban-wide applications. More information about the default option parameters can be found in the ISC3 User's Guide (U.S. EPA, 1995b).

The option to vary the emissions by season and hour-of-day should be selected, unless the objectives of the application or the form of the emissions inventory data dictate otherwise.

For best estimates, the use of the wet and dry deposition and plume depletion options should also be selected. Deposition estimates are very useful in multi-pathway exposure assessments. Note that the selection of the plume depletion option will increase model run time. To utilize the wet and dry deposition option, the model requires additional data for the meteorological and chemical parameters. For meteorological input, the user should consult the meteorological data preprocessors' user's guides (see above).

To determine whether the modeling domain satisfies the criteria for an "urban" or "rural" area, Section 8.2.8 of the Guideline on Air Quality Models (40CFR51) should be followed. The domain can be subdivided into urban and rural areas based on land use data. Sources in these areas are modeled separately and concentrations from each model run are then added at each receptor.

2.3 Averaging Period

The ISCST3 model computes an hourly concentration for each receptor. Other averaging periods, e.g., 3-hour, daily, seasonal and annual can also be aggregated (U.S. EPA, 1995b). The averaging period selected is based on the intended use. Annual average air concentrations are generally needed for use in chronic (long-term) exposure studies. Shorter term ambient concentrations are usually needed for determining acute exposure. However, it should be noted that sometimes the input data (i.e., emissions) may not have the temporal resolution needed for short term concentrations.

2.4 Receptors

A receptor is any location where ambient concentration estimates are needed. Receptors are usually placed in "ambient air" which is outside of inaccessible plant property. For point and area sources, placement is usually at the fence line and for mobile sources placement is near roadways. The ISCST3 model requires the coordinates of the specified receptors. Receptor locations should be selected based on a case-by-case determination with expert judgement on the needs of the study. Often, receptors are selected at coordinates provided in the census data (census block, census block groups or census tracts). Other receptor locations include ambient air quality monitoring site locations.

Census data and urban land use information can be used to identify locations (potential receptors) where individuals live, work, attend school, and spend time in recreation. Since model run time is proportional to the number of receptors, a degree of care is needed to select the optimal number of receptors. In the example study, receptor selection was based in part, on the input needs of the Hazardous Air Pollutant Exposure Model (HAPEM4) exposure model (U.S. EPA, 1999a). The receptor points were defined as the population weighted centroid of each census tract.

2.5 Terrain

Terrain elevation at each source and receptor must be input into ISCST3. Digitized terrain elevation data are available through the U.S. Geological Survey (USGS) web site at http://edcwww.cr.usgs.gov/doc/edchome/ndcdb/ndcdb.html. Their 1:24,000-Scale (7.5-minute) Digital Elevation Model (DEM) data can be downloaded directly, at no cost, from the GeoComm International Corporation (GCIC) at http://gisdatadepot.com/dem and from MapMart.com at http://www.mapmart.com. Data can also be ordered and shipped on CD ROM for a nominal cost from these vendors. The free and purchasable data from GCIC are in the new USGS Spatial Data Transfer Standard (SDTS) format and must be converted to the old DEM file format to work in the EPA terrain preprocessor AERMAP (U.S. EPA, 1998). Data in the old DEM format are available for relatively nominal cost from MAPMART. MAPMART does offer a limited number of the old DEM formatted data files to be downloaded for free. ISCST3 model users can use AERMAP to enter the receptor locations and retrieve the elevation data from the AERMAP output[1]. In the AERMAP download package, there is a conversion procedure for converting SDTS formatted data to the old DEM format for input into AERMAP.

Source (stack) elevation is usually provided in the inventory. For many urban areas, the majority of emission sources are near ground level. In these cases, terrain can be assumed to be flat and source and receptor elevations set to zero. Where the urban area is in mountainous terrain, terrain effects are important for sources with stacks. First, the impact of individual plumes on elevated terrain results in higher air concentration (through placing the receptor at the correct higher air concentration, vertical location within the plume and estimating the impaction of the plume upon intervening terrain). Second, wind channeling due to terrain can cause higher air concentrations. The ISCST3 model does not address wind channeling effects other than if these effects are captured by the available meteorological data. If the urban area contains complex terrain features that are expected to significantly affect the modeled concentrations, a dispersion model that handles such situations should be selected from those listed in the Guideline on Air Quality Models (40CFR51).

2.6 Meteorological Data

Meteorological data must be preprocessed before use in ISCST3. The ISCST3 model

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[1]The AERMAP format must be slightly modified to eliminate extraneous data.

requires two meteorological data sets, surface and upper air. Hourly surface and twice-daily upper air meteorological data files can be purchased online from the National Climatic Data Center (NCDC) (http://www.ncdc.noaa.gov). The data can also be purchased on CDs. The CDs with surface data are SAMSON (Solar and Meteorological Surface Observation Network), HUSWO (Hourly U.S. Surface Weather Observations), INSWO (International Surface Weather Observations), and ISHD (Integrated Surface Hourly Data). The CD with upper air data is titled Radiosonde Data of North America. The EPA meteorological preprocessors are currently designed to process meteorological data from the CDs. For data purchased online, reformatting is required before use in the EPA preprocessors.

If wet deposition estimates from ISCST3 are required, precipitation data are necessary. The ISHD data contains hourly precipitation measurements.

In urban areas, on-site meteorological data are not often available. The closest NWS stations may not be the most representative due to the influences of terrain or water bodies. Consult with the State/Regional meteorologist for the most applicable NWS stations for your area.

Mixing heights are computed using surface and upper air data (Radiosonde Data of North America) via the mixing height program provided on the SCRAM web site (http://www.epa.gov/scram001).

The PCRAMMET and MPRM meteorological data preprocessors use surface and mixing height data as input to create ISCST3 input files. PCRAMMET and MPRM can accept data directly from the SAMSON and HUSWO CDs. In addition, MPRM can also accept INSWO and ISHD data. MPRM should be used to prepare the input files necessary for applying the gas deposition algorithm in ISCST3. Values for additional parameters needed in applying the gas deposition algorithms for the case study city are presented in Section 4.2.6.2. MPRM can also be used for setting up a meteorological data file for ISCST3 to use in estimating both particle dry deposition, and gas and particle wet deposition.

Both MPRM and PCRAMMET meteorological data preprocessors can occasionally produce very low mixing heights (less than 10 meters) based on the twice-daily values from the mixing height data file and the interpolation scheme used to provide hourly values of mixing height. Anomalously low calculated mixing heights may be associated with a midday cold frontal passage. While the occurrence of very low mixing heights is more likely for the rural mixing heights than for the urban mixing heights, due to differences in the interpolation routines, low mixing heights may occur for both rural and urban conditions. The application of a very low mixing height with a near-surface level area source can produce anomalously high air concentrations due to the treatment of limited mixing effects in the ISCST3 model; expert judgement is needed to determine the minimum mixing height for a given urban area. For the example study, a minimum value of 100 meters was applied to the hourly mixing heights produced by MPRM to avoid this anomaly from influencing the results. For urban areas,

building heights will limit the lower mixing heights and the 100-meter value was considered the upper limit to the minimum value for the depth of the well-mixed boundary layer in a large urban area (Sutton, 1953).

2.7 Chemistry

The ISCST3 model provides concentration estimates due to primary emissions and has a limited capability to consider atmospheric transformations by exponential decay (half-life). Some pollutants (e.g., formaldehyde, acetaldehyde, and acrolein) are also formed in the atmosphere due to reactions among other pollutants (i.e., formed by secondary production). Thus, in addition to estimating concentrations due to primary emissions, an estimate of concentrations based on secondary production is necessary and should be added to the ISCST3 output in order to avoid large underpredictions. EPA's OZIPR screening model (Gery and Crous, 1991) may be used to estimate the secondary transformation of acetaldehyde, formaldehyde and acrolein. U.S. EPA, 1999c describes an approach where secondary HAP production is estimated with the stand-alone OZIPR model that incorporates only nondispersive processes, such as photochemistry and the results from this model are then coupled with output from the ISCST3 model, that accounts for dispersion but not for chemical transformation. The study results were encouraging because, in comparisons with available monitoring data, this simple approach seems to perform as well as more complex models.

2.8 Background Concentrations

Background air quality includes pollutant concentrations due to natural sources, nearby sources other than those under consideration, and unidentified sources. For typical exposure assessments, background concentrations should be added to the modeled concentrations to provide total ambient air concentrations for estimating exposure. Air quality data from a HAP monitoring network in the vicinity of the analysis area are often used to establish background concentrations. Also, background concentrations of some air toxics may be found in the literature.

The following approach for estimating background concentrations in the absence of measured or other reported values can be used. An expanded point source inventory can be obtained for an area surrounding each city from the National Toxic Inventory (NTI). The domain for this expanded point source inventory should extend beyond the domain of the inventory being explicitly modeled in the analysis. An estimate of background concentrations at each receptor within the modeling domain is obtained by multiplying the point source emission rate by a distance dependent factor; sources less than 50 km are excluded. The modeled background concentration can be based on a summation of concentrations computed from a grid across the modeling domain. These background concentrations can then be added to the modeled concentrations. See Section 4.2.8 and Appendix A for details of estimating background concentrations for the Houston study.

2.9 Monitoring Data

Monitoring data can be used to check the validity of the modeled concentration estimates or determine background concentrations. Ideally, the monitoring and modeling data should span the same time period. Air toxics monitoring data are available from EPA's Aerometric Information Retrieval System (AIRS) web site at http://www.epa.gov/airs. In most instances, ambient data are collected at a frequency of one in six days. A variety of statistical tests can be used to compare modeled with observed estimates. Statistical tests, such as root mean square (RMS) errors, can be used to evaluate the model performance against monitor values. How the model estimates compare to annual average monitored data is useful for determining the suitability of the estimates. For comparisons in urban areas, there are many uncertainties in all facets of the comparison effort. For model evaluation studies, a factor of two agreement between modeled and observed values is generally considered to be acceptable.

2.10 Study Limitations

As part of the conclusions in an urban-wide air toxics modeling study report, the limitations of the modeling effort should be clearly stated. The important limitations of the ISCST3 model are provided in the User's Guide (U.S. EPA, 1995b) and the Guideline on Air Quality Models (40CFR51). Limitations due to data availability and other factors should also be described.

3. SOURCE CHARACTERIZATION

3.1 Modeling Domain

The urban area domain should be selected based on case-by-case determination with expert judgement. The urban area domain can include a city center or multiple counties. It should be carefully defined because the larger the modeling domain, the greater the number of sources and receptors to be considered and thus the greater the required computational resources. Guidance in the Integrated Urban Air Toxics Strategy (U.S. EPA, 1999b online at http://www.epa.gov/ttn/uatw/urban/fr19jy99.html) should be consulted.

3.2 Emission Inventories

The first step of the urban-wide dispersion modeling process is the assembly of the emissions inventory with the specific air toxics emitted and the sources of their airborne emissions. Ideally, the emission estimates are from direct measurements of representative source emissions. Although such measurements are likely to provide the most accurate data for an emission source, these data are typically not available because such sampling is often too time and resource-intensive. When specific emission measurements are not feasible or available, other emission estimation methods, including material balances and emission factors, are sometimes used as an alternate method. Emission factors indicate the quantity of a pollutant typically released to the atmosphere for a particular source operation, and are usually considered

to be representative of an industry or emission type as a whole. Each approach to estimating emissions, including use of direct measurement data, has an inherent level of uncertainty, which adds to the overall uncertainty of a risk analysis.

A national emissions inventory of toxic pollutants developed by EPA is a good starting point for gathering the necessary emissions data for an urban-scale assessment. The national toxics inventories compiled by EPA contain emissions of the 188 air toxics listed in section 112(b) of the CAA. The 1996 National Toxics Inventory (NTI)[2] is the first national modeling emission inventory constructed using state and local HAP inventory data and containing stationary and mobile source data. EPA prepared the 1996 NTI using five primary sources of data: (1) state and local air toxics inventories developed by state and local air pollution control agencies, (2) existing databases related to EPA's Maximum Achievable Control Technology (MACT) program which requires emission standards under Section 112(d) of the CAA. (www.epa.gov/ttn/uatw/eparules.html) (3) Toxics Release Inventory (TRI) data (www.epa.gov/tri/), (4) emissions estimated by using mobile source methodology developed by experts in EPA's Office of Transportation and Air Quality, and (5) emission estimates for 30 of 500 non-point source categories generated using emission factors and activity data. Much of the state/local, TRI, and EPA MACT emissions data may have been generated by the sources themselves. Documentation for all emissions estimates in the 1996 NTI is available on http://www.epa.gov/ttn/chief/nti/index.html#nti. The following provides a brief summary of the data contained in the NTI.

All of the raw inventory inputs in the NTI exist as estimates for point sources, non-point stationary sources, and mobile sources. "Point" sources provide emissions data at the facility and sub-facility level and include location coordinates (e.g., latitude and longitude). "Non-point" stationary source and "mobile" source data exist as emissions estimates for an entire source category aggregated to the county level. Inventory data files for these different types of sources are generally maintained separately and include different data elements. For the purpose of aggregating air toxics emission sources in the urban wide assessment in the example application, all emissions inventory inputs were grouped into four sectors: "major," "area and other," "onroad," and "nonroad." Each sector is further defined as follows:

> **Major** sources are large stationary sources that emit more than 10 tons per year of any listed air toxic (CAA, section 112(b)) or a combination of listed air toxics of 25 tons per year or more. Typical examples of major sources include electric utility plants, chemical plants, steel mills, oil refineries, and large hazardous waste incinerators. These sources may release air toxics from equipment leaks, when materials are transferred from one location to another, or during discharge through emissions stacks or vents.

> **Area and Other** sources are smaller stationary sources that emit less than 10 tons per year of a single air pollutant or less than 25 tons per year of a combination of air toxics. The

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[2]At the time of writing this report, the NTI has been replaced with the National Emissions Inventory (NEI).

emission inventory includes facility data for some area sources and aggregated emission estimates at the county level for the remaining area sources. Typical examples of area sources include neighborhood dry cleaners and gas stations. Though emissions from individual area sources are often relatively small, collectively their emissions can be of concern particularly where large numbers of sources are located in heavily populated areas. "Other" stationary sources are sources that may be more appropriately addressed by other programs rather than through regulations developed under certain air toxics provisions (sections 112 or 129) in the Clean Air Act. Examples of other stationary sources include wildfires and prescribed burning, which have emissions that are being addressed through the burning policy agreed to by the EPA and the USDA. For this assessment, the "area" and "other" sectors have been combined in the calculations and presentation of the current national-scale assessment.

Onroad mobile sources comprise vehicles used on roads and highways (e.g., cars, trucks, buses).

Nonroad mobile sources are all remaining mobile sources (e.g., trains, lawnmowers, construction vehicles, farm machinery). Note that airport data are handled separately as major sources.

In the NTI, major and area source facilities are drawn from the "point" source inventory files, meaning those with known geographic locations (i.e., latitude and longitude). Area and other source categories that are aggregated as county-level emissions are drawn from the "non-point" source inventory files, meaning those stationary sources that do not have location coordinates but instead exist as county-wide total emissions by source category. Onroad and nonroad sources exist as distinct sectors in the "mobile" source inventories and are also aggregated to the county level.

As explained earlier, a primary source of data in EPA's toxics emission inventory is an inventory developed by state and/or local air pollution control agencies. Thus, the data in EPA's inventory is, meant to be, at least in theory, locale-specific. However, a number of states and local agencies do not submit inventories and therefore, the data are from the other sources and thus to some extent, based on National estimates. In addition, the facility-specific data submitted may be lacking geographic coordinates or have erroneous ones, and may also not have facility-specific emission release source characteristics. Furthermore, the level of specificity may still not be sufficient for an accurate urban scale modeling assessment. For example, large industrial sources (e.g., paper mills, refineries, etc.) may be grouped together so that hundreds of individual release points are assumed to exit from a few groups of stacks. If an inventory does not contain the individual location and release parameters, the analyst has little choice but to model the source as a group. Ambient concentrations from such facilities should be viewed with caution, especially at nearby receptors. If one assumes that ground level fugitive releases (e.g., leaks from pumps, seals or compressors, spilled liquids that form a puddle and then evaporate, lagoons, etc.) exit through an elevated stack, ground level concentrations will be significantly underestimated.

Thus the existing information should be analyzed and, to the extent possible, more detailed information should be gathered at the local scale. Such additional information includes the temporal pattern of emissions (e.g., periodic "puffs" vs. constant emission rates), the specific locations and emission release characteristics of individual small sources such as dry cleaners and gas stations (which for many local areas are represented by a county sum in the national inventory), and more detailed information on the individual specific release characteristics for large sources with hundreds of release points (e.g., whether release is from a stack or fugitive source, and the associated required release parameters).

In summary, while the national inventory is a starting point, it should be used with considerable analysis and supplemented with local data. It is important to understand the national inventories developed by EPA, determine the extent that local data exists for the urban-scale domain of interest, analyze the data for missing or erroneous features, and supplement/correct it.

3.3 Processing emissions data into ISCST3

Before emissions are used as input to the ISCST3 dispersion model, the emissions data require significant preparation. Some of this preparation occurs during the compilation of the inventory and some occurs in the Emissions Modeling System for Hazardous Air Pollutants (EMS-HAP), which is a series of computer programs that process emission inventory data for subsequent air quality modeling (U.S. EPA, 2000a). The necessary inventory preparation steps are described below:

7   Compiling detailed, quality assured, air toxics emissions inputs for all known stationary and mobile sources.

7   Grouping individual pollutant species into compound groups. The NTI contains approximately 400 different species representing the 188 air toxics listed in section 112(b) of the CAA. Many of the species belong to compound classes. Grouping of these species is necessary for many reasons. One reason is that the individual chemical species belonging to groups are not geographically representative. For example, "lead oxide" may have been reported in just a few counties, whereas other counties aggregated their lead oxide emissions into "lead compounds." Second, grouping allows for pollutants with similar characteristics to be modeled together for purposes of efficiency. For example, specific lead species and compounds reported as the broad group "lead compound" are grouped to be subsequently modeled as "lead compounds-fine" and "lead compounds-coarse." Third, grouping decisions made for urban-scale assessment reflect "downstream" data needs, such as making the resultant concentration estimates reflect compounds for which health benchmark information exists.

7   Temporally allocating emission values by season and day of week to 24-hours emission rates. Emissions are temporally allocated based on the type of source using a database of temporal profiles by source classification code.

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7 Grouping into desired source category groups to be able to determine relative contribution of concentrations for each, e.g., major, area, onroad and nonroad.

7 Spatially allocating county-level emissions to1 km grid cells using surrogate data, such as population, industrial land or roadway miles. Note that the appropriate surrogate data for the urban area need to input into EMS-HAP (U.S. EPA, 2000a) and EPA has developed available surrogates for national scale modeling assessments. For Urban wide analysis, users should develop local scale surrogates using site-specific information. Emissions for a source category are computed based on the percentage of the matching surrogate in the grid cell for that county. For example, the consumer products usage source category is matched to population. If 10 percent of the population of the county is in grid cell A, then this grid cell gets 10 percent of the county's consumer products usage emissions. However, allocation is unnecessary where local activity data is available (i.e., travel demand models or local business surveys).

3.4 Source Characterization for ISCST3

Generating the source inventory for modeling is intertwined with the creation of the pollutant inventory. Each emissions source and the constituents each source emits must be specifically identified. For the ISCST3 dispersion model, each source will need to be classified as a point, area, volume, or line source. Building the source inventory usually begins with mapping the locations of emission sources, receptors and the study domain.

The selection of either urban or rural dispersion coefficients is based on commercial and industrial land use classifications (Guideline on Air Quality Models). For large individual major sources, the selection is based on land use classification within a 3 km radius. For other more numerous area and mobile sources, the designation can be made based on the predominant land use type in the 1 km grid cell in which the source resides[3]. Sources located in an area defined as urban should be modeled using urban dispersion parameters and sources located in areas defined as rural are modeled with rural dispersion parameters and resulting concentrations at each receptor are added together.

The ISCST3 model can accommodate a large number of sources and receptors, however, an optimum configuration is needed in order to minimize computer resources. Because source inputs vary with the type of source modeled, an important first step in creating the inventory is to identify each source of emissions as a point, area, volume, or line source. In ISC, line sources are not modeled, so line sources are modeled as a series of area sources as explained below. With the source types established, the appropriate model inputs can be determined. The following subsections describe the various source types and associated inputs for modeling. EMS-HAP

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[3]In making these determinations, the user should examine land use in adjacent grid cells and use judgement to create a "broad brush" view of the land use in the urban area; a "checkerboard" pattern is not meaningful.

(U.S. EPA, 2000a) has been designed to assist in the preparation of the NTI data as input in ISCST3. Additional information is available from the EMS-HAP user's guide (U.S. EPA, 2000a).

ISCST3 Point Source Characterization

Point sources involve the release of emissions from a well-defined stack or vent, at known physical stack parameters and operational conditions. Consequently, characterizing point sources for modeling is fairly straightforward. The basic model inputs for any point source are: stack location coordinates, the physical stack parameters (height above ground level and inside diameter at stack exit); operational conditions (gas velocity and temperature at stack exit); building dimensions (height, width, depth), and emission rate. In situations where a major source has multiple stacks and buildings, the individual locations of each should be used in the model.

ISCST3 Area Source Characterization

The definition of an area source for ISCST3 modeling is not the same as the CAAA area source definition in Section 3.2. Area sources are sources of air toxic pollutants that are emitted at or near ground level (e.g., landfills, waste lagoons, evaporation and settling ponds, nonroad mobile sources, etc.). Onroad mobile sources can also be characterized as area sources when specific roadway emissions are not available. The sizes of these sources can range from a few square meters in the case of settling ponds, to a few square kilometers or larger in the case of landfills. Emissions from area sources are assumed to be of neutral buoyancy. Therefore, plume phenomena such as downwash and impaction on elevated terrain features are not considered relevant for modeling area sources. The emission rate for area sources is in units of mass per unit time per unit area [e.g., $g\ s^{-1}\ m^{2}$]. It is an emission flux rather than an emission rate. As an example, assume the pollutant emission rate from a small lagoon is $150\ g\ s^{-1}$. The dimensions of the lagoon are 10 m by 20 m (total area is $200\ m^{2}$). If this source were modeled as a single, square area source, then the modeled emission flux would be $0.75\ g\ s^{-1}m^{-2}$ ($150\ g\ s^{-1} \div 200\ m^{2}$).

In ISCST3, area sources can be modeled in two ways: 1) with known locations and dimensions (e.g., landfills, airports, etc.); and 2) allocated to 1 km grid cell locations in the county when the actual location is not available (e.g., dry cleaners). Obtaining the actual location of the latter type sources and modeling them as point sources will result in better air quality estimates.

For dispersion modeling, the important parameters used to characterize area sources are location, geometry (this includes SW corner, initial vertical dimension, and angle of rotation), and release height. If the area source is not at ground level, a height for the source may be entered (for example, a non-zero value would typically be entered for the height of a land fill). If the release height of the source is greater than approximately 10 m, it should probably be

modeled as a volume source.

There are two basic types of volume sources: surface-based or ground-level sources that may also be modeled as area sources, and elevated sources. As with area sources, emissions from volume sources are assumed to be of neutral buoyancy. The effective emission height of a surface-based volume source, such as a surface rail line, is usually set equal to zero. An example of an elevated volume source is an elevated conveyor with an effective emission height set equal to the height of the conveyor. A source may be defined as a volume source for modeling when its emissions can be considered to occur over a certain area and within a certain depth of space. At refineries, fugitive exhaust from on-site structures such as tanks, or a treatment facility may be modeled as a volume source. Release area, base elevation and area are needed for modeling. A roadway over which contaminated soil is hauled may also be modeled as a series of volume sources.

The important parameters used to characterize volume sources for dispersion modeling are location, release height and initial lateral and vertical dimensions. The ISCST3 model user's guide has instructions on defining the initial lateral and vertical dimensions of the source. The length of the side of the volume source will need to be known, as will the vertical height of the source, and whether it is on or adjacent to a structure or building. The north-south and east-west dimensions of each volume source must be the same. For refined modeling, the location is simply expressed by a single east-west (X) and north-south (Y) coordinate.

ISCST3 Line Source Characterization

Line sources are typically used to represent roadways. For specifically estimating concentrations of nonreactive pollutants from highway traffic at adjacent receptors (hot spots) a dispersion model that handles such situations should be selected from those listed in the Guideline on Air Quality Models (40CFR51). Basic model inputs are the overall source length, width, and height

In ISCST3, toxic pollutants from line sources are simply modeled as a series of area or volume sources. In the case of a long and narrow line source, it may be impractical to divide the source into N volume sources, where N is given by the length of the line source divided by its width. Dividing the length of the line source by its width effectively splits the line source into a string of squares (for example, if the length of the line source was 100 m, and the width was 5 m, then the line source could be split into twenty, adjacent square volume sources). An approximate representation of the line source can be obtained by placing a smaller number of volume sources at equal intervals along the line source (for example, for the line source of length 100 m and width 5 m, a total of 10 square volume sources separated from one another by 5 m could be

defined). With this option, the spacing between individual volume sources should not be greater than twice the width of the line source. A larger spacing can be used, however, if the ratio of the minimum source-receptor distance and the spacing between individual volume sources is greater than about three. Previous model evaluation studies with roadways have shown that in ISCST3 modeling roads as volume sources gave similar results to modeling the roads as area sources (EPA, 1995c). However, modeling as area sources is more resource efficient. Additional sensitivity studies (Personal Communication, Brode, 2001) showed that the aspect ratios (ratio of roadway length to roadway width) can be increased from the present 1 to 10 up to 1 to 100 without degrading model performance. For the above reasons, in this example application, roads are modeled as ISCST3 area sources with aspect ratios up to 100.

Typically, onroad mobile sources are considered line sources. However, the NTI mobile source emissions are based on county-wide totals and allocating the emissions to all roads is impractical. Onroad emissions are modeled in ISCST3 in two ways. The first was to assign onroad mobile emissions to 1 km grid cells (see Section 4.3.1.1). A second method was to allocate onroad mobile emissions to major road segments such as Interstate, U.S. and State Highways using Geographical Information System (GIS) software. Onroad mobile emissions not specifically allocated to these roads were interpolated to 1 km grid cells (see Section 4.3.1.2). Nonroad mobile emissions, also reported as a county-wide total, are typically allocated to 1 km grids based on surrogates and also modeled as area sources in ISCST3.

3.5 Default Source Parameters

Besides the emission rate, the parameters needed to model emissions from point sources include source location coordinates, physical release height, stack diameter, exit velocity and temperature. These parameters should available in the NTI which employs an extensive data default assignment (see http://www.epa.gov/ttn/chief/net/nei_plan_feb2001.pdf).
Since most modeling analyses include a large number of sources over a relatively large area, it is inevitable that there will be gaps in the data for some of the sources. It is necessary to determine values for all the missing source characteristics, substitute them, and document the substitutions before the sources can be modeled.

Latitude and longitude are necessary to correctly place facility release points and associated emissions into specific geographic domains. Many instances have been reported where state and county codes do not correspond to the latitude and longitude values and/or the zip code supplied with each facility. The first stage in the verification of non-missing data is to use GIS overlays to determine if the latitude and longitude of each release point is within the study domain (i.e., the county). This ensures that sources supposed to be located within a physical representation associated with a county are sited within the boundaries of that county. This step includes coordination with local agencies.

Valid parameters for the physical characteristics of each point release (stack height, diameter, temperature and velocity) are necessary for proper air quality modeling. However, not all of the physical characteristics of each release point are reported. Also, fugitive or vent release locations are often not reported. Sometimes point source release values reported are physically implausible, suggesting that a misunderstanding regarding the meaning of the data field or the units of measure, or a mistranscription of data. The user should contact the local agency for better data or replace these unreasonable parameters with conservative values that are related to the type of emissions source.

For point sources with missing data, the following conservative values are recommended for use in air toxics modeling analyses:

Stack height	10 meters
Stack diameter	1 meter
Exit temperature	295 K
Exit velocity	1 meter/second

If the NTI does not contain building dimension information, and since building wake effects (building downwash) influences can significantly increase concentrations for receptors located close to the point source, the following approach may be used to set default values of building height and building width in the ISCST3 model. Default building dimensions of $H_b = 0.625 * H_s$ and $H_w = 2 * H_b$ (where H_b is building height, H_w is building width and H_s is stack height) may be used for stack heights of less than or equal to 65 meters, with a minimum building height of 3.05 meters, representative of a one-story structure. The value used for H_b places the stack height just above the Schulman-Scire criterion, except for stack heights that are less than about 4.6 meters, which is 1.5 times the minimum building height of 3.05 meters. The application of the Schulman-Scire downwash algorithm is therefore limited to the shorter stacks for which it is more likely to be applicable. The use of the Huber-Snyder downwash algorithm for stacks that are taller than 4.6 meters also avoids the potential for unrealistically increasing predicted impacts for these stacks based on relatively arbitrary building information, which could occur if the Schulman-Scire algorithm were to be applied to those stacks. For stack heights of greater than 65 meters, assume no building downwash occurs, since stacks of that height are likely to satisfy good engineering practice (GEP) stack height requirements to avoid building downwash influences.

Non-buoyant sources are sources with plume height equal stack height (e.g., from isolated vents), are likely to be from building vents or similar emission points. A building height equal to the stack height should be assumed, with building width equal to twice the building height. This automatically triggers the ISCST3 building downwash algorithm, and is a conservative approach.

3.6 Pollutants

The ISCST3 model is run for one pollutant at a time. The number of pollutants should be carefully defined to minimize resources. Section 112 of the Clean Air Act lists 188 hazardous air pollutants (HAPs). The Integrated Air Toxics Strategy has identified 33 HAPs that are of primary concern in urban areas (U.S. EPA, 1999b).

3.7 Source Grouping

From a post-analysis viewpoint, by grouping similar sources (e.g., mobile emissions), the analyst can more easily look at the impact of different source types. These groupings can be further subdivided into onroad and nonroad mobile source groupings. ISCST3 provides methods for grouping sources for these purposes.

3.8 Quality Assurance

In a complex analysis such as urban area wide modeling, there are many opportunities for error. Also, there many people are involved in the analysis and making decisions. It is recommended that all decisions be documented.

4. EXAMPLE CASE STUDY

4.1 Introduction

This section documents the methodology and results of an example case study. For this example, the Houston urban area is selected. The model domain covers several counties with the Houston urban area and Harris County in the center of the domain. The area covered by the study, along with key roadways and the location of the surface meteorological data site, is shown in Figure 4.1-1a. Emissions data for 1996 are used in this example. For illustration, example estimated concentrations are presented for five HAPs: benzene, cadmium, chromium, formaldehyde, and lead. There are three sets of model results/illustrations. The first set shows ambient concentrations when all highway emissions are allocated to 1 km grid cells (see section 4.3.1.1 for more detail on how emissions are allocated). For the second set, benzene and formaldehyde emissions from onroad mobile emissions are allocated to road segments (see 4.3.1.2 for an explanation of emission allocation). A third set was created to examine the effects of receptor placement on concentrations. In this example, benzene emissions using the latter emissions are used to calculate concentrations at receptors on a 500 m in a subset of the Houston domain (Fig. 4.1-1b). Since benzene is the most extensive of the HAPs, benzene's model results are presented in Section 4.4.1. A summary of results for the remaining HAPS, cadmium, chromium, formaldehyde, and lead are then presented in Section 4.4.2.

4.2 Model Methodology

4.2.1 Model Selection

The model used for this study was the EPA Industrial Source Complex Short Term (ISCST3) dispersion model. The ISCST3 model is a steady-state Gaussian plume model which can be used to assess pollutant impacts from a wide variety of sources such as multiple point, area and mobile sources. This model was selected for this application to demonstrate what can be done with off the shelf modeling tools. For this modeling application annual average, daily average, and by hour-of-day concentrations were calculated. This selection for the temporal resolution of the modeling results was based on the type of data that might be needed for use in a typical long term human exposure assessment. The ISCST3 model is applicable to receptors within about 50 km from the source and does not directly simulate the effects of pollutant chemistry (i.e., chemical transformation and reactivity).

The ISCST3 dispersion model includes the capability of handling multiple point, area, and mobile sources, incorporates building downwash effects, includes an urban dispersion option, and also contains considerable flexibility for specifying receptor locations and for grouping of source impacts. The ISCST3 model also includes algorithms to treat the effects of elevated and/or complex terrain, and the effects of dry and wet deposition of gaseous and particulate emissions. The ISCST3 model includes an option to vary emissions by season and hour-of-day, which was useful in meeting one of the design criteria for this modeling analysis, since the available emissions inventories reflect variations in emission rates by season and hour-of-day as inputs. This temporal resolution has also been selected for the model outputs based on the needs of a typical long term exposure assessment.

At the time of report preparation, EPA is developing and testing another steady state plume model, AERMOD which could be used as an alternative to the ISC3 model. AERMOD is actually a modeling system with three separate components: AERMOD (AERMIC Dispersion Model), AERMAP (AERMOD Terrain Preprocessor), and AERMET (AERMOD Meteorological Preprocessor). Special features of AERMOD include its ability to treat the vertical inhomogeneity of the planetary boundary layer, special treatment of surface releases, irregularly-shaped area sources, a three plume model for the convective boundary layer, limitation of vertical mixing in the stable boundary layer, and fixing the reflecting surface at the stack base. A treatment of dispersion in the presence of intermediate and complex terrain is used that improves on that currently in use in ISCST and other models, yet without the complexity of the Complex Terrain Dispersion Model-Plus (CTDMPLUS). To the practicable extent, the structure of the input or the control file for AERMOD is the same as that for the ISCST3.

4.2.2 Averaging Period

In order to ascertain the long term exposure to the pollutants being modeled, annual average concentrations were calculated. Hourly and daily averages were also calculated for further study.

4.2.3 Receptor Selection Strategy

Receptors in the Houston domain were selected to coincide with census tract centroids as shown in Figure 4.2-1. This would allow the receptors to represent the impact concentrations would have on urban population areas. The selection of the locations of the receptors was made so that modeled results can be input into the EPA's HAPEM exposure model (U.S. EPA, 1999a).

In the present analysis, our receptors are located at the centroid of each census tract; typically several kilometers apart. There is interest in determining if there are any geographical variations in concentrations within the census tract. Since adding additional receptors to the entire domain increases model run time and analysis resources, we selected a smaller subdomain for testing. This subdomain encompassed sources of high emissions, which could result in localized high concentrations and may not be represented by the largely spaced census tract receptors. In this case, the emissions are stationary sources in industrial areas located in the southeast section of Houston where there were fewer census tracts (receptors) to calculate concentrations. In this subdomain, we added receptors at 500 m intervals in order to see the locally high concentrations.

4.2.4 Treatment of Terrain Influences

The ISCST3 model may be run without terrain influences, i.e., flat terrain, or alternatively, the ISCST3 model will adjust the plume heights by the receptor elevation above or below stack base to account for the effects of elevated and complex terrain. The ISC3 User's Guide (U.S. EPA, 1995b) contains information for handling terrain. The flat terrain option was used for the Houston analysis. The terrain within the Houston modeling domain is relatively flat with maximum height variations of about 50 feet. Given that a significant portion of the emissions for these pollutants is from area sources, and the ISCST3 model ignores terrain influences for area sources, the flat terrain assumption is considered adequate for Houston.

4.2.5 Land Use Classification

Since the Houston study domain is large, it encompasses both rural and urban regions. Emissions input into ISCST3 must be assigned either all rural or all urban dispersion "flags" for use in ISCST3. The "flag" was based on the presence of man-made objects likely to affect the surface roughness characteristics. For efficiency, the Houston domain was divided into urban and rural grid cells (1 km resolution). Grid cells were classified as urban or rural based on

Commercial/Industrial Land Use Classification. A grid cell was classified urban that contained Commercial/Industrial surrogates. Otherwise, it was classified as rural. All sources in an urban grid cell are modeled with urban dispersion and all sources in a rural grid cell are modeled with rural dispersion. Once the land use is classified, separate ISCST3 model runs were made for the rural dispersion and rural emissions and for urban dispersion and urban emissions. The results from the two separate runs were then combined to give concentrations at receptors from both urban and rural sources. Figure 4.2-1 shows the land use classification used in ISCST3 for Houston.

The effects of the land use was noticeable for near-source low-level sources during stable meteorological conditions. Under these conditions, because of the reduced mechanical mixing in the lower atmosphere with rural dispersion, a source assigned rural dispersion would yield higher near source concentrations than for a similar source with urban dispersion.

4.2.6 Meteorological Data

4.2.6.1 Selection of Surface and Upper Air Stations

The ISCST3 model requires hourly surface observations of wind speed, wind direction, ambient temperature, and stability category, in addition to mixing heights derived from twice-daily upper air soundings as meteorological inputs. The mixing height data was calculated by the Mixing Heights program on the SCRAM web site. The hourly surface data for major National Weather Service (NWS) stations were obtained from NCDC.

Houston is located in flat coastal plains about 70 km from the Gulf of Mexico and about 40 km from Galveston Bay. The climate is predominantly marine and is influenced by land/sea breezes. This effect is likely to decrease across the city. Meteorological data are collected at two NWS sites in Houston: George Bush Intercontinental Airport (IAH) located north of the city and Hobby Field (HOU) located south of the city. In a large urban area such as Houston meteorological conditions are likely to vary across the city and ideally, emission sources should be modeled with the most representative meteorological data. In this case, Hobby Field reported a large amount of missing meteorological data and for computational efficiency and simplicity, only the George Bush airport data were used. It is assumed that annual average concentrations based on the two data sets are likely to be very similar and any effects due to land/sea breeze circulation are negligible. The location of IAH can be seen in Figure 4.1-1a.

The selection of the upper air stations for deriving mixing heights was based on the station considered to be the most representative for the city. For Houston, the Lake Charles upper air station is located about 135 miles away, while the upper air station at Victoria, TX is about 120 miles away. However, the Victoria station was relocated to Corpus Christi, TX in January 1990. Since Victoria is located about the same distance inland from the Gulf of Mexico as both Houston

and Lake Charles, and the distance from Houston to Victoria is comparable to the distance from Houston to Lake Charles, both stations would be equally representative for use with the Houston surface data. However, given the fact that the Victoria station was moved to Corpus Christi, and the fact that Corpus Christi is located nearer to the Gulf coast, Lake Charles was considered to be the better choice for use with Houston. The selections of the upper and surface stations also corresponds with the recommendation of the Texas Natural Resource Conservation Commission (TNRCC) for modeling in Harris County, where Houston is located (TACB, 1992). Table 4.2-1 gives the names and locations of the stations used for the study.

4.2.6.2 Meteorological Parameters for Deposition Calculations

Several additional meteorological parameters are needed as inputs to the Meteorological Processor for Regulatory Models (MPRM) in order to implement the dry deposition algorithms in the ISCST3 model for particulate and gaseous emissions. For this study, the TOXICS option was selected in ISCST3 which included dry deposition. Additional parameters related to wet deposition were not needed, since wet deposition was not included in the analysis. The additional dry deposition parameters are listed below with values based on guidance in Section 3.3 of the MPRM User's Guide (U.S. EPA, 1996a):

Houston:	Winter	Spring	Summer	Fall
Albedo	0.20	0.14	0.16	0.18
Bowen Ratio	1.5	1.0	2.0	2.0
Roughness Length (measurement site) (m)	0.15	0.15	0.15	0.15
Roughness Length (application site) (m)	1.00	1.00	1.00	1.00
Minimum Monin-Obukhov Length (m)	50.0	50.0	50.0	50.0
Surface Heat Flux (fraction of net)	0.25	0.25	0.25	0.25
Anthropogenic Heat Flux (Wm^{-2})	10.0	10.0	10.0	10.0
Leaf Area Index	1.0	1.0	1.0	1.0

4.2.6.3 Meteorological Preprocessing

The MPRM program was used to preprocess the meteorological data for use with the ISCST3 model. The source of the surface meteorological data used in MPRM was the Integrated Surface Hourly Data (ISHD), available from NCDC, for the year 1996. Both the MPRM (U.S. EPA, 1996a) and PCRAMMET (U.S. EPA, 1996b) meteorological preprocessors can be used to preprocess NWS surface and mixing height data for use with the ISCST3 model. Only MPRM was used. PCRAMMET does not allow for specifying temporal (e.g., seasonal) or spatial variations of the surface parameters identified in the previous section and does not support the additional parameters needed to utilize the dry deposition algorithm for gaseous pollutants. These additional parameters are leaf area index (input by the user), and incoming solar radiation (calculated by MPRM). An estimate of minimum mixing depth for both study areas was

determined based on guidance in Section 2.6.

4.2.6.4 Meteorological Statistics for Houston

Meteorological statistics were calculated for the Houston domain in order to further understand model results. A wind rose shown in Figure 4.2-2 was created for Houston using the WRPLOT program which is available on the SCRAM web site. The wind rose showed that in 1996, the wind direction for Houston was predominantly from the south-southeast. There were 1,599 calm hours reported in the data or about 18% of the hours in a year (8,784 hours for a leap year).

Table 4.2-2 shows the average daily maximum and minimum temperatures, averages hourly wind speed, average hourly wind direction, and annual accumulated rainfall for 1996 and climatology. Climatological values for wind speed and temperature were obtained from the EPA SCRAM web site for the years 1984 through 1992. Thirty year (1961-1990) climatological annual rainfall was obtained from http://www.met.utah.edu/jhorel/html/wx/climate/normrain.html. From Table 4.2-2, it can be seen that 1996 did not deviate from climatology for wind speed and direction, and temperatures. However, it did appear that 1996 was a dry year when compared to climatology.

4.2.7 Chemistry

Estimating ambient concentrations of pollutants that undergo secondary transformation such as formaldehyde requires three steps. In the first step, the ISCST3 model is used to estimates concentrations from sources that directly emit formaldehyde. Decay can be estimated by using a half life for the modeled HAP. A value of 155,520 seconds was used for the half life of formaldehyde and for exponential decay. See Section 3 of the ISC3 User's Guide (U.S. EPA, 1995b) for decay calculations in ISCST3. Concentration estimates are obtained at all receptors in the domain. In the second step, estimates from the screening level photochemical model (OZIPR) are obtained. In the third step, estimates for steps 1 and 2 are added to obtain the total formaldehyde concentration. For this analysis, OZIPR was not run, and instead tabular values in U.S. EPA, 1999c were used. This is consistent with recommendations in the report. The tables in U.S. EPA, 1999c are organized by season, for the hours between 8am and 8pm local time. Secondary contributions during overnight hours, 9pm to 7am, are obtained by linearly interpolating 8pm to 8am secondary concentrations when the 8pm value exceeds the 8am value; when the 8pm value is smaller than the 8am value, all overnight values are assigned the 8pm value.

4.2.8 Background

The methodology used to calculate background concentrations is described in Appendix A.

The methodology described is for diesel PM but the same approach was used for benzene and lead.

Annual average background concentrations were calculated for benzene and lead. Benzene background concentrations are presented in Figure 4.2-3a. The higher background concentrations are southwest, northwest, and northeast of Houston. The high background concentrations in these areas are from sources in Houston and Galveston. Note that lower concentrations are in Houston because the large sources located there do not impact within Houston but their impact is seen elsewhere in the domain. In the southeast part of the domain, there is overlap of lower background concentrations. This is because the 50 km radius ring for both Houston and Galveston, TX overlap. This is an area where sources less than 50 km away from Houston are not considered and sources less than 50 km from Galveston are not considered.

Lead annual average background concentrations are shown in Figure 4.2-3b. Higher background concentrations are located west of the Houston area. The lowest background concentrations are located in the northwest part of the Houston downtown area. The two circular regions are representative of the 50 km ring associated with the two airports in the Houston region.

4.2.9 Model Evaluation Procedure

In order to evaluate the results for the Houston study, benzene, formaldehyde, and lead modeled annual average concentrations are compared to observed annual average concentrations from monitors in the domain. The locations of the monitors are shown in Figure 4.1-1. There are no monitors in the Houston area for cadmium and chromium. Note that Monitor 3 is missing. This monitor had sparse data and appeared to have been dropped from the monitor dataset for Houston.

4.2.10 Study Limitations

Some limitations of the study involve the following:

1.   Data availability/reliability. Emissions data can have uncertainties in magnitude of emissions but also in other parameters such as location. These issues are addressed by user quality assurance of the data and EMS-HAP quality assurance programs. Meteorological data, terrain inputs and site selection also contribute to uncertainty in model results. Care should be taken in selecting the meteorological data and sites as outlined in Section 2.6. Meteorological preprocessors, such as MPRM should be used to perform additional quality assurance on data as well.

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2. Computational resources. Computational resources can limit the number of receptors chosen for model simulations (See Section 2.4) since increasing the number of receptors can increase runtime. Also, the number of sources as well as averaging times for concentrations can also increase runtime.

3. Model Limitations. ISCST3 model formulation also contributes to uncertainty in modeled results. See ISC3 User's Guide (U.S. EPA, 1995b) for ISCST3 model limitations.

4.3 EMISSIONS

4.3.1 Processing of Emission Data for ISCST3

Emissions data was processed with two methods. The first method was to process all sources, major, area/other, onroad mobile, and nonroad mobile, and interpolate to 1 km grid cells. A second method was to interpolate major, area/other, and nonroad mobile emissions to 1 km grid cells as in the first method. However, in order to better model onroad mobile emissions, the emissions were allocated to road segments in the Houston domain. Onroad mobile emissions not specifically allocated to road segments were allocated to 1 km grid cells. Emission processing for the 1 km gridded emissions (method one) are discussed in 4.3.1.1 while the allocation of onroad emissions to road segments is discussed in Section 4.3.1.2. Emissions for ISCST3 were processed using EMS-HAP (U.S. EPA, 2000a). The processing steps of the gridded emissions can be seen in Figure 4.3-1. Once processed by EMS-HAP, the emissions data were put into a format necessary for input to the source (SO) pathway of ISCST3 (see U.S. EPA, 1995b for source input format). Also, emissions were split into urban and rural sources for the urban and rural dispersion in ISCST3. Details follow in Section 4.3.1.1. It should be noted that the emissions inventories processed through EMS-HAP contained emissions for several pollutants, including those not presented in this report (i.e., butadiene, diesel particulate matter, etc.).

4.3.1.1 Gridded emissions

Mobile Sources Processing

For mobile sources, the first preprocessing step was to separate the airport emissions from the mobile inventory using AirportProc (Chapter 2 of the EMS-HAP User's Guide, 2000a). This program separated the airport emissions from the mobile inventory and prepared the airport emissions for input into the point source processing programs. AirportProc allows for modeling airport emissions as point sources instead of spatially allocated mobile sources. This capability was built into the program because airport locations are readily available.

Once the airport emissions are split from the mobile inventory, the remaining mobile

inventory is processed through a series of programs to create ISCST3 ready emission source files. The first step is that the sources within the Houston domain are extracted from the mobile inventory. These sources are then processed through the EMS-HAP MobilePrep program (Ch 9 of EMS-HAP User's Guide, 2000a). This program splits the mobile inventory into onroad and nonroad mobile inventories and also creates variables needed for the AMProc program.

After the onroad and nonroad inventories are created, they are then processed through Mobile_addDPM.SAS® which concatenates diesel-PM emissions with the onroad inventory and the nonroad inventory, resulting in onroad and nonroad inventories containing diesel-PM emissions. Next, each inventory, onroad and nonroad mobile, are processed through AMProc (Ch. 10, EMS-HAP User's Guide, 2000a). AMProc selects pollutants, groups and assigns characteristics to each pollutant, spatially allocates county level emissions, temporally allocates emissions, determines model parameters, and other functions (see Ch. 10 of EMS-HAP User's Guide, 2000).

Output from AMProc is processed through AMFinalFormat which creates SAS® datasets and ISCST3 emission source files (SO pathway) to be included in the ISCST3 runstream input file.

Area Sources Processing

The 1996 area source inventory initially includes landfills. The area source inventory was then split into landfills and remaining county level area sources. Landfills were to be modeled as ISCST3 area sources. This was because ISCST3 area sources are used to model low level or ground level emissions with no plume rise. See Section 3.4 for a review of ISCST3 area source characterization.

The first step in processing the landfills was to obtain location and size data about the landfills. TNRCC provided landfill data for Texas. Landfills were selected by county and area converted from acres to square meters. Since counties contained more than one landfill, allocation factors were calculated as the ratio of the area of a specific landfill and the total area of all landfills in a county. This was done by the program landfill2point.SAS® (Figure 4.3-1). The landfill inventory was then used as input into the ISCST3 major sources.

The remaining county level area sources were processed by EMS-HAP. The first step was the AreaPrep program (Ch. 8 of EMS-HAP User's Guide) which prepares the area source inventory for AMProc. AreaPrep assigns spatial surrogates for each area source category for subsequent spatial allocation of county level emissions. The program also assigns codes to source categories for matching to temporal profiles and creates inventory variables needed by AMProc. After processing by AreaPrep, the area source inventory was processed by AMProc and AMFinalFormat resulting in 1 km gridded area source emissions. These emissions were written

to source (SO pathway) files ready for ISCST3.

Major Sources Processing

The 1996 point source inventory was first processed through a program (extract_Houston.SAS®) that extracted sources within the Houston domain (state county FIPS 48201, 48473, 48339, 48291, 48071, 48167, 48039, 48157) that have defaulted site locations or questionable FIPS. The data were from the output from PtDataProc (see description below) when it was used to prepare data for the ASPEN model. Sites extracted had the LFLAG variable set to "county", indicating a defaulted site. A site's location is defaulted when the location coordinates are missing or incorrect. See the EMS-HAP User's Guide, Chapter 3 for a more detailed explanation (U.S. EPA, 2000a). Once the sites were extracted, they were then manually checked. Sites in which the correct location could be determined readily were corrected. Remaining defaulted sites were sent to TNRCC for correct locations. A list of corrected sites is shown in Table 4.3-1.

The next step was to process the entire major source inventory, airport emissions inventory, and landfill emissions through the program Houston_ISCpreproc.SAS®. This program combined the three inventories, initialized certain ISCST3 variables (ISCtype, arelhght, axlen, etc.), corrected the suspect sites, and performed quality assurance on the inventories. Output included the corrected point sources (no landfills or airports) and data ready for PtDataProc. The PtDataProc ready data contained point sources, landfills, and airport emissions.

PtDataProc (Ch.3 EMS-HAP User's Guide) performed quality assurance on point source locations and stack parameters. The program also removed inventory variables not needed for further processing. After processing by PtDataProc, the point source inventory was processed by PtModelProc (PtAspenProc in EMS-HAP User's Guide, Ch. 4). PtModelProc selected pollutants, grouped or partitioned pollutants and determined their characteristics. Rural/urban dispersion parameters were assigned and vent type and building parameters were also assigned. Output from PtModelProc was used as input into PtTemporal.

PtTemporal temporally allocated annual emissions to hourly profiles. These hourly profiles are then used to produce eight three-hour emission rates. Output from PtTemporal was input into PtFinal_ISC (PtFinalFormat in EMS-HAP User's Guide, Ch. 7) which created the ISCST3 ready source files (SO pathway).

Final Processing of Gridded Emissions

The source files created by EMS-HAP contained both rural and urban sources. Since ISCST3 is run for urban and rural separately, the source files had to be split into all rural

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emissions and all urban emissions. The splitting was done by a SAS® program that processed the source files and split them into rural or urban files based on the locations of the sources in the Houston domain. The cells were designated urban or rural based on the Commercial/Industrial land use classification. After the splitting, the source files were ready for input into ISCST3. The source files consisted of the emissions, building dimension files, hourly emission files, and gas and particle deposition information files. See the ISC3 User's Guide (U.S. EPA, 1995b) for information about the format of these files. Values for particle deposition (particle diameter, etc.) were obtained from EMS-HAP, Appendix E (U.S. EPA, 2000a). Fine particle diameters were 1.58 : m and coarse particle diameters were 6.93 : m. Mean particle density for cadmium and chromium was 1.0 g cm^{-3}. Values for other deposition parameters for both particles and gases can be found in Wesely et al., 2002.

4.3.1.2 Allocation of onroad mobile emissions to road segment emissions

Previous methodologies for preparing ISCST3 model-ready mobile emissions inventories are based on using spatial surrogates to allocate the county level emissions to each grid cell. These surrogates are meant to represent areas where mobile source emissions are likely to occur. Population is used as the surrogate for neighborhood roads and roadway types are used for the major roads. Surrogate values are calculated for each grid cell by using Geographic Information System (GIS) software to spatially overlay a grid onto census block areas and TIGER roads. Census blocks boundaries and roads are obtained from the U.S. Census TIGER/Line data (http://www.census.gov/geo/www/tiger) and population counts from the U.S. Census of population and housing (http://www.census.gov/mp/www/rom/msrom6ae.htm). Census block areas are joined with population data to determine the number of people living within each block. A modeling grid is overlayed onto census blocks and the total population in each grid cell is calculated. The ratio of the cell population to the total county population is then applied to the county emissions to obtain grid cell level emissions. Roads consist of contiguous arcs which are coded according to road type. The total length of each road type is calculated for each cell. Ratios to the total length of each road type in the county are calculated and applied to the county emissions for that road type. The emissions from the population and roads are then summed to obtain the total mobile emissions for each grid cell.

A drawback to this methodology is that the spatial distribution of emissions are not always represented accurately. First, surrogates may not adequately represent the census block's mobile source activity correctly. Secondly, distributing mobile source emissions throughout an area may underestimate emissions density on transportation features such as roadways or parking lots. Road emissions are spread evenly throughout a cell instead of occurring along actual road locations. As a result, air dispersion modeling can not capture high concentrations that often occur next to roadways and at intersections. This study demonstrates an alternative methodology using link-based emissions generated for the major roadways in Harris County, Texas. Harris County emissions are calculated for each major roadway link using traffic counts and vehicle emission data. Roads are then modeled as ISCST3 area sources with aspect ratios (ratio of

roadway length to roadway width) up to 100. Road emissions for local and neighborhood streets are processed using the previous gridding methodology due to the lack of traffic counts on the local facilities. The process for creating link based emissions for Harris County is described below.

Data Sources

The data required for generating link based emissions include 1) city specific traffic counts 2) a base map of road locations and 3) mobile emissions factors.

Local Traffic Counts - City specific traffic counts may be obtained from the State Department of Transportation (DOT) or from local sources such as the Metropolitan Planning Organization (MPO) or a Regional Planning Council/Council of Governments. State DOTs' may also provide access to local travel data. These data are usually part of the Highway Performance Monitoring System (HPMS), administered by the U.S. Department of Transportation (http://www.fhwa.dot.gov/ohim/hpmspage.htm). It is preferable that the traffic counts are in a spatial database, suitable for import into a GIS. Traffic counts will usually be provided as Annual Average Daily Traffic (ADT). The ADT represents the total number of vehicles crossing a measured point during an average day. The traffic counts for the Houston study are from the Houston/Galveston Area Planning Council.

As an alternative to traffic counts for inventory calculations, many MPOs use travel demand models (TDMs) to predict the number of vehicle trips in a transportation network TDMs use local economic and demographic data to determine trip originations and destinations in travel analysis zones (TAZs), often the same as Census blocks. TDMs also calculate the optimum number of trips along each roadway in a simulation network.

TDMs have several advantages in modeling air toxics, including placement of vehicle starts in TAZs. Start emissions from mobile sources may constitute the majority of toxic releases. Because TAZs often use Census-defined boundaries, vehicle start emissions and their locations can be estimated with greater accuracy and imported into air quality models as area sources using GIS software. Users familiar with emission budgeting and conformity applications of the MOBILE model will find that geographically resolved toxic emissions inventories can be created using many techniques already in place.

Road Locations - A base map of road locations in the study area can usually be acquired from the sources identified above. These should be in electronic form and, at a minimum, contain geographic coordinates and road names. If possible, these data should contain information on roadway attributes including road width, number of lanes, median width and surface type. If an electronic map is not available, then a paper map can be converted to digital form by digitizing which will assign geographic coordinates to the road links. Ideally, the digital map would be in a

format that can be easily imported into a GIS. Examples are ArcInfo® export files or ArcView® shape files that are used by those software packages. If local sources are not available, U.S. Census TIGER roads can be used, although they may not be as accurate and up to date.

   Emission Factors - In the Houston modeling analysis, emission factors for benzene, 1,3-butadiene and formaldehyde are obtained from the EPA toxic emission factor model, MOBTOX5b, developed by the Office of Transportation and Air Quality (Cook et al., 1998; U.S. EPA, 1999d; Cook et al., 2000). The emission factors are expressed in grams emitted per vehicle mile traveled (g mi^{-1}). MOBTOX5b generates emissions factors for total organic gas (TOG) and speciates TOG into individual air toxics based on vehicle and fleet parameters. The TOG speciation fractions in the model depend on technology types, driving cycles, and normal versus high emitters. The toxic fraction of TOG is also highly dependent on fuel parameters included in the Complex Model for reformulated gasoline and a draft fuel effects model for MTBE. Emission factors are generated for the vehicle classes shown in Table 4.3-2. They are based on an average vehicle speed of 19.6 miles per hour for all vehicles. In reality, speeds will vary significantly among different roadway links, and can have a large impact on emission factor estimates (U.S. EPA, 2000b). These emission factors also assume a distribution of operating modes with 20.6% of VMT assigned to cold starts, and 27.3% to hot starts[4]. Using parameters more appropriate for individual roadway links will result in more accurate link specific emissions. In the Houston analysis, for instance, a higher average vehicle speed and assignment of more VMT to running mode would have been more representative of major roadways. Of course, these parameters also vary by time of day, which is not reflected in this analysis. However, the use of default parameters are adequate for the purposes of methodology development and evaluation of the impacts of a link based approach on dispersion modeling results.

   EPA has recently integrated gaseous toxic and PM emission factor estimations into the MOBILE6 model (U.S. EPA, 2000c; U.S. EPA, 2002). MOBILE6 estimates emission factors by highway functional system (freeway, arterial collector, local roadway, freeway ramp). When the user specifies an average speed for roadway functional type, MOBILE6 applies a speed distribution for that roadway type. Thus, MOBILE6 can be used to develop emission factors more appropriate for specific links.

   MOBILE6 calculates toxic emission factors as a fraction of total organic gas (TOG). The toxic fraction of TOG for each species is highly dependent on fuel properties. Therefore, MOBILE6 requires more detailed fuel parameter descriptions for calculating toxic emission factors than for criteria pollutant emission factors. Detailed fuel composition data is available for

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[4]A cold start is defined as the first 3.5 miles traveled by vehicles after a "cold-start", and a hot start as the first 3.5 miles after a hot start."

some areas through the Alliance of Automobile Manufacturers' North American Fuel Survey[5]. Where Alliance survey data is unavailable, TRW Petroleum Technologies Survey gathers regional fuel data which may be substituted for local survey data[6]. In particular, the fuel properties required by the MOBILE6.2 and MOBTOX5b models are:

- % Aromatic of gasoline on volume basis
- % Olefin of gasoline on volume basis
- % Benzene of gasoline on volume basis
- E200 - % of vapor a gasoline produces at 200°F
- E300 - % of vapor a gasoline produces at 300°F
- Oxygenate type and content on volume basis

Emission factors for diesel PM are based on modeling done for EPAs' recent regulation promulgating 2007 heavy duty vehicle standards (U.S. EPA, 2000c). The emission factors used are as follows:

LDDV – 253 mg/mi
LDDT – 309 mg/mi
HDDV (urban interstate/ freeway) – 985 mg/mi
HDDV (other urban facilities) – 921 mg/mi)

Generally, particulate emission factors can be estimated using the MOBILE6 emissions model, which calculates particulate emission rates using similar fleet and fuel parameters as discussed above. However, particulate emissions do not require fuel parameter specifications of the same detail as the gaseous toxics component of the model.

Users with access to a TDM should make use of roadway specific speeds, informed by TDM results. Since some TDMs often produce speeds only to ensure optimum distribution of traffic volume, speeds in inventory calculations should be based on other means of calculating speed (For more detailed discussion of travel demand modes in, consult "Procedures for Emission Inventory Preparation. Volume IV: Mobile Sources." EPA report number EPA420-4-92-009. Available at http://www.epa.gov/otaq/invntory/r92009.pdf.)

In the Houston modeling study, toxic emissions factors for each pollutant are calculated using local data on Houston fuel and fleet parameters. These emissions factors are applied to the

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[5]The Alliance's fuel survey can be accessed via http://www.autoalliance.org/fuelquality.htm or (202)326-5533

[6]The TRW fuel survey data can be accessed from: TRW Petroleum Technologies, Attn: Cheryl L. Dickson, P.O. Box 2543, Bartlesville, OK 74005. Telephone: (918)338-4419

annual Vehicle Miles Traveled (VMT) for each road segment as described later in this section. Traffic counts by vehicle class are determined by a vehicle split table that apportions the total traffic into 12 vehicle types as seen in Table 4.3-2. This type of table is specific to every locality as each city has its own particular vehicle mix. Emission rates are also specific for each area. Those for the Houston study are estimated as described above.

<u>Data processing</u>

Road segments

The Houston study uses roads extracted from TIGER data because road data from local sources do not contain the necessary geographic information. Once the data are acquired they are imported into the ArcInfo® GIS. The road data must then be edited to obtain a layer of major roads which meet the following ISCST3 model criteria. First, local and neighborhood roads are deleted so that only the major roads for which VMT will be calculated remain. Refer to Figure 4.1-1 for road locations. Next, road segments must be processed to meet minimum and maximum length requirements for use in the ISCST3 model. A roadway link cannot have less than a 1:100 ratio or greater than a 100:1 ratio with the road width. Table 4.3-3 shows the number of lanes assumed for each road class and the associated length parameters. In order to create road segments with correct lengths, the segments are first joined together to form pieces of the maximum possible length, thereby eliminating segments shorter than the minimum threshold. Vertices, x and y locations along the line, are then added at specified intervals along the segments and used to split them into sections that do not exceed the maximum length threshold.

Traffic counts

Each road segment must be associated with a traffic count in order to calculate the traffic volumes and related mobile emissions. In the Houston study area there are discrepancies between the traffic count locations and the road segments; this becomes apparent when these two data sources are overlayed using the GIS. The traffic counts are collected at discrete point locations which do not always align with the roads. The points contain no attribute information, such as address location, to link them to road segments. In order to link traffic counts with the closest road segment, a buffer is generated around each traffic count point. In the Houston study a 100 meter buffer proved the optimum size but this may vary depending on the area modeled. The traffic count buffers serve to convert point locations to polygon areas which can then be overlayed with road segments. The overlay process joins traffic counts to individual road segments.

Traffic counts assigned using the method described above are linked to discrete locations along a road. Counts must be interpolated along the entire length of the road in order to calculate continuous traffic flows. To do this, the dynamic segmentation capabilities of the GIS are used to create a file containing ordered road segments and their ADT counts. Dynamic segmentation is a

layered system of pointers which can associate attributes to geographic locations along a linear feature. In this study, it is used to determine the order of segments along each road by creating a route. Each route is comprised of sections which are identified by their starting and ending position along the road. The starting point is the "from node" and the ending point is the "to node"; therefore each section is a vector which imparts a direction of flow. As long as all of the sections along a road run or flow in the same direction, it is possible to create an ordered table of road segments with attached ADT value. This ordered table can then be used to interpolate the ADT along the route by creating ratios of distances between segments with known traffic counts. The ratios are used to apportion ADT based on distance and direction from known values assuming a constant rate of change between traffic count locations. The road segments containing road name, unique ID number, segment length, traffic count, road type and State/County FIPs codes are then written out into an ASCII file and imported into SAS® software for calculation of emissions.

Calculation of link based emissions

The ASCII records generated in the steps above are read into SAS® software for calculation of road emissions. First, the vehicle split factors shown in Table 4.3-2 are applied to each record by road type. These distributions are national defaults used in the EPA Emission Trends report to characterize the vehicle types present on the 12 different roadway types included in the HPMS.

Applying the vehicle split table divides the traffic along each road among the 12 vehicle types and assigns a proportionate amount of the total ADT to each road segment. Once the vehicle split ADT counts are determined, the emissions factor table is used to calculate emissions by vehicle type, pollutant and road type by performing the following operations:

Annual VMT = ADT * Roadway Length * 365

Emissions = (VMT * emissions factor)

After the emissions along each road segment are calculated, the data are brought back into ArcInfo and the emissions are merged with the road segment locations. The results for benzene and formaldeyde are presented in Section 4.4. A final step is to write out a formatted file for input into the ISCST3 model. This file contains the UTM coordinates which define the starting and end points of each segment as well as the information needed to model the road segments which include emissions, total segment length, road classification code, and road width. Road segment emissions are modeled in ISCST3 as rural sources while the remaining onroad mobile emissions not specifically allocated to road segments are processed through EMS-HAP as for gridded emissions and modeled in ISCST3 as rural or urban sources.

In applications in which a TDM is used, it may also be necessary to match vehicle traffic counts to specific roadways, as transportation models often express vehicle counts at nodes between roadways, rather than on specific roadways. TDM users may also need to generate a number of emission factors for each vehicle type, corresponding to different transportation facility categories and vehicle speeds predicted through use of the model.

One problem with the approach described here is that county level VMT estimates from the Highway Performance Modeling System (HPMS) used in the National Emissions Inventory and National Toxics Inventory do not always match local traffic count data. For example, the link based approach was tried on several adjoining counties in the Houston metropolitan area. The link based emissions calculated for major roadways in these counties exceeded the total county emissions in the NTI. This may be due to disparities in the way in which traffic data are collected but further investigation is necessary.

One consideration in implementing link-based roadway emissions inventories are parameters for the "release height" above the roadway of interest. In the Houston analysis, a zero release height was used. However, for some heavy-duty trucks, a higher release height may be warranted to reflect greater stack height. Due to uncertainties introduced by turbulence on roadways, however, it is unclear which release height is most appropriate. For elevated highways, a higher release height may also be warranted. However, highway elevation data were not available.

Another concern is the treatment of link emissions as area sources or as volume sources. The Houston model analysis implemented roadways as rectangular area sources. Common air quality models such as ISCST3 also allow specification of volume sources. Given the turbulent roadway meteorology, it is unclear whether volume or area source treatment of mobile sources is most appropriate. It will improve understanding of model output stability for users to employ both approaches for sensitivity analysis.

Users employing TDMs may also use starts per TAZ to locate start emissions more accurately. In this case a map of the TAZs, including number of starts, can be imported into a GIS database system. The distribution of vehicle types in each TAZ throughout the modeling domain are likely to be similar to those in the link based methodology. However, it is anticipated that local registration databases will more accurately reflect the composition of "start" fleets. MOBILE6 can determine start emissions for each hour of the day. The distribution of vehicle soak emissions can be determined by the ends of trips as predicted by travel demand models. The total emissions for each TAZ can be gridded using a GIS, or imported directly into air quality model input files, however, it is anticipated that grid cells will be easier to program as area sources into air quality models.

4.4 HOUSTON DOMAIN EMISSIONS AND MODELING RESULTS

This section describes the results of emissions preprocessing and ISCST3 simulations for Houston. Section 4.4.1 will describe the results for benzene and Section 4.4.2 will give overviews of results for the other HAPs. Simulations using all mobile sources modeled as area sources are referred to as ISCST3 BASE. For simulations using the road segment emissions (benzene and formaldehyde), results will be referred to as ISCST3 ROADS. ISCTST3 results using the 500 m receptor density are referred to as ISCST3 FINE GRID. For each simulation, modeling is performed for all source categories at one time, but model results can be output for each source category separately, so that concentration estimates can be attributed to each category.

For all HAPs, concentrations were calculated at 711 receptors (700 census tract centroids and 11 monitors sites) by ISCST3. For purposes of displaying ISCST3 results, the receptor concentrations were averaged over a 1 km grid cell containing that receptor. If there was more than one receptor in a grid cell, concentrations among the receptors were summed and then averaged within the grid cell; if there were no receptors in a cell, then the cell average was zero. This process resulted in 692 grid cells. See Figure 4.4-1 as an example showing the 1 km grid cells.

Table 4.4-1 gives the maximum annual averaged total (all sources) concentration and southwest corner of the grid cell in which it is located for each pollutant. The concentrations for each source category in that grid cell are also given. Table 4.4-2 gives the maximum concentration and location of each source category for each pollutant.

4.4.1 Benzene

4.4.1.1 Emissions

One kilometer gridded benzene emissions for total emissions, major, and onroad sources are shown in Figures 4.4-1 and 4.4-2. The emissions are high along the roadways leading into and around Houston, showing the contribution of onroad emissions. Other roadways can be seen as long segments in which the emissions are higher than the surrounding areas. The major emissions (Figure 4.4-2a) are mostly located in eastern Harris County. Most of the emissions range from 1-25 tons year^{-1}. However, there are five sources with emissions greater than 80 tons year^{-1}.

Figure 4.4-3a shows the contributions from the different source categories to the emissions for Houston. Also shown are the distributions for the 1996 national inventory, the Houston major source emissions, Houston area source emissions, and Houston mobile emissions. Onroad mobile emissions comprised most of the emissions (41%). A more detailed breakdown of the emissions by source category can be seen in Figure 4.4-3f for Houston.

Road segment emissions for benzene are shown in Figure 4.4-4a. Some of the higher emissions can be seen along the interstate highways (> 0.4 tons year^{-1} km^{-2}). Once the emissions on the road segments were allocated to those segments, the road segment emissions could be subtracted from the NTI onroad mobile gridded emissions. The remaining onroad gridded emissions are those onroad emissions not specifically allocated to the roadways shown in Figure 4.4-4a. These gridded remaining onroad mobile emissions are shown in Figure 4.4-4b. The highest emissions are clustered around the center of the city. Compared to Figure 4.4-2b, the roads were no longer as obvious in the remaining onroad gridded emissions as in the onroad mobile emissions shown in Figure 4.4-2b.

4.4.1.2 ISCST3 RESULTS

ISCST3 BASE

Annual average concentrations (background concentrations not included) from all sources were highest north of the city center (Fig 4.4-5). These higher concentrations correspond to the areas where there were high emissions (see Figure 4.4-1). Other high values were scattered around the region, northwest Galveston County and in eastern Harris County. The concentrations for each source category are presented in Figure 4.4-6. For major source concentrations, values increased from west to east. The highest concentrations are located near the major source emissions. The higher onroad concentrations appeared to be concentrated near high onroad emissions. Nonroad concentrations were mostly located within the city.

ISCST3 ROADS

The total concentrations for the ISCST3 ROADS run are shown in Figure 4.4-7a. The higher concentrations were mostly located within the city urban area. The onroad concentrations (Figure 4.4-7b) were also higher in the city than the surrounding areas. This pattern differs from the ISCST3 BASE onroad mobile concentrations (See Figure 4.4-6c) in which the onroad mobile concentrations are more widespread in the city. In order to compare the concentrations from the two different model runs, percent differences between ISCST3 ROADS and ISCST3 BASE were calculated. Figure 4.4-8 shows the percent differences between ISCST3 ROADS and ISCST3 BASE for total and onroad concentrations respectively (major, area, and nonroad mobile concentrations were not affected by the road segment emissions allocation). Allocating the onroad mobile emissions to road segments resulted in higher concentrations for most receptors. In north and northwest Harris County, the ISCST3 ROADS total concentrations are lower than ISCST3 BASE total concentrations. This same pattern also holds for percent differences between the onroad source concentrations. The lower ISCST3 ROADS concentrations in north Harris County were a result of the allocation of emissions to road segments. There were actually lower traffic counts in this area, resulting in lower emissions, and subsequently lower concentrations.

Figure 4.4-9 shows the largest source contributor to total concentrations for each receptor for ISCST3 BASE (Figure 4.4-9a) and ISCST3 ROADS (Figure 4.4-9b). For ISCST3 BASE concentrations, the total concentrations in each grid cell were composed in most part to the contribution from onroad mobile source concentrations (Figure 4.4-9a). The location of the maximum total concentration was an exception, in that the major source concentration contributed the most to the total concentration. As for the ISCST3 BASE run for benzene, the onroad concentrations contributed most to the total concentration at a majority of receptors. A comparison of maximum total concentrations for ISCST3 BASE and ISCST3 ROADS is shown in Table 4.4-3. The maximum concentration for ISCST3 ROADS is higher than for ISCST3 BASE. Also, the location of maximum concentration for ISCST3 ROADS was southwest of the maximum concentration of ISCST3 BASE.

ISCST3 FINE GRID

ISCST3 was run for benzene using a set of receptors spaced 500 m apart in an area shown in Figure 4.1-1. Onroad segment emissions and gridded emissions for all other sources (major, area, nonroad, and nonallocated onroad) were input into ISCST3. As previously noted, this area was chosen because of the location of major and onroad emissions. Concentrations from the model were analyzed in two ways: 1) scaling the color bar on the plots to the 98th percentile of the concentrations to see the concentration gradient; 2) scaling the color bar on the plots to the maximum concentration so that higher concentrations, "hot spots" could be detected.

The total concentrations are presented in Figure 4.4-10. Figure 4.4-10a shows the concentrations scaled to the 98th percentile. The most noticeable concentration gradients can be seen along the roadways. Figure 4.4-10b shows the concentrations scaled to the maximum value. Most concentrations were 5 : g m^{-3} or lower. The maximum concentration was over 40 : g m^{-3}.

Figure 4.4-11 through Figure 4.4-14 show the concentrations for major, area, onroad, and nonroad concentrations. For major concentrations, there appear to be three local maxima in the concentrations (Figure 4.4-11a). Figure 4.4-11b shows a similar pattern as for total concentrations, the highest concentration was in the western part of the domain with a concentration over 40 : g m^{-3}, although the local maxima can still be seen. Area source concentrations were low, less than 1 : g m^{-3}, with a maximum concentration at the eastern edge of the domain (Figure 4.4-12). Local maximum onroad concentrations are located along the roadways with the maximum concentration located near the interstate highways (Figure 4.4-13). As for area concentrations, nonroad concentrations are less than 1 : g m^{-3} (Figure 4.4-14). Several local maxima are evident from the concentration with the maximum concentration, approximately 0.8 : g m^{-3} was located in the southwest corner of the domain.

4.4.2 Other HAPs

For the other pollutants, cadmium, chromium, formaldehyde, and lead, the methodology for modeling and displaying used for benzene was applied to each pollutant.

Cadmium

Cadmium emissions were less than 2 tons year^{-1}. Area emissions were the largest contributors to the emissions by source categories, with incinerators being the largest sources (Figure 4.4-3b). Figure 4.4-15 shows the gridded total (all sources) emissions and the area source emissions. The pattern between both emission categories was similar. Emissions that appeared in the total emissions (for example, in northeast Harris County) but not in area source emissions were due to nonroad and major source emissions, which were few in number.

Total concentrations for cadmium (Figure 4.4-16a) were composed of concentrations from three source categories: major, area/other, and nonroad mobile. The highest total concentrations were located near the city center and in Galveston County. The area source concentrations were the largest components of the total concentration at most locations as seen in Figure 4.4-16b with the exception of the maximum total concentration (Table 4.4-1) where the major source concentration was the largest component.

Chromium

Figure 4.4-3c shows that major source emissions are the largest of the total emissions for chromium. Analysis of the gridded emissions for total emissions (Figure 4.4-17), major emissions, area emissions, onroad, and nonroad emissions (not shown) show that for the most part, the total emissions at each 1 km cell were composed of onroad, nonroad, and area sources. In other words, the major sources were few in number but were large emitters.

Highest total concentrations were in eastern Harris County (Figure 4.4-18a) near high emissions. Also, high total concentrations were modeled in Galveston County. Figure 4.4-18b shows the largest source contributors for each grid cell. In eastern Harris County, the major sources contributed the most to the total concentration. This was also true for the location of highest total concentration (Table 4.4-1).

Formaldehyde

Gridded total emissions for formaldehyde are shown in Figure 4.4-19. The higher emissions are along and around the roadways. Also, high emissions are located at the airports in northern and southern Harris County. These are primarily due to aircraft emissions which are large

nonroad mobile emitters. Figure 4.4-3d shows that nonroad mobile sources are in fact, the largest contributor to the total emissions.

Road segment emissions for formaldehyde are presented in Figure 4.4-20. A pattern in the location of the higher emissions is seen that is similar to the benzene road segment emissions pattern. As with benzene, the higher gridded remaining onroad mobile emissions are near the center of the city (Figure 4.4-21a). Compared to the all gridded onroad emissions (Figure 4.4-21b), more detail of the emissions can be seen in the city and in northwest Harris County, as well as northern Brazoria County.

ISCST3 BASE total concentrations for formaldehyde (including secondary concentrations of 8.8 : g m^{-3}) are shown in Figure 4.4-22a. As with other pollutants, high concentrations were modeled in northern Houston. Also high concentrations were calculated in the southern part of the city. The high secondary concentrations gave the total concentrations a more uniform distribution. Onroad mobile concentrations are shown in Figure 4.4-22b. High onroad concentrations were calculated in the northern part of the city and also in the southwest part of the city near high emission sources.

For ISCST3 ROADS, highest total (including secondary) concentrations for formaldehyde were mostly located within the city (Figure 4.4-23a) and in northern Harris County. The onroad concentrations also show a similar pattern (Figure 4.4-23b). The percent differences between ISCST3 ROADS and ISCST3 BASE are shown in Figures 4.4-24. Total concentration percent differences were positive at a majority of receptors with a few negative differences. For onroad concentrations, at most locations, the differences are positive, indicating that ISCST3 ROADS concentrations were higher than ISCST3 BASE. The exceptions were mainly in northern Harris County, in northeast Harris County and, southwest Harris County.

Figure 4.4-25 shows the largest source category contributing to the total concentrations for ISCST3 BASE (Figure 4.4-25a) and ISCST3 ROADS (Figure 4.4-25b). The pattern is similar for both model results but along some of the roadways within Houston, the onroad concentrations contribute more than nonroad, due in part to the increased onroad concentrations from ISCST3 ROADS. Table 4.4-4 compares the locations of the maximum total concentrations for ISCST3 and ISCST3 ROADS. Only the value of the total concentration changed as did the value of the onroad mobile concentration. Note that the position of the maximum total concentration did not change.

Lead

Figure 4.4-3e shows the breakdown of emissions for lead. The nonroad emissions are the largest contributors to the emissions (44%). The nonroad mobile emissions are due to piston engine aircraft. The gridded emissions for lead are shown in Figure 4.4-26. For the most part, the

spatial distribution of the gridded total emissions (Figure 4.4-26a) appears similar to the gridded area emissions (Figure 4.4-26b). The nonroad emissions (Figure 4.4-26c) show only a few sources but they are large emissions relative to area emissions. The nonroad emissions consist mainly of the two major airports in the domain.

Total concentrations for lead are shown in Figure 4.4-27a. The higher concentrations are in southern Harris County with another area of high concentrations in the northern part of the county. The area, and nonroad mobile concentrations are shown in Figure 4.4-27a-b. Higher area concentrations are located in the center of Houston eastward to the Harris County line. High nonroad concentrations are clustered in southern Harris County. For most receptors, the nonroad concentrations contribute the most to total concentrations (Figure 4.4-28).

4.4.3 Model to Monitor Comparisons

In order to ascertain the performance of the model concentrations, the annual average model concentrations at monitor sites were compared to annual average concentrations from the monitors. Only three of the HAPs had reported monitor values: benzene, formaldehyde, and lead. However, there was only one monitor for lead and four for formaldehyde. Only benzene will be discussed. Figure 4.4-29 gives the annual average concentrations for individual monitors and ISCST3 and ISCST3 ROADS for benzene. Also shown on the graph are the average concentration among all monitors for ISCST3 BASE, ISCST3 ROADS, and the monitor values. Root mean square (RMS) errors were calculated for ISCST3 BASE and ISCST3 ROADS. Allocating the onroad mobile emissions to road segments increased the average model concentration and decreased the RMS errors. Since benzene is dominated by onroad mobile sources, these findings suggest that allocating onroad emissions to road segments improves the model results. At the individual monitors, ISCST3 ROAD concentrations are higher than ISCT3 BASE concentrations. Observed concentrations are higher than ISCST3 BASE at all monitors except one monitor. ISCST3 ROADS concentrations are higher than observed concentrations at four of the monitors.

5. SUMMARY AND CONCLUSIONS

Emissions for the Houston region were processed through EMS-HAP and annual average concentrations were calculated using the ISCST3 model. Emissions were processed with two methods: 1) all sources were modeled as 1 km grid cells, and 2) onroad mobile emissions were allocated to road segments. In method two, onroad mobile emissions not specifically allocated to road segments were modeled to 1 km grid cells. Other sources (major, area/other, and nonroad mobile) were modeled as in method one. After emission processing by EMS-HAP, sources were divided into rural and urban sources. ISCST3 was then run for each source type and concentrations added together at each receptor during postprocessing. ISCST3 was run for five pollutants: benzene, cadmium, chromium, formaldehyde, and lead. There were 711 receptors

used in the model (700 census tract centroids and 11 monitors). For benzene and formaldehyde, ISCST3 was also run using the road segment emissions. Additionally, for benzene, ISCST3 was run in an area of high major/onroad emissions with receptors every 500m.

Several conclusions can be drawn from the results of this study:

1. Increasing the receptor density near high emission sources changed the location of maximum concentrations between ISCST3 BASE and ISCST3 FINE GRID. The ISCST3 FINE GRID results also illustrated the concentration gradients that can occur near high emission sources. These findings illustrate the importance in of the receptor placement and density to model performance.

2. Allocating the onroad mobile emissions to road segments can improve the model predicted concentrations when compared to monitor observations. The benzene ISCST3 BASE underpredicted the average concentrations at the seven monitors. Road segment allocation (ISCST3 ROADS) resulted in better model-monitor agreement and also changed the location of maximum concentrations when compared to ISCST3 BASE. Allocating onroad mobile emissions to road segments also increased the maximum total concentration for formaldehyde but as seen in Table 4.4-2, the nonroad mobile concentrations still dominated the maximum total concentration.

3. It can be seen that higher concentrations are located near the higher emissions for the five HAPS presented. It appeared that a majority of the high emissions were located in eastern and northern Harris County, as were the higher concentrations. Also among the five HAPs, the trend is that the HAPs with higher emissions also have higher maximum concentrations.

4. It is important that emissions inventory development continue to be refined in order to define emission parameters, sources, emissions amounts, and locations for input into dispersion models. This will aid in predicting accurate model concentrations for assessing exposure to toxic pollutants.

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Table 4.2-1 Surface and upper air stations used in Houston study.

Station, Identifier	Type	Identifier, Number	Lat(°N), Lon(°W)	Elevation (m)
George Bush Airport, TX	surface	IAH, 722430	29.99; 95.36	33
Lake Charles, LA	upper air	LCH, 3937	30.12; 93.22	5

Table 4.2-2. 1996 and climatological wind speed, wind direction, average daily maximum temperature, minimum daily temperature, and annual total rainfall.

Variable	1996	Climatology
Wind speed (ms^{-1})[1]	3.3	3.6
Wind direction (°)[1]	138	153
Average maximum daily temperature(°C)[1]	26.2	25.9
Average minimum daily temperature(°C)[1]	15.1	15.3
Annual accumulated rainfall (mm)[2]	748.5	1,170
1. Climatology based on 1984-1992. **2. Climatology based on 1961-1990.**		

Table 4.3-1. Corrected Location Coordinates of Point Sources in Houston Domain

Site Name	ACT-ID	Corrected Point Source Inventory Location Variables			
		Coordinate System	UTM Zone	X	Y
Simpson Paper	48201-12359	UTM	15	285900	3289700
Champion International	48201-12405	UTM	15	296363	3307528
BASF Corporation	48039-12765	UTM	15	266202	3210415
Ethyl Corporation	48201-50029	UTM	15	290143	3291068
Ethyl Corporation	48201-50027	UTM	15	290143	3291068
Hoescht Celanese	48201-12733	UTM	15	300334	3278837
Occidental Chemical	48201-12749	UTM	15	298400	3290970
Texaco Chemical Company	48339-12759	UTM	15	270737	3355860
Rolling Environmental Services	48201-15980	UTM	15	297414	3290047
Huntsman Petrochemical Corporation	48201-53638	NC	NC	NC	3275.68
Ethyl Corporation	48201-50000	NC	NC	NC	3292.29
Exxon Comp USA	48201-50253	NC	15	NC	NC
Citgo Pipeline	48201-47361	NC	15	NC	NC
NC= No Change UTM = Universal Transverse Mercator					

Table 4.3-2. Houston/Vehicle Split Table for Allocation of Road Segment Emissions.

National	1997 VMT (millions of Miles Traveled)											
Vehicle Type[1]												
Road Type[2]	**LDGV**	**LDGT1**	**LDGT2**	**HDGV**	**MC**	**LDDV**	**LDDT**	**2B HDDV**	**Light HDDV**	**Medium HDDV**	**Heavy HDDV**	**Buses**
Rural INT	55.06%	21.00%	10.70%	2.81%	0.42%	0.76%	0.26%	0.01%	0.24%	0.91%	7.37%	0.46%
Rural OF	55.06%	21.00%	10.70%	2.81%	0.42%	0.76%	0.26%	0.01%	0.24%	0.91%	7.37%	0.46%
Rural MA	55.06%	21.00%	10.70%	2.81%	0.42%	0.76%	0.26%	0.01%	0.24%	0.91%	7.37%	0.46%
Rural MJC	55.06%	21.00%	10.70%	2.81%	0.42%	0.76%	0.26%	0.01%	0.24%	0.91%	7.37%	0.46%
Rural MNC	55.06%	21.00%	10.70%	2.81%	0.42%	0.76%	0.26%	0.01%	0.24%	0.91%	7.37%	0.46%
Rural LOC	55.06%	21.00%	10.70%	2.81%	0.42%	0.76%	0.26%	0.01%	0.24%	0.91%	7.37%	0.46%
Urban INT	60.39%	21.95%	11.18%	1.63%	0.38%	0.83%	0.27%	0.00%	0.09%	0.34%	2.76%	0.17%
Urban OF	60.39%	21.95%	11.18%	1.63%	0.38%	0.83%	0.27%	0.00%	0.09%	0.34%	2.76%	0.17%
Urban OP	60.39%	21.95%	11.18%	1.63%	0.38%	0.83%	0.27%	0.00%	0.09%	0.34%	2.76%	0.17%
Urban MA	60.39%	21.95%	11.18%	1.63%	0.38%	0.83%	0.27%	0.00%	0.09%	0.34%	2.76%	0.17%
Urban COL	60.39%	21.95%	11.18%	1.63%	0.38%	0.83%	0.27%	0.00%	0.09%	0.34%	2.76%	0.17%
Urban LOC	60.39%	21.95%	11.18%	1.63%	0.38%	0.83%	0.27%	0.00%	0.09%	0.34%	2.76%	0.17%

1.
LDGT1 - Light Duty Gasoline Trucks (<= 6,000 lbs.)
LDGT2 - Light Duty Gasoline Trucks (6,000 - 8,500 lbs.)
HDGV - Heavy Duty Gasoline Vehicles
MC - Motorcycles
LDDV - Light Duty Diesel Vehicles
LDDT - Light Duty Diesel Trucks
2B HDDV - Heavy Duty Diesel Vehicles (6,001 - 10,000 lbs.)
Light HDDV - Heavy Duty Diesel Vehicles (10,001 - 19,500 lbs.)
Medium HDDV - Heavy Duty Diesel Vehicles (19,501 - 33,000 lbs.)
Heavy HDDV - Heavy Duty Diesel Vehicles (> 33,000 lbs.)

2.
INT - Interstate
OF - Other Freeway or Expressway
MA - Minor Arterial
MJC - Major Collector
MNC - Minor Collector
OP - Other Principal
LOC - Local
COL - Collector

Table 4.3-3. Types and Dimensions of Roadway Segments.

Roadway Type	Lanes	Width (Lane=3.65m)	Min. Length(m)	Max Length(m)
Interstate Roads	8+5 median/shoulder	47.45	0.4745	4745
U.S. Highways	6+3 median/shoulder	32.85	0.3285	3285
State Highways	4+2 median/shoulder	21.90	0.2190	2190

Table 4.4-1. Maximum Annual Average Total (From All Sources) Concentration and Southwest Corner of Grid Cell For Each HAP in Study[1].

HAP	Maximum Concentration (: g m⁻³)	(X,Y) (UTM)	Major Source Concentration (: g m⁻³)	Area/Other Source Concentration (: g m⁻³)	Onroad Mobile Concentration (: g m⁻³)	Nonroad Mobile Concentration (: g m⁻³)
Benzene	5.245	(285,000,3,290,000)	4.317	0.193	0.4848	0.2633
Cadmium	0.002935	(314,000,3,252,000)	0.00283	0.0001	N/A[2]	0
Chromium	0.01578	(314,000,3,252,000)	0.01551	0.00008	0.00001	0.00018
Formaldehyde	5.41(14.2)[3]	(279,000,3,281,000)	0.0516	0.0865	0.251	5.06
Lead	0.3651	(279,000,3,281,000)	0.00011	0.00346	0.00006	0.3618

1. Background not included.
2. Not/Applicable
3. Value in Parentheses includes secondary contribution

Table 4.4-2. Maximum Concentrations and Southwest Corner of Location For Each Category and HAP.

HAP	Major Concentration ($\mu g\ m^{-3}$) (x;y)	Area/Other Concentration ($\mu g\ m^{-3}$) (x;y)	Onroad Mobile Concentration ($\mu g\ m^{-3}$) (x;y)	Nonroad Mobile Concentration ($\mu g\ m^{-3}$) (x;y)
Benzene	4.32 (285,000;3,290,000)	0.505 (305,000;3,290,000)	3.68 (274,000;3,304,000)	1.03 (279,000; 3,281,000)
Cadmium	0.003 (314,000;3,252,000)	0.0014 (273,000;3,299,000)	N/A	0.0001 (306,000;3,284,000)
Chromium	0.0155 (314,000;3,252,000)	0.0025 (231,000; 3,276,000)	0.0003 (274,000; 3,304,000)	0.004 (306,000; 3,284,000)
Formaldehyde	1.01 (293,000;3,281,000)	0.328 (288,000;3,268,000)	1.84 (274,000;3,304,000)	5.06 (279,000;3,281,000)
Lead	0.0083 (314,000;3,252,000)	0.0204 (289,000;3,293,000)	0.0004 (274,000;3,304,000)	0.3618 (279,000;3,281,000)

Table 4.4-3. Benzene Maximum Total Concentration and Southwest Corner of Location for ISCST3, ISCST3 ROADS, ISCST3 FINE GRID.

Model	Maximum Concentration ($\mu g\ m^{-3}$)[1]	(X,Y) (UTM)	Major Source Concentration ($\mu g\ m^{-3}$)	Area/Other Source Concentration ($\mu g\ m^{-3}$)	Onroad Mobile Concentration ($\mu g\ m^{-3}$)	Nonroad Mobile Concentration ($\mu g\ m^{-3}$)
ISCST3	5.245	(285000,3290000)	4.317	0.193	0.4848	0.2633
ISCST3 ROADS	7.09	(262000,3286000)	0.0761	0.159	6.43	0.466

Table 4.4-4. Formaldehyde Maximum Concentrations and by concentration source category for ISCST3 and ISCST3 ROADS.

Model	Maximum Concentration ($\mu g\ m^{-3}$)[1]	(X,Y) (UTM)	Major Source Concentration ($\mu g\ m^{-3}$)	Area/Other Source Concentration ($\mu g\ m^{-3}$)	Onroad Mobile Concentration ($\mu g\ m^{-3}$)	Nonroad Mobile Concentration ($\mu g\ m^{-3}$)
ISCST3	5.41(14.2)	(279000,3281000)	0.0516	0.0865	0.251	5.06
ISCST3 ROADS	5.59(14.4)	(279000,3281000)	0.0516	0.0865	0.413	5.06
1. Value in Parentheses includes secondary contribution						
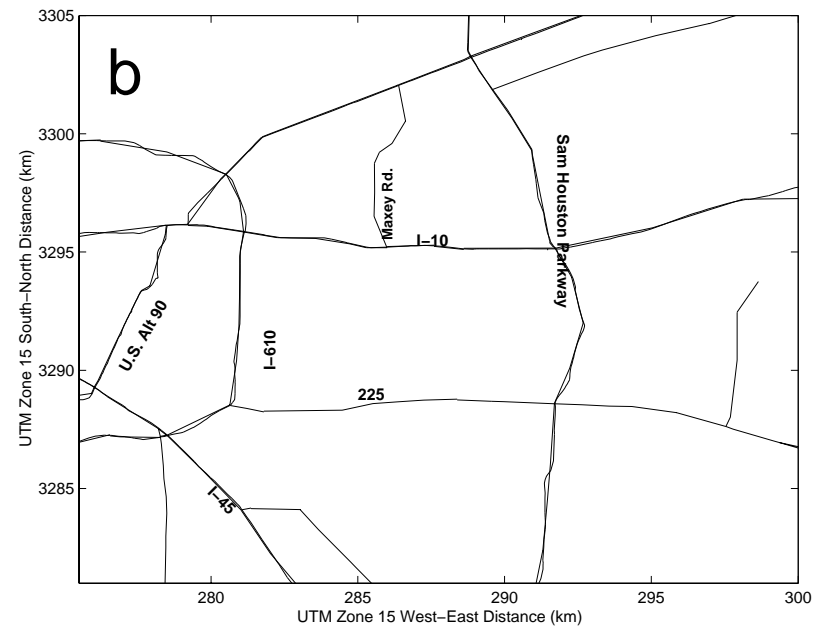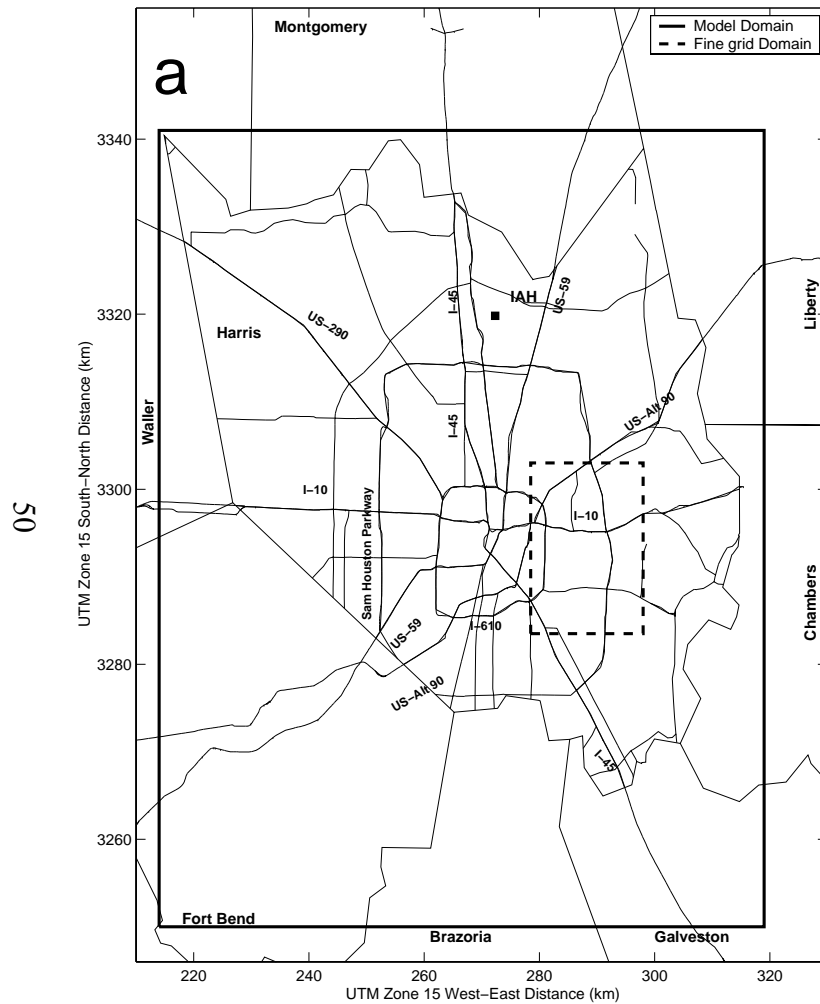
Figure 4.1-1. a) Houston domain with key roads and location of airport and b) ISCST3 FINE GRID with key roads.
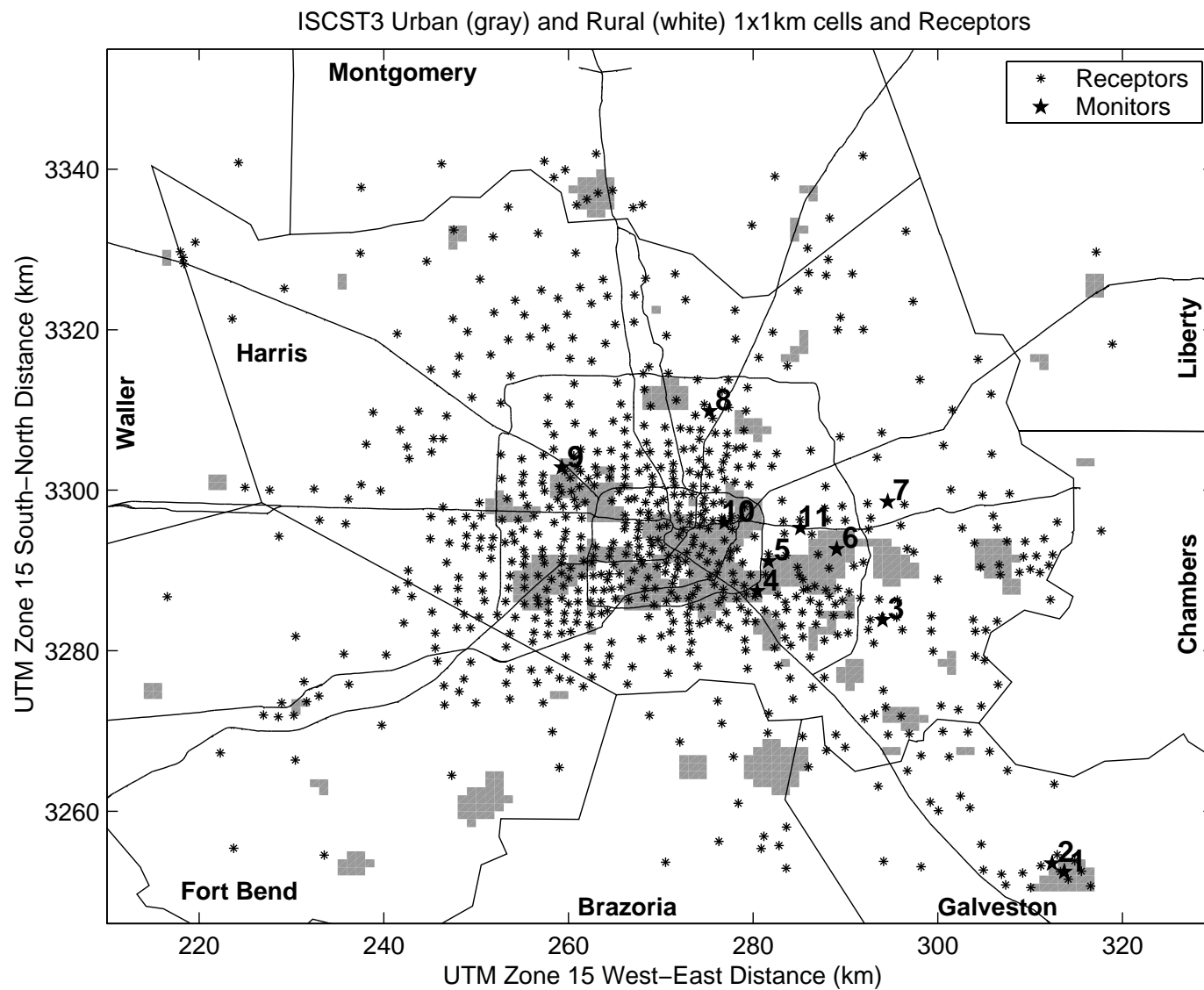
Figure 4.2-1. Locations of urban and rural grid cells, ISC receptors, and monitors.
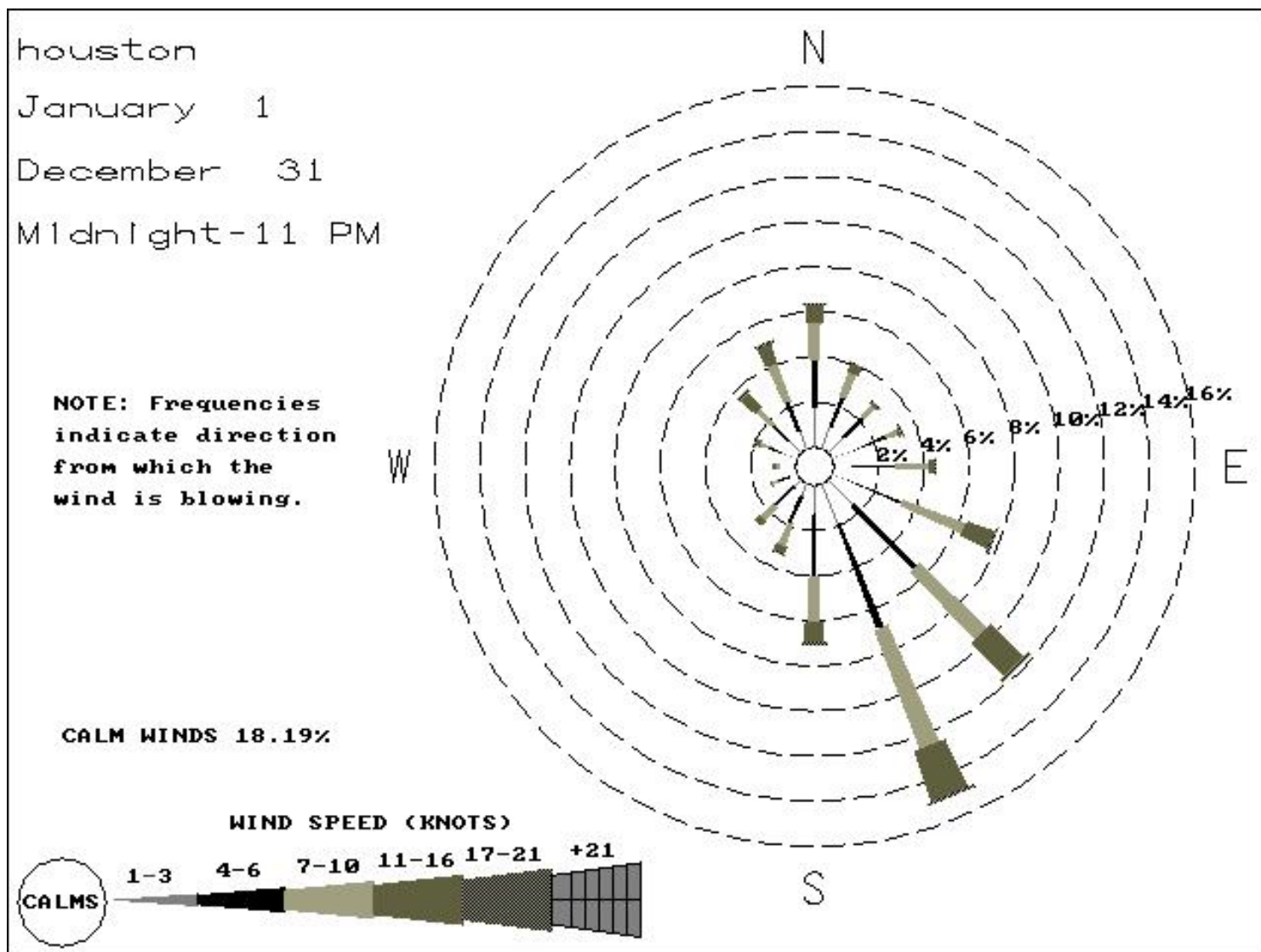
Figure 4.2-2. Wind rose of winds for Houston, 1996.
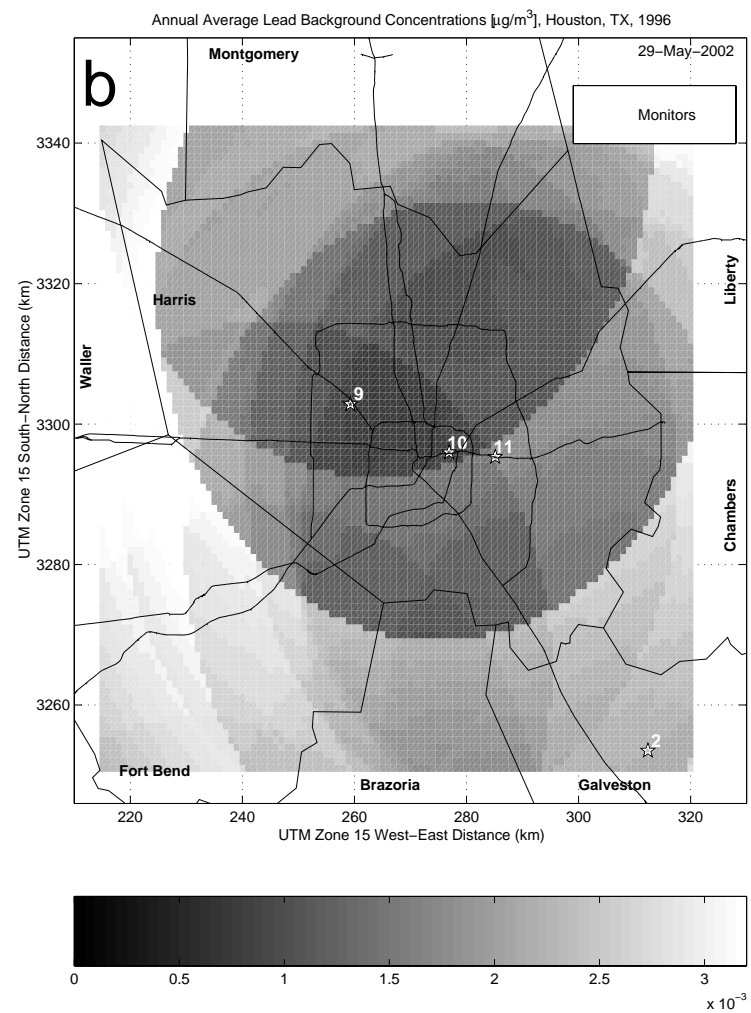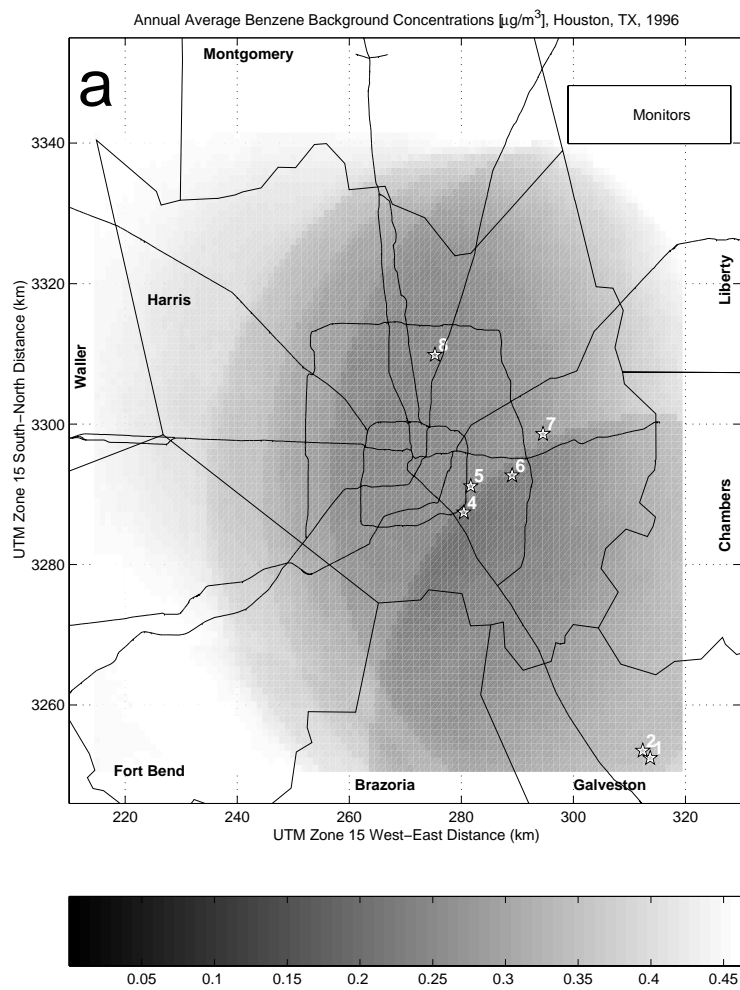
Figure 4.2-3. Annual average background concentrations (μg m⁻³) for a) benzene and b) lead.
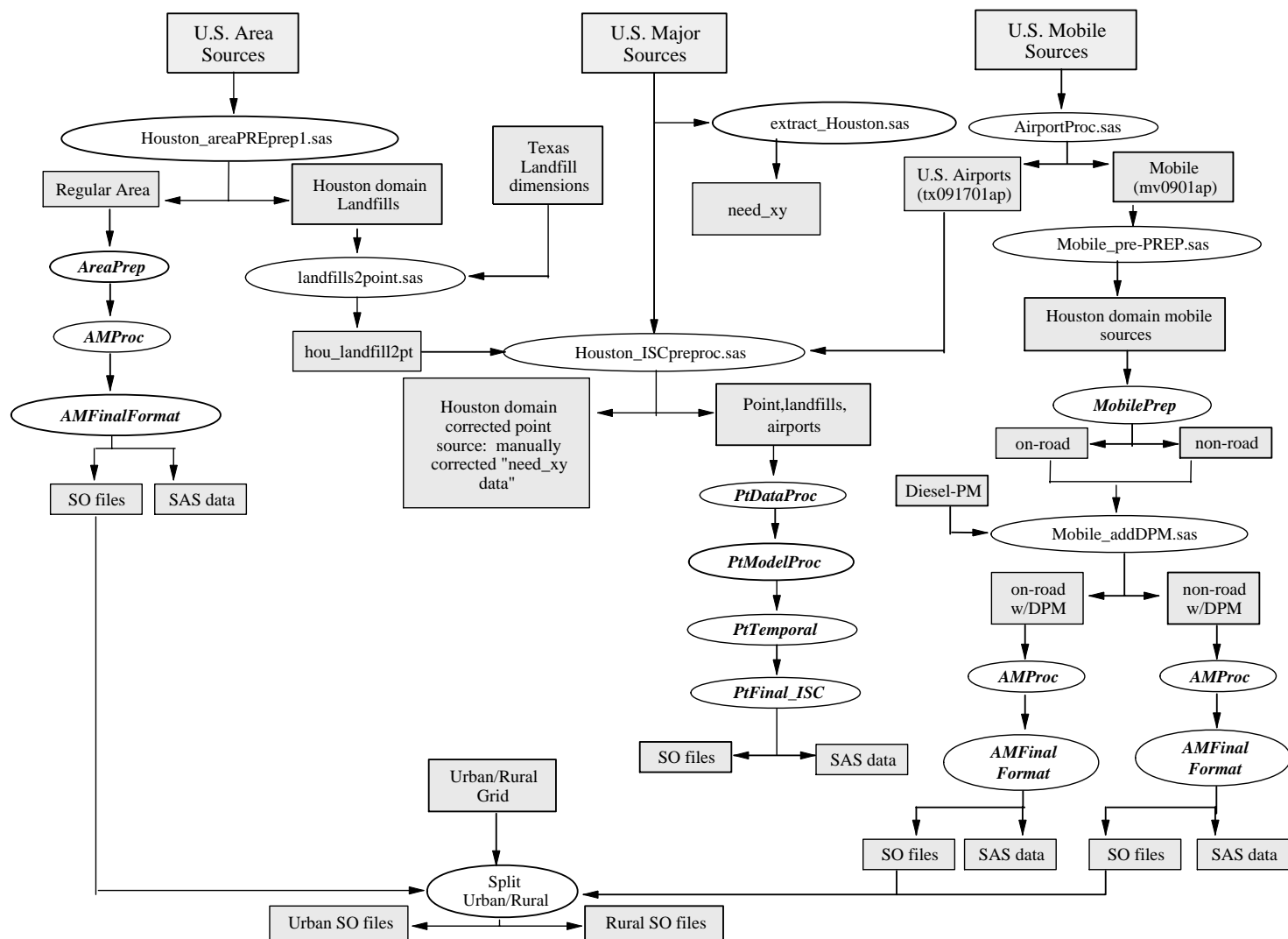
Figure 4.3-1. Flowchart of gridded emissions processing for Houston.

ISC−ready Benzene Total 1x1km Emissions [tons/yr], Houston, TX, 1996
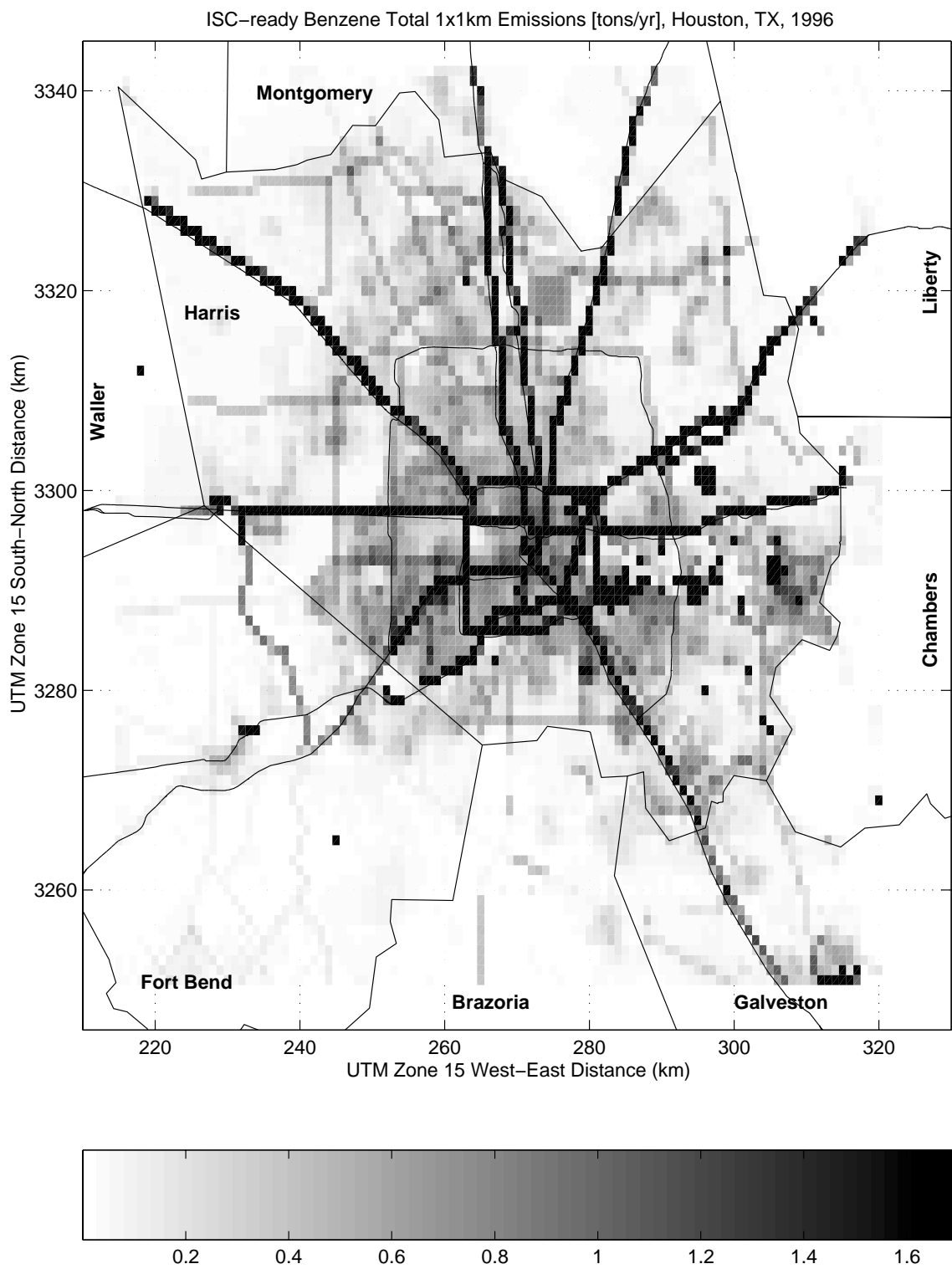
Figure 4.4-1. Benzene 1 km gridded emissions (tons yr^{-1}) from all sources.

55

ISC−ready Benzene Major Source 1x1km Emissions [tons/yr], Houston, TX, 1996

ISC−ready Benzene Onroad Mobile Source 1x1km Emissions [tons/yr], Houston, TX, 1996
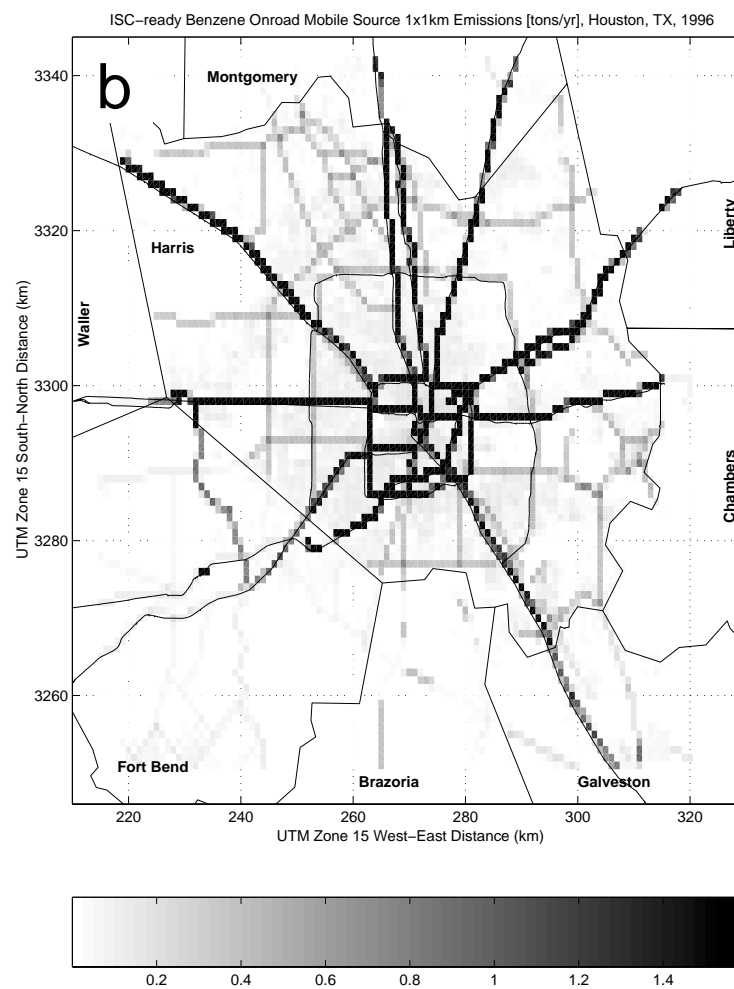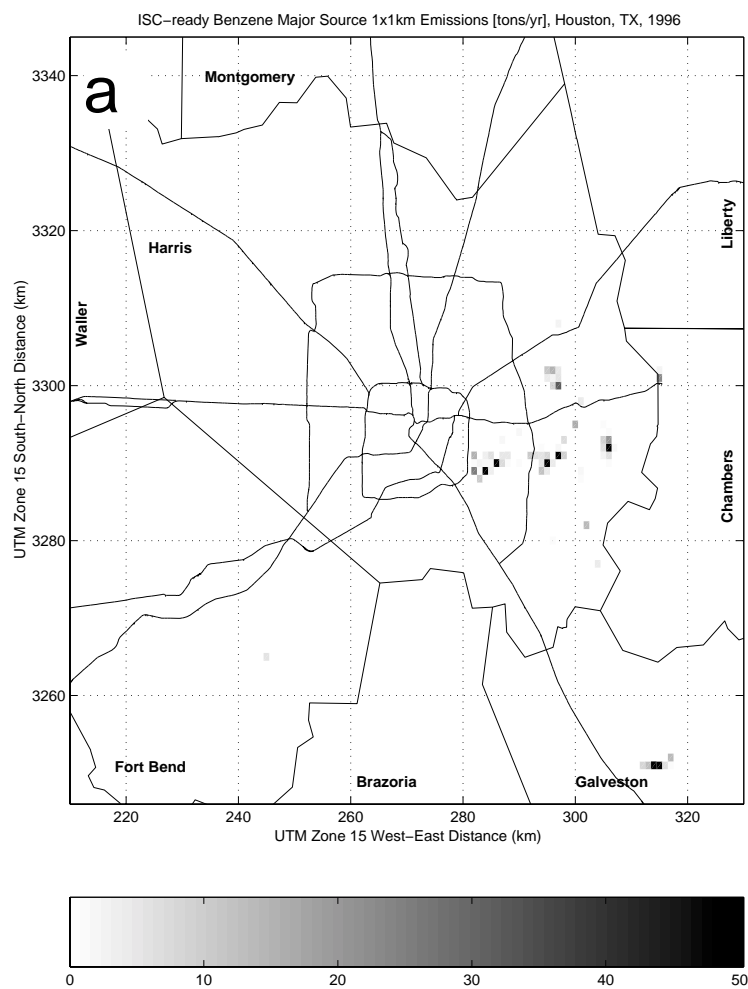
Figure 4.4-2 Benzene 1 km gridded a) major source emissions, and b) onroad mobile emissions. Emissions are in tons yr^{-1}.

Houston Benzene Emissions: 4,368 tons

U.S. Benzene Emissions: 336,544 tons

Petroleum/Coal Products 4%

Chemical & AlliedProducts 5%

Remaining Sources 11%

Petroleum Refineries 15%

Onroad Mobile Sources 41%

Nonroad Mobile Sources 24%

Oil & Nat. Gas Prod. 2%

Gasoline Dist. Stages 1 & 2 2%

Remaining Sources 6%

Fires 12%

Onroad Mobile Sources 50%

Nonroad Mobile Sources 28%

57

Ethylene Processes 4%

POTW 5%

Remaining Sources 11%

Petroleum/Coal Products 12%

Petroleum Refineries 51%

Chemical & AlliedProducts 17%

Houston Benzene
Major Emissions: 1,255 tons

Chemical & Allied Products 5%

Fires (Forest/Wildfires) 8%

Nat. Gas. Trans. & Stor. 18%

Oil & Nat. Gas Prod. 29%

Gasoline Dist. Stages 1 & 2 20%

Remaining Sources 20%

Houston Benzene
Area Emissions: 229 tons

Nonroad Mobile 36%

Onroad Mobile 64%

Houston Benzene
Mobile Emissions: 2,883 tons

Figure 4.4-3a. Distribution of emissions for Houston and U.S. inventories for benzene.
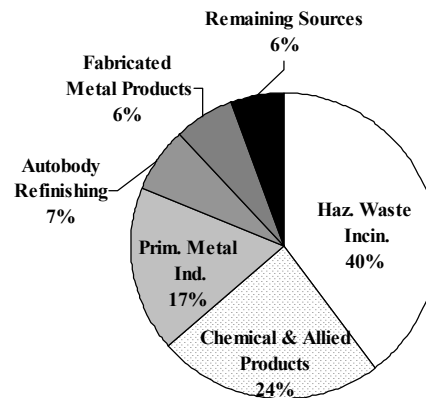
Houston Cadmium Emissions: 1.4 tons

Chromium
Metal Plating
4%

Portland
Cement Manu.
5%

Remaining
Sources
6%

Utility Boilers
16%

Haz. Waste
Incin.
44%

Petroleum
Refineries
25%
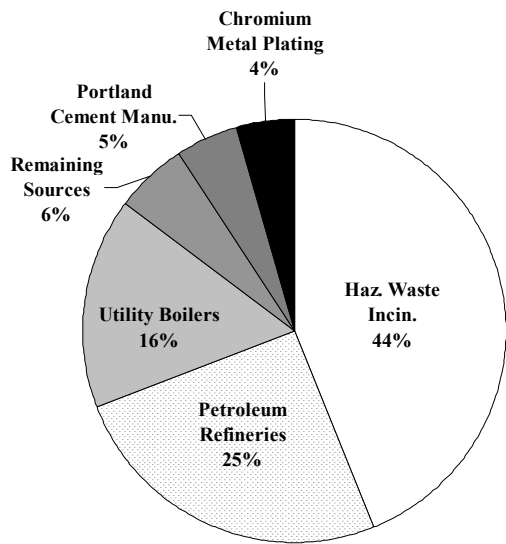
U.S. Cadmium Emissions: 157 tons

Haz. Waste
Incin.
5%

Uknown
Sources
4%

Primary
Copper
Smelting
7%

Utility
Boilers
13%

Remaining
Sources
43%

Secondary
Lead
Smelting
28%

58

Pulp and Paper
1%

Haz. Waste Incin.
7%

Portland Cement
Manu.
9%

Petroleum
Refineries
51%

Utility Boilers
32%

Residental Heat.:
Distillate Oil
2%

Boilers
3%

Remaining Sources
1%

Chromium Metal
Plating
9%

Waste Incin.
Haz/Medical
85%
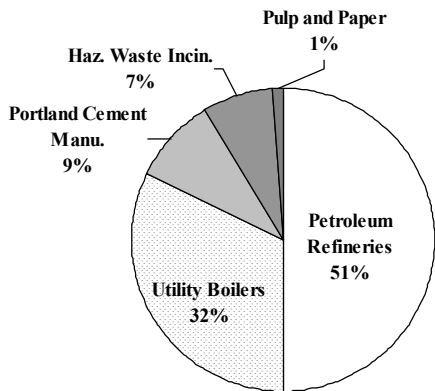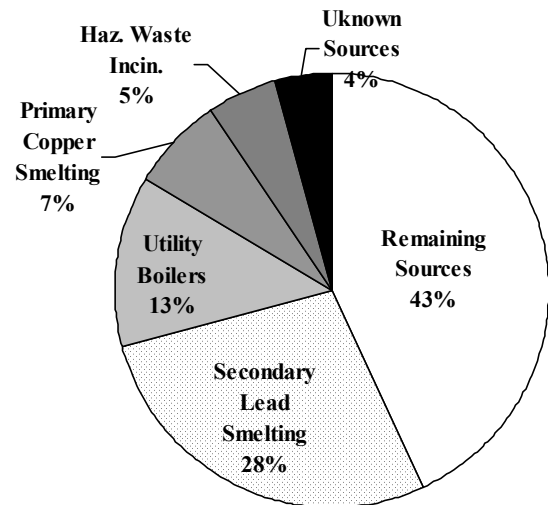
Houston Cadmium Major Emissions: 0.7 tons
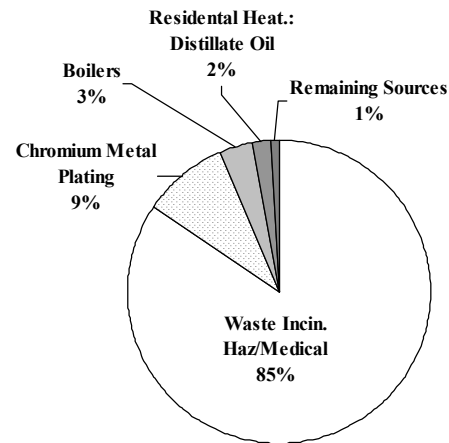
Houston Cadmium Area Emissions: 0.7 tons

Figure 4.4-3b. Distribution of emissions for Houston and U.S. inventories cadmium. Mobile chart not included since cadmium emissions do not include onroad mobile emissions.

Houston Chromium Emissions: 6.4 tons
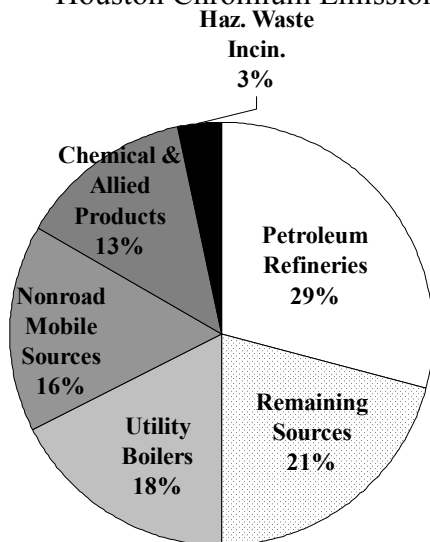
U.S. Chromium Emissions: 1,037 tons
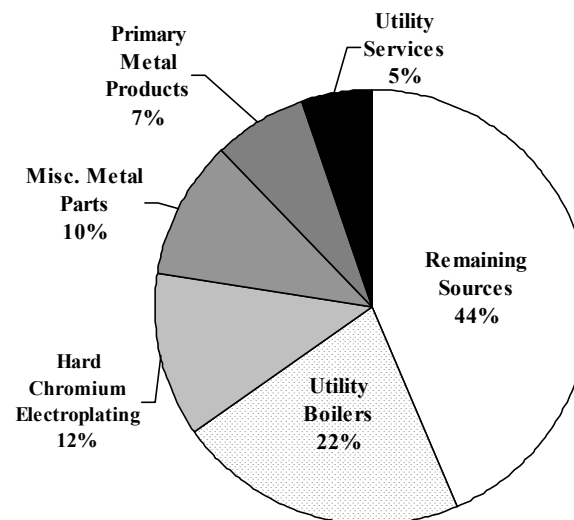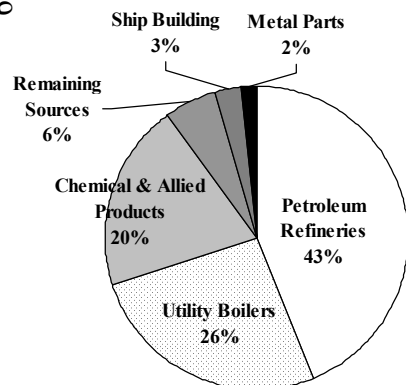
Houston Chromium
Major Emissions: 4.3 tons
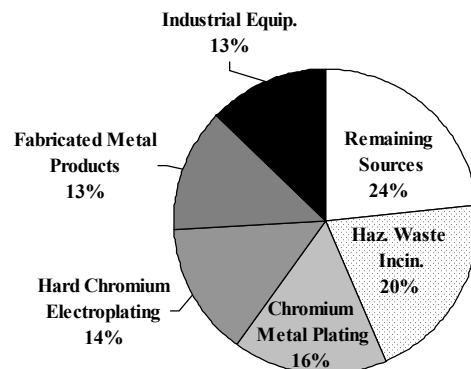
Houston Chromium Area Emissions: 1 tons
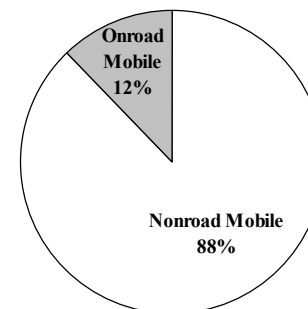
Houston Chromium
Mobile Emissions: 1.1 tons

59

Figure 4.4-3c. Distribution of emissions for Houston and U.S. inventories for chromium.

Houston Formaldehyde Emissions: 2,811 tons

Chemical & Allied Products 2%

Oil and Gas Extraction 4%

Stationary Recip. Internal Comb. Engines 5%

Remaining Sources 8%

Nonroad Mobile Sources 46%

Onroad Mobile Sources 35%
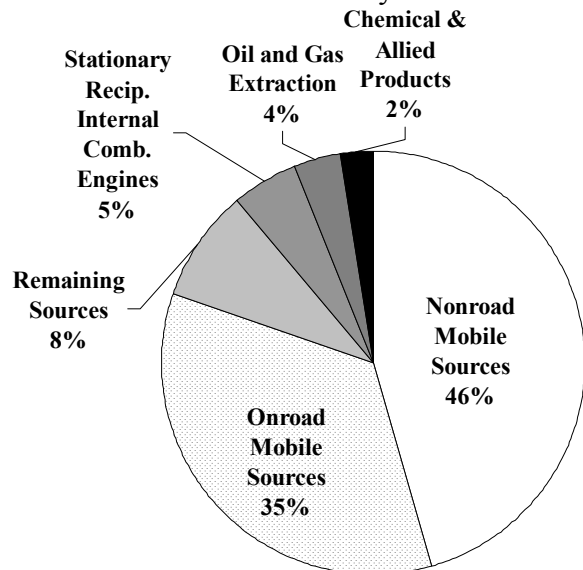
U.S. Formaldehyde Emissions: 301,708 tons

Petroleum/ Coal Products 1%

Remaining Sources 6%

Stationary Recip. Internal Comb. Engines 7%

Fires 29%

Onroad Mobile 28%

Nonroad Mobile 29%

Utility Services 3%

Utility Boilers 3%

Remaining Sources 4%

Chemical & Allied Products 25%

Oil and Gas Extraction 40%

Petroleum Refineries 25%
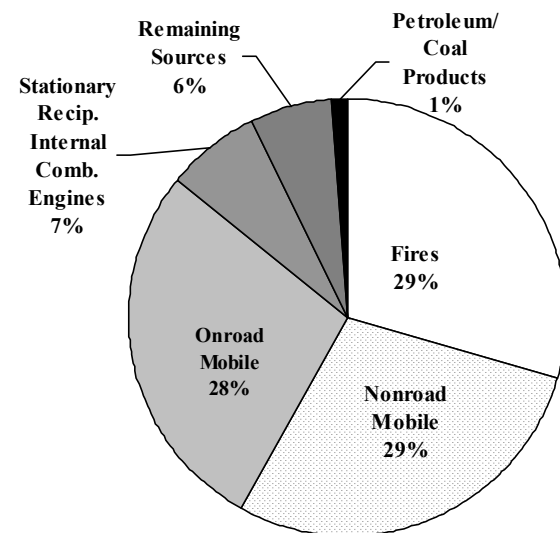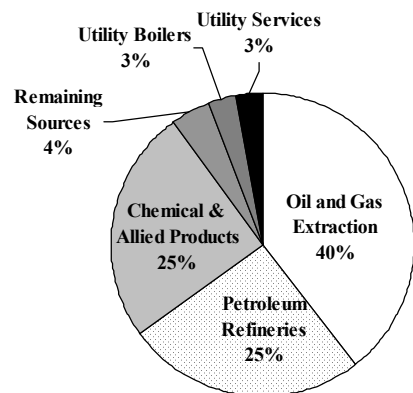
Houston Formaldehyde
Major Emissions: 252 tons

Chemical & Allied Products 2%

Utility Boilers 2%

Remaining Sources 3%

Stationary Comb. Turbines 22%

Stationary Recip. Internal Comb. Engines 48%

Fires(Forest/Wild/ Presc.) 23%
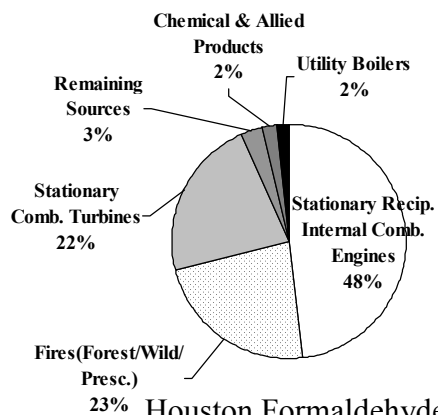
Houston Formaldehyde
Area Emissions: 300 tons

Onroad Mobile 43%

Nonroad Mobile 57%
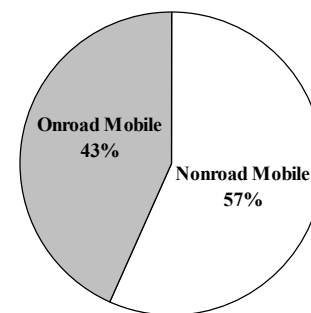
Houston Formaldehyde
Mobile Emissions: 2,259 tons

Figure 4.4-3d. Distribution of emissions for Houston and U.S. inventories for formaldehyde.

Houston Lead Emissions: 29 tons
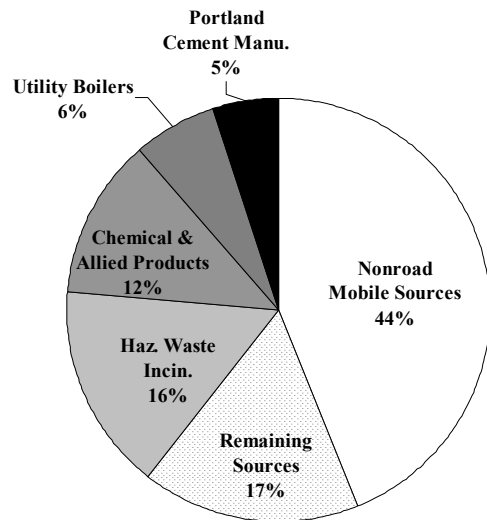
U.S. Lead Emissions: 2,613 tons

Portland Cement Manu. 5%

Utility Boilers 6%

Chemical & Allied Products 12%

Haz. Waste Incin. 16%

Nonroad Mobile Sources 44%

Remaining Sources 17%

Primary Lead Smelting 12%

Primary Metal Industries 4%

Unknown Sources 12%

Remaining Sources 39%

Utility Boilers 13%

Nonroad Mobile Sources 20%

Remaining Sources 7%

Petroleum Refineries 13%

Haz. Waste Incin. 17%

Utility Boilers 24%

Chemical & Allied Products 20%

Portland Cement Manu. 19%

Houston Lead
Major Emissions: 7.7 tons

Remaining Sources 6%

Fabricated Metal Products 6%

Autobody Refinishing 7%

Prim. Metal Ind. 17%

Haz. Waste Incin. 40%

Chemical & Allied Products 24%

Houston Lead
Area Emissions: 8.1 tons

Onroad Mobile 2%
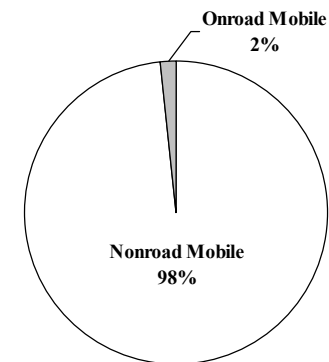
Nonroad Mobile 98%

Houston Lead
Mobile Emissions: 13 tons

Figure 4.4-3e. Distribution of emissions for Houston and U.S. inventories for lead.

	TYPE	CODE	BENZENE	CADMIUM	CHROMIUM	FORMALDEHYDE	LEAD
Emissions (tons)			4368.00	1.36	6.38	2811.00	28.57
Source Category							
Nonroad Mobile Sources			23.55%	1.30%	15.69%	45.65%	43.97%
Onroad Mobile Sources			42.46%	0%	2.21%	34.73%	0.70%
Hazardous Waste Incineration	MACT	0801	0%	43.81%	3.42%	0%	15.82%
Petroleum Refineries	MACT	0502	0.11%	25.28%	29.29%	2.28%	3.53%
Utility Boilers: Coal, Oil, and Natural	MACT	1808	0.13%	16.19%	17.61%	0.27%	6.35%
Chemicals and allied products	SIC	28xx	5.08%	0%	13.35%	2.48%	12.20%
Petroleum Refineries - Other Sources	MACT	0503	14.65%	0%	0%	0%	0%
Portland Cement Manufacturing	MACT	0410	0%	4.69%	0.66%	0%	5.11%
Chromium Metal Plating	CAT	9069	0%	4.41%	2.51%	0%	0%
Primary metal industries	SIC	33xx	0%	0%	0.40%	0%	4.97%
Stationary Reciprocating Internal Combustion Engines	MACT	0105	0.11%	0.03%	0.01%	5.12%	0%
Petroleum and coal products	SIC	29xx	3.55%	0%	0%	0%	0.42%
Fabricated metal products	SIC	34xx	0%	0%	2.00%	0.01%	1.90%
Oil and gas extraction	SIC	13xx	0.02%	0%	0%	3.54%	0%
Industrial/Commercial/ Institutional Boilers	MACT	0107	0.03%	1.71%	0.93%	0.18%	0.35%
Stationary Combustion Turbines	MACT	0108	0.02%	0%	0%	2.37%	0%
Pulp and Paper	MACT	1626	0.17%	0.64%	0.29%	0.16%	1.12%
Industrial machinery and equipment	SIC	35xx	0.20%	0%	1.96%	0%	0%
Hard Chromium Electroplating	MACT	1615	0%	0%	2.15%	0%	0%
Autobody Refinishing Paint Application	CAT	9027	0%	0%	0%	0%	1.97%
Stone, clay, glass, and concrete products	SIC	32xx	0.01%	0%	1.88%	0%	0.03%
Shipbuilding & Ship Repair (Surface Coating)	MACT	0715	0.02%	0%	1.73%	0%	0.12%
Oil & Natural Gas Production	MACT	0501	1.86%	0%	0%	0%	0%
Open Burning: Forest and Wildfires	CAT	9306	0.40%	0%	0%	1.42%	0%
Pubicly Owned Treatment Works (POTW)	MACT	0803	1.56%	0%	0%	0%	0%
Residential Heating: Distillate Oil	CAT	9380	0%	0.98%	0.21%	0.05%	0.18%
Miscellaneous Metal Parts & Products	MACT	0710	0.02%	0%	1.16%	0.01%	0.02%
Open Burning: Prescribed Burnings	CAT	9307	0.25%	0%	0%	0.88%	0%
Ethylene Processes	MACT	1635	1.07%	0%	0%	0%	0%
Residential Heating: Wood/Wood Residue	CAT	9382	0%	0.29%	0.41%	0.05%	0.28%
Medical Waste Incinerators	MACT	1801	0%	0.60%	0.01%	0%	0.39%
Natural Gas Transmission & Storage	MACT	0504	0.99%	0%	0%	0%	0%
Gasoline Distribution (Stage I)	MACT	0601	0.98%	0%	0%	0%	0%
Asphalt roofing and Processing	MACT	0418	0.01%	0%	0.83%	0%	0.12%
Steel Foundries	MACT	0309	0.02%	0%	0.90%	0%	0%
Motor freight transportation and warehousing	SIC	42xx	0.69%	0%	0%	0%	0%
Hydrogen Fluoride Production: GENERIC	MACT	1409	0.40%	0%	0%	0.07%	0%
Industrial Cooling Towers	MACT	1619	0.43%	0%	0%	0%	0%
Marine Vessel Loading Operations	MACT	0603	0.31%	0%	0%	0%	0%
Gasoline Distribution Stage II	CAT	9166	0.30%	0%	0%	0%	0%
Electric, gas, and sanitary services	SIC	49xx	0.02%	0%	0%	0.26%	0%
Petroleum Refining and Natural Gas Support	CAT	9327	0.22%	0%	0%	0%	0%
Surface Coatings: Architectural	CAT	9427	0.18%	0%	0%	0%	0%
Iron Foundries	MACT	0308	0%	0%	0%	0%	0.18%
Structure Fires	CAT	9425	0%	0%	0%	0.17%	0%
MON - combined	MACT	1640	0.02%	0.01%	0.08%	0.02%	0.01%
Residential Heating: Bituminous and Lignite Coal	CAT	9379	0%	0.04%	0.04%	0%	0.02%
Municipal Solid Waste Landfills - NSPS&	MACT	0802	0.10%	0%	0%	0%	0%
Residential Heating: Natural Gas	CAT	9381	0%	0%	0%	0.09%	0%
Consumer Products Usage	CAT	9087	0%	0%	0%	0.08%	0%
Lumber and wood products	SIC	24xx	0%	0%	0.08%	0%	0%
Primary Copper Smelting	MACT	0203	0%	0%	0%	0%	0.08%
Open Burning: Scrap Tires	CAT	9308	0.04%	0%	0.03%	0%	0%
Off-Site Waste and Recovery Operations	MACT	0806	0%	0%	0%	0%	0.07%
Refractories Products Manufacturing	MACT	0406	0%	0%	0.07%	0%	0%
Rubber and miscellaneous plastics products	SIC	30xx	0%	0%	0.02%	0%	0.05%
Transportation equipment	SIC	37xx	0.04%	0%	0%	0.03%	0%
Chromic Acid Anodizing	MACT	1607	0%	0%	0.06%	0%	0%
Residential Heating: Anthracite Coal	CAT	9378	0%	0.02%	0.02%	0%	0.01%
Transportation services	SIC	47xx	0.01%	0%	0%	0.01%	0%
Metal Can (Surface Coating)	MACT	0707	0%	0%	0%	0.01%	0%
Asphalt Concrete Manufacturing	CAT	9023	0%	0%	0%	0%	0.01%
Primary Lead Smelting	MACT	0204	0%	0%	0%	0%	0.01%
Wood Furniture (Surface Coating)	MACT	0716	0%	0%	0%	0.01%	0%
Metal Coil (Surface Coating)	MACT	0708	0%	0%	0%	0.01%	0%
Pipelines, except natural gas	SIC	46xx	0.01%	0%	0%	0%	0%
Automotive repair, services, and parking	SIC	75xx	0%	0%	0%	0.01%	0%
Aviation Gasoline Distribution: Stage I & II	CAT	9032	0%	0%	0%	0%	0.01%

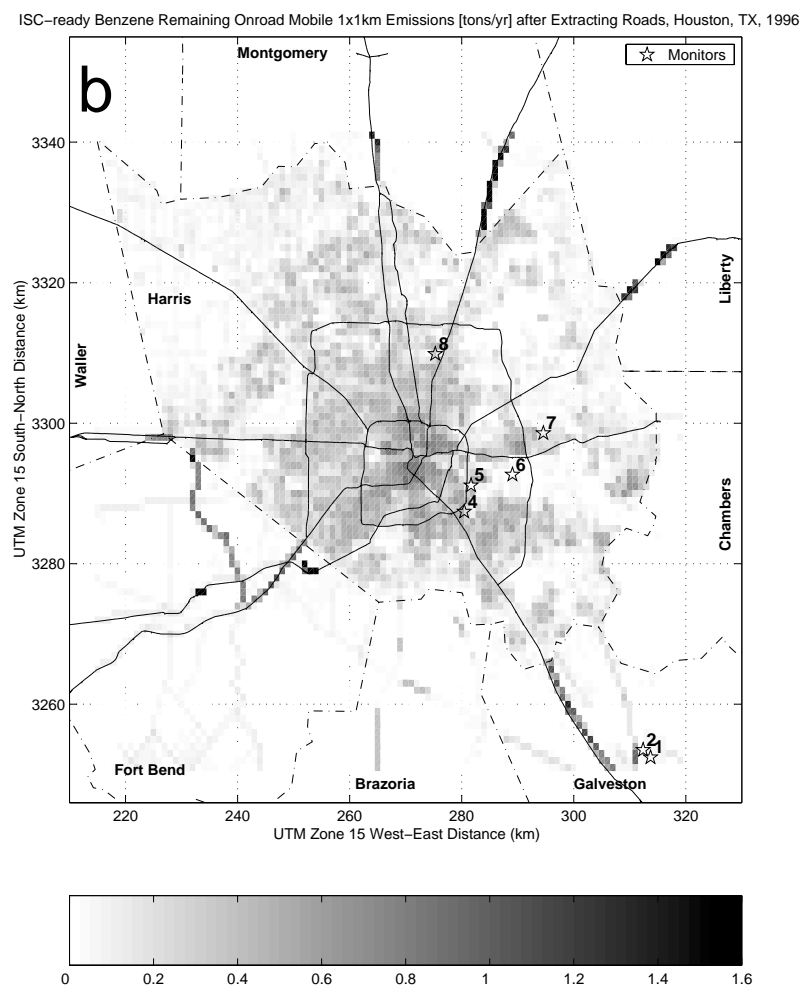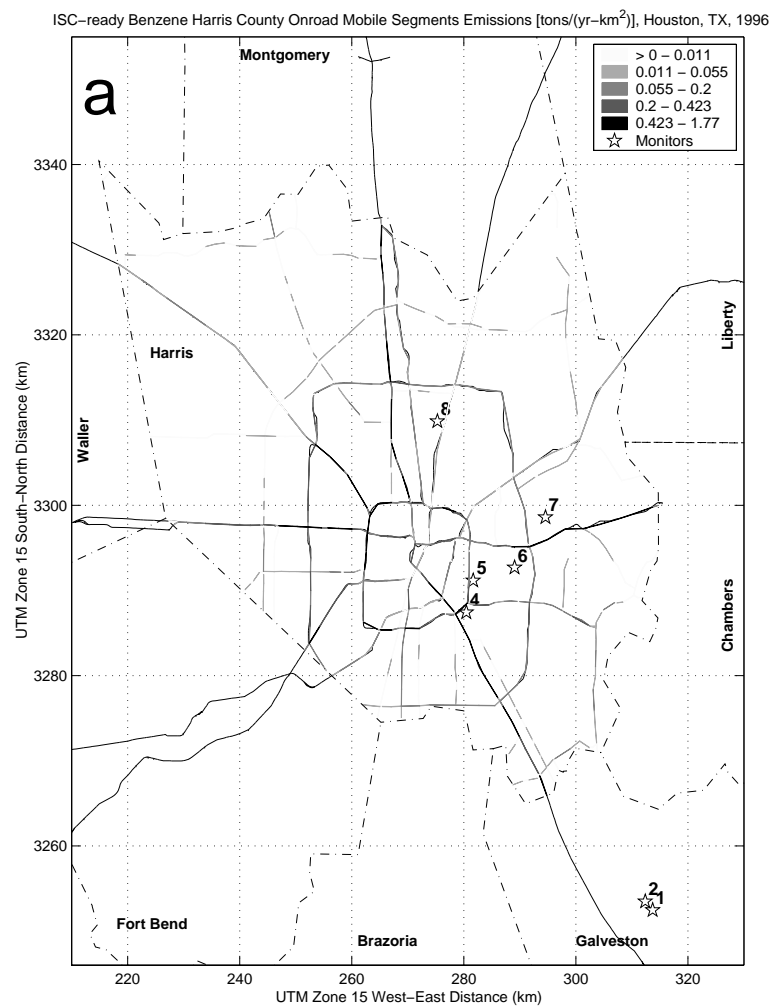Figure 4.4-3f. Percent contribution of individual source categories for each pollutant in the Houston domain.

ISC–ready Benzene Harris County Onroad Mobile Segments Emissions [tons/(yr–km^2)], Houston, TX, 1996

ISC–ready Benzene Remaining Onroad Mobile 1x1km Emissions [tons/yr] after Extracting Roads, Houston, TX, 1996

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Figure 4.4-4. Benzene a) road segment emissions (tons yr^{-1} km^{-2}) b) remaining 1 km gridded onroad mobile emissions (tons yr^{-1}) after extracting road segment emissions.
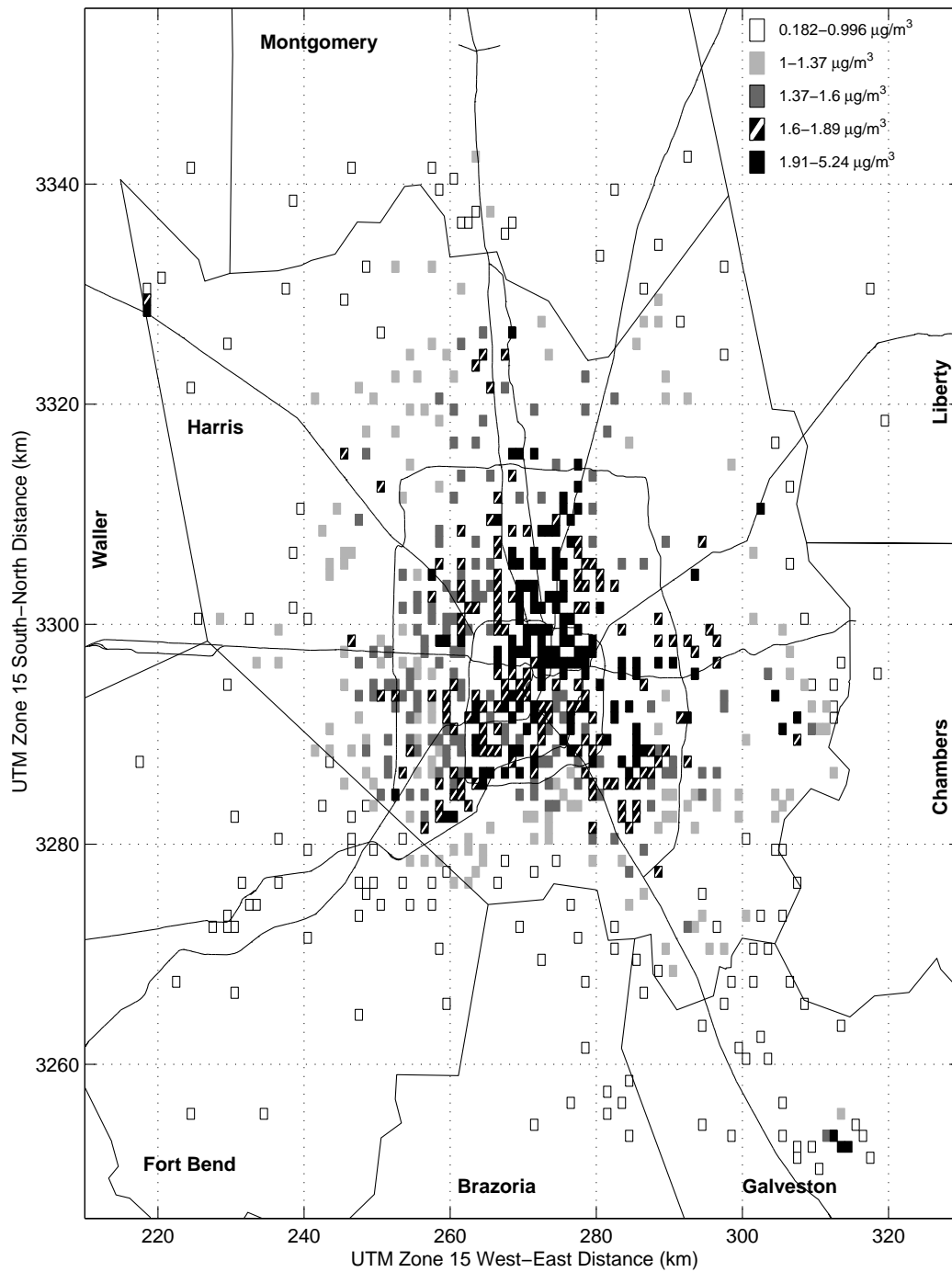
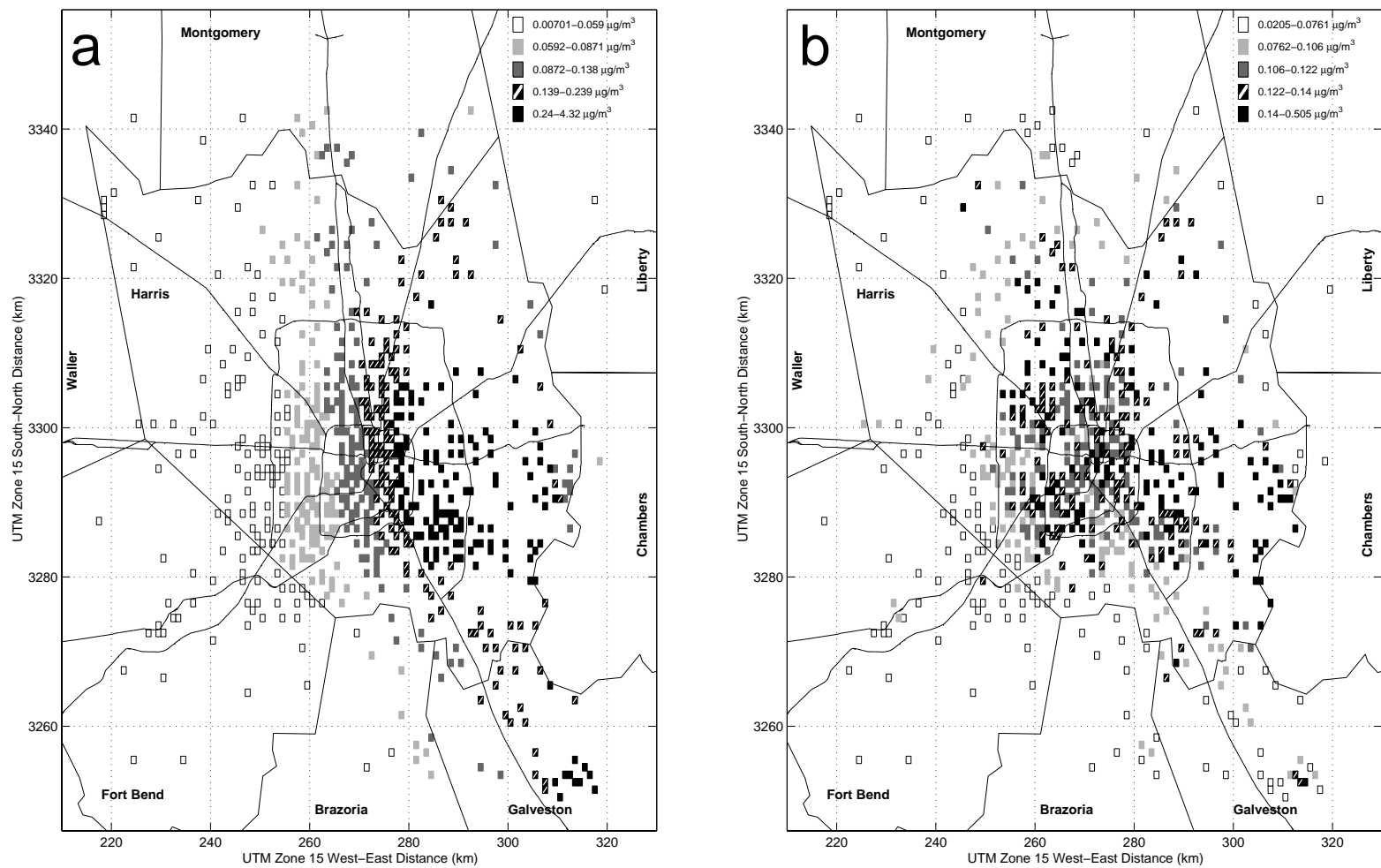Figure 4.4-5 Benzene ISCST3 BASE annual average total concentrations ($\mu g\ m^{-3}$).

Figure 4.4-6. Benzene annual average ISCST3 BASE concentrations ($\mu g\ m^{-3}$). a) major sources, b) area and other sources, c) onroad mobile, and d) nonroad mobile sources.
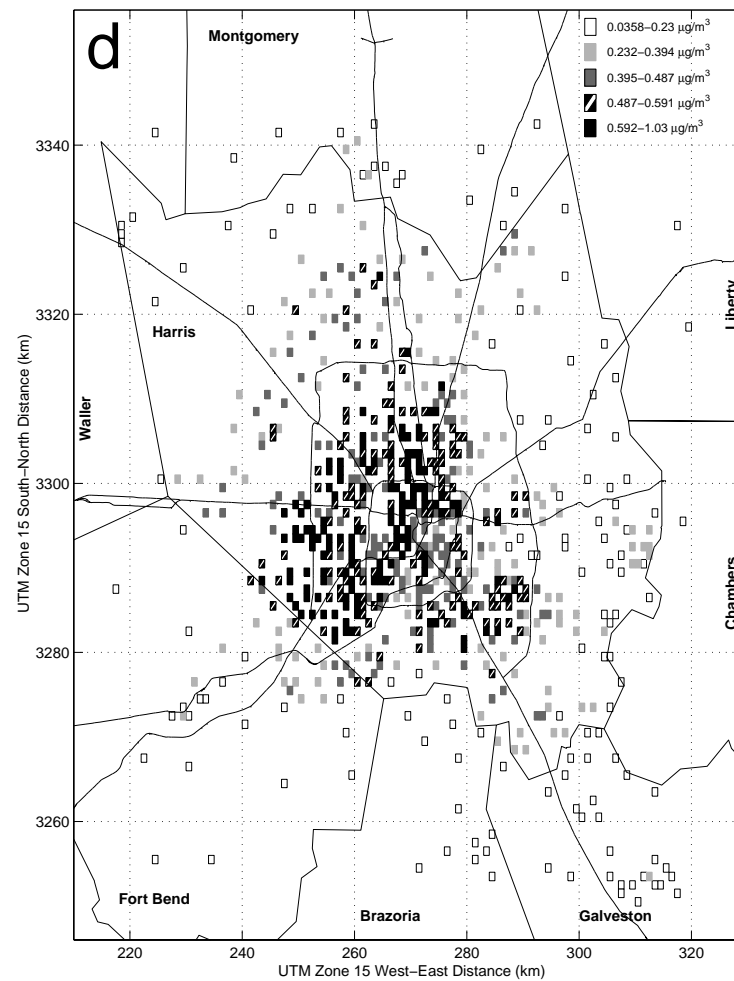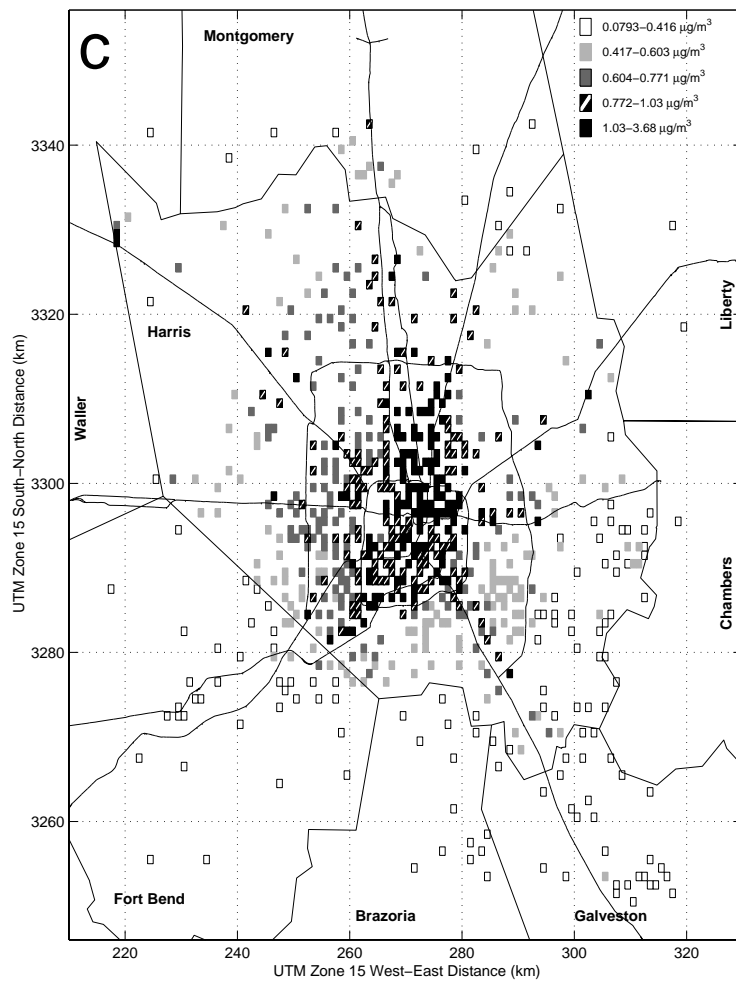
Figure 4.4-6. Continued.
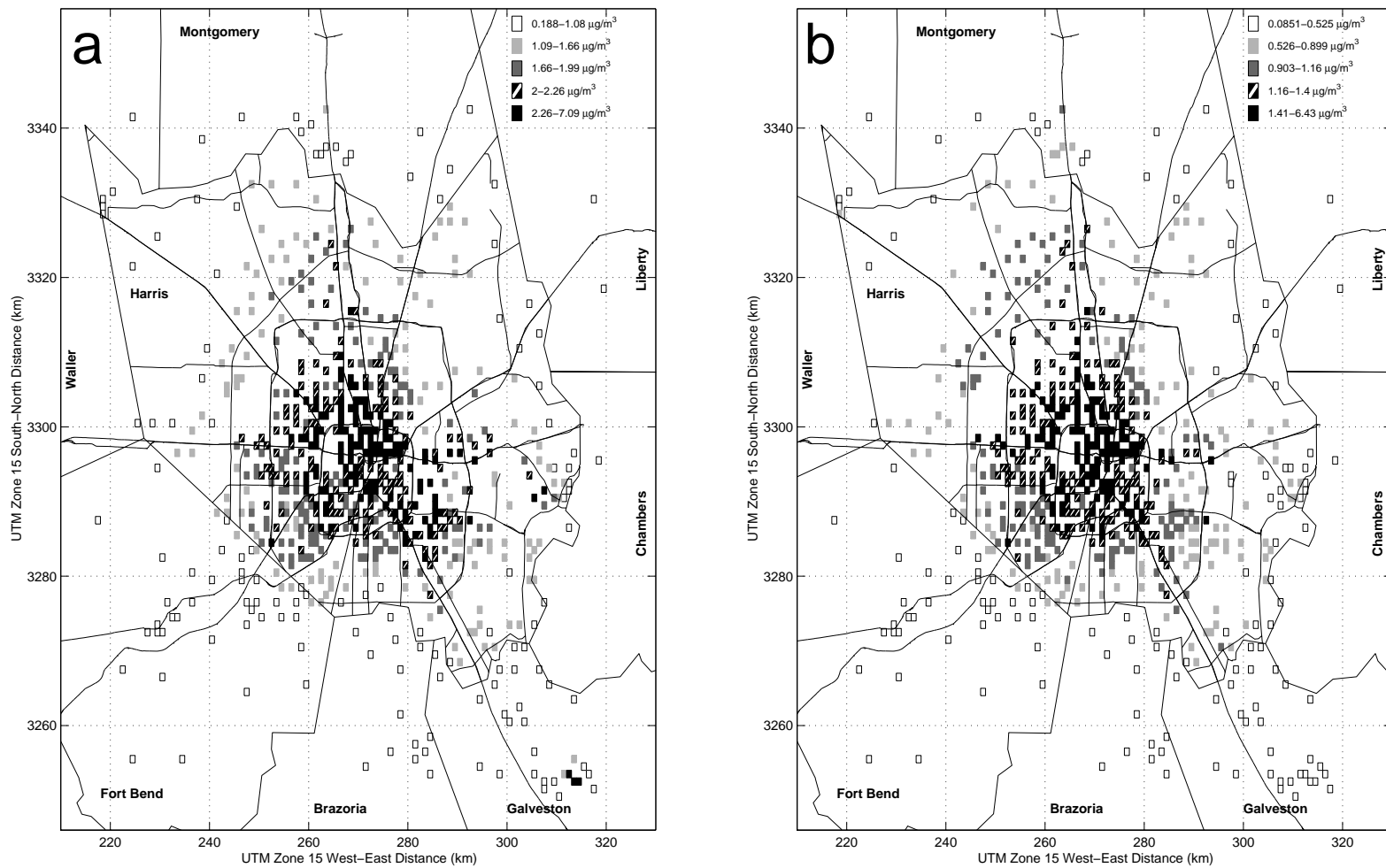
Figure 4.4-7. Benzene annual average ISCST3 ROADS concentrations (μg m^{-3}) for a) total (all sources) concentrations, and b) onroad mobile concentrations.
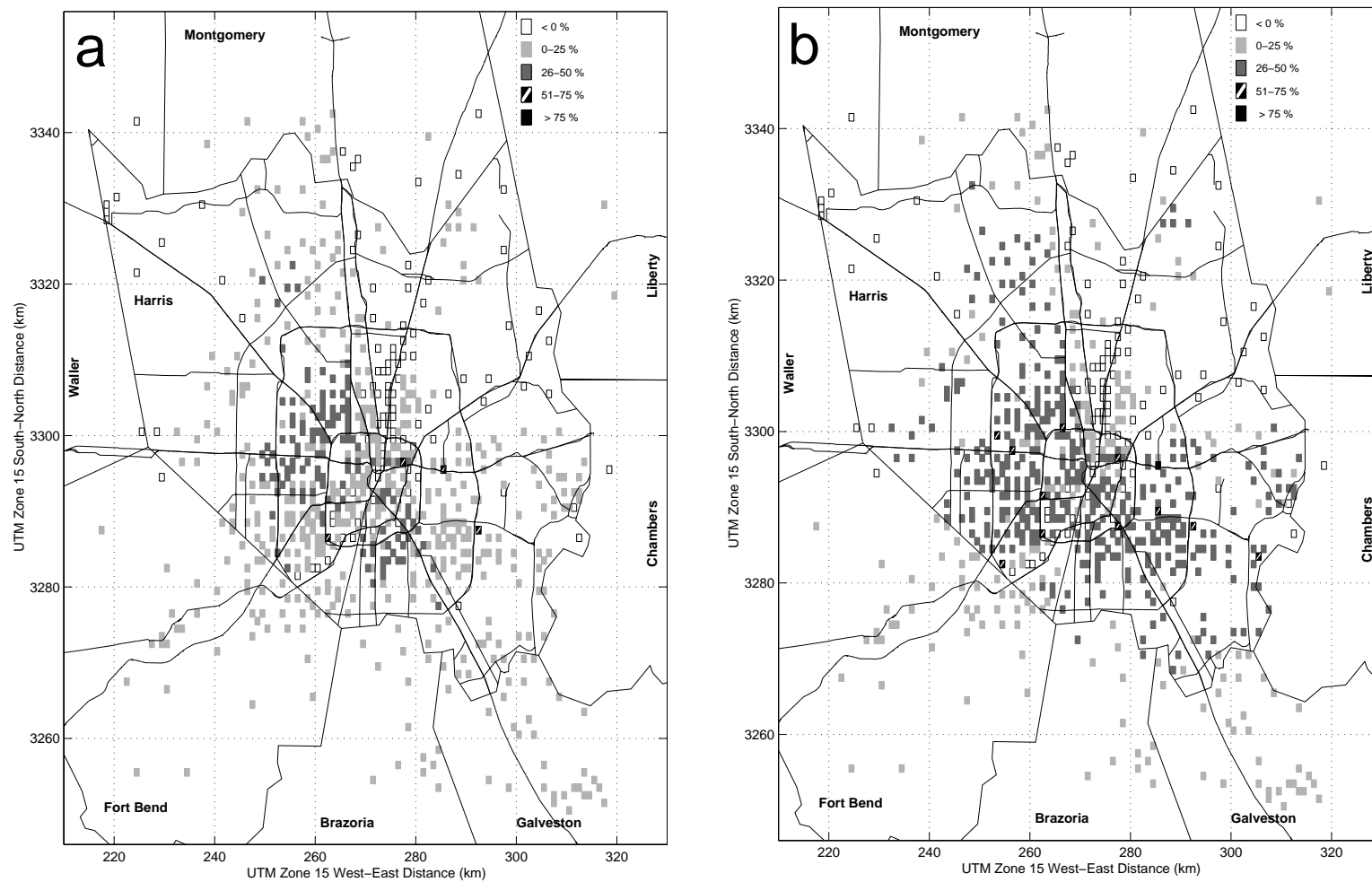
Figure 4.4-8. Benzene percent differences for ISCST3 ROADS minus ISCST3 BASE for a) total (all sources) concentrations and b) onroad mobile concentrations.
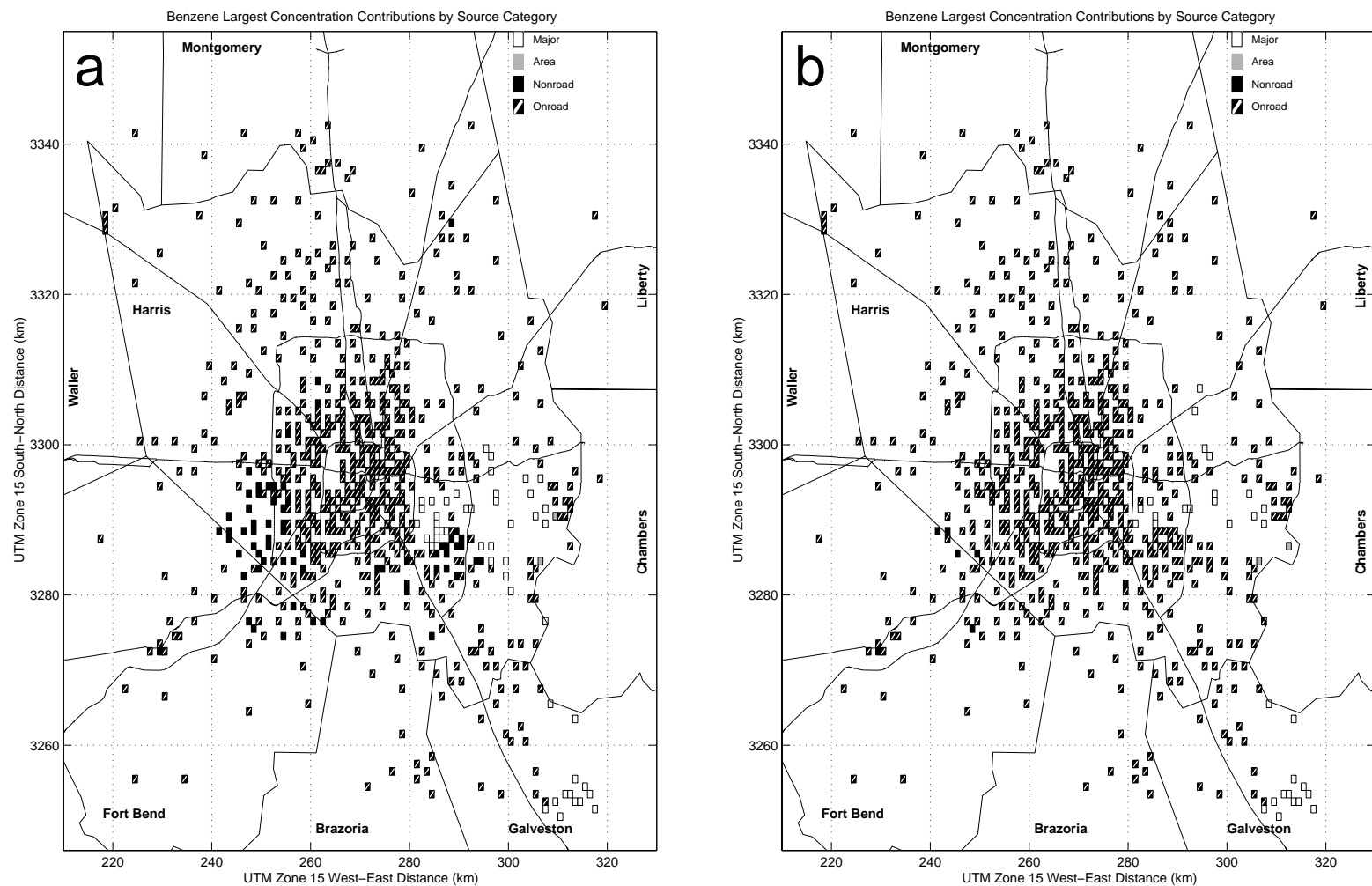
Figure 4.4-9. Largest source contributor at each receptor for benzene total concentrations for a) ISCST3 BASE and b) ISCST3 ROADS.

Annual Average Concentrations [μg/m^3], ISCST3 ROADS, Houston, TX, 1996
Benzene, with Near–Source Receptors, All Sources– Incl. Background
COLORBAR SCALED TO 98TH–PERCENTILE TO SHOW CONCENTRATION GRADIENTS, NOT BIGGEST HOTSPOT

a

11–Mar–2002

UTM Zone 15 South–North Distance (km)

UTM Zone 15 West–East Distance (km)

Annual Average Concentrations [μg/m^3], ISCST3 ROADS, Houston, TX, 1996
Benzene, with Near–Source Receptors, All Sources– Incl. Background
COLORBAR SCALED TO MAX CONCENTRATION SHOWS BIGGEST HOTSPOTS

b

11–Mar–2002

UTM Zone 15 South–North Distance (km)

UTM Zone 15 West–East Distance (km)

Figure 4.4-10. Benzene ISCST3 FINE GRID annual average total concentrations (μg m^{-3}). a) scaled to 98th percentile of concentrations and b) scaled to maximum concentration.
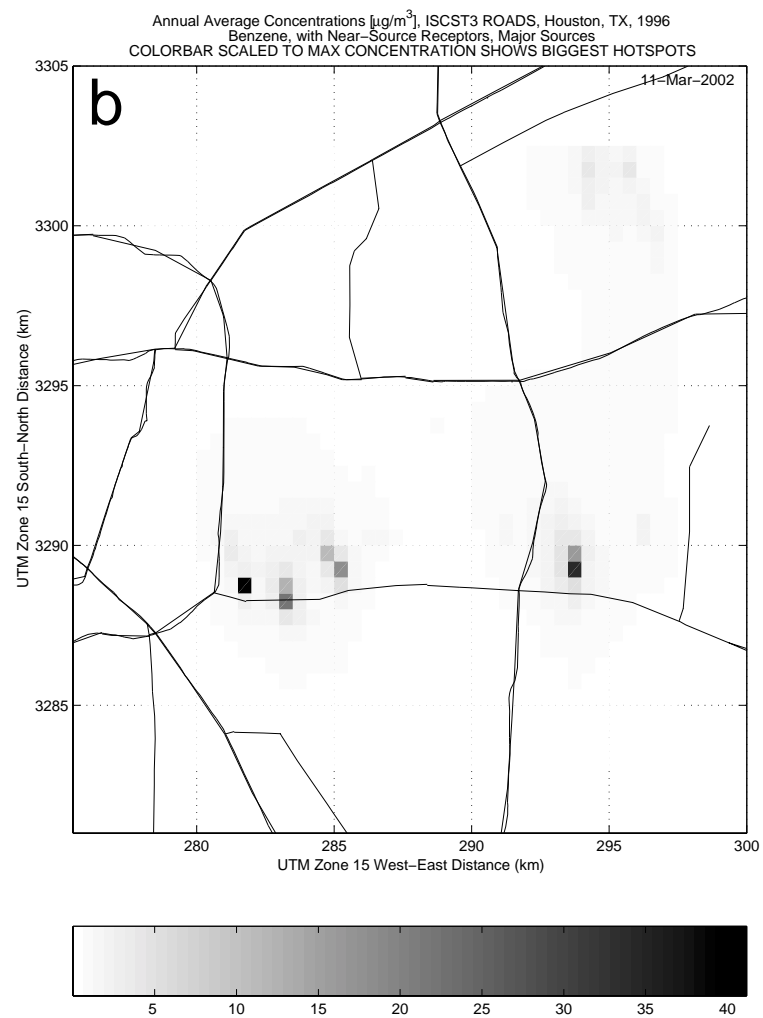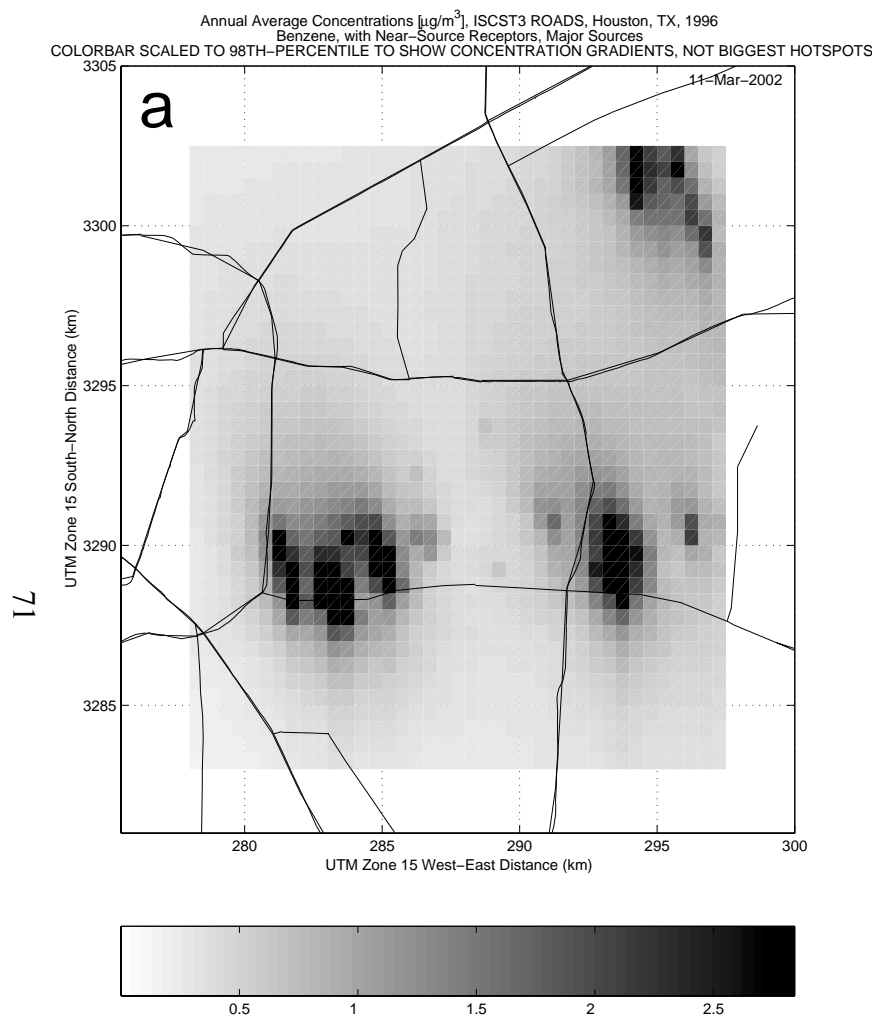
Figure 4.4-11. Benzene ISCST3 FINE GRID annual average major source concentrations ($\mu g\ m^{-3}$) a) scaled to 98th percentile of concentrations and b) scaled to maximum concentration.

Figure 4.4-12. Benzene ISCST3 FINE GRID annual average area source concentrations ($\mu g\ m^{-3}$) a) scaled to 98th percentile of concentrations and b) scaled to maximum concentration.
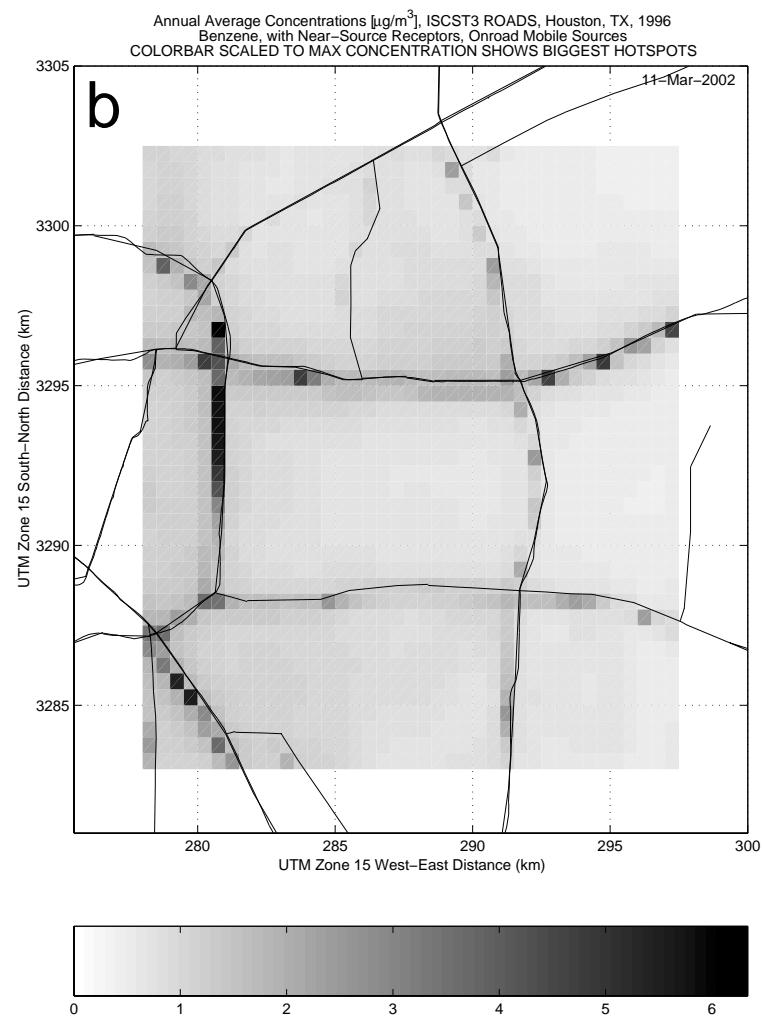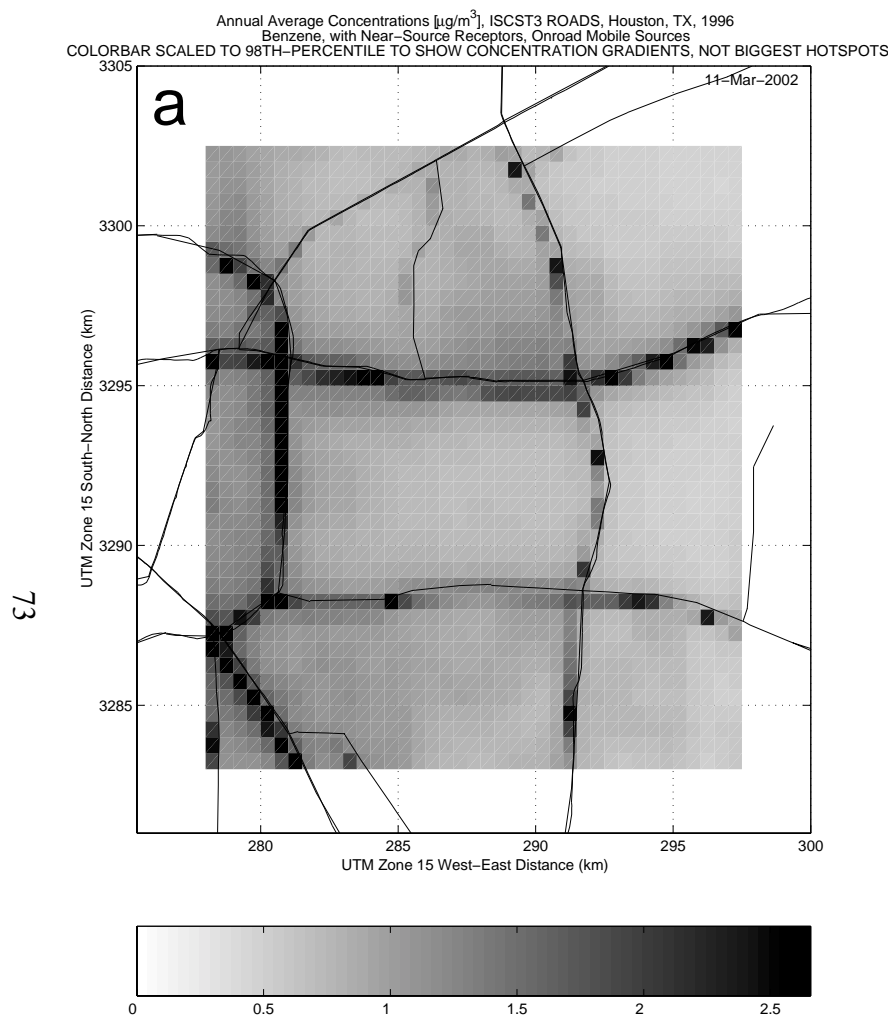
Figure 4.4-13. Benzene ISCST3 FINE GRID annual average onroad mobile source concentrations (μg m^{-3}) a) scaled to 98th percentile of concentrations and b) scaled to maximum concentration.
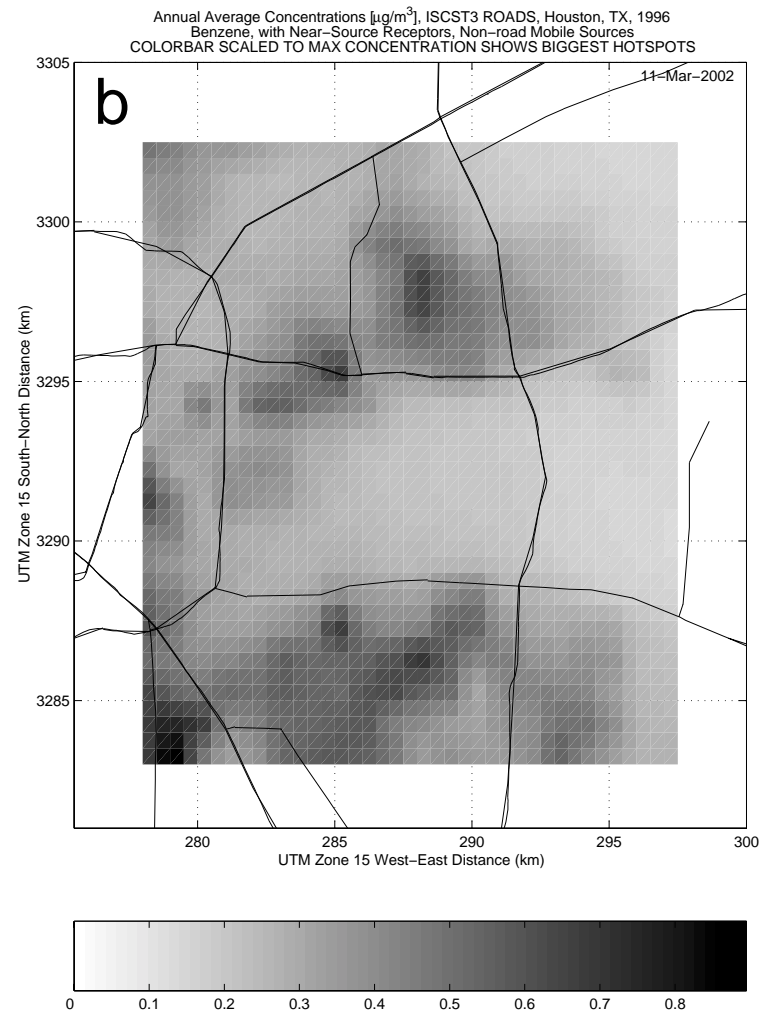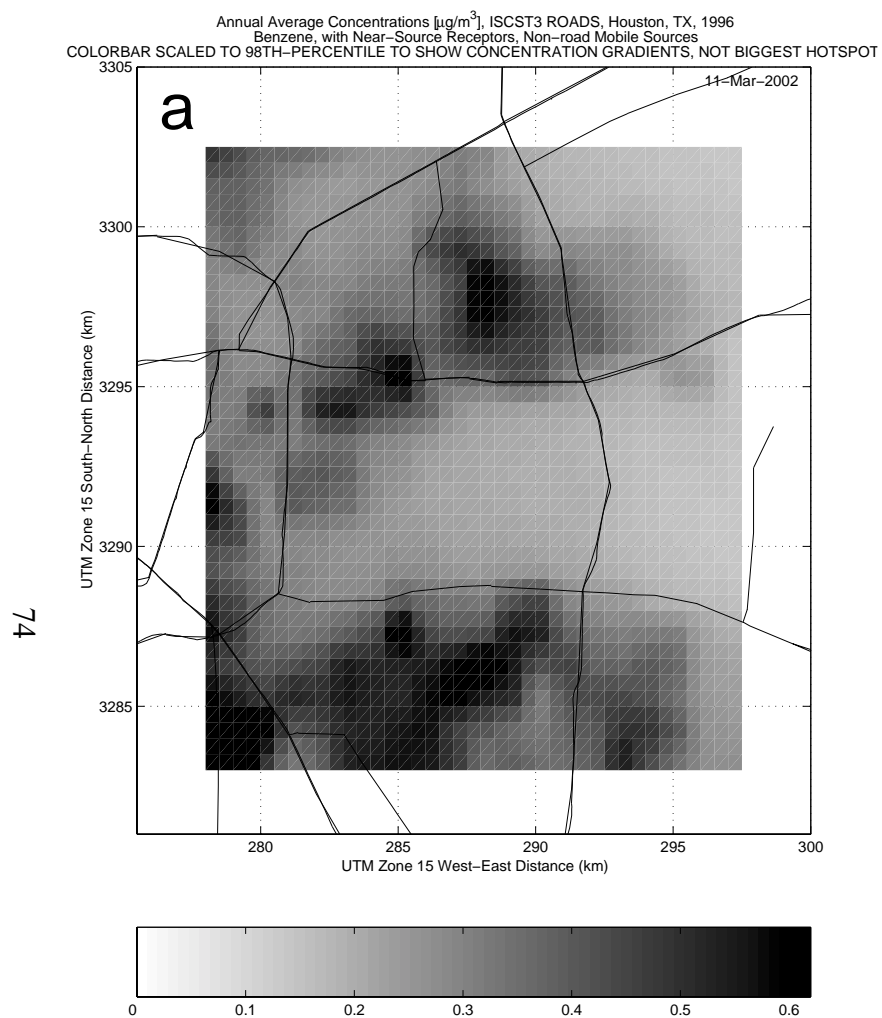
Figure 4.4-14. Benzene ISCST3 FINE GRID annual average nonroad mobile source concentrations (μg m^{-3}) a) scaled to 98th percentile of concentrations and b) scaled to maximum concentration.
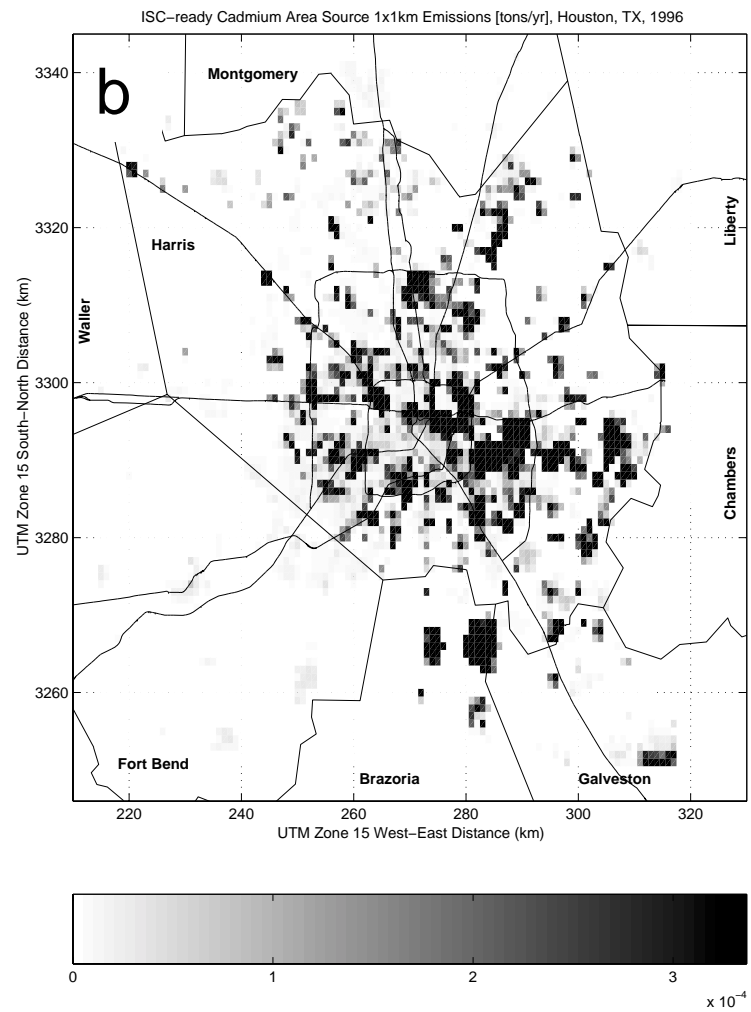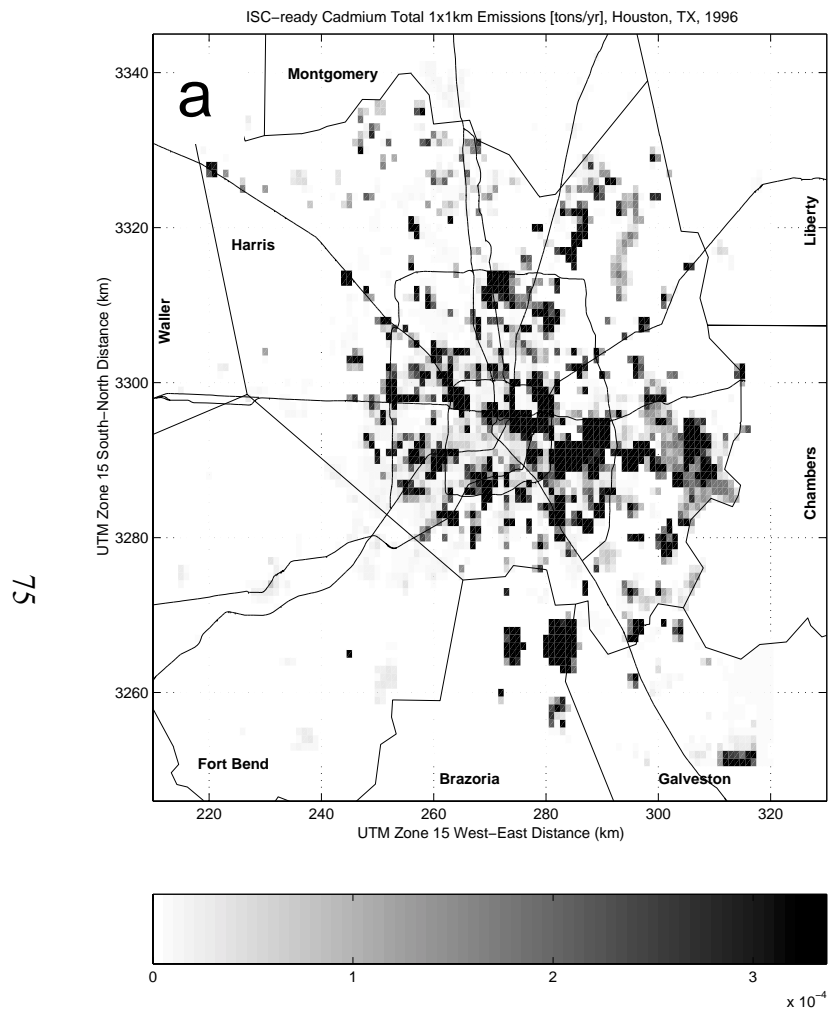
Figure 4.4-15 Cadmium 1 km gridded emissions (tons yr^{-1}) for a) all sources, and b) area/other sources.
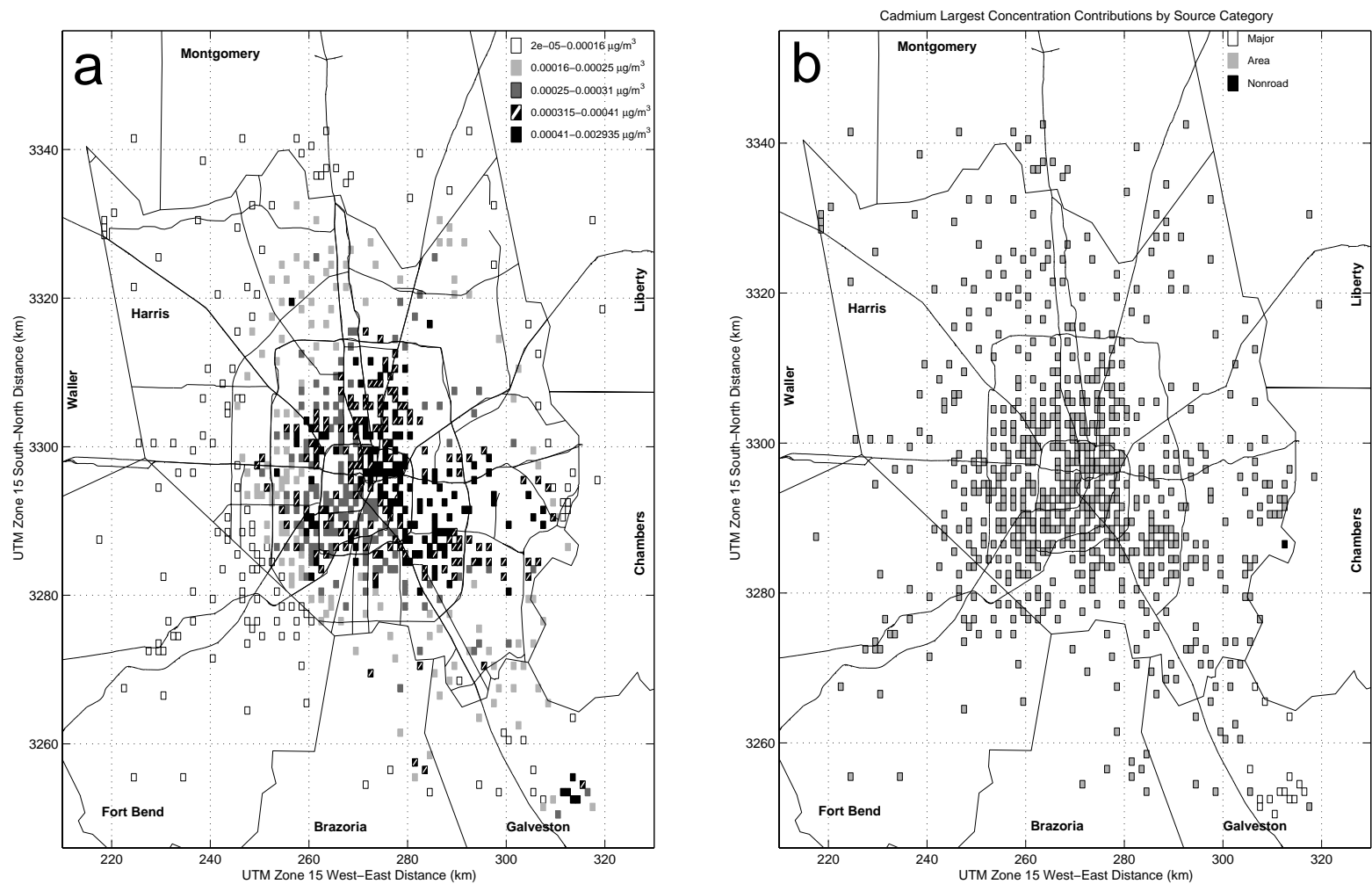
Figure 4.4-16. Cadmium ISCST3 annual average a) total concentrations (μg m^{-3}) and b) largest source contributor at each receptor.

ISC−ready Chromium Total 1x1km Emissions [tons/yr], Houston, TX, 1996

Figure 4.4-17. Chromium 1 km gridded emissions (tons yr^{-1}) from all sources.

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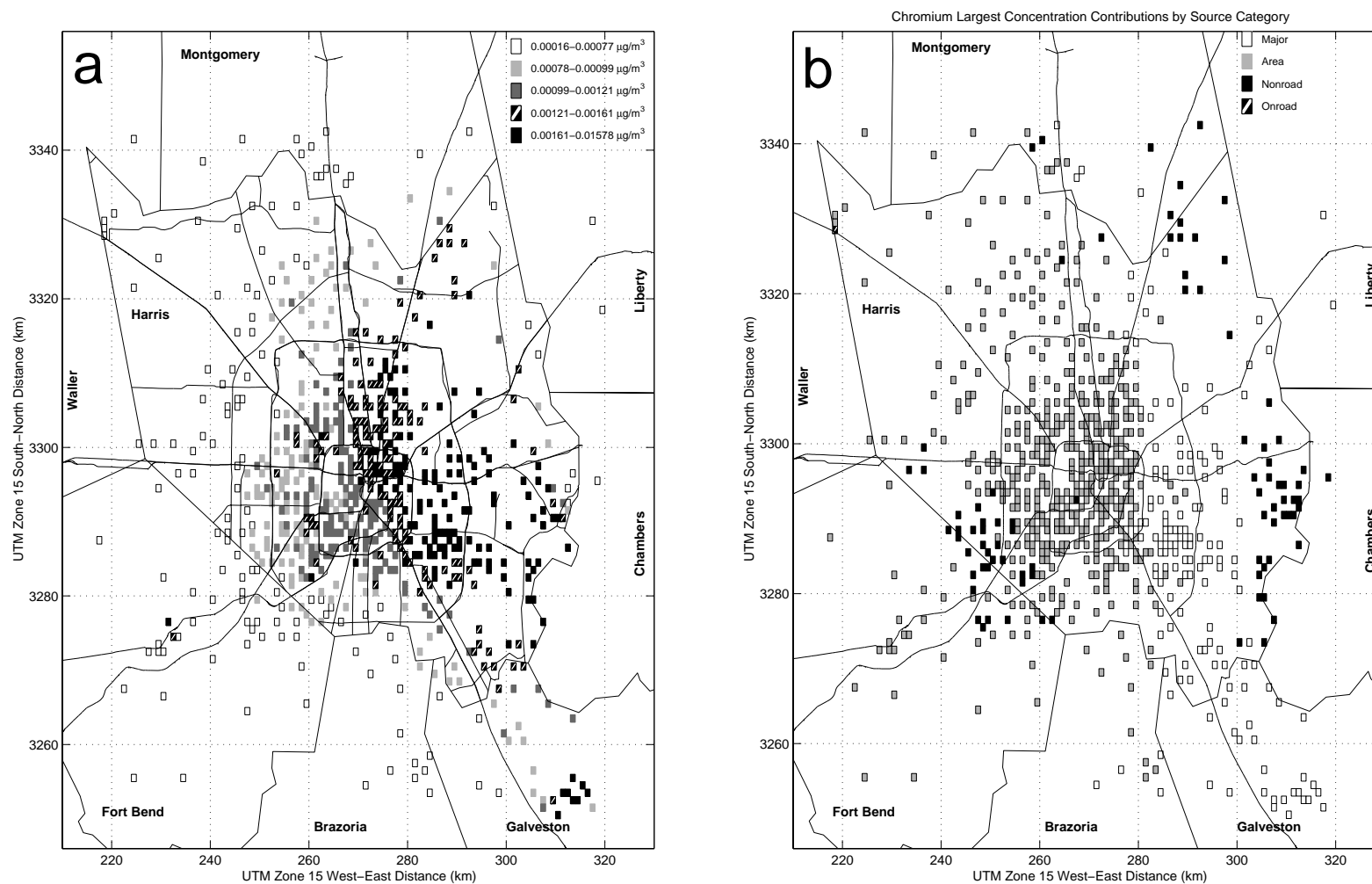
Figure 4.4-18. Chromium ISCST3 annual average a) total concentrations ($\mu g\ m^{-3}$) and b) largest source contributor at each receptor.
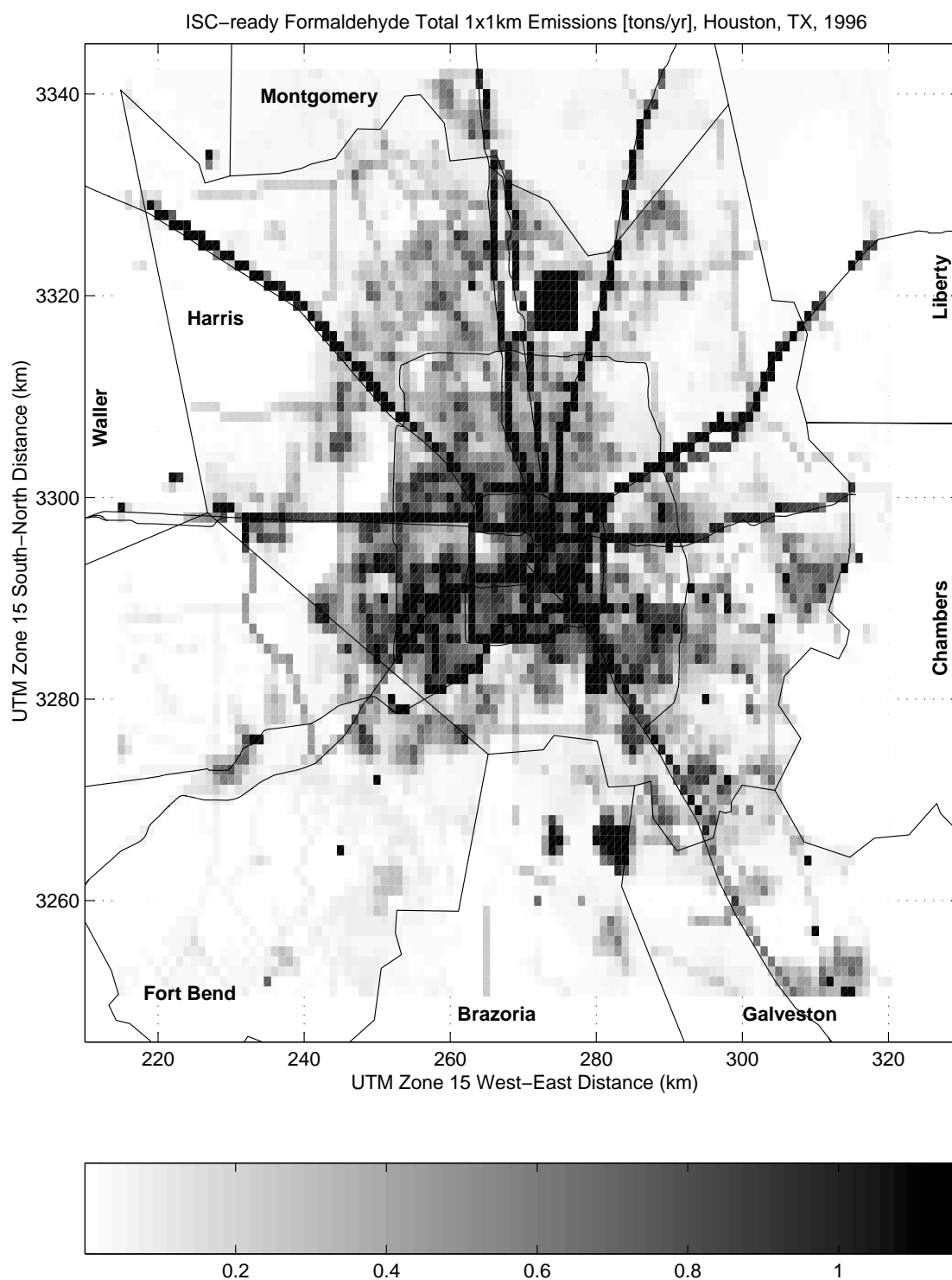
Figure 4.4-19. Formaldehyde 1 km gridded emissions (tons yr^{-1}) from all sources.

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ISC−ready Formaldehyde Harris County Onroad Mobile Segments Emissions [tons/(yr−km^2)], Houston, TX, 1996
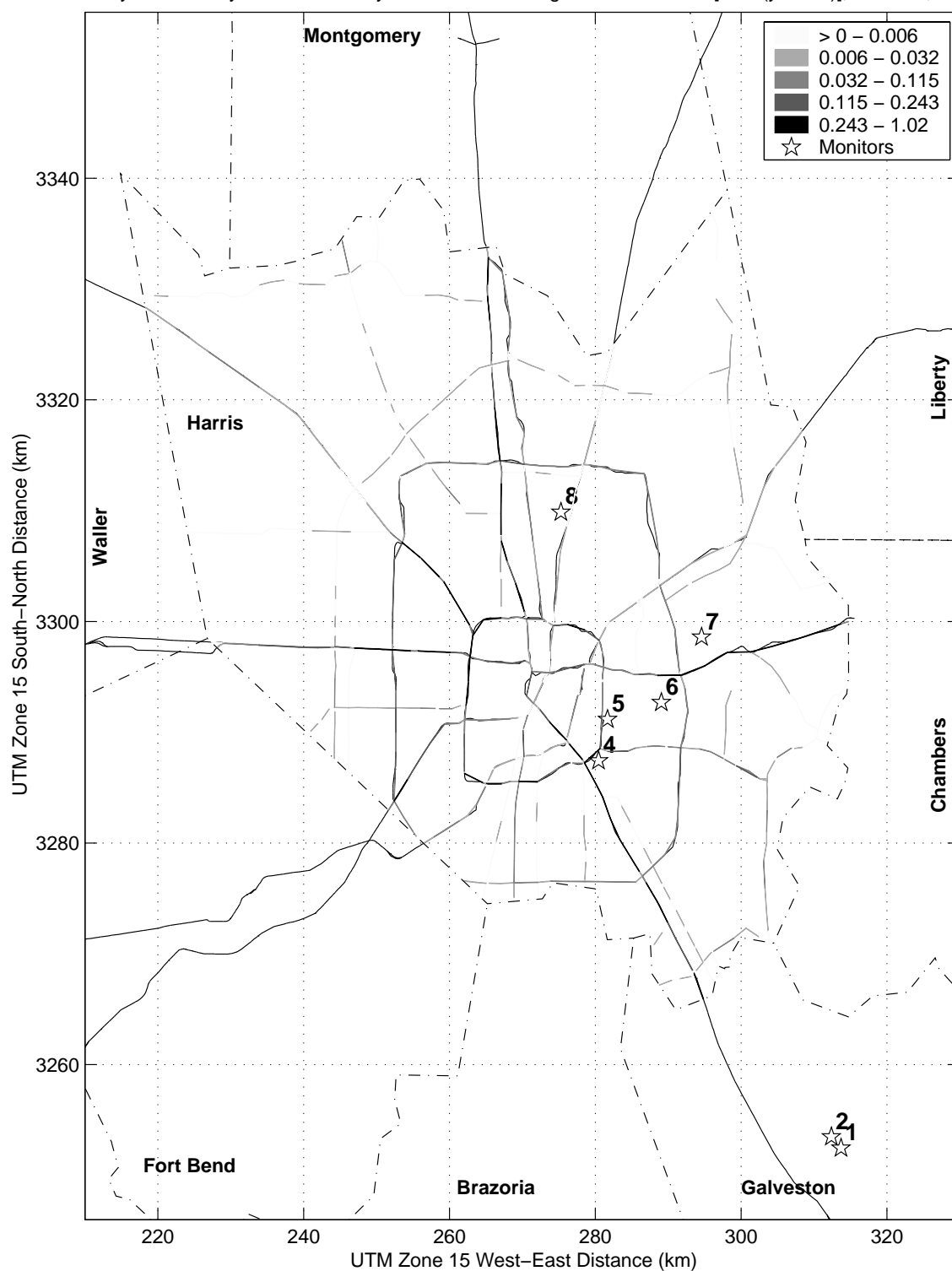
Figure 4.4-20. Formaldehyde road segment emissions (tons yr^{-1} km^{-2}).
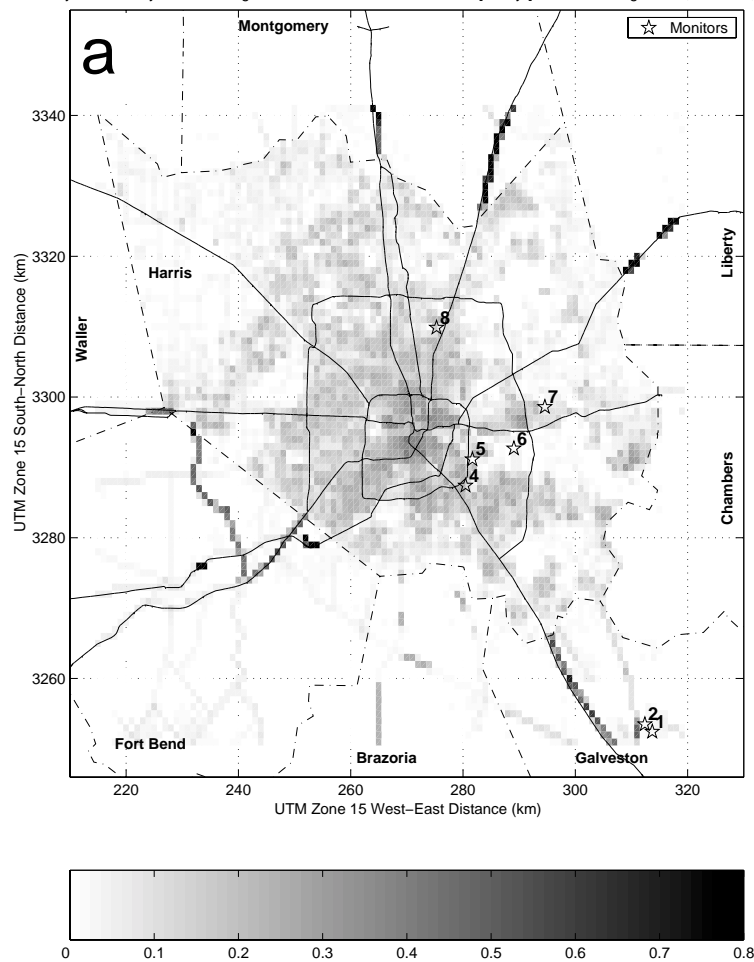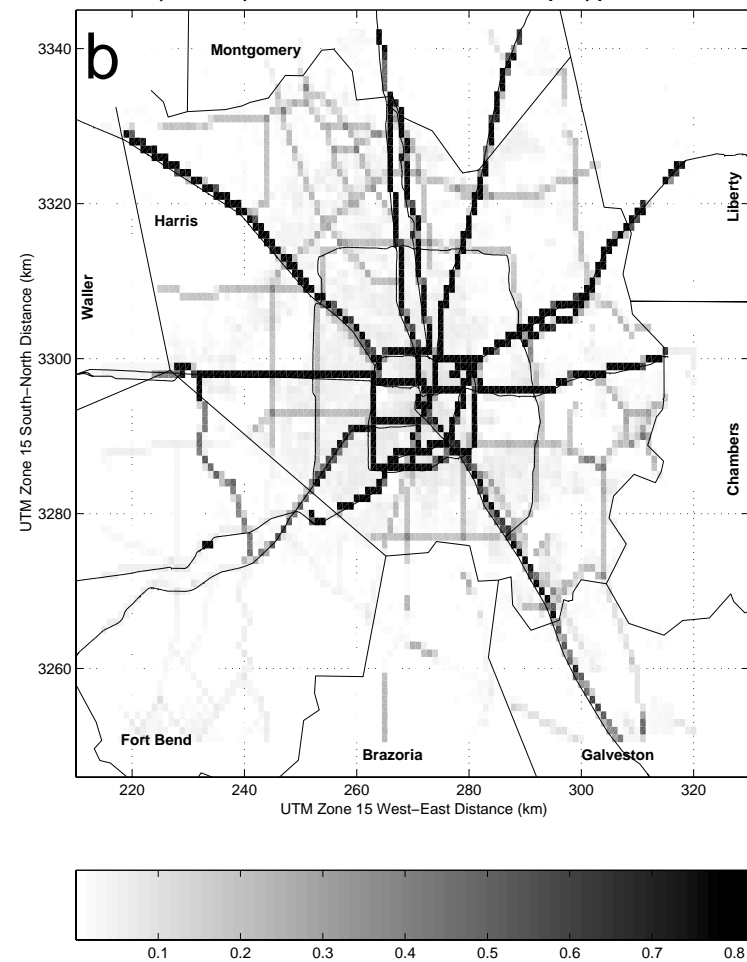
Figure 4.4-21. Formaldehyde 1 km onroad mobile gridded emissions (tons yr^{-1}) for a) remaining onroad emissions after extracting road segment emissions and b) ISCST3 BASE onroad mobile gridded emissions.

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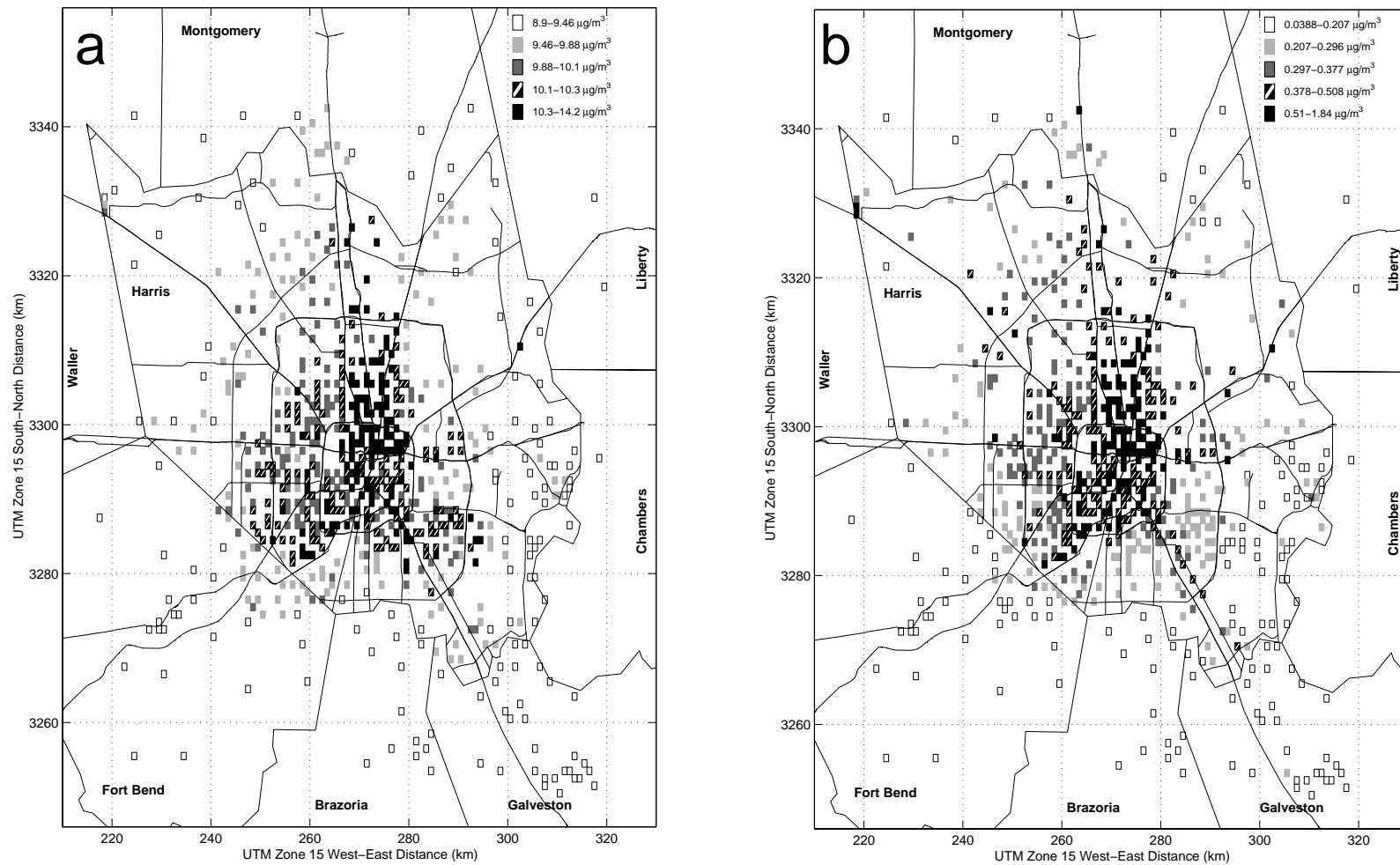
Figure 4.4-22. Formaldehyde ISCST3 BASE annual average concentrations ($\mu g\ m^{-3}$) for a) all sources, and b) onroad mobile sources.
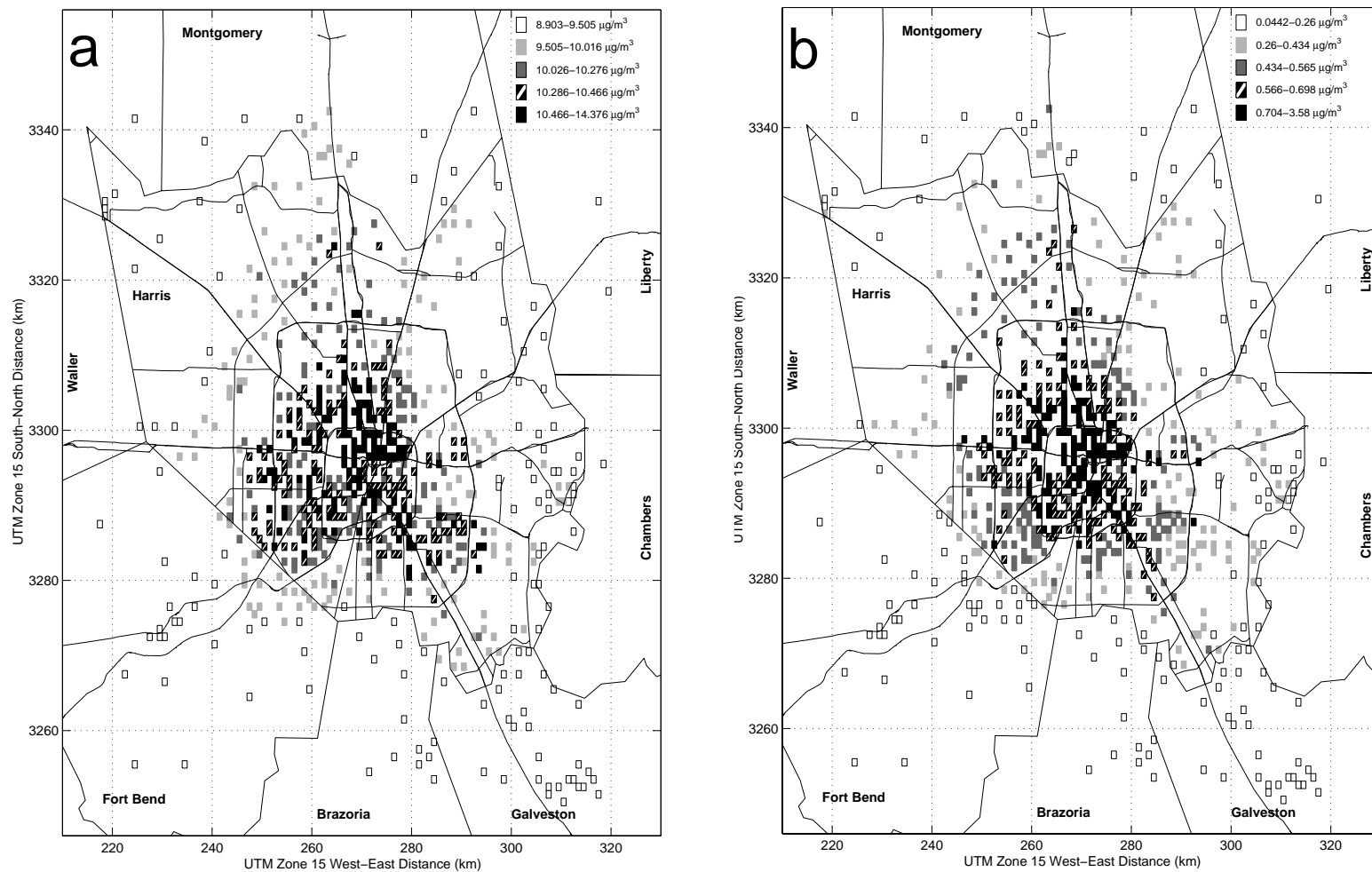
Figure 4.4-23. Formaldehyde ISCST3 ROADS annual average concentrations ($\mu g\ m^{-3}$) for a) all sources, and b) onroad mobile sources.
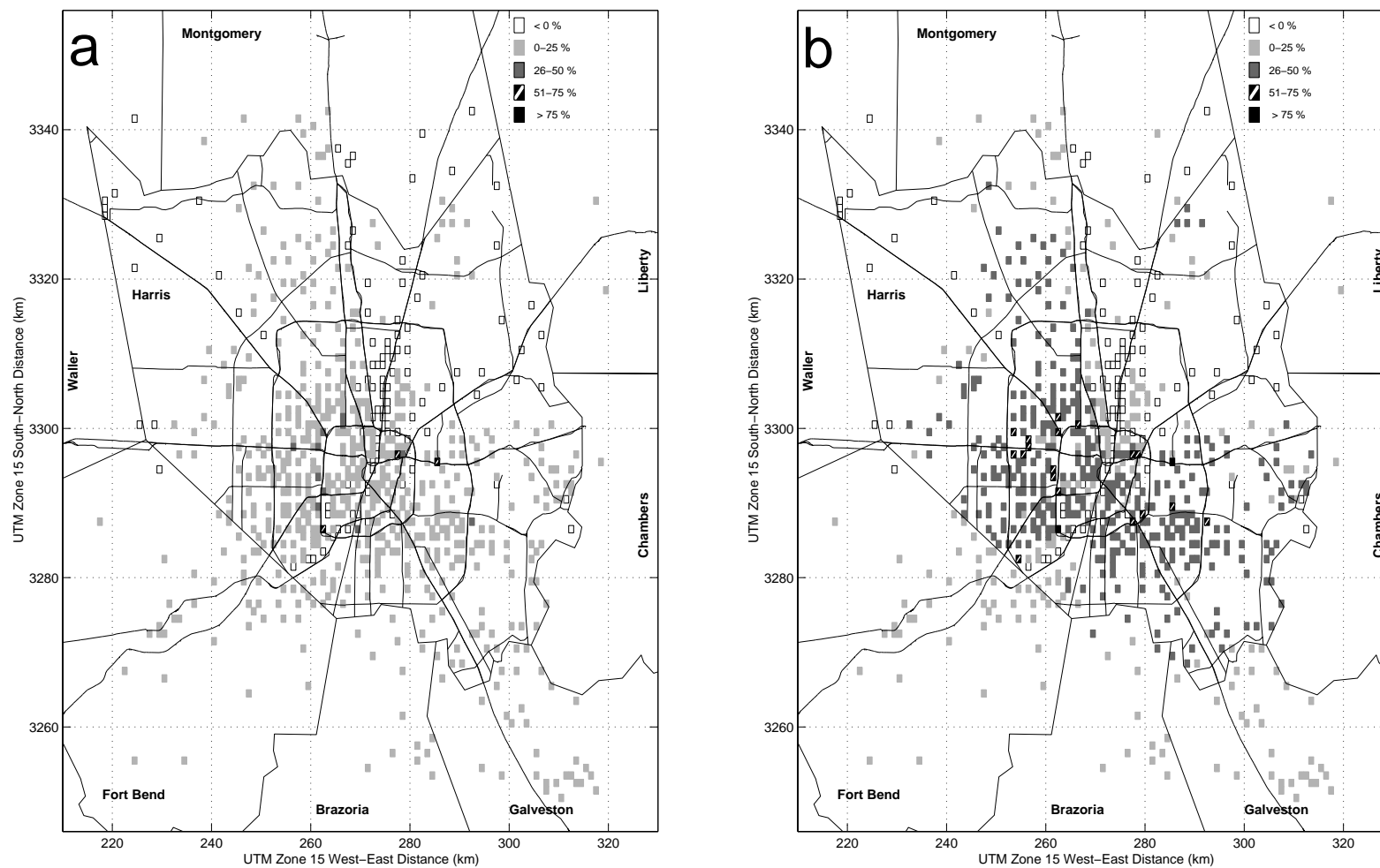
Figure 4.4-24. Formaldehyde percent differences for ISCST3 ROADS minus ISCST3 BASE for a) total concentrations and b) onroad mobile concentrations.
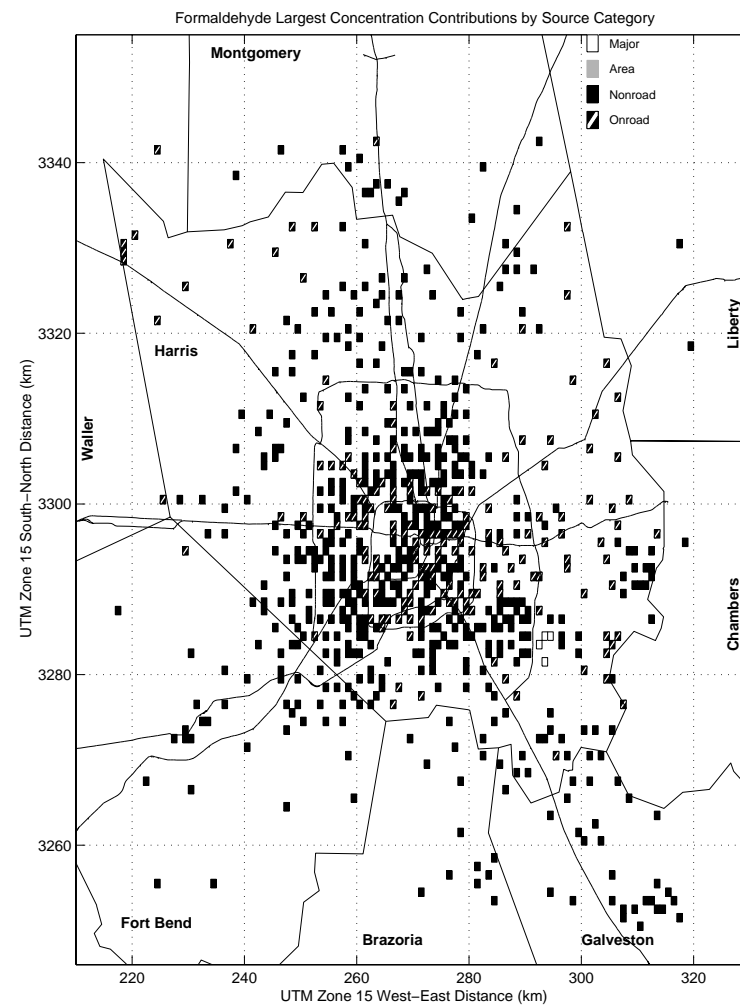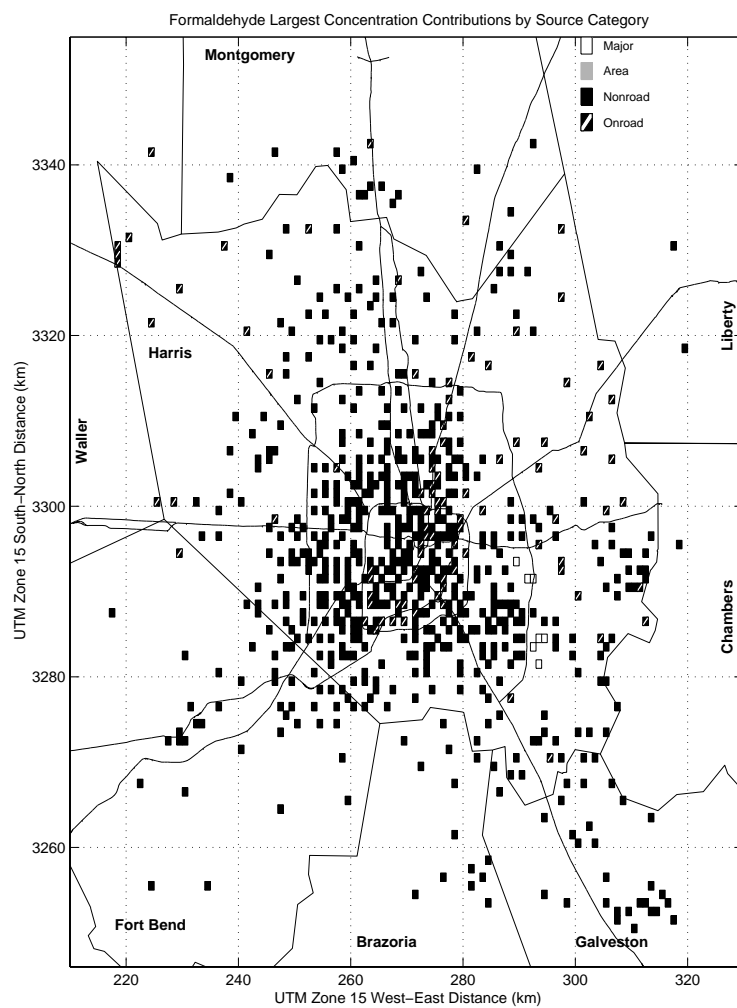
Figure 4.4-25. Largest source contributor for each recptor for formaldehyde for a) ISCST3 BASE and b) ISCST3 ROADS.
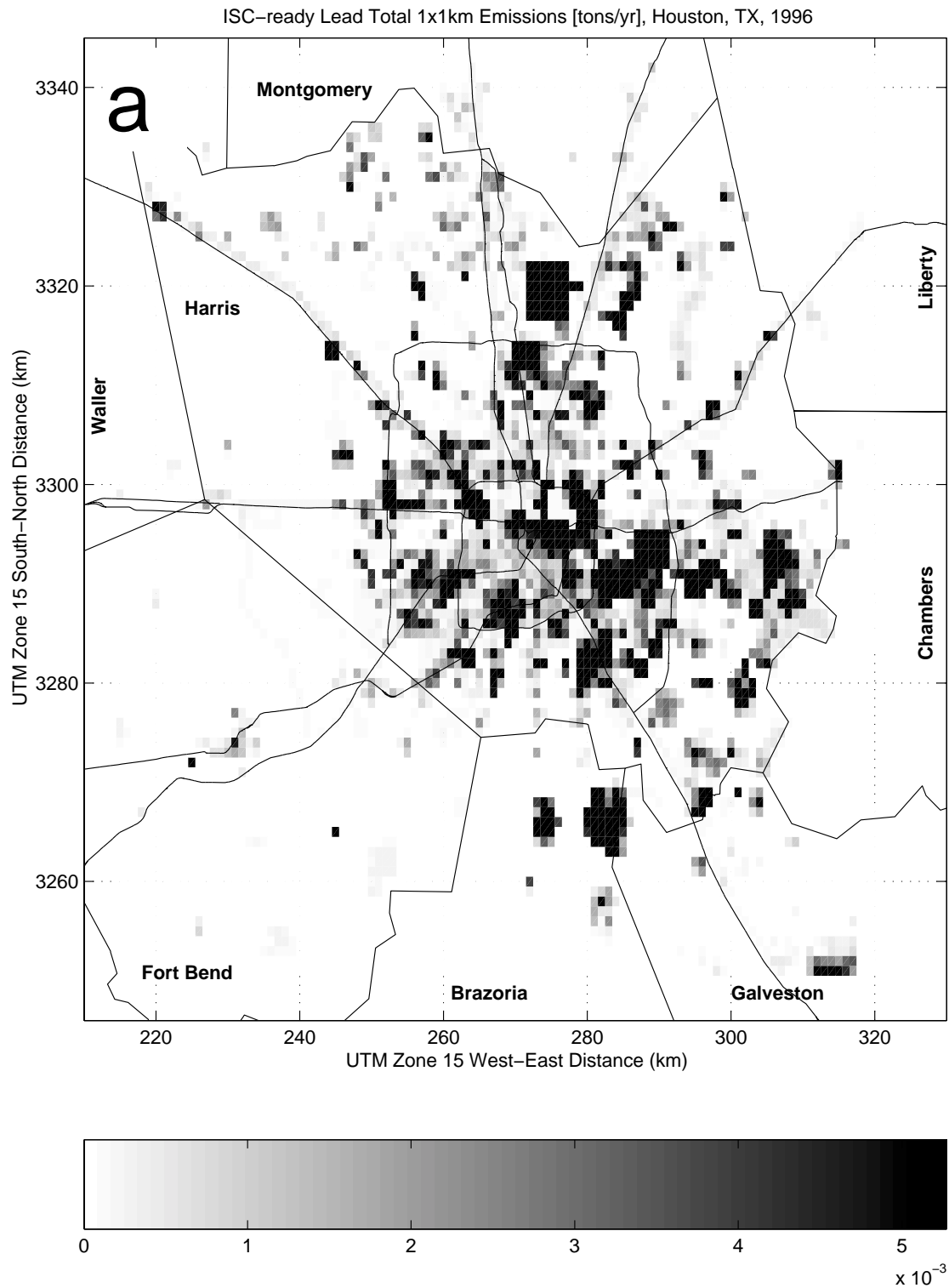
Figure 4.4-26. Lead 1 km gridded emissions (tons yr^{-1}) for a) all sources,
b) area/other sources., and c) nonroad mobile sources.
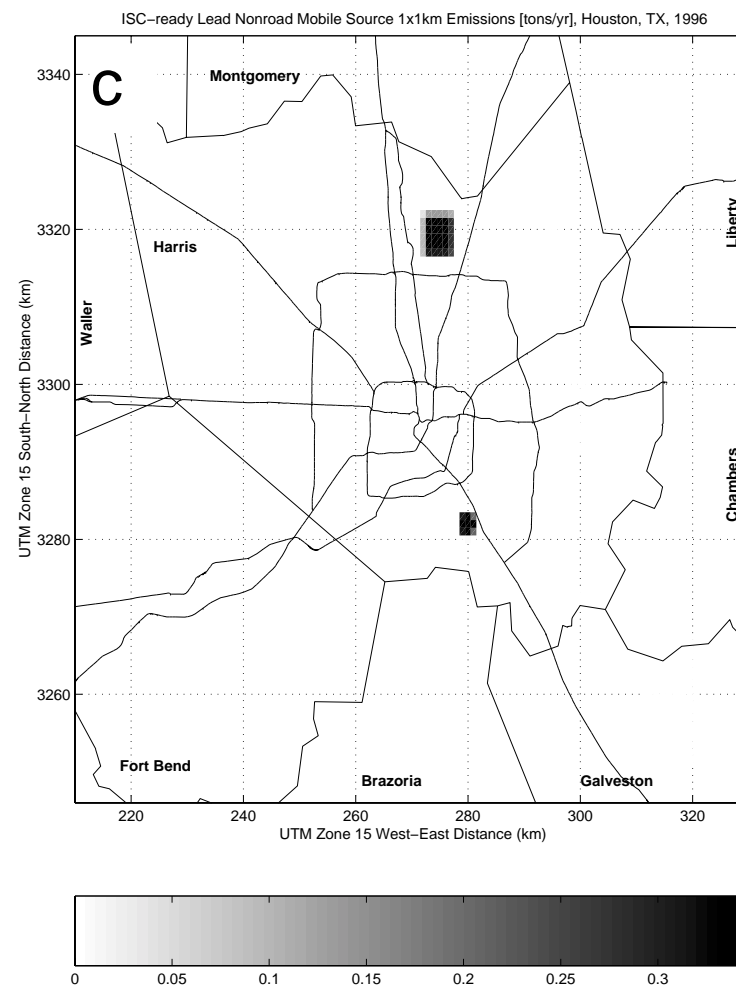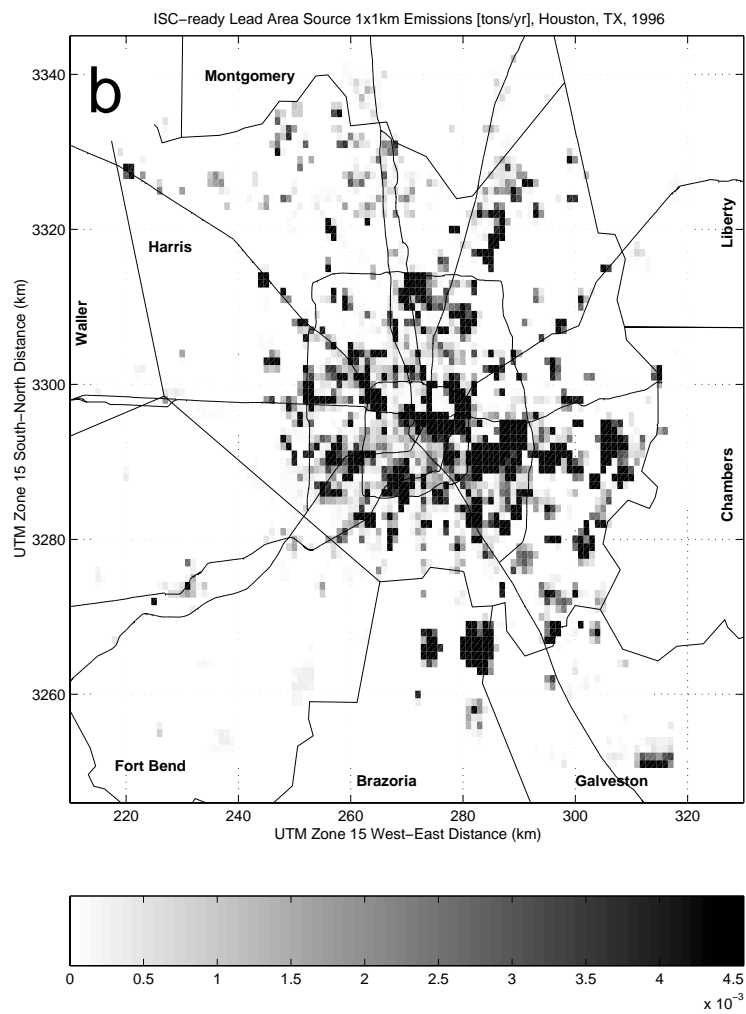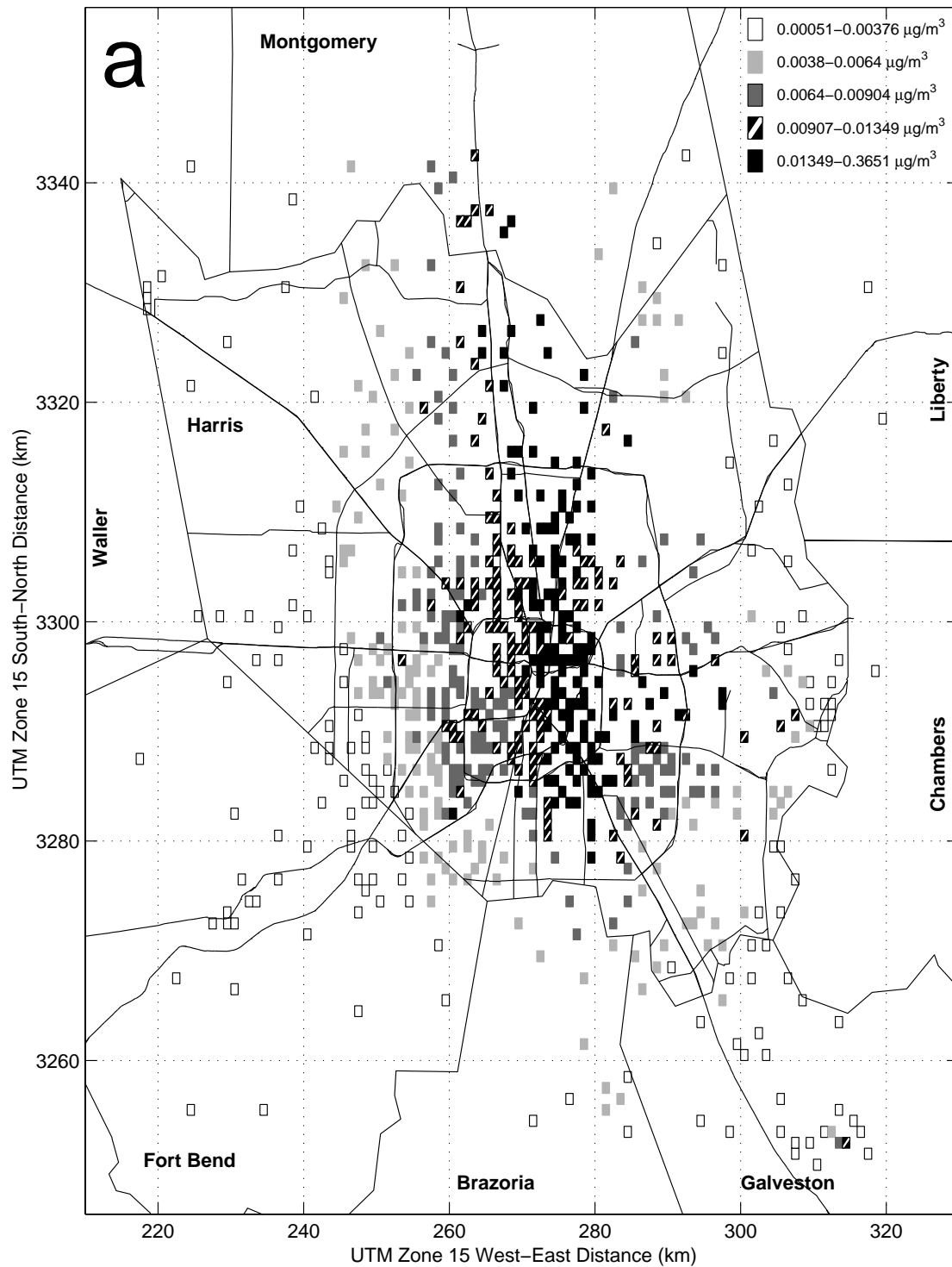
Figure 4.4-26. Continued.

Figure 4.4-27. Lead annual average ISCST3 concentrations ($\mu g\ m^{-3}$) for a) all sources, b) area/other sources, and c) nonroad mobile sources.
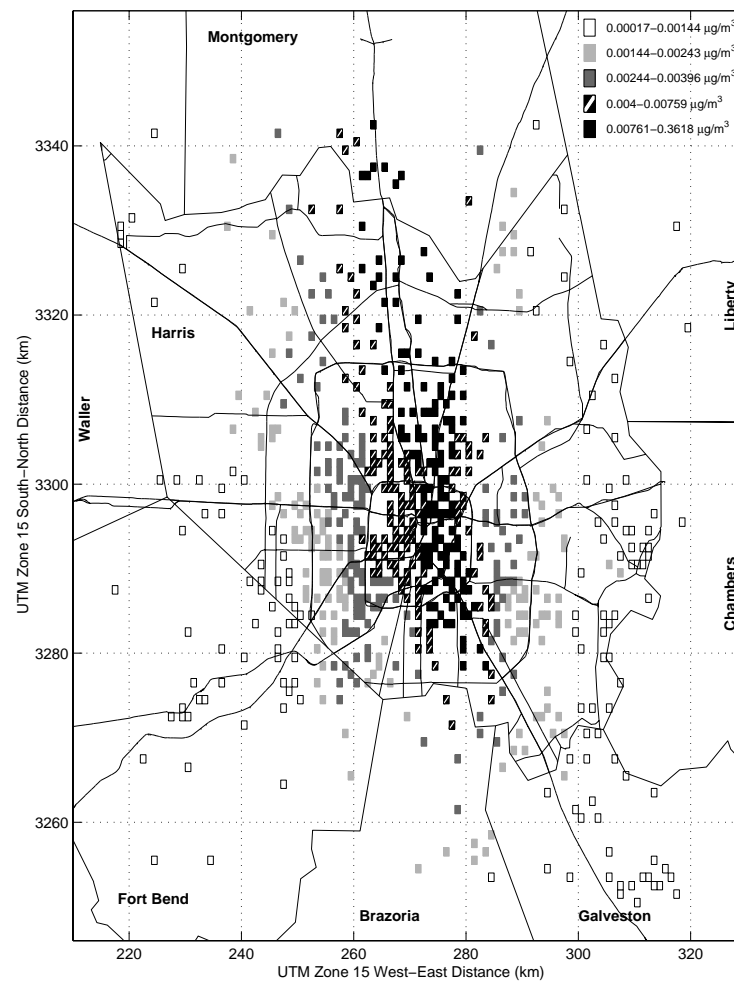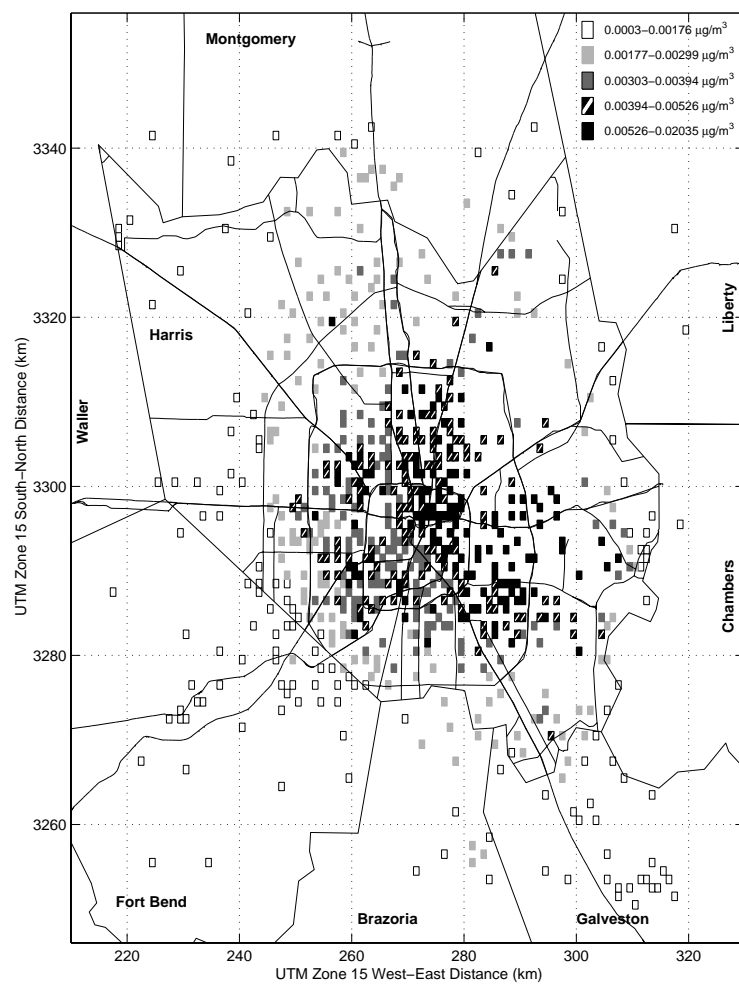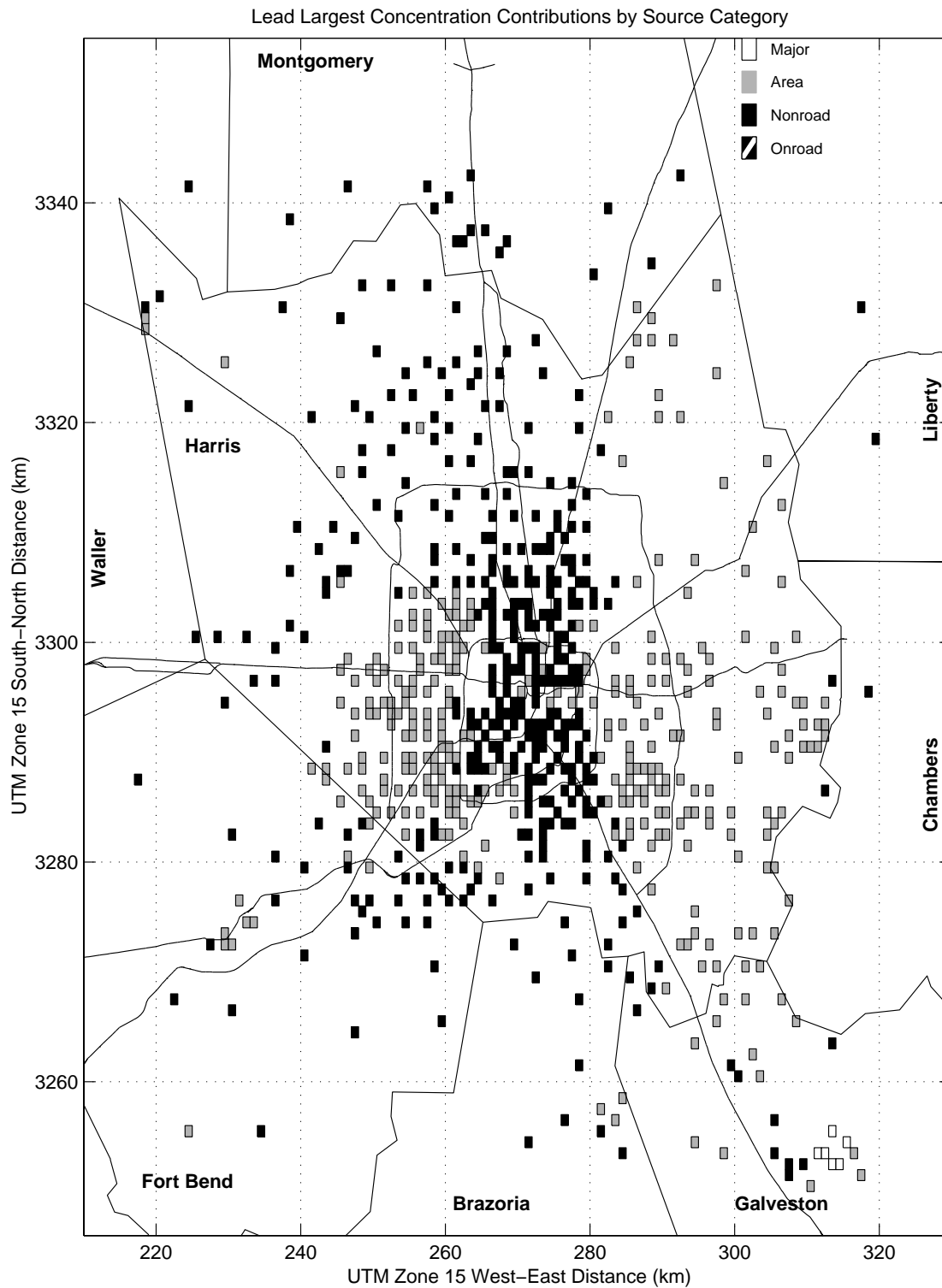
Figure 4.4-27. Continued.

Figure 4.4-28. Largest source contributor at each receptor for lead.
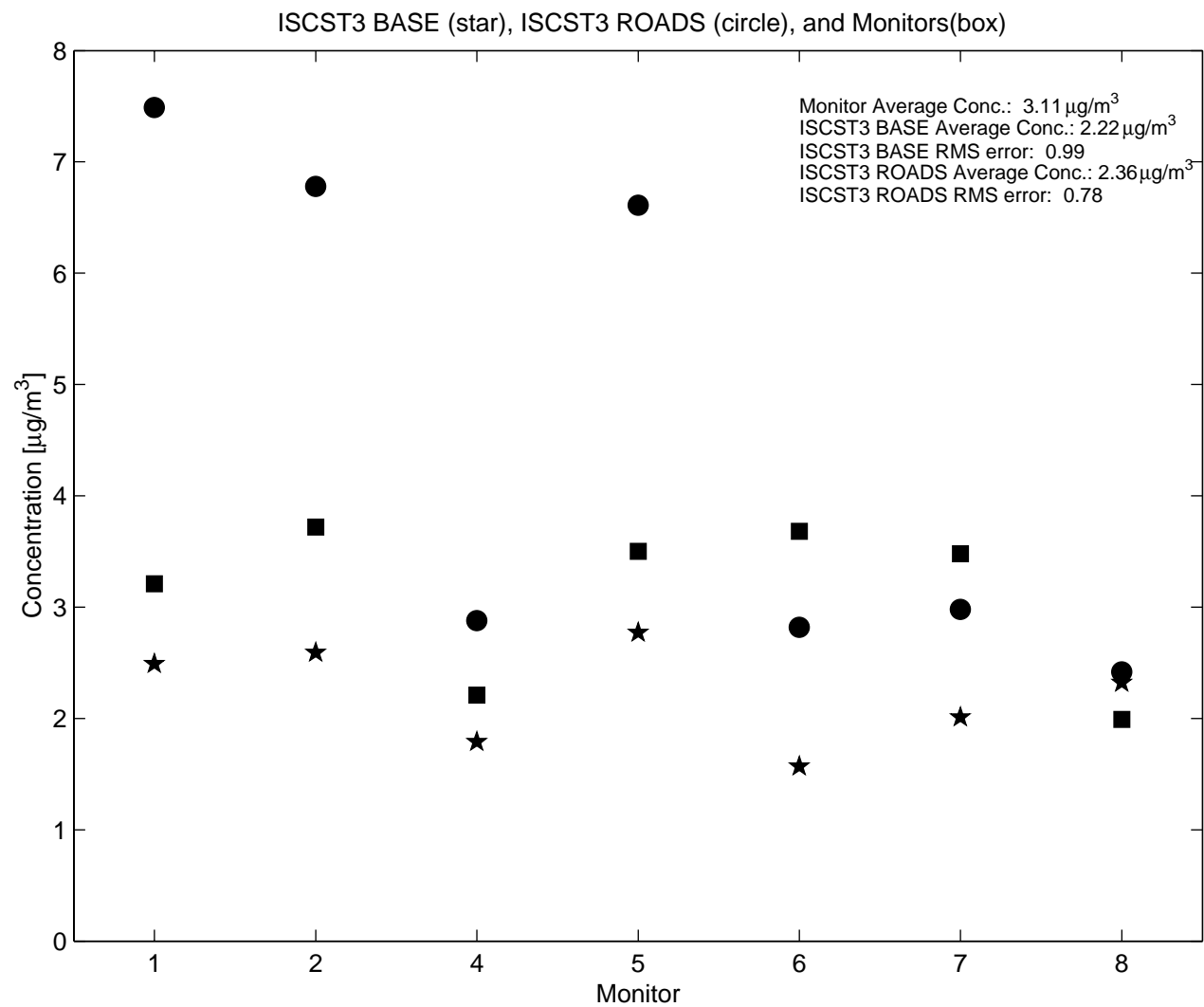
ISCST3 BASE (star), ISCST3 ROADS (circle), and Monitors(box)

Monitor Average Conc.: 3.11 $\mu g/m^3$
ISCST3 BASE Average Conc.: 2.22 $\mu g/m^3$
ISCST3 BASE RMS error: 0.99
ISCST3 ROADS Average Conc.: 2.36 $\mu g/m^3$
ISCST3 ROADS RMS error: 0.78

Figure 4.4-29. ISCST3 BASE (star), ISCST3 ROADS (circles) and monitor (box) annual average concentrations ($\mu g\ m^{-3}$) for benzene.

Appendix A

Estimating Background Concentration for Diesel PM

APPENDIX A - TABLE OF CONTENTS

LIST OF FIGURES

1. INTRODUCTION:

Background concentrations are an essential part of the total air quality concentration to be considered in determining source impacts. Background air quality includes pollutant concentrations due to: 1) natural sources; 2) nearby sources that are unidentified in the inventory; and 3) long range transport into the modeling domain. Typically, monitored air quality data should be used to establish background concentrations.

The ISCST3 model calculates concentrations at receptors with a maximum distance of 50 km. Gaussian type models are not applied for distances greater than 50 km. However, sources at distances more than 50 km from the receptor contribute to the total concentration at the receptor location.

For diesel PM, a modeling based approach was developed to provide a rough approximation of concentrations due to transport from sources located between 50 km and 300 km from the receptor. This approximation was based on results from existing CALPUFF simulations from an elevated source (35 m) and a surface release (2 m) for three geographical areas: Boise, ID, Medford, OR, and Pittsburgh, PA. These simulations were made as part of a series of simulations to compare ISC results with CALPUFF results (U.S. EPA, 1993). CALPUFF is a Lagrangian puff model, which was originally designed for mesoscale applications, and it can operate in a range of 0-300 km from the source (U.S. EPA, 1995). For these CALPUFF simulations, CALPUFF was run using ISC meteorology. Therefore, these CALPUFF results are not the result of a full-scale refined analysis, in which the meteorological conditions are allowed to vary in space and time.

2. APPROACH TO DEVELOP CONCENTRATION VS DISTANCE

The annual average CALPUFF concentration estimates, normalized by the emission rate, are shown in Figure A-1 as a function of distance from the source for 3 cases. A spline polynomial approximation was used to get analytical representation for the results shown in Figure A-1. These parameterizations provide annual average concentrations in (μg m^{-3}) at a distance 50 km < x < 300 km from a low release source (Eq.1a) and an elevated source (Eq.1b).

$$C=6.18022\times10^{-10}\times x^4-5.2255\times10^{-7}\times x^3+1.61998\times10^{-4}\times x^2-2.22567\times10^{-2}\times x+1.215630 \qquad (1a)$$
$$C=3.37367\times10^{-10}\times x^4-2.91373\times10^{-7}\times x^3+0.32310\times10^{-5}\times x^2-1.3411\times10^{-2}\times x+0.784964 \qquad (1b)$$

Average curves for all 3 geographical areas are shown in Figure A-2. The approximations 1(a-b) are also shown in the figure for a low level release and a release from the elevated source. The source emission rate is assumed to be equal 100 g s^{-1}.

3. ESTIMATING BACKGROUND CONCENTRATION

We introduce a method to calculate the "background" concentrations due to contribution from emission sources located farther then 50 km. The method is based on a simplistic

approach: first, a receptor grid is set up for the entire U.S. with a spatial resolution of 0.2 degree latitude by 0.5 degree longitude. Second, for each receptor, all emission sources located at a distance greater than 50 km and less than 300 km from the center of a grid box are considered. These census tract emissions are based on the 1996 NTI. The emissions from each census tract located from 50 to 300 km away from the center of the grid box are multiplied by a distance dependent factor defined in equation 1a and summed up to obtain a concentration at the center of the grid box. In this analysis, diesel PM emissions are from onroad and nonroad mobile sources, which are released at ground level. Therefore, equation 1a is applicable. In these estimates, no adjustment has been made to account for the variation in transport due to the climatology of wind direction for the area being modeled.

A schematic plot showing the relationship between the census tract centroids at a distance 50 - 300 km and the grid box centroid is shown in Figure A-3. Here the center of the grid box is shown as a star and a contribution from emission sources within a ring of 50 – 300 km is considered. The "background" concentration at each grid box center is the sum of concentrations resulting from all sources within the 50-300 km radius.

4. STUDY LIMITATIONS

The approach described above has several limitations. The estimates assume a complete and accurate inventory. Use of the ISC meteorology in CALPUFF does not account for wind flow in rivers and valleys as in mountainous terrain. The local wind flow patterns could cause concentrations to be significantly different at specific locations. Some uncertainty is introduced when averaging results over grid boxes instead of specific tracts. Using three specific locations to obtain a national average parameterization is simplistic. Finally, using CALPUFF with site specific information on emission release height, stack parameters, wet and dry deposition, meteorological wind field, etc. would give different estimates. Thus, these estimates of the impact of emissions located greater than 50 km but less than 300 km are considered as an approximation of "background" concentration until more reliable estimates can be obtained from monitoring data or when improved modeling techniques are developed.

This analysis suggests that the limitations of the ISCST3 model to calculate dispersion not farther than 50 km model may cause underestimates of concentrations in certain areas, where many sources with a high emission rate are located close to each other. Using a constant value for the "background" concentrations does not seem to be accurate enough and these results suggest a value for "background" should be computed for each receptor.

5. REFERENCES

U.S. EPA,1993. Interagency Workgroup on air Quality Modeling (IWAQM), Phase 1 Report: Interim Recommendation for Modeling Long Range Transport and Impacts on Regional Visibility, EPA-454/R-93-015; U.S. Environmental Protection Agency; Research Triangle Park, 1993.

U.S. EPA, 1995. A User's Guide for the CALPUFF Dispersion Model, EPA-454/B-95-006; U.S. Environmental Protection Agency; Research Triangle Park, 1995.
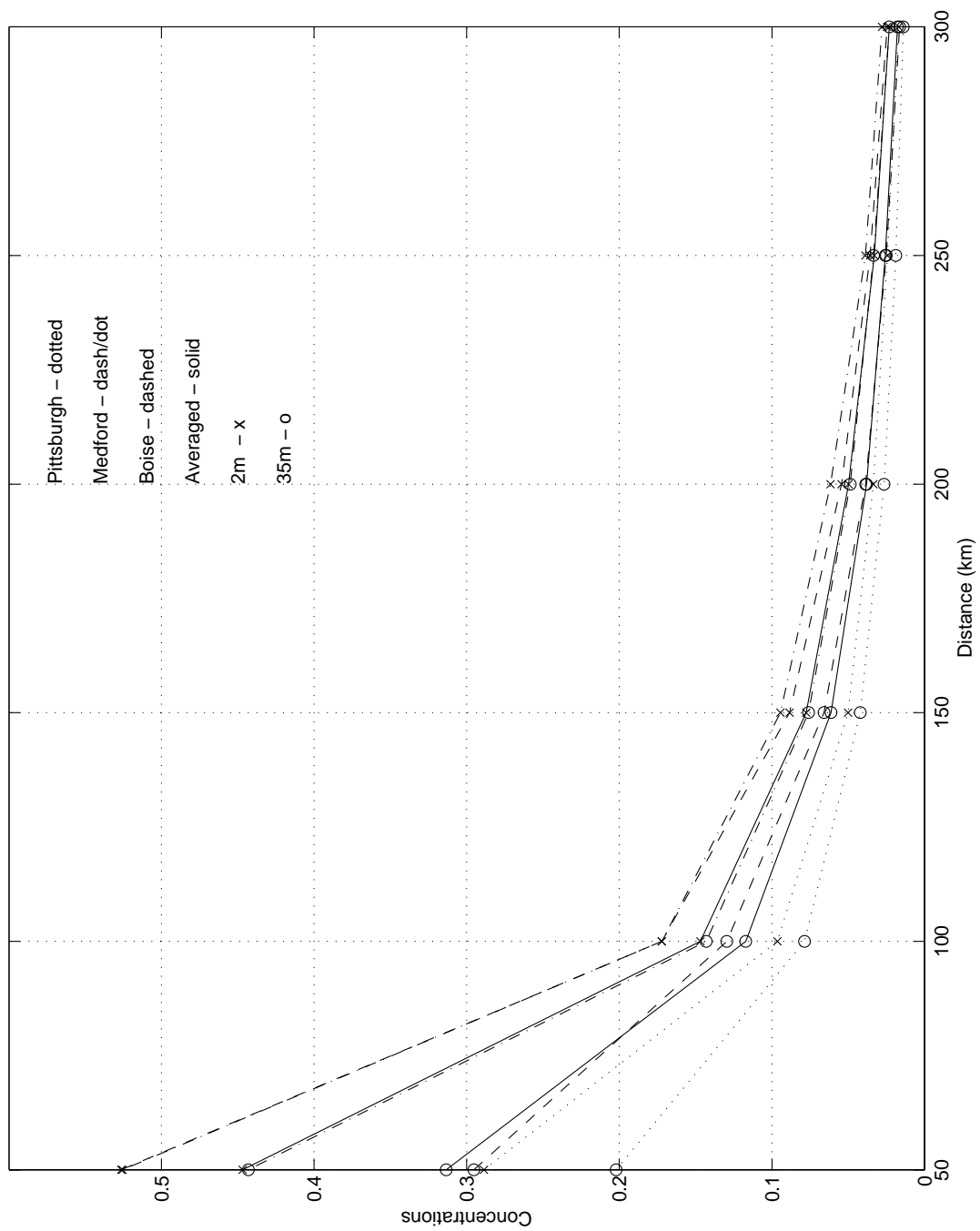
Figure A-1. Annual average CALPUFF concentrations for Pittsburgh, Boise, and Medford
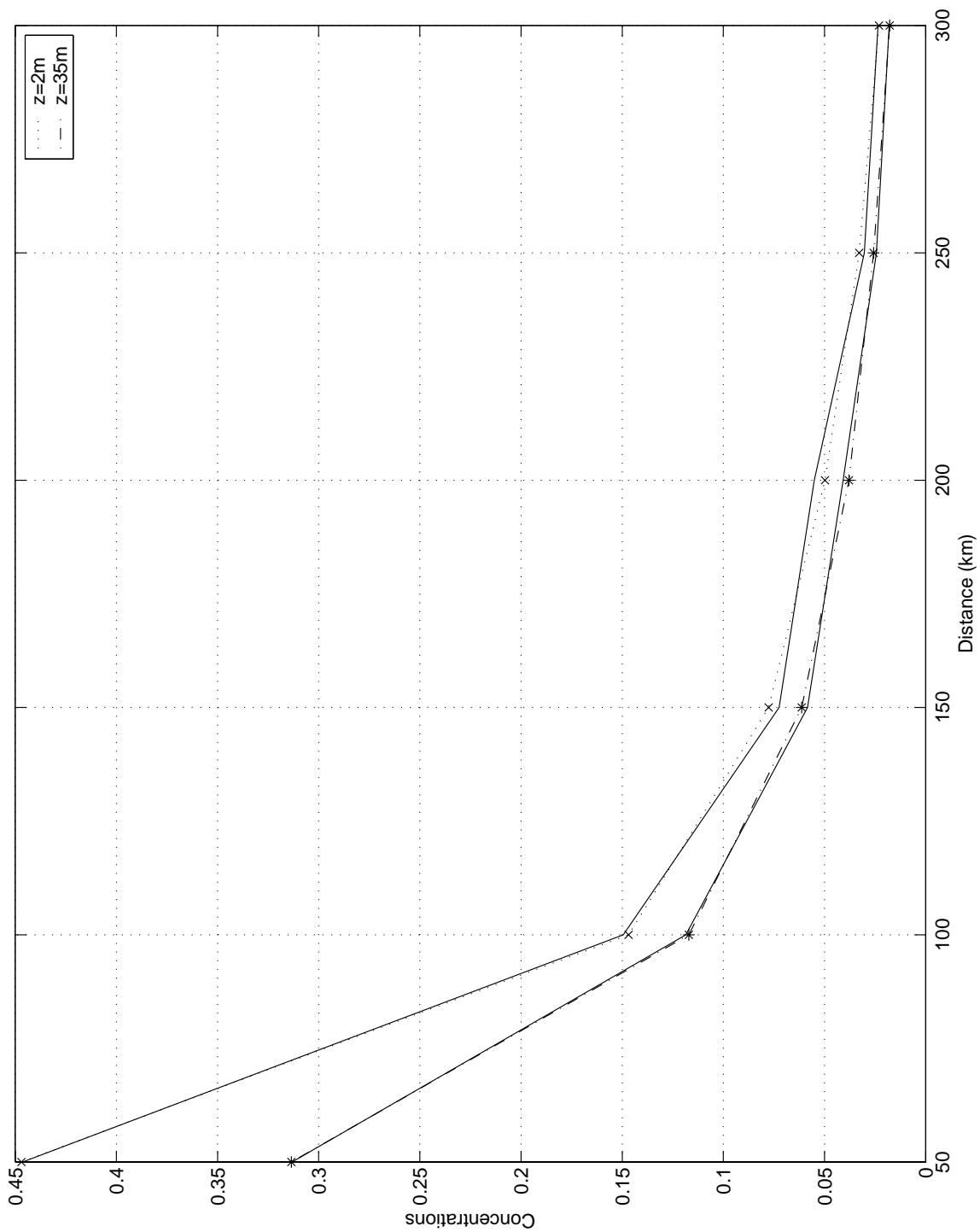
Figure A-2. Average concentration curves averaged among Pittsburg, Medford, and Boise for release heights of 2 and 35 meters.
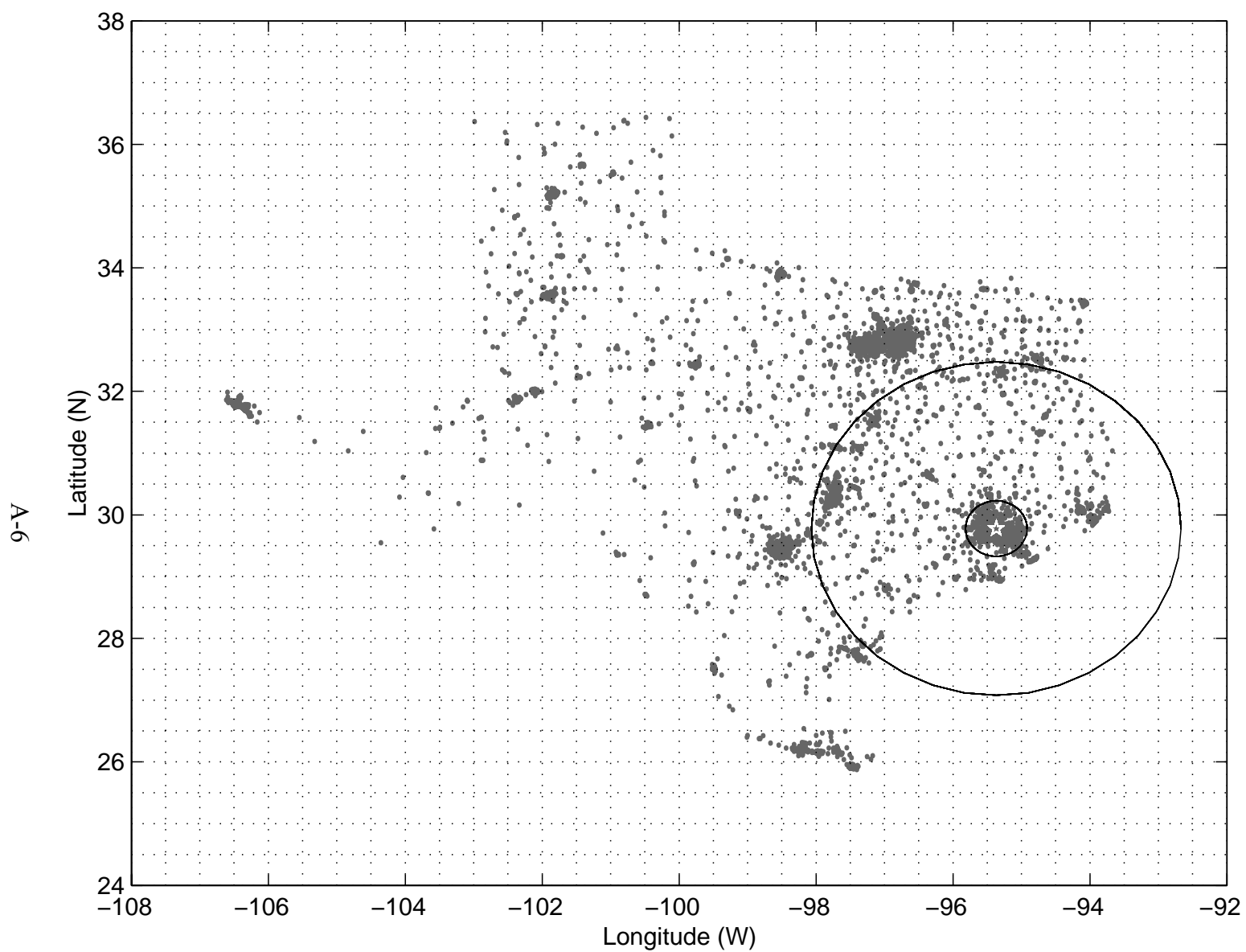
Figure A-3. Census tract centroids (dots) and rings of 50 and 300 km centered over Houston, TX (star) used for calculation of background concentrations.

TECHNICAL REPORT DATA
(Please read Instructions on reverse before completing)

1. REPORT NO. **EPA-454/R-02-003**	2.	3. RECIPIENT'S ACCESSION NO.

4. TITLE AND SUBTITLE **Example Application of Modeling Toxic Air Pollutants in Urban Areas**	5. REPORT DATE **June 2002**
	6. PERFORMING ORGANIZATION CODE

7. AUTHOR(S)	8. PERFORMING ORGANIZATION REPORT NO.

9. PERFORMING ORGANIZATION NAME AND ADDRESS	10. PROGRAM ELEMENT NO.
	11. CONTRACT/GRANT NO.

12. SPONSORING AGENCY NAME AND ADDRESS **U.S. Environmental Protection Agency** **Office of Air Quality Planning and Standards** **Emissions, Monitoring and Analysis Division** **Research Triangle Park, NC 27711**	13. TYPE OF REPORT AND PERIOD COVERED **Final Report**
	14. SPONSORING AGENCY CODE

15. SUPPLEMENTARY NOTES

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16. ABSTRACT

Urban areas contain major sources and numerous smaller area sources and, as a result, air quality modeling analyses posses special challenges. This document deals with the applications of the Industrial Source Complex (ISCST3) model which can estimate close distance impacts from industrial facilities. ISCST3 has been extensively used in analyzing impacts from a single or a few facilities and this document provides a transition to the more complex issues associated with urban-wide applications. This document: 1) provides a demonstration of a methodology for modeling air toxics for use in city-specific analyses and an example application, 2) updates techniques described in Dispersion Modeling of Toxics Pollutants in Urban Areas, EPA-454/R-99-021 and, 3) incorporates techniques described in A Simplified Approach for Estimating Secondary Production of Hazardous Air Pollutants (HAPs) Using the OZIPR Model, EPA-454/R-99-054.

17.	KEY WORDS AND DOCUMENT ANALYSIS	
a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution, Air Quality Dispersion Models, Meteorology, Air Toxics, Urban Area Modeling		

18. DISTRIBUTION STATEMENT	19. SECURITY CLASS *(Report)* **Unclassified**	21. NO. OF PAGES **109**
Release Unlimited	20. SECURITY CLASS *(Page)* **Unclassified**	22. PRICE

EPA Form 2220-1 (Rev. 4-77) **PREVIOUS EDITION IS OBSOLETE**