



Air Dispersion Modeling
Component of the Portland
Air Toxics Assessment
(PATA)

Draft Report

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Prepared for:

Peter Murchie
US EPA
Office of Air Quality Planning and Standards

Prepared by:

Arlene Rosenbaum, Ed Carr, and Jonathan Cohen
ICF Consulting
60 Broadway
San Francisco, CA 94111
(415) 677-7100

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1. Introduction

The 1990 Clean Air Act Amendments provided the foundation for EPA's current air toxics program. This program is designed to characterize, prioritize, and equitably address the serious impact of hazardous air pollutants (HAPs) on the public health and environment through a strategic combination of regulatory approaches, voluntary partnerships, on-going research and assessments, and educational outreach.

One of these assessments, the Portland air Toxics Assessment (PATA), will help EPA and Oregon DEQ (ODEQ) identify areas of concern, characterize risks, and track progress toward meeting air toxics program goals at the State and National levels. The PATA is planned to include several components:

- 1999 emission inventories
- Air monitoring data
- Air dispersion modeling
- Population exposure assessment
- Risk characterization

The PATA is designed to characterize risk, understand source contribution to exposure and risk, and support reduction efforts in Portland, while also providing relevant information for Oregon Department of Environmental Quality (ODEQ) air toxics program development.

This report describes the meteorological and air dispersion modeling portion of PATA. As described below the model selected for this study was CALPUFF. Meteorological inputs were developed with the CALMET model. Another component of PATA, the 1999 emission inventory, was prepared by ODEQ and Portland's Metropolitan Regional Government Organizations (METRO) and provided for input to CALPUFF. Some supplementary emissions data were also taken from the 1996 National Toxics Inventory (NTI) and the 1999 National Emissions Inventory (NEI), as described below. In addition, the results of the air monitoring component were provided by ODEQ for the model performance evaluation.

2. Goals of PATA Air Dispersion Modeling

2.1 Modeling and Monitoring

There are two distinct but complimentary approaches commonly used to assess air quality: ambient monitoring and air dispersion modeling. Ambient monitoring provides direct measurements of airborne pollutant concentrations. Uncertainties of these measurements arise because of measurement errors and limitations in the sampling technology, such as minimum detection levels that may be higher than pollutant concentrations. However, if these uncertainties and limitations are minimized and properly characterized, monitoring results can be considered to represent the best estimate of pollutant concentrations at the locations and during the time periods of sampling.

There may be other important limitations of ambient monitoring results for some uses. For example, because of the expense of monitoring, the number of sampling locations is generally small for most studies. To use the results to characterize population exposure commonly entails invoking simplifying assumptions about the uniformity of pollutant concentrations over large areas. This may be appropriate for some pollutants that typically display small concentration gradients (e.g., ozone); but it is more problematic for most air toxics, which tend to exhibit large spatial variations in concentrations.

Modeling studies provide indirect evidence for exposures, since exposures are calculated and rely on the quality of input data and the validity of modeling assumptions and model formulation. Despite their uncertainties, modeling approaches have several advantages.

- Lower expense. Modeling studies typically provide concentration estimates at a much larger number of locations for a lower budget, than do monitoring studies.
- Temporal flexibility. Modeling can be performed for any past, present, or future year, whereas measurements reflect only current conditions.
- Source attribution. Individual sources and/or source categories can be tracked throughout the modeling process to yield information on the importance of each source or source category to overall concentrations.
- Consideration of hypothetical situations. Modeling can address situations such as impacts of planned facilities, controls on existing facilities, or alternative meteorological conditions.
- Inclusion of more chemical species. Accurate monitoring techniques do not exist for all HAPs at the present time; and the concentrations of some HAPs may be below the minimum detection limits of the sampling technology.

All of these advantages of modeling approaches assume that model results portray actual concentrations with a reasonable degree of accuracy. Thus, model performance evaluation is a key component to any modeling study.

Because of their complementary strengths and weaknesses, monitoring and modeling approaches can usefully be integrated in the design of an air quality study. For this study we used monitoring data, collected by ODEQ from 18 July 1999 to 17 July 2000 at five locations on metropolitan Portland, to evaluate the performance of the model, and thus to estimate the uncertainty of the model predictions.

2.2 Goals

The goals of the air dispersion modeling component of PATA were as follows.

- Estimate air quality concentrations at locations in the Portland metropolitan area without monitors, i.e. provide finer spatial resolution of air quality in Portland than is available from ODEQ's monitoring study
- Use local emissions and meteorological data and more in-depth modeling to provide more accurate and finely resolved model predictions for Portland than those available from US EPA's National Air Toxics Assessment (NATA) national-scale assessment (US EPA 2001), so as to provide better estimates of the spatial patterns of concentrations across the domain and the variation of exposure concentrations across the population
- Evaluate the relative contributions to air pollutant concentrations from different emission sources (onroad mobile, nonroad mobile, major stationary, area) to guide risk reduction strategies

3. Scope of PATA

3.1 Target Pollutants

Twelve air toxic pollutants were selected for air dispersion modeling, based on a review of the 1996 NATA national-scale assessment for the Portland area. These were:

- 1,3-butadiene
- primary acetaldehyde
- primary acrolein
- arsenic
- benzene
- chloroform
- chromium
- diesel particulate matter (diesel PM as PM₁₀)
- primary formaldehyde
- nickel
- polycyclic organic matter (POM as 16-PAH¹)
- tetrachloroethylene

Airborne acetaldehyde, acrolein, and formaldehyde have both primary² and secondary³ components. However, because the accurate estimation of secondary pollutant formation requires a photochemical grid model, it was judged to be beyond the scope of this project as discussed below in section 3.4.1 on alternative models. Therefore, the air dispersion modeling predictions were limited to the primary components only.

3.2 Modeling Time Frame

The health risk information available for the target HAPs relates risk to long-term concentration averages, either annual or lifetime (i.e., 70-year). Therefore, the modeling study was designed to estimate annual average outdoor concentrations. Because outdoor HAP concentrations are known to vary seasonal, due to seasonal patterns of both emissions and meteorology, a full year modeling simulation was selected.

In order to utilize HAP monitoring data collected by ODEQ for model performance evaluation, the time frame for the simulation was collected to coincide with the period during which the most monitoring data was collected: 18 July 1999 – 17 July 2000.

¹ The set of 16 polycyclic aromatic hydrocarbonss (PAHs) are taken from the 1996 NATA national-scale assessment. They are acenaphthene, acenaphthylene, anthracene, benzo(a)anthracene, benzo(a)pyrene, benzo(b)fluoranthene, benzo(ghi)perylene, benzo(k)fluoranthene, chrysene, dibenzo(a,h)anthracene, fluoranthene, fluorene, indeno(1,2,3-cd)pyrene, naphthalene, phenanthrene, and pyrene.

² Primary pollutants are directly emitted into the atmosphere.

³ Secondary pollutants are formed in the atmosphere from the chemical transformation of precursor compounds, which may or may not be hazardous air pollutants themselves.

3.3 Modeling Domain

The Portland metropolitan area is comprised of the urbanized portions of the three Oregon counties Multnomah, Washington, and Clackamas counties. The modeling domain was selected to include the locations of all emissions sources likely to have a large influence on concentrations in this metropolitan area. As a result the urbanized portion of Clark County, across the Columbia River in Washington, was also included in the domain. No other specific areas likely to play an important role in the air quality of the Portland metropolitan area were identified.

The modeling domain is shown in Figure 1. Note that in order to make the domain rectangular and still include the entire metropolitan area of interest it was necessary to include small portions of Columbia and Yamhill Counties as well.

The size of the domain, 60 km by 50 km, is sufficiently small that the flat earth approximation is valid and the UTM coordinate system was used in the assessment. The southwest corner of the domain is located at UTM coordinate 495 Easting and 5015 Northing and the northeast corner at 555 Easting and 5065 Northing (Zone 10), as indicated in Figure 1.

3.4 Model Selection

The extent to which a specific air dispersion model is suitable for the evaluation of air toxic source impacts depends upon several factors, such as the nature of the pollutant (e.g., gaseous, particulate, reactive, inert), the meteorological and topographic complexities of the area, the complexity of the source distribution, the spatial scale and resolution required for the analysis, and the level of detail and accuracy required for the analysis. For example, steady-state Gaussian plume models are not considered appropriate for downwind distances outside of the 0.1 km to 50 km range. Because of the assumption in Gaussian models of a steady wind speed and direction over the entire modeling domain for each hour, the 50 km distance may be inappropriately long in many areas, especially where complex terrain or meteorology is present.

3.4.1 Alternative Models

3.4.1.1 Industrial Source Complex (ISC) model and AERMOD

The most commonly used model for air quality modeling is the US EPA's Industrial Source Complex model, now in its third version (ISC3). The ISC3 model is a steady-state Gaussian plume model, which can be used to assess primary pollutant concentrations and depositions from a wide variety of sources. It may be applied in urban or rural areas, and has optional features to account for settling and dry deposition of particles, reactive decay, and limited terrain elevations. US EPA has proposed a more advanced steady-state Gaussian plume replacement model, AEROMOD, to provide improved accuracy compared to ISC3. However, in its current form AEROMOD does not include wet deposition, so it would not be appropriate for environmental exposure assessment of

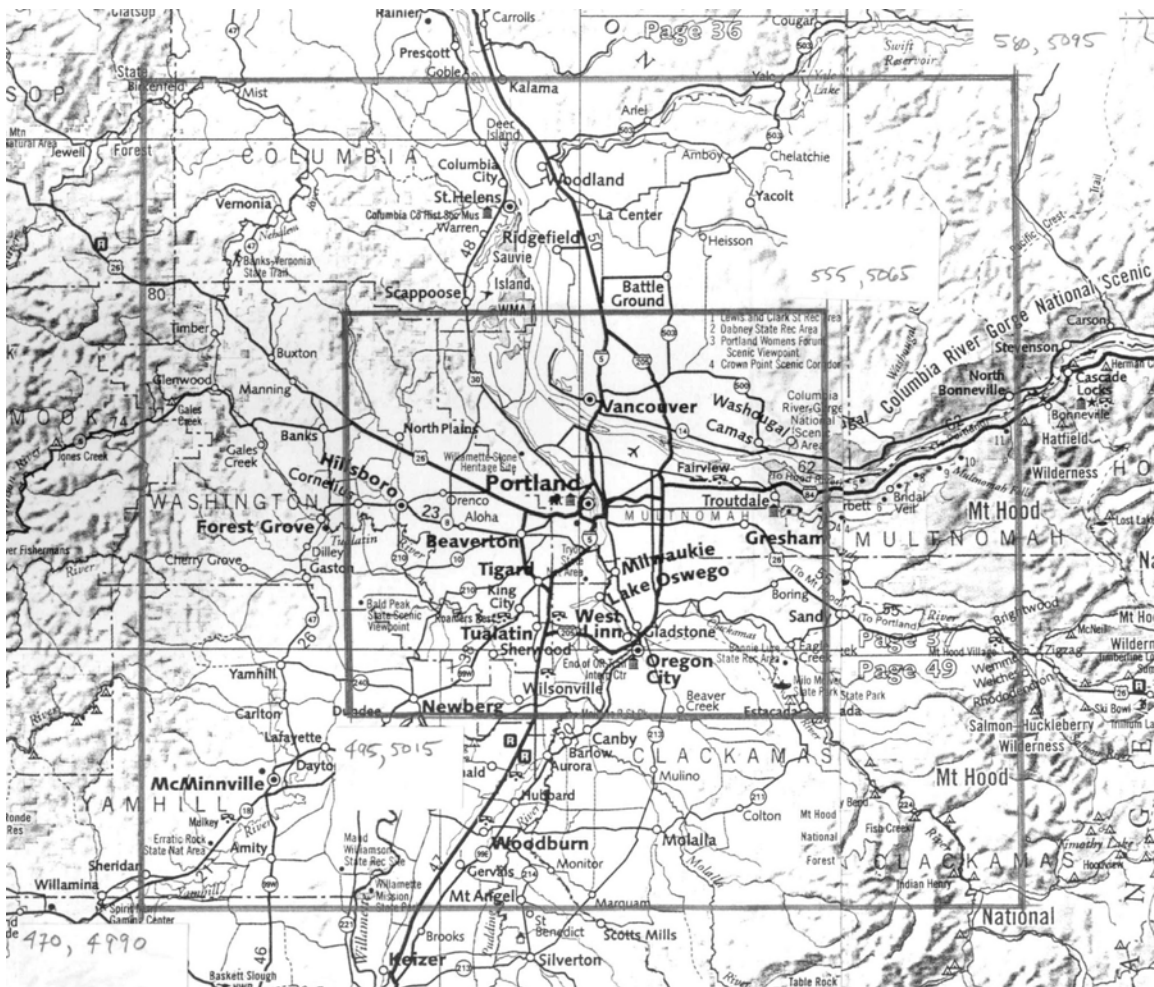


Figure 1. Portland Air Toxics Assessment (PATA) modeling domain.
(inner rectangle)

pollutants subject to deposition (e.g., particulate-bound air toxics, such as chromium, arsenic, and nickel). Also ISC3, AEROMOD and similar models only have very limited capability for treating chemical transformation, so would be unsuitable for estimating secondary formation of the pollutants such as formaldehyde, acetaldehyde, and acrolein. Additionally, because of the Gaussian plume model formulation these models can only consider wind data from a single location and they cannot directly simulate near stagnation conditions (i.e., very low wind speeds). These important limitations make ISC3 unsuitable for the Portland Area, with its complex wind patterns.

3.4.1.2. Assessment System for Population Exposure Nationwide (ASPEN)
US EPA and others have developed other air dispersion models, not included in the Guideline, for a variety of purposes. The Assessment System for Population Exposure Nationwide (ASPEN) was developed for the inhalation component of US EPA's

Cumulative Exposure Project (CEP; Rosenbaum et al.1999), and was recently used by the Office of Air Quality Planning and Standards (OAQPS) for the NATA national-scale assessment. ASPEN includes an air dispersion module similar to the long-term average version of ISC, i.e., ISCLT2. It includes treatment of wet and dry deposition for particles, and more detailed treatment of chemical transformation than ISC, although less detailed than UAM-Tox (see below). The concentration estimates from ASPEN are designed to represent population-weighted averages over a size scale of one to several square kilometers (i.e., middle-scale to neighborhood-scale), which is slightly larger than the desired spatial goal for this study. In contrast to ISC, ASPEN can utilize meteorological information from several locations, and includes a simplified treatment of secondary formation of gaseous air toxics. It was designed to efficiently simulate the dispersion of emissions for an unlimited number of pollutant/source combinations. It however lacks the capability to fully incorporate 3-dimensional wind fields. Thus wind fetches from the point of emission release are assumed to be straight lines, regardless of the patterns at downwind locations; and wind patterns in upper layers are derived from surface patterns based on atmospheric stability and land use (i.e., urban or rural), rather than being independently estimated. Given the significant terrain features and the likely disparate wind patterns among several monitoring stations (e.g., Troutdale versus Hillsboro) suggest that ASPEN's assumption of straight wind fetches will be inadequate for Portland.

3.4.1.3 Urban Airshed Model for Toxics (UAM-Tox)⁴

The UAM-Tox is an enhanced version EPA's UAM model. It is a three-dimensional grid model designed to simulate all-important physical and chemical processes that occur in the atmosphere. The model incorporates mathematical representations of the processes of transport, diffusion, chemical reaction and deposition. Based upon inputs of emissions, 3-dimensional wind fields, mixing heights, initial concentration and boundary conditions the model computes concentrations for each species for each grid cell for each hour of simulation. UAM-Tox incorporates explicit chemical reactions for key photochemically active pollutants, such as 1,3-butadiene, formaldehyde, and acetaldehyde, and tracks primary and secondary fractions separately. UAM-Tox has been used in other air toxic studies, such as the Southern California MATES-II study and a USEPA study of reformulated gasoline in Baltimore and Houston.

However, because UAM-Tox is a grid model, all emissions are characterized as being spread uniformly over a 3-dimensional grid cell. This characterization may result in a significant loss of spatial resolution information for the primary pollutants included in this study, and the maximum concentration may be significantly underestimated. Given the goals of improving the spatial resolution for onroad mobile sources, a grid model would not be appropriate for estimating concentrations of primary pollutants.

However this model would be useful for estimating concentrations of secondary pollutants, if a suitable emission inventory were available. Development of an emissions

⁴ UAM-Tox is available to the public on request from ICF Consulting, on condition that the source code not be modified.

inventory is particularly resource intensive, since the non-linear chemistry requires estimation of the many precursor compounds, as well as other compounds that influence the non-linear atmospheric chemistry that leads to formation of formaldehyde, acetaldehyde, and acrolein.

3.4.1.4 CALPUFF

While not currently a guideline model, CALPUFF is in the process of being proposed by US EPA as a guideline model for long-range transport of primary pollutants and for sulfates and nitrates. The model is a multi-layer, multi-species non-steady-state Gaussian puff dispersion model. CALPUFF is designed to be applied on scales of tens of meters to tens of kilometers (near-field) and from tens of kilometers to hundreds of kilometers (far-field). It includes algorithms for sub-grid scale effects, such as terrain impingement, as well as, longer range effects, such as pollutant removal due to wet scavenging, dry deposition, and reactive decay. CALPUFF can handle various types of emission source characterization, such as points and area. Like UAM, the model accounts for spatially varying meteorological conditions with a three-dimensional wind field. However, it does not include treatment of secondary formation.

3.4.2 Selection of CALPUFF

Due to their inability to treat complex wind patterns, ISC, AERMOD, and ASPEN were judged to be unsuitable for application to the Portland area.

UAM-Tox and CALPUFF are each able to simulate Portland's complex wind patterns with 3-dimensional wind fields. UAM-Tox is also able to simulate secondary formation (unlike CALPUFF), but lacks CALPUFF's ability to provide fine spatial resolution of air quality predictions, and requires an emission inventory of precursor compounds that was not available at the time of this study. CALPUFF also has somewhat lower resource requirements and is easier to operate.

Based on these considerations, CALPUFF was selected as the air dispersion model for this study. This selection precluded the estimation of secondary components of formaldehyde, acetaldehyde, and acrolein.

4. Application of CALPUFF

Application of the CALPUFF model requires 3 types of input data:

- Geophysical data
- Emissions
- Meteorology

The development of these inputs is described in this section, as well as the choice of modeling options and receptor locations.

4.1 CALPUFF Modeling Options

The CALPUFF modeling options specify variables and algorithms for representing physical processes that are important for accurate predictions of air concentrations. The options for this study were selected to maximize performance in predicting long term average concentrations at the spatial scales of the PATA study.

The key modeling options used in this study were:

- Gaussian vertical distribution in the near-field;
- Buoyancy induced dispersion;
- Vertical wind shear modeled above stack top;
- Use of similarity theory to determine crosswind and vertical components of turbulence (dispersion option 2);
- Near-field puffs modeled as elongated slugs;
- Puff splitting allowed i.e., if puffs stay within the modeling domain after being initially split they will be allowed to be split again at 5:00 pm local time before nocturnal shear develops;
- Transitional plume-rise modeled, stack-tip downwash included;
- No building wake effects;
- Partial plume penetration;
- Plume path coefficient terrain adjustment;
- No subgrid-scale terrain adjustment;

-
- First-order reactive decay rates assigned to 1,3-butadiene (half-life 3 hours⁵), primary formaldehyde (half-life 12 hours⁶), primary acetaldehyde (half-life 15 hours⁷), and primary acrolein (half-life 12 hour⁸); all other pollutants characterized as inert;
 - Wet and dry deposition applied to the particulate pollutants - chromium, nickel, arsenic, POM, and diesel PM⁹; and
 - Minimum wind speed (m/s) for non-calm conditions of 0.5 m/s.

Another important feature of the air dispersion simulations for this study was the separate modeling of each aggregate emission source category (i.e., major stationary, area, onroad mobile, nonroad mobile, and special nonroad mobile¹⁰, as discussed below), following the approach taken in the 1996 NATA national-scale assessment¹¹. This approach permits analysis of the separate contributions of each category to total ambient concentration predictions; this information will facilitate design of risk reduction strategies.

4.2 Model Receptors

As noted above, one of the goals of PATA is to provide more finely resolved model predictions for Portland than those available from US EPA's NATA national-scale assessment, so as to provide better estimates of the spatial patterns of concentrations across the domain and the variation of exposure concentrations across the population. The NATA national-scale assessment predictions are representative of US Census tract average concentrations.

This study used a total of 943 modeling receptors. For the portion of the modeling domain of primary interest (i.e., the portions of Multnomah, Clackamas, and Washington Counties that fall within the modeling domain), the receptors were located at the 877 US Census block group centroids. In order to shorten model run times, however, receptors for the remainder of the modeling domain were located at the 61 US Census tract centroids for the portions of Yamhill, Columbia, and Clark (WA) Counties that fall within the modeling domain. Figure 2 shows the block group and tract boundaries.

⁵ Based on reaction with hydroxyl radicals at a concentration of 8×10^{-5} molecules/cm³ (Howard, 1989).

⁶ Based on the average of sunlight photolysis rate and reaction rate with hydroxyl radicals in clean air (Howard, 1989).

⁷ Based on reaction with hydroxyl radicals (CARB, 2001).

⁸ Based on reaction with hydroxyl radicals (Howard, 1989).

⁹ For some emission sources and source categories particle size distributions (i.e., PM_{2.5} and PM₁₀) were provided by ODEQ. Where this information was absent default assumptions from the NATA national-scale assessment were used. These specify fine and coarse fractions by pollutant and aggregate source category (point, area, onroad mobile, and nonroad mobile).

¹⁰ Special nonroad emission sources include commercial marine vehicles (CMV), recreational marine vehicles (RMV), railroads, and airports.

¹¹ In the 1996 NATA national-scale assessment the nonroad mobile aggregate category included all the sources that comprise PATA's nonroad mobile and special nonroad mobile categories, so that there are only 4 aggregate source categories in the NATA study.

In addition, a receptor was located at each of the five monitoring locations to facilitate comparison of model-to-monitor comparisons for the model performance evaluation.

Receptor elevations were interpolated from the terrain information file described below.

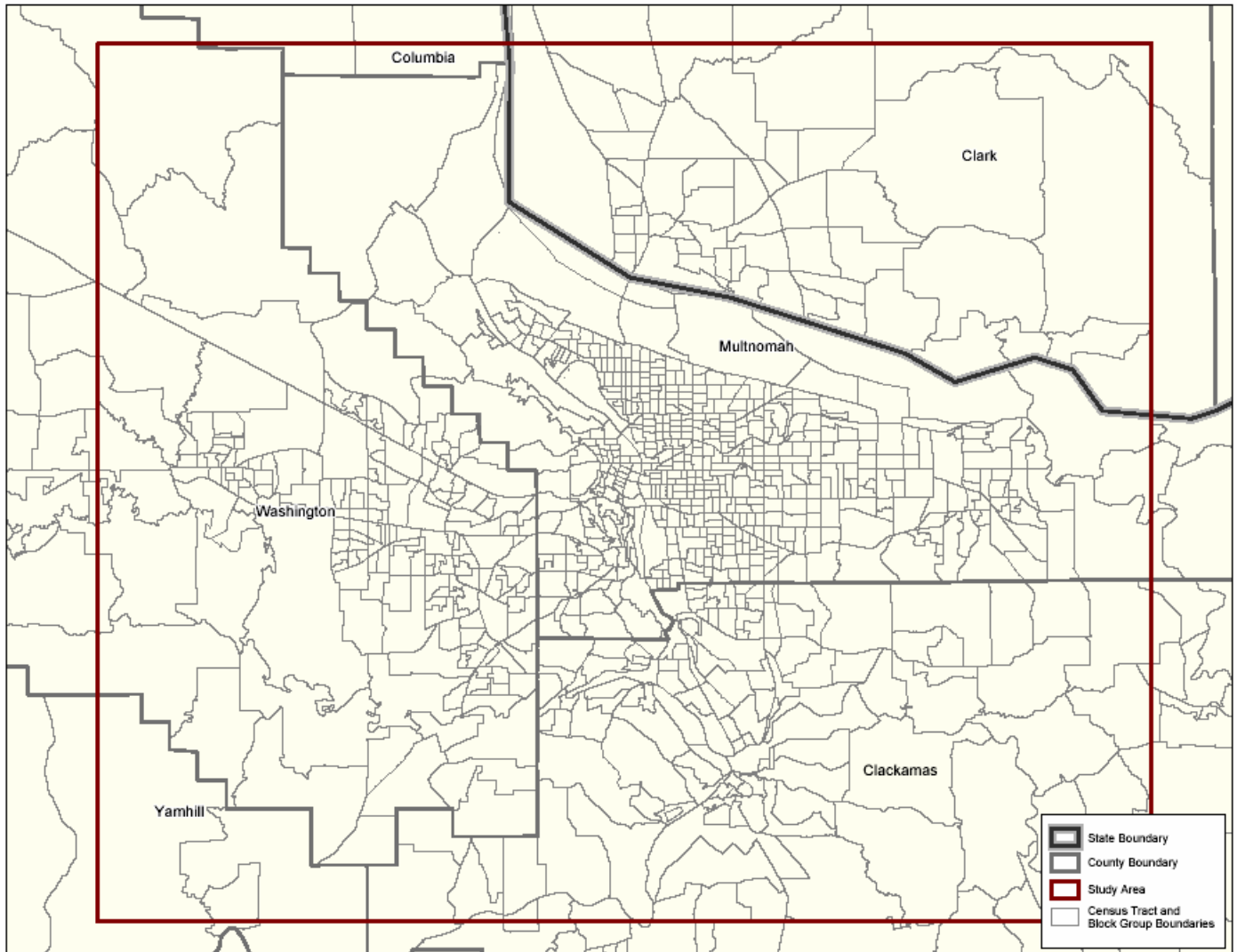


Figure 2. US Census block group boundaries (Multnomah, Clackamas, and Washington Counties) and tract boundaries (Yamhill, Columbia, and Clark [WA] Counties) within the PATA modeling domain.

4.3 Geophysical Data

4.3.1 Land Use

The U.S. Geological Survey (USGS), in cooperation with the U.S. Environmental Protection Agency, has produced an updated land cover dataset for the conterminous United States on the basis of 1992 Landsat thematic mapper imagery and supplemental data. The National Land Cover Dataset (NLCD; July 2000) is a component of the USGS Land Cover Characterization Program. The NLCD contains 21 categories of land cover information gridded at 30-meter resolution. These data were used in preparing the land-use for the PATA domain, and deriving the spatial patterns of other variables required for developing meteorological data, as well as deposition velocities.

4.3.2 Terrain Elevations

The terrain elevation inputs to CALPUFF were derived from the USGS digital elevation model (DEM) with 90-meter horizontal resolution.

4.4 Emissions

4.4.1 Data Sources

ODEQ provided 1999 county total emissions by source classification code (SCC) for area and nonroad mobile emissions for Multnomah, Washington, and Clackamas counties. Data for these sources included temporal patterns if available. ODEQ also provided the major stationary emission source estimates for these counties. These included actual or estimated stack parameters (i.e., release height, release velocity, release temperature), as well as seasonal and diurnal adjustments. In addition, ODEQ provide data on the exact locations of 170 dry cleaners so that they could be modeled at point sources rather than area sources.

Area, nonroad mobile, and major stationary source emissions for Columbia, Yamhill, and Clark (WA) counties were taken from the 1999 NEI prepared by US EPA.

Portland's Metropolitan Regional Government Organization (METRO) provided on-road emission estimates for Multnomah, Washington, and Clackamas counties, as well as Clark County (WA), developed using the EMME/2 travel demand model and US EPA's MOBILE6.2 emission factor model (METRO 2002). These included annual emission rates by roadway link for freeway and primary arterials, and by traffic analysis zone for secondary roads. METRO also provided temporal profiles.

Onroad emissions for the small portions of Columbia and Yamhill counties that fall in the modeling domain were taken from US EPA's 1996 NTI, because this portion of the 1999 NEI was not yet released at the time of this study. These included annual emission rates for gasoline and diesel fueled vehicles, by county.

Table 1 summarizes the agency or database providing emissions estimates for each county and emission source type. The processing of these data for model input is discussed below.

Table 1. Data sources for 1999 PATA emissions estimates, by county and emission source category .

COUNTY	On-Road Mobile	Non-Road Mobile	Major Stationary Sources	Area Sources
Multnomah	METRO	ODEQ	ODEQ	ODEQ
Clackamas	METRO	ODEQ	ODEQ	ODEQ
Washington	METRO	ODEQ	ODEQ	ODEQ
Columbia	1996 NTI	1999 NEI	1999 NEI	1999 NEI
Yamhill	1996 NTI	1999 NEI	1999 NEI	1999 NEI
Clark (WA)	METRO	1999 NEI	1999 NEI	1999 NEI

4.4.2 Spatial Resolution of Area and Nonroad Emissions

In order to provide sufficient spatial resolution in emissions to support the block group resolution of the model receptors in Multnomah, Clackamas, and Washington Counties, all area and nonroad emissions, other than marine vessels, railway yards, and aircraft were allocated to 1-km by 1-km grid cells in the inner portion of the domain. The inner fine-resolution portion of the domain has a southwest corner at UTM coordinate 511 Easting and 5031 Northing, and northeast corner of 537 km Easting and 5051 km Northing.

In the remainder of the modeling domain these emission categories were allocated to 2-km by 2-km grid cells.

Commercial marine vessel (CMV) emissions were allocated to 59 special polygons developed to represent shipping routes along the Columbia and Willamette Rivers designated by ODEQ, as described below. Recreational marine vessels (RMV) were similarly allocated to 118 special polygons (including the 59 CMV polygons) developed to represent the areas of recreational boating designated by ODEQ.

Railway yards and airports were allocated to special polygons developed to represent the actual locations and extent of the facilities, as described below.

As explained above Portland's METRO provided onroad mobile emissions for Multnomah, Clackamas, Washington, Clark (WA) Counties. Emissions from freeways and primary arterials were provided for each of 1,095 two-way roadway links. These links were represented with special polygons. Emissions for secondary roadways were reported by traffic analysis zone. The boundaries of these zones were used to specify 1,194 special polygons.

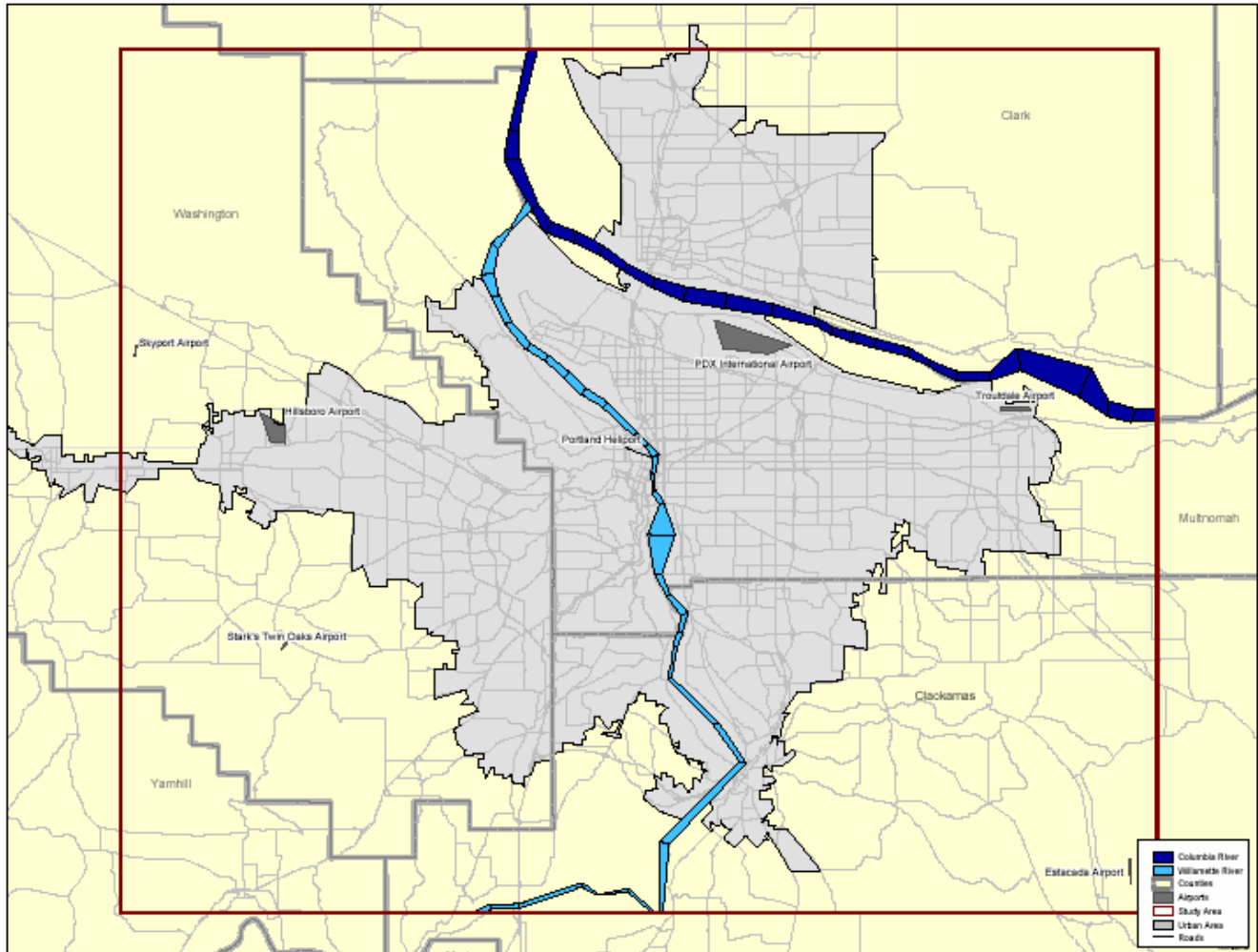


Figure 3. Special polygons developed to represent locations of emissions from commercial marine vessels, recreational marine vessels, and airports.

Onroad mobile source emissions in the small parts of Yamhill and Columbia Counties that fall within the modeling domain were allocated to the same grid cells as the area sources.

4.4.3 Emission Processing

4.4.3.1 Major Stationary Sources

Emissions data for the 102 major stationary sources received from ODEQ and taken from the 1999 NEI required no special processing for input to CALPUFF, except for formatting. Figure 4 shows the locations of the major stationary sources of benzene.

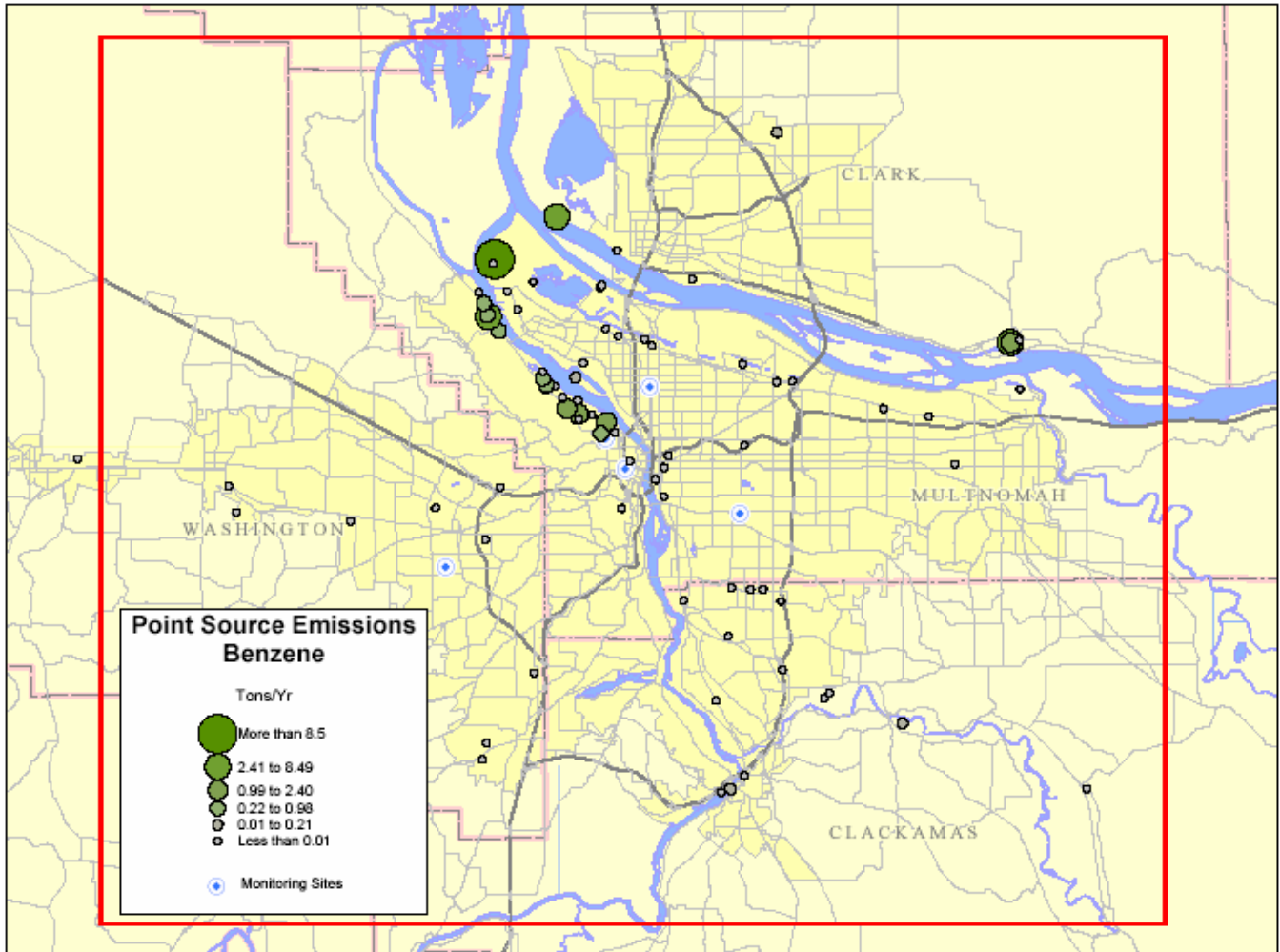


Figure 4. Locations and magnitudes of benzene emissions from major stationary sources.

4.4.3.2 Dry Cleaners

Although dry cleaner emissions are typically characterized as area sources in modeling studies, ODEQ was able to provide location parameters for the 170 individual dry cleaning establishments in the modeling domain so that they could be characterized as point sources. Each was modeled as a volume source with effective release height of 1.5-m, an initial sigma-y of 2.2-m, and initial sigma-z of 1.4-m. These values were derived based on the assumption of fugitive emissions (non-stack) from a one-story building of 1,000 sq feet.

4.4.3.3 Area Sources

Area source emissions were spatially allocated from county total to model grid cells using spatial surrogates based on land use and population, following the methods applied

in the 1996 NATA national-scale assessment. First, each SCC was assigned to a spatial surrogate. For example, industrial fuel combustion SCCs were assigned to industrial land use, and solvent utilization from consumer products was assigned to population. Then the emissions for the SCC were distributed among the county's grid cells in the same proportions as the corresponding surrogate.

Residential population patterns were derived from the 2000 US Census. Land use patterns were derived from the 21 categories in the USGS National Landcover Dataset described above. However, this dataset aggregates several land use categories that were reported separately in the 1990 USGS *Landuse and Landcover* data used for the 1996 NATA national-scale assessment. For example, commercial, industrial, and transportation landuses are combined into a single category in the 2000 dataset, but comprise all or part of 6 different landuse categories in the 1990 dataset. Therefore, in order to maintain the level of detail in spatial allocation used in the NATA national-scale assessment, we subdivided the 2000 commercial-industrial-transportation category into three separate land use categories on the basis of the 1990 dataset proportions.

For area sources each model grid cell was modeled as an area source with an effective emission height of 5.0-m and an initial sigma-z of 2.32-m. These values were derived based on the assumption of a typical vertical dimension of a buoyant release associated with residential combustion of wood from a one-story building, one of the more important area sources in Portland.

4.4.3.4 Nonroad Mobile Sources: Commercial and Recreational Marine Vessels

Emissions from commercial marine vessels (CMV) and recreation marine vessels (RMV) were spatially allocated to polygons representing shipping and boating routes on the Columbia and Willamette Rivers as described above.

The CMV emissions were temporally allocated according to patterns provided by ODEQ based on actual shipping records. RMV emissions were also temporally allocated according to patterns provided by ODEQ.

Both types of emissions were modeled as area source with an effective emission height of 0.0-m and initial sigma-z of 1.5-m.

4.4.3.5 Nonroad Mobile Sources: Railroads

Railroad line-haul emissions were spatially allocated to model grid cells according to railroad miles derived from the US Census Topologically Integrated Geographic Encoding and Referencing (TIGER®/Line) files. Railroad yard emissions were allocated to 10 specific locations as designated by ODEQ. Both these types of emissions were modeled as area sources

4.4.3.6 Nonroad Mobile Sources: Aircraft

Aircraft emissions were spatially allocated to the locations of the seven airports within the modeling domain, and temporally allocated according to profiles provided by ODEQ based on landing and takeoff records.

Each airport was modeled as a volume source with the initial sigma-y based on the size of airport. Except for commercial aircraft at Portland International (PDX), all emissions were modeled with an effective release height of 1.5-m and an initial sigma-z set at 2.32-m, based on a typical wingspan for general aviation aircraft of 10-m.

PDX commercial aircraft emissions were modeled in three operating modes - taxi, takeoff, and climb out/approach - with appropriate values for initial sigma-y, sigma-z and release height to reflect the mode and size of larger aircraft with average wingspan of 50-m and tail height of 15-m.

4.4.3.7 Nonroad Mobile Sources: Construction Equipment

ODEQ estimated county total construction equipment emissions with US EPA's NONROAD model. The NONROAD model allocates emissions from construction equipment to counties based on expenditures for construction activity in each county. To maintain consistency for this study, construction equipment emissions were similarly spatially allocated from modeling domain totals to model grid cells according to spatial and temporal surrogates of estimated expenditures on construction equipment activity for buildings and roadways.

Building construction expenditures by date, location, and structure type were provided by METRO in a database of building permits from throughout the modeling domain. It was assumed that 20% of building construction cost was associated with diesel equipment activity, primarily for site preparation. Building construction expenditures derived from building permits do not include the costs of installing associated utilities and private roads, however, although these activities typically rely heavily on diesel equipment. Therefore, an additional 25% of building costs for residences were attributed to diesel activity, and an additional 15% of building costs for other types of buildings.

State, county and local transportation agencies provided data about their expenditures on road construction and maintenance during the modeling period. All expenditures for roadway construction and maintenance were attributed to diesel equipment activity.

These same data were also used to temporally allocate the emissions to seasons: Dec-Feb, Mar-May, Jun-Aug, Sep-Nov.

Once the construction equipment emissions were allocated to grid cells, each grid cell was modeled as an area source with an effective release height of 2.0-m and an initial sigma-z of 2.32-m.

4.4.3.8 Other Nonroad Mobile Sources

All other nonroad mobile source categories were spatially allocated from county totals to the grid cells using surrogates of land use and population following the method used in the 1996 NATA national-scale assessment, as described in 4.1.2.3, and modeled as area sources with an effective release height of 2.0-m and an initial sigma-z of 2.32-m.

4.4.3.9 Onroad Mobile Sources

As explained above onroad mobile source emissions for Multnomah, Clackamas, Washington, and Clark (WA) Counties were allocated to either special polygons developed to represent roadway links (freeways and primary arterials) or traffic analysis zones (TAZs; secondary and local roadways). The spatial allocations were provided by METRO from their travel demand model, EMME/2. METRO also provided a temporal profile.

Onroad mobile source emissions for Yamhill and Columbia Counties were allocated to the same grid cells as the area sources. The spatial surrogates were adapted from the NATA national-scale assessment, and consisted of a combination of roadway miles and population. The same temporal profile provided by METRO for the other 4 counties was used for these as well.

All onroad mobile emissions were modeled as area sources with an effective release height of 2.0-m, and an initial sigma-z of 2.32-m to account for buoyant plume rise and turbulent mixing from the vehicle wake.

Figure 5 shows the spatial pattern of benzene emissions from onroad emission sources.

4.5 **Meteorology**

Given the model options selected for CALPUFF, the following types of hourly meteorological information are required.

- 3-dimensional wind fields
- 3-dimensional temperature fields
- 2-dimensional mixing heights fields
- 2-dimensional Pasquill-Gifford-Turner stability class fields (optional)
- 2-dimensional surface friction velocity fields
- 2-dimensional convective velocity scale fields
- 2-dimensional Monin-Obkhov scaling length fields
- 2-dimensional precipitation rate fields

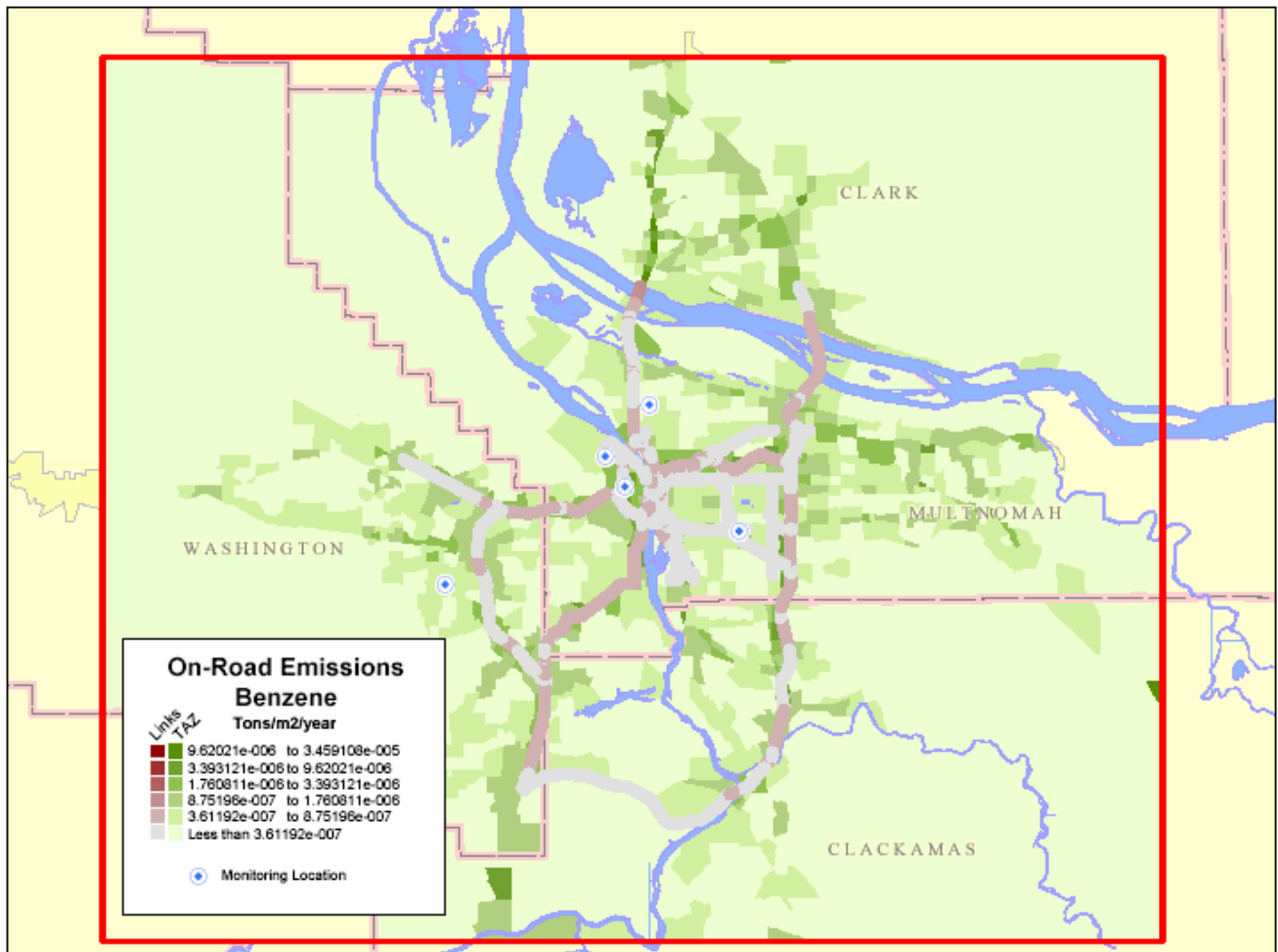


Figure 5. Spatial patterns of benzene emissions from onroad mobile sources.

In addition, CALPUFF requires information on temperature, air density, solar radiation, relative humidity and precipitation at a random set of locations throughout the modeling domain¹². For these variables CALPUFF assigns each grid cell the values at the nearest location with such specifications.

The meteorological modeling approach selected for this study was the CALMET model (Version 5; EarthTech, 2000). CALMET includes a diagnostic wind field generator containing an objective analysis and parameterization treatments of slope flows,

¹² Although gridded versions of some of these variables (e.g., temperature, precipitation) were also provided to CALPUFF by CALMET, requirements for these gridded inputs depend on the CALPUFF options selected. But CALPUFF always requires these data at the more sparse set of locations in the modeling domain.

kinematic terrain effects, terrain blocking effects and a divergence minimization procedure, and a micrometeorological model for overland and overwater boundary layers.

A 3-dimensional prognostic model was also considered. However, the level of improvement over a diagnostic approach at high spatial resolution (1-km) was considered minimal, given (1) the significant amount of meteorological data available, and (2) the fact that most of the emissions of interest are released at or near the surface.

4.5.1 Meteorological Monitoring Data

4.5.1.1 Surface Data

Six surface meteorological monitoring sites provided data for this study. Three were located at airports - Hillsborough, Troutdale and Portland International Airport. Variables reported from the airport stations include hourly wind speed, wind direction, temperature, dewpoint temperature (from which relative humidity can be determined), rainfall, surface pressure, cloud cover and ceiling height. Three ODEQ sites that also provided meteorological data are: SE Lafayette, Sauvie Island, and Carus. The ODEQ meteorological data include hourly wind speed, wind direction, and standard deviation of the horizontal wind direction (sigma-theta). These data were used as input to the CALMET model as part of the objective analysis procedure following the diagnostic analysis.

The Jefferson High School monitoring data was not included because historical data were not available for that site.

A US Department of Energy meteorological site located at NE 45th and Highway 99 in Vancouver, WA was also considered. However, because significant data gaps were found in the historical records, and because the site only archived the scalar wind speed and direction, these data were not used.

Data from the Portland State University's sponsored meteorological monitoring program were reviewed for possible use in this analysis. In all cases, the stations showed frequent and broad data gaps in the monitoring record, and there were non-uniform periods of data recording. Because of the additional effort that would be required to process these data and their expected limited contribution to the analysis, it was decided not to include them.

4.5.1.2 Upper Air data

The upper-air data as measured in Salem, Oregon during the simulation period were used in the CALMET analysis. The variables included of wind direction, wind speed, temperature, pressure, and geopotential height, which are required by CALMET to develop 3-dimensional wind and temperature fields, as well as the spatially-varying mixing height.

The KPTV tower located in the West Hills was also considered for use in the upper-air analysis, but since the tower only measured temperature at three fixed heights, and did not measure air pressure, the data set was not adequate for specifying a sounding profile.

4.5.2 CALMET Modeling Options

The diagnostic wind module contained within the CALMET system was used for this study. The module uses the information on terrain and atmospheric stability to parameterize treatments of slope flows, kinematic terrain effects and terrain blocking effects. Following the diagnostic analysis an objective analysis procedure using the observations is used to estimate meteorological fields. Finally, the divergence minimization procedure is applied to conserve mass.

The grid resolution was chosen at 500-m so as to simulate the larger-scale microscale flows (on the order of 1-2 km). Nine vertical layers were specified for the vertical distribution of winds and temperature. The vertical layer structure was defined as: 0-20 m, 20-40 m, 40-80 m, 80-160 m, 160-320 m, 320-650 m, 650-1000 m, 1000-2000 m, 2000-3000 m. This structure balances the computational and space resources of the model within the needed resolution of the wind profile.

Other important wind field modeling options used in the analysis include:

- The O'Brien scheme to minimize the loss of mass through the top of the model.
- Similarity theory to vertically extend the use of hourly surface data within the mixed layer.
- A maximum radius of influence over land within the surface layer of 50 km.
- A maximum radius of influence over land within the upper layers of 50 km.
- A minimum radius of influence within the surface layer of 0.1 km.
- A radius of influence of terrain of 2.0 km.
- Where no stations are found within the maximum radius of influence, use of the closest station.
- Relative weighting of the first guess field and observations in the surface and aloft layers set at 10 and 50 km.
- No barriers used in wind field development.
- Mixing heights spatially averaged using an upwind looking cone.

-
- Minimum and maximum mixing heights of 50 and 2500-m, respectively.

Other modeling options were set to CALMET default values.

5. Modeling Results

5.1 Background Concentrations

To accurately estimate outdoor ambient concentrations, it is necessary to account for contributions to ambient concentrations from sources not addressed by the CALPUFF simulations. These include natural sources, historical emissions (i.e., material released into the environment before the simulation period but still present), and/or transported emissions from outside the modeling domain.

The background concentrations used for this study were taken from the 1996 NATA-NSA. Except for diesel PM, background concentrations are based on values reported in the technical literature for 13 air toxic pollutants; for the rest, EPA assumed a value of zero. In the NATA national-scale assessment these values were applied uniformly throughout the country. The same approach was followed for this study. Table 2 presents the non-zero background concentrations used in this study.

For diesel PM, instead of using monitored air quality data to estimate background concentrations, a modeling-based approach was used to provide a rough approximation of concentrations due to transport from sources located between 50 km and 300 km from the receptors. Consequently, the diesel PM background concentration estimates vary across the country. For this study the 1996 NATA national-scale assessment estimate of background diesel PM for census tracts in the PATA modeling domain were adopted.

Table 2. Background air toxic concentrations
(Source: US EPA, 2001)

Pollutant	Annual Average ($\mu\text{g}/\text{m}^3$)
Benzene	0.48
Formaldehyde	0.25
Chloroform	0.083
Tetrachloroethylene	0.14
Diesel PM	0.24 – 0.42 (varies by location in domain)

5.2 Types of Concentration Prediction Summaries

In this section we review the PATA ambient concentration predictions from the CALPUFF modeling. Unless otherwise noted all the results presented are for annual average concentrations.

Several types of summaries are provided for each of the target HAPs in Appendix A.

5.2.1 Range of Concentration Predictions

First, boxplots are presented to show the range of concentration predictions across all the receptors in the domain. Because the air dispersion modeling was conducted for each aggregate source category separately, the boxplot summaries are presented for the total concentration predictions, as well as by aggregate source category: major, area, onroad mobile, special nonroad mobile (CMV, RMV, railways, airports), other nonroad mobile, and background.

The concentration level corresponding to a 1 per million cancer risk or a 1.0 hazard quotient (acrolein) is also indicated in the figure with a dashed line. These concentration levels were specified for the PATA by ODEQ and are presented in Table 3.

Table 4 presents a summary of CALPUFF model predictions for all the US Census tracts in the PATA modeling domain. For Multnomah, Clackamas, and Washington counties, the annual average model predictions at the block group centroids were combined to create tract averages.

Table 3. Risk concentration levels.
(source: ODEQ, 2003)

Pollutant	Risk Concentration ($\mu\text{g}/\text{m}^3$)
1,3-Butadiene	0.033 [*]
Acetaldehyde	0.45 [*]
Acrolein	0.020 ^{**}
Arsenic	0.00023 [*]
Benzene	0.13 [*]
Chloroform	0.043 [*]
Chromium	0.000083 [*]
Diesel Particulate Matter (diesel PM)	0.0033 [*]
Formaldehyde	0.077 [*]
Nickel	0.0021 [*]
Polycyclic Organic Matter (POM as 16-PAH)	0.018 [*]
Tetrachloroethylene	0.18 [*]

* Concentration corresponding to an upper-bound estimate of increased cancer risk of 1 per million for continuous exposure over a 70-year lifetime. EPA defines an upper bound as a plausible upper limit to the true value of a quantity. Thus, the risk at this concentration is likely to be lower than 1 per million, but may be greater.

** Concentration corresponding to a 1.0 hazard quotient, i.e., the reference concentration (RfC). The RfC is an estimate (with uncertainty spanning perhaps an order of magnitude) of a continuous inhalation exposure to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious effects during a lifetime.

Table 4. Summary of CALPUFF predictions of annual average concentrations ($\mu\text{g}/\text{m}^3$) for all US Census tracts in the PATA modeling domain, by aggregate emission source category.

Pollutant	Source Category	Mean	Percentiles								
			Min	5	10	25	50	75	90	95	Max
1,3-Butadiene	point	6.9E-06	1.1E-07	2.6E-07	4.5E-07	1.0E-06	2.2E-06	5.5E-06	1.0E-05	1.5E-05	6.7E-04
	area	4.3E-04	5.3E-05	8.4E-05	8.9E-05	1.0E-04	1.5E-04	3.4E-04	9.1E-04	1.2E-03	2.0E-02
	onroad	1.3E-01	2.2E-03	1.6E-02	3.4E-02	7.2E-02	1.0E-01	1.5E-01	2.5E-01	3.1E-01	6.1E-01
	nonroad	9.1E-02	2.4E-03	1.2E-02	2.0E-02	5.5E-02	9.4E-02	1.2E-01	1.5E-01	1.7E-01	3.6E-01
	total	2.2E-01	5.3E-03	3.0E-02	6.2E-02	1.4E-01	2.2E-01	2.7E-01	3.5E-01	4.2E-01	7.8E-01
Primary Acetaldehyde	point	9.9E-04	5.4E-05	1.2E-04	1.7E-04	2.7E-04	4.4E-04	7.3E-04	1.5E-03	2.9E-03	5.5E-02
	area	1.3E-03	1.0E-04	3.1E-04	4.1E-04	6.3E-04	8.1E-04	1.3E-03	2.5E-03	4.5E-03	1.3E-02
	onroad	3.5E-01	1.0E-02	4.9E-02	9.6E-02	2.1E-01	3.1E-01	4.3E-01	6.7E-01	8.3E-01	2.0E+00
	nonroad	1.4E-01	4.0E-03	2.3E-02	3.3E-02	8.3E-02	1.2E-01	1.6E-01	2.2E-01	2.6E-01	1.2E+00
	total	4.9E-01	1.5E-02	7.3E-02	1.5E-01	3.3E-01	4.4E-01	5.8E-01	8.1E-01	1.0E+00	2.5E+00
Primary Acrolein	point	5.0E-05	8.6E-06	1.4E-05	2.0E-05	3.1E-05	4.0E-05	5.1E-05	8.0E-05	1.4E-04	4.5E-04
	area	1.9E-01	2.3E-03	1.1E-02	1.7E-02	3.9E-02	1.6E-01	3.2E-01	4.0E-01	4.4E-01	5.5E-01
	onroad	2.5E-02	6.9E-04	3.5E-03	6.7E-03	1.4E-02	2.1E-02	3.0E-02	4.6E-02	5.8E-02	1.4E-01
	nonroad	2.4E-02	7.0E-04	3.2E-03	4.9E-03	1.4E-02	2.2E-02	2.8E-02	3.6E-02	4.3E-02	2.0E-01
	total	2.3E-01	3.7E-03	1.9E-02	3.0E-02	7.2E-02	2.3E-01	3.8E-01	4.6E-01	4.9E-01	5.9E-01
Arsenic	point	3.5E-07	1.3E-08	3.5E-08	5.4E-08	1.3E-07	2.0E-07	3.2E-07	6.9E-07	1.1E-06	7.3E-06
	area	5.6E-05	9.4E-07	6.0E-06	1.1E-05	3.0E-05	5.4E-05	7.7E-05	1.0E-04	1.2E-04	1.8E-04
	onroad	8.8E-05	1.5E-06	9.2E-06	2.1E-05	4.9E-05	7.2E-05	1.1E-04	1.7E-04	2.3E-04	5.5E-04
	nonroad	2.6E-05	5.6E-07	4.5E-06	6.8E-06	1.3E-05	1.9E-05	3.1E-05	4.3E-05	5.7E-05	2.6E-04
	total	1.7E-04	3.3E-06	2.2E-05	4.4E-05	1.1E-04	1.6E-04	2.0E-04	3.0E-04	3.6E-04	8.0E-04
Benzene	point	1.1E-03	5.7E-05	1.8E-04	2.2E-04	3.4E-04	6.0E-04	1.2E-03	2.3E-03	3.4E-03	2.0E-02
	area	1.1E+00	2.5E-02	1.6E-01	2.6E-01	5.8E-01	1.1E+00	1.4E+00	1.9E+00	2.2E+00	3.0E+00
	onroad	1.4E+00	4.8E-02	2.3E-01	4.3E-01	8.6E-01	1.2E+00	1.7E+00	2.7E+00	3.2E+00	6.2E+00
	nonroad	5.6E-01	1.4E-02	8.0E-02	1.5E-01	3.3E-01	5.5E-01	6.8E-01	1.0E+00	1.2E+00	1.7E+00
	background	4.8E-01	4.8E-01	4.8E-01	4.8E-01	4.8E-01	4.8E-01	4.8E-01	4.8E-01	4.8E-01	4.8E-01
	total	3.5E+00	5.7E-01	1.0E+00	1.4E+00	2.4E+00	3.6E+00	4.5E+00	5.4E+00	5.9E+00	8.6E+00

(continued)

Table 4. Summary of CALPUFF predictions of annual average concentrations ($\mu\text{g}/\text{m}^3$) for all US Census tracts in the PATA modeling domain, by aggregate emission source category.

Pollutant	Source Category	Mean	Percentiles								
			Min	5	10	25	50	75	90	95	Max
Chloroform	point	2.4E-03	9.1E-05	2.0E-04	2.6E-04	4.4E-04	8.4E-04	1.4E-03	3.1E-03	6.1E-03	2.6E-01
	area	2.5E-03	3.1E-04	9.6E-04	1.3E-03	2.0E-03	2.5E-03	2.9E-03	3.5E-03	3.9E-03	6.1E-03
	background	8.3E-02	8.3E-02	8.3E-02	8.3E-02	8.3E-02	8.3E-02	8.3E-02	8.3E-02	8.3E-02	8.3E-02
	total	8.8E-02	8.4E-02	8.4E-02	8.5E-02	8.6E-02	8.7E-02	8.7E-02	8.9E-02	9.0E-02	3.4E-01
Chromium	point	2.4E-05	8.4E-07	2.1E-06	3.1E-06	6.7E-06	1.9E-05	2.9E-05	4.4E-05	5.9E-05	6.4E-04
	area	1.9E-03	2.7E-05	8.9E-05	1.4E-04	6.4E-04	1.6E-03	2.3E-03	4.0E-03	5.1E-03	1.1E-02
	onroad	3.9E-05	1.2E-06	6.3E-06	1.3E-05	2.2E-05	3.3E-05	4.8E-05	7.3E-05	9.0E-05	2.1E-04
	nonroad	8.2E-05	1.3E-06	4.2E-06	6.9E-06	3.4E-05	6.7E-05	1.0E-04	1.4E-04	1.7E-04	9.3E-04
	total	2.1E-03	3.1E-05	1.1E-04	1.7E-04	7.6E-04	1.8E-03	2.5E-03	4.3E-03	5.9E-03	1.1E-02
Diesel PM	point	1.1E-05	9.1E-07	1.5E-06	2.0E-06	3.1E-06	5.3E-06	1.0E-05	2.2E-05	3.9E-05	2.5E-04
	onroad	8.8E-01	2.9E-02	1.4E-01	2.7E-01	5.2E-01	7.7E-01	1.1E+00	1.6E+00	2.1E+00	4.8E+00
	nonroad	1.4E+00	4.5E-02	2.0E-01	3.5E-01	7.7E-01	1.1E+00	1.6E+00	2.2E+00	3.1E+00	1.5E+01
	background	2.9E-01	2.4E-01	2.5E-01	2.6E-01	2.7E-01	2.8E-01	3.1E-01	3.3E-01	3.3E-01	3.8E-01
	total	2.6E+00	4.4E-01	6.9E-01	1.0E+00	1.7E+00	2.2E+00	2.9E+00	3.9E+00	5.0E+00	1.8E+01
Primary Formaldehyde	point	5.6E-04	4.1E-05	8.0E-05	1.3E-04	2.5E-04	3.8E-04	5.5E-04	9.0E-04	1.4E-03	1.2E-02
	area	5.7E-02	1.2E-03	7.1E-03	1.1E-02	2.0E-02	5.4E-02	8.9E-02	1.1E-01	1.2E-01	1.4E-01
	onroad	5.5E-01	1.5E-02	7.9E-02	1.5E-01	3.2E-01	4.8E-01	6.6E-01	1.1E+00	1.3E+00	3.1E+00
	nonroad	4.3E-01	1.8E-02	6.1E-02	1.0E-01	2.7E-01	3.9E-01	5.0E-01	6.9E-01	8.6E-01	2.6E+00
	background	2.5E-01	2.5E-01	2.5E-01	2.5E-01	2.5E-01	2.5E-01	2.5E-01	2.5E-01	2.5E-01	2.5E-01
	total	1.3E+00	2.9E-01	4.1E-01	5.3E-01	9.4E-01	1.3E+00	1.5E+00	1.9E+00	2.2E+00	4.9E+00
Nickel	point	2.3E-05	7.3E-07	1.9E-06	2.9E-06	6.2E-06	1.7E-05	2.8E-05	4.2E-05	5.6E-05	6.5E-04
	area	7.6E-04	1.8E-05	9.9E-05	1.7E-04	4.1E-04	6.8E-04	9.1E-04	1.5E-03	1.8E-03	2.8E-03
	onroad	7.3E-05	2.3E-06	1.1E-05	2.1E-05	4.2E-05	6.3E-05	8.8E-05	1.3E-04	1.7E-04	4.0E-04
	nonroad	4.9E-05	8.4E-07	4.5E-06	6.8E-06	2.2E-05	4.2E-05	6.0E-05	8.7E-05	1.1E-04	4.2E-04
	total	9.0E-04	2.2E-05	1.2E-04	2.1E-04	5.1E-04	8.3E-04	1.1E-03	1.7E-03	2.0E-03	3.1E-03

(continued)

Table 4. Summary of CALPUFF predictions of annual average concentrations ($\mu\text{g}/\text{m}^3$) for all US Census tracts in the PATA modeling domain, by aggregate emission source category.

Pollutant	Source Category	Mean	Percentiles								
			Min	5	10	25	50	75	90	95	Max
POM	point	3.2E-05	1.4E-06	3.5E-06	5.2E-06	1.0E-05	1.8E-05	2.9E-05	6.2E-05	9.4E-05	5.4E-04
	area	2.8E-01	1.9E-03	1.7E-02	3.3E-02	8.0E-02	2.8E-01	4.3E-01	5.4E-01	5.9E-01	9.9E-01
	onroad	7.4E-03	5.4E-05	6.3E-04	1.4E-03	3.4E-03	5.6E-03	8.6E-03	1.5E-02	2.1E-02	5.5E-02
	nonroad	3.8E-03	2.1E-05	2.4E-04	4.4E-04	1.1E-03	1.6E-03	2.7E-03	3.8E-03	5.8E-03	2.6E-01
	total	2.9E-01	2.0E-03	2.0E-02	3.8E-02	8.5E-02	2.9E-01	4.4E-01	5.6E-01	6.0E-01	1.0E+00
Tetrachloroethylene	point	2.0E-02	4.8E-04	9.1E-04	1.3E-03	2.9E-03	7.1E-03	1.7E-02	3.6E-02	5.8E-02	6.1E-01
	area	4.0E-02	2.0E-03	6.9E-03	1.3E-02	2.8E-02	4.2E-02	5.2E-02	6.1E-02	6.6E-02	1.0E-01
	background	1.4E-01	1.4E-01	1.4E-01	1.4E-01	1.4E-01	1.4E-01	1.4E-01	1.4E-01	1.4E-01	1.4E-01
	total	2.0E-01	1.4E-01	1.5E-01	1.6E-01	1.7E-01	1.9E-01	2.1E-01	2.3E-01	2.5E-01	8.0E-01

(concluded)

5.2.2 Spatial Pattern of Concentration Predictions

The second figure presented for each HAP is an isopleth diagram showing the spatial pattern of concentration predictions over the modeling domain. An isopleth is a line that indicates a set of locations with concentration predictions of equal value.

5.2.3 Model-to-Monitor Comparisons

The third figure for each HAP shows the concentration predictions compared to measured values at the 5 monitoring locations. (Exceptions are acrolein and diesel PM). The measured values are presented on the graph as a set of 3 horizontal lines. The middle line represents the annual average of the measured concentrations, calculated by averaging all 24-hour sample values for the HAP/monitor combination, after replacing all concentrations reported as below the minimum quantitation level (MQL) with half the MQL. The number of 24-hour samples for each HAP/monitor combination ranged from 11 to 56.

The top and bottom horizontal lines represent the upper and lower bounds, respectively, of the 95% confidence interval for the annual average concentrations. They are calculated as follows:

1. Average all the 24-hour sample values, after replacing the concentrations reported as below the MQL with zero for the lower bound and with the MQL for the upper bound: X_0 and X_1 .
2. Calculate the standard deviations, S_0 , $S_{0.5}$, and S_1 , corresponding to substitution for values reported below the MQL of 0, half MQL, and MQL, respectively. Select the highest (S_{MAX})
3. Calculate the bounds as

$$\text{Lower bound} = X_0 - t * S_{MAX} / \text{sqrt}(N)$$

$$\text{Upper bound} = X_1 + t * S_{MAX} / \text{sqrt}(N)$$

where t = the t-statistic = 1.96 to 2.23, depending on the number of samples, and
 N = the number of samples = 11 to 63.

Thus, the 95% confidence interval of the monitored annual average increases as the fraction of samples below the MQL increases, and as the standard deviation (i.e., variability) of the sample values increases.

For many of the target HAPs a substantial number of the measurement values were below the MQL. These included 1,3-butadiene, arsenic, chloroform, chromium, nickel, and tetrachloroethylene. The influence of the MQLs on the comparisons is discussed in the pollutant-specific sections below.

Because model predictions pertain to groundlevel concentrations, for the model-to-monitor comparisons an adjustment was made to concentrations measured at the downtown monitor, which was located at the top of a 15-meter building. Because the bulk of emissions in the PATA domain are released at ground level, ground level concentrations would be expected to be higher than those above ground. EPA's SCREEN3 air dispersion model was used to estimate the ratio between concentrations at ground level and concentrations at 15-meters elevation for a ground level release. The adjustment factor applied to the downtown monitor measurements for the model-to-monitor comparison was 1.37.

The annual average concentration prediction at the exact location of the monitor is shown as a large red dot. However, because the monitors are considered neighborhood-scale, according to US EPA monitoring guidelines the measurements are expected to be representative for a distance of 0.5 km to 4 km. Therefore, for comparison purposes all the receptor concentration predictions within 4 km of the monitoring location are also indicated on the figure with small black dots.

The annual average concentrations from the measurements and the model predictions are presented in Table 5, as well as a summary of the model-to-monitor ratios.

According to US EPA (2001) studies of the performance of long-term air quality models suggest that 90 percent of the estimated concentrations should be within a factor of 2 of those observed, if the emissions are well characterized and the meteorological data are representative. Since this study used very detailed meteorological data, any large discrepancies between modeled and monitored concentrations are likely to be due to uncertainties in emissions estimates.

5.2.4 Emissions Source Category Contributions

As noted above separate CALPUFF simulations were performed for each aggregate emission source category: major stationary, area, onroad mobile, nonroad mobile, and special nonroad mobile. This approach allows the analysis of the contribution of each category to the total ambient concentration predictions, as presented in the fourth figure for the annual average predictions at the monitor locations.

5.2.5 Comparison of PATA Predictions to 1996 NATA Predictions

The fifth and last figure for each HAP shows a comparison between the frequency distribution of CALPUFF model predictions over the PATA domain and the corresponding frequency distribution for the PATA domain as predicted by the Assessment System for Population Exposure Nationwide (ASPEN) for the 1996 NATA national-scale assessment. Because the NATA predictions were reported for census tracts only, for this comparison the CALPUFF predictions for block groups in each census tract were averaged together to create a tract average, and it is the distribution of tract averages that is depicted in the figure.

Table 5. Annual average concentrations ($\mu\text{g}/\text{m}^3$) derived from measurements and predicted by CALPUFF for 5 locations in the PATA modeling domain.

Pollutant	Site	Monitored Concentration			CALPUFF Prediction			Model-to-Monitor Ratios*	
		Mean	Std Error**	%<MQL	At Site	Within 4 Km of Site		Mean	Std Dev
						Mean	Std Dev		
1,3-Butadiene	Beaverton	0.11	0.06	97%	0.31	0.30	0.08	2.6	1.6
	Downtown	0.19	0.08	85%	0.84	0.35	0.16	1.8	1.1
	N Roselawn	0.14	0.06	84%	0.23	0.29	0.11	2.0	1.1
	NW Post Office	0.14	0.06	84%	0.37	0.38	0.17	2.6	1.6
	SE Lafayette	0.14	0.05	79%	0.23	0.27	0.09	1.8	0.9
Acetaldehyde***	Beaverton	1.9	0.1	0%	0.7	0.6	0.2	0.3	0.1
	Downtown	3.0	0.2	0%	2.2	1.0	0.6	0.3	0.2
	N Roselawn	2.4	0.2	0%	0.5	0.6	0.5	0.3	0.2
	NW Post Office	2.1	0.1	0%	0.7	1.1	0.7	0.5	0.3
	SE Lafayette	2.0	0.1	0%	0.5	0.5	0.2	0.3	0.1
Arsenic	Beaverton	0.0021	0.0023	90%	0.0003	0.0002	0.0001	0.1	0.1
	Downtown	0.0018	0.0012	100%	0.0007	0.0003	0.0002	0.2	0.2
	N Roselawn	0.0023	0.0012	93%	0.0002	0.0002	0.0001	0.1	0.1
	NW Post Office	0.0015	0.0008	89%	0.0004	0.0004	0.0002	0.2	0.2
	SE Lafayette	0.0029	0.0030	75%	0.0002	0.0002	0.0001	0.1	0.1
Benzene	Beaverton	1.4	0.1	0%	6.1	5.1	1.1	3.7	0.8
	Downtown	2.6	0.2	0%	7.7	4.7	1.4	1.8	0.6
	N Roselawn	2.1	0.2	0%	4.0	4.1	1.1	1.9	0.6
	NW Post Office	1.9	0.1	0%	4.7	5.1	1.4	2.6	0.7
	SE Lafayette	2.5	0.2	0%	3.7	4.5	1.0	1.8	0.4
Benzene (June-August)	Beaverton	1.1	0.1	0%	2.2	2.2	0.5	1.9	0.5
	Downtown	1.9	0.1	0%	5.4	2.7	1.0	1.4	0.5
	N Roselawn	1.4	0.1	0%	1.9	2.1	0.7	1.4	0.5
	NW Post Office	1.4	0.1	0%	2.8	2.7	1.0	1.9	0.7
	SE Lafayette	1.5	0.1	0%	2.1	2.3	0.6	1.5	0.4

(continued)

Table 5. Annual average concentrations ($\mu\text{g}/\text{m}^3$) derived from measurements and predicted by CALPUFF for 5 locations in the PATA modeling domain.

Pollutant	Site	Monitored Concentration			CALPUFF Prediction			Model-to-Monitor Ratios*	
		Mean	Std Error**	%<MQL	At Site	Within 4 Km of Site		Mean	Std Dev
						Mean	Std Dev		
Chloroform	Beaverton	0.24	0.14	100%	0.09	0.09	0.00	0.4	0.2
	Downtown	0.34	0.20	100%	0.09	0.09	0.00	0.3	0.1
	N Roselawn	0.25	0.14	100%	0.09	0.09	0.00	0.3	0.2
	NW Post Office	0.26	0.14	98%	0.09	0.09	0.00	0.3	0.2
	SE Lafayette	0.24	0.14	100%	0.09	0.09	0.00	0.4	0.2
Chromium	Beaverton	0.0007	0.0005	100%	0.0080	0.0068	0.0028	9.9	7.7
	Downtown	0.0017	0.0007	75%	0.0045	0.0033	0.0015	1.9	1.1
	N Roselawn	0.0014	0.0004	69%	0.0020	0.0023	0.0011	1.6	0.9
	NW Post Office	0.0024	0.0005	56%	0.0063	0.0036	0.0015	1.5	0.7
	SE Lafayette	0.0016	0.0005	64%	0.0016	0.0022	0.0008	1.3	0.6
Formaldehyde***	Beaverton	1.9	0.1	0%	1.5	1.5	0.3	0.7	0.2
	Downtown	3.8	0.3	0%	4.7	2.2	1.1	0.6	0.3
	N Roselawn	3.2	0.5	0%	1.4	1.7	0.7	0.5	0.2
	NW Post Office	2.5	0.2	0%	1.6	2.4	1.2	0.9	0.5
	SE Lafayette	2.4	0.1	0%	1.4	1.5	0.3	0.6	0.1
Nickel	Beaverton	0.0009	0.0004	93%	0.0018	0.0017	0.0009	1.9	1.4
	Downtown	0.0032	0.0010	42%	0.0017	0.0015	0.0007	0.5	0.3
	N Roselawn	0.0021	0.0004	48%	0.0010	0.0013	0.0006	0.6	0.3
	NW Post Office	0.0044	0.0006	26%	0.0033	0.0017	0.0007	0.4	0.2
	SE Lafayette	0.0027	0.0006	42%	0.0008	0.0010	0.0004	0.4	0.2
POM (as 16-PAH)	Beaverton	0.022	0.003	n/a****	0.889	0.455	0.196	20.7	9.4
	Downtown	0.076	0.008	n/a****	0.528	0.459	0.191	6.1	2.6
	N Roselawn	0.042	0.005	n/a****	0.611	0.467	0.194	11.1	4.8
	NW Post Office	0.068	0.009	n/a****	0.195	0.455	0.228	6.6	3.4
	SE Lafayette	0.036	0.004	n/a****	0.434	0.477	0.134	13.2	4.0

(continued)

Table 5. Annual average concentrations ($\mu\text{g}/\text{m}^3$) derived from measurements and predicted by CALPUFF for 5 locations in the PATA modeling domain.

Pollutant	Site	Monitored Concentration			CALPUFF Prediction			Model-to-Monitor Ratios*	
		Mean	Std Error**	%<MQL	At Site	Within 4 Km of Site		Mean	Std Dev
						Mean	Std Dev		
POM (as 16-PAH) (June-August)	Beaverton	0.012	0.003	n/a****	0.014	0.012	0.003	1.0	0.3
	Downtown	0.061	0.010	n/a****	0.115	0.020	0.019	0.3	0.3
	N Roselawn	0.024	0.007	n/a****	0.010	0.014	0.008	0.6	0.4
	NW Post Office	0.055	0.007	n/a****	0.016	0.022	0.022	0.4	0.4
	SE Lafayette	0.023	0.004	n/a****	0.010	0.011	0.004	0.5	0.2
Tetrachloroethylene	Beaverton	0.34	0.19	98%	0.22	0.22	0.12	0.6	0.5
	Downtown	0.53	0.26	93%	0.19	0.21	0.02	0.4	0.2
	N Roselawn	0.38	0.18	92%	0.20	0.20	0.02	0.5	0.3
	NW Post Office	2.29	0.33	28%	0.29	0.20	0.03	0.1	0.0
	SE Lafayette	0.46	0.20	91%	0.23	0.24	0.03	0.5	0.2

* Ratios of CALPUFF annual average concentration from receptors within 4 km of the monitoring site to the average monitored concentration.

** When there are no concentration measurements below the MQL, the standard error of the mean is calculated as $\text{std error} = \text{std dev} / \sqrt{N}$.

When there are concentration measurements below the MQL, 3 annual averages and std deviations are calculated.

- X0 is the annual average, and S0 is the std dev, assuming all measurements below the MQL = 0.
- X0.5 is the annual average, and S0.5 is the std dev, assuming all measurements below the MQL = 0.5* MQL.
- X1 is the annual average, and S1 is the std dev, assuming all measurements below the MQL = MQL.

In that case the mean is specified as X0.5, and the std error is approximated as

$$\text{std error} = \sqrt{\frac{\max^2(S0, S0.5, S1)}{N} + \frac{(X1 - X0)^2}{12}}$$

The second term on the right-hand side represents the variance of a uniform distribution between X1 and X0, and therefore accounts for the uncertainty due to the concentration measurements below the MQL.

*** CALPUFF predictions for acetaldehyde include the primary component only, and for formaldehyde include the primary and background components only.

**** The number of concentration measurements below the MQL varies among the 16 PAH constituents of POM.

The differences between the CALPUFF and ASPEN predictions result from differences in emissions inputs, meteorological inputs, and modeling algorithms. The most important of these factors is likely to be the differences in emissions. Therefore, a comparison between the two studies of emissions by aggregate source category is also provided in the figure.

5.3 Pollutant-Specific Concentration Predictions

5.3.1 1,3-Butadiene

Figure A-1 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of 1,3-butadiene. The total boxplot indicates that the average prediction is about $0.2 \mu\text{g}/\text{m}^3$, the 95th percentile value about $0.4 \mu\text{g}/\text{m}^3$, and approximately 95% of the model predictions exceed the 1 per million risk level of $0.033 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to about $0.8 \mu\text{g}/\text{m}^3$.

The figure suggests that the total concentration prediction is dominated by the contribution from onroad mobile emission sources, with a smaller but substantial contribution from nonroad mobile sources (about half from lawn and garden equipment) and special nonroad mobile sources (primarily RMV). Both onroad mobile and special nonroad mobile sources show a large number of extreme individual receptor values.

Consistent with the boxplots, the isopleths in Figure A-2 show elevated concentrations near major roadways, particularly in the downtown area, and around the special nonroad mobile sources of Portland International Airport and Hillsboro Airport.

The wide 95% confidence intervals around the annual averages of the monitoring data in Figure A-3 indicate that the bulk of measured concentrations were below the MQL at all monitors, ranging from 84% to 97%. The figure shows that the model predictions were consistent with the measurements. In all cases the range of annual average predictions within 4 km of the monitor location substantially overlapped the 95% confidence interval of the average of the measured values. Table 5 shows that the ratio of the mean concentration within 4 km to the mean measured concentration ranged from 1.8 to 2.6, but given the uncertainty of the measurement values, the true ratios could be somewhat higher or lower.

Figure A-4 shows that at the monitor locations about 60% to 75% of the total concentration predictions are contributed by onroad mobile sources. The remainder comes from a combination of special nonroad sources (primarily RMV) and other nonroad sources (about half from lawn and garden equipment).

Figure A-5 shows that the set of concentration predictions from CALPUFF are consistently about twice as high as the corresponding ASPEN predictions from the 1996 NATA national-scale assessment, due to higher contributions from both onroad mobile emissions and nonroad mobile emissions (including special nonroad sources).

5.3.2 Primary Acetaldehyde

As noted above ambient acetaldehyde is comprised of both primary and secondary components. Due to limitations of the CALPUFF model only the primary components were simulated in this study.

Although it is not possible to determine the secondary fraction of ambient acetaldehyde concentrations directly from monitoring data some estimates are available from previous modeling studies. One such study applied UAM-Tox in Houston and Baltimore-Washington to project ambient concentration for 1988, 1995, and 1999 (Ligocki et al., 1992). The results for Baltimore-Washington (which is more similar to Portland than is Houston with respect to air toxics emissions) suggest that the secondary fraction of acetaldehyde is approximately 70%-80% in winter and 90%-95% in summer. US EPA's CEP found that ASPEN predicted approximately 60% of total acetaldehyde was secondary. Given these findings it is likely that total acetaldehyde concentrations in Portland are substantially higher than the concentration predictions for the primary component alone.

Figure A-6 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of primary acetaldehyde. The total boxplot indicates that the average prediction is about $0.5 \mu\text{g}/\text{m}^3$, the 95th percentile value about $1.0 \mu\text{g}/\text{m}^3$, and about half of the model predictions exceed the 1 per million risk level of $0.45 \mu\text{g}/\text{m}^3$. "Hot spot" concentration predictions range up to about $2.5 \mu\text{g}/\text{m}^3$.

The figure suggests that the total concentration prediction is dominated by the contribution from onroad mobile emission sources, with a smaller but substantial contribution from nonroad mobile sources (about 60% from construction equipment). Onroad mobile sources show a large number of extreme individual receptor values.

Consistent with the boxplots, the isopleths in Figure A-7 shows elevated concentrations near major roadways, particularly in the downtown area.

In Figure A-8 a comparison of annual average model predictions with measured values shows a general underprediction, as expected, since the predictions include only the primary component of total acetaldehyde, while the measured values also include secondary components. Table 5 shows that for all the monitor locations, the ratio of the mean primary acetaldehyde concentration within 4 km to the mean measured total acetaldehyde concentration ranged from 0.26 to 0.50.

Consistent with the boxplots, Figure A-9 shows that at the monitor locations 75% to 85% of the total concentration predictions are contributed by onroad mobile sources. The remainder comes from a combination of special nonroad sources and other nonroad sources.

Figure A-10 shows that the set of concentration predictions from CALPUFF are consistently about half as high as the corresponding ASPEN predictions from the 1996 NATA national-scale assessment. This large discrepancy is expected since the ASPEN predictions include secondary acetaldehyde as well as primary.

5.3.3 Primary Acrolein

As noted above ambient acrolein is comprised of both primary and secondary components. Due to limitations of the CALPUFF model only the primary components were simulated in this study.

Although it is not possible to determine the secondary fraction of ambient acrolein concentrations directly from monitoring data some estimates are available from previous modeling studies. The 1996 NATA national-scale assessment found the average fraction ambient acrolein that was secondary according to ASPEN predictions was 44%. Given these findings it is likely that total acrolein concentrations in Portland are substantially higher than the concentration predictions for the primary component alone.

Figure A-11 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of primary acrolein. The total boxplot indicates that the average prediction is about $0.25 \mu\text{g}/\text{m}^3$, the 95th percentile value about $0.50 \mu\text{g}/\text{m}^3$, and virtually all of the model predictions exceed the reference concentration of $0.02 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to about $0.60 \mu\text{g}/\text{m}^3$.

The figure suggests that the total concentration prediction is dominated by the contribution of area sources (virtually all from structural fires), although onroad, nonroad, and special nonroad sources each independently generate concentrations above the reference concentration as well.

The isopleths in Figure A-12 show a pattern of elevated concentrations that appear to be correlated with residential land use.

There is no model-to monitor comparison figure for primary acrolein, because ODEQ indicated that they consider their acrolein measurements taken during the simulation period to be flawed.

Consistent with the Figure A-11 boxplots, Figure A-13 shows that at the monitor locations from 30% to 90% of the concentration predictions are contributed by area sources. At the downtown monitor there is also about a 30% contribution from onroad mobile sources.

Figure A-14 shows that the set of concentration predictions from CALPUFF are much more variable than the corresponding ASPEN predictions from the 1996 NATA national-scale assessment, with much higher CALPUFF predictions at the upper end of the

distribution. These higher concentrations occur despite the exclusion of secondary acrolein from the CALPUFF predictions and its inclusion in the ASPEN predictions. Thus the implied discrepancy for total acrolein is even greater. As is evident in the figure the discrepancy is the result of much higher PATA estimates for area sources, specifically structural fires.

Because of the importance of the structural fire emission category to the concentration predictions of primary acrolein, and the lack of monitoring data for evaluating model performance for this pollutant, we recommend a thorough review of the emissions estimates for this source category.

5.3.4 Arsenic

Figure A-15 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of arsenic. The total boxplot indicates that the average prediction is about $0.0002 \mu\text{g}/\text{m}^3$, the 95th percentile value about $0.0004 \mu\text{g}/\text{m}^3$, and approximately 20% of the model predictions exceed the 1 per million risk level of $0.00023 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to about $0.0008 \mu\text{g}/\text{m}^3$.

The figure suggests that the total concentration prediction is the aggregate of contributions from area sources (primarily distillate oil combustion and natural gas combustion), onroad mobile sources, and nonroad mobile sources. Onroad mobile sources show a large number of extreme individual receptor values.

The isopleths in Figure A-16 show elevated concentrations in the inner core of the urbanized area, with an extreme “hot spot” in the downtown area.

The monitoring data presented in Figure A-17 is for arsenic as $\text{PM}_{2.5}$, which was the particle size fraction collected by ODEQ during the modeling time frame. The size fraction of the arsenic model predictions depends on the size fraction of the arsenic emissions in the PATA inventory. This was unspecified. The emissions, and thus the model predictions, are likely to include particles above the 2.5 micron size range that were omitted from the measurement data. The largest emission sources of arsenic in the PATA inventory were combustion of distillate oil and natural gas. The 1996 NATA national-scale assessment adopted particle size fractions from the earlier Cumulative Exposure Project national emission inventory. In that inventory arsenic from industrial area sources was assumed to be comprised of 72% particles of size 2.5 microns or less. Therefore, the model predictions should be somewhat higher than the measured values.

The wide 95% confidence intervals around the annual averages of the monitoring data in Figure A-17 indicate that the bulk of measured arsenic concentrations were below the MQL at all monitors, ranging from 70% to 100%. The figure shows that the model predictions are consistent with the measurements. In all cases the range of annual average predictions within 4 km of the monitor location fell within the wide 95% confidence interval of the average of the measured values. Table 5 shows that for all the monitor locations, the ratio of the mean concentration within 4 km to the mean measured

concentration ranged from 0.07 to 0.24. However, given the uncertainty of the measured values, the true ratios may be higher or lower.

Figure A-18 shows that at the monitor locations about 10% to 50% of the total concentration predictions are contributed by area sources. Another 30% to 50% is contributed by onroad mobile sources, and the remainder from nonroad mobile sources.

Figure A-19 shows that the set of concentration predictions from CALPUFF are consistently higher than the corresponding ASPEN predictions from the 1996 NATA national-scale assessment, due to inclusion of arsenic emissions from onroad mobile sources in the PATA inventory.

5.3.5 Benzene

Figure A-20 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of benzene. The total boxplot indicates that the average prediction is about $3.5 \mu\text{g}/\text{m}^3$, the 95th percentile value about $6.0 \mu\text{g}/\text{m}^3$, and all the model predictions exceed the 1 per million risk level of $0.13 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to about $8.5 \mu\text{g}/\text{m}^3$.

The figure suggests that the onroad mobile sources and area sources (primarily residential wood combustion) are the largest contributors, but all the source categories except point, each independently generate concentrations above the 1 per million risk level as well – even background. Onroad mobile sources show a large number of extreme individual receptor values.

The isopleths in Figure A-21 shows a complex pattern of elevated concentrations throughout the modeling domain, with a large “hot spot” in the downtown area.

The model-to-monitor comparison in Figure A-22 shows a consistent tendency to overpredict, especially at the Beaverton monitor, suggesting that some of the benzene emissions in the PATA inventory may be overestimated. Table 5 shows that for all the monitor locations, the ratio of the mean concentration within 4 km to the mean measured concentration ranged from 1.8 to 3.7.

Figure A-23 shows that at the monitor locations about 30% to 70% of the total concentration predictions are contributed by onroad mobile sources. Another 10% to 40% is contributed by area sources. The remainder is a combination of nonroad mobile, special nonroad mobile, and background.

In order to assess why the benzene concentrations appear to be overestimated we examined the largest contributors to the concentration predictions. Because onroad mobile emissions of other HAPs, such as 1,3-butadiene and primary acetaldehyde, do not appear to be significantly overestimated judging by model performance, it seemed unlikely that the onroad mobile contribution was the cause of the discrepancy. However, as discussed below, POM concentrations were also appear to be overpredicted; POM

concentrations are dominated by residential wood combustion emissions. Therefore, we turned our attention to the residential wood combustion category.

Since no residential wood combustion emissions were temporally allocated to the third quarter (June-August), we were able to examine the model performance for benzene in the absence of residential wood combustion contributions by limiting our model-to-monitor comparison to the third quarter. (See Figure A-24.) The third quarter comparison shows much improved model performance, with the average concentration predictions within 4 km of each monitor overlapping the 95% confidence intervals for the monitored values. Table 5 shows that for the third quarter the ratios of the mean concentration within 4 km to the mean measured concentration ranged from 1.4 to 1.9. These findings suggest that benzene emissions from residential wood combustion are likely to be overestimated in the PATA inventory.

Figure A-25 shows that the set of concentration predictions from CALPUFF are consistently higher than the corresponding ASPEN predictions from the 1996 NATA national-scale assessment, due to the higher emission estimates for area sources (i.e., residential wood combustion) in the PATA inventory.

5.3.6 Chloroform

Figure A-26 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of chloroform. The figure indicates concentration predictions that are extremely uniform at about $0.09 \mu\text{g}/\text{m}^3$, dominated by background sources, with all concentration predictions exceeding the 1 per million risk level. However, there is one extreme “hot spot” value at $0.34 \mu\text{g}/\text{m}^3$.

The isopleths in Figure A-27 show no elevated concentrations, except for a large “hot spot” in Clark County, associated with a major stationary source.

In Figure A-28 the extremely large 95% confidence intervals around the annual averages for monitored values indicate a large number of concentrations below the MQL at all monitors. In fact, only one 24-hour sample at one monitor exceeded the MQL. All the annual average concentration predictions at the monitor locations and within 4 km fall within the confidence intervals for the average of the measured values. Table 5 shows that for all the monitor locations, the ratio of the mean concentration within 4 km to the mean measured concentration ranged from 0.26 to 0.36. However, given the uncertainty of the measured values, the true ratios may be somewhat higher or lower.

Figure A-29 shows that at the monitor locations about 95% of the predicted concentrations are attributable to background concentrations.

Figure A-30 shows that the set of concentration predictions from CALPUFF nearly identical to the corresponding ASPEN predictions from the 1996 NATA national-scale assessment, except for a small fraction of receptors at the upper end of the distribution. CALPUFF predictions are higher for these receptors due to a major stationary source in

Clark County that appears to have been omitted from the 1996 NATA emission inventory.

5.3.7 Chromium

Figure A-31 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of chromium. The total boxplot indicates that the average prediction is about $0.002 \mu\text{g}/\text{m}^3$, the 95th percentile value about $0.006 \mu\text{g}/\text{m}^3$, and almost all of the model predictions exceed the 1 per million risk level of $0.000083 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to about $0.011 \mu\text{g}/\text{m}^3$.

The figure suggests that the total concentration prediction is dominated by area sources (primarily surface coating of plastic parts).

The isopleths in Figure A-32 show elevated concentrations in the inner core of the urbanized area, with an extreme “hot spot” in the industrial/commercial area of Washington County and a moderate one in the downtown area.

The monitoring data presented in Figure A-17 is for trivalent chromium as $\text{PM}_{2.5}$, which was the valence state and particle size fraction collected by ODEQ during the modeling time frame. The model predictions are for total chromium (trivalent, hexavalent, and un-compounded chromium metal) and the size fraction depends on the size fraction of the chromium emissions in the PATA inventory, which was unspecified. The emissions, and thus the model predictions, are likely to include some hexavalent chromium and some particles above the 2.5 micron size range, both of which were omitted from the measurement data.

The largest emission sources of chromium in the PATA inventory were surface coating of plastic parts. The predominant valence of chromium from this source is unknown. However, ambient field studies have suggested that airborne chromium in rural areas is 99% trivalent and in urban areas averages about 75% trivalent.

The 1996 NATA national-scale assessment adopted particle size fractions from the earlier Cumulative Exposure Project national emission inventory. In that inventory chromium from industrial area sources was assumed to be comprised of 70% particles of size 2.5 microns or less.

Given the discrepancies in valence states and size fractions, the model predictions should be somewhat higher than the measured values, perhaps by as much as 60%.

The wide 95% confidence intervals around the annual averages of the monitoring data in Figure A-33 indicates that many of the measured chromium concentrations were below the MQL at all monitors, ranging from 56% to 100%. Except for the Beaverton monitor the figure shows that the annual average model predictions are consistent with the measured values, with the sets of receptor concentrations within 4 km of each monitor substantially overlapping the wide 95% confidence intervals for the average of the

measured values. Table 5 shows that for these four monitor locations, the ratio of the mean concentration within 4 km to the mean measured concentration ranged from 1.3 to 1.9. This slight overestimate is consistent with the valence state and size fraction discrepancies discussed above. However, given the uncertainty of the measured values, the true ratios may be somewhat higher or lower.

Concentrations at the Beaverton monitor, near the Washington County “hot spot” appears to be considerably overpredicted. Table 5 shows that the ratio of the mean concentration within 4 km to the mean measured concentration at Beaverton of 9.9.

Figure A-34 shows that at the monitor locations about 85% to 98% of the total concentration predictions are contributed by area sources. The remainder comes from a combination of onroad, nonroad, and point sources. Given the apparent overprediction at the Beaverton monitor, we recommend a thorough review of the chromium emissions estimates for surface coating of plastic parts, especially in the vicinity of that monitor.

Figure A-35 shows that the range of concentration predictions from CALPUFF is very similar to the corresponding ASPEN predictions from the 1996 NATA national-scale assessment, with ASPEN predictions slightly higher at the upper end of the range. This small discrepancy appears to result from a larger nonroad source contribution to the ASPEN predictions, suggesting a change in the NONROAD emissions model with respect to chromium since the 1996 NATA study.

5.3.8 Diesel Particulate Matter

Figure A-36 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of diesel PM. The total boxplot indicates that the average prediction is about $2.6 \mu\text{g}/\text{m}^3$, the 95th percentile value about $5.0 \mu\text{g}/\text{m}^3$, and all of the model predictions exceed the reference concentration of $0.0033 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to more than $17 \mu\text{g}/\text{m}^3$.

The figure suggests that the bulk of the total concentration prediction comes from a combination of nonroad (about 75% from construction equipment), onroad, and special onroad sources (more than half from RMV).

The isopleths in Figure A-37 show a pattern of elevated concentrations throughout the urbanized area, with an extreme “hot spot” in the downtown section.

There is no model-to-monitor comparison figure for diesel PM, because of the limitations of monitoring technology for this pollutant, which is actually a mixture of compounds.

Consistent with the Figure A-36 boxplots, Figure A-38 shows that at the monitor locations from 25% to 50% of the concentration predictions are contributed by onroad sources, about 30% to 60% from nonroad sources, and about 2% to 20% from special nonroad sources.

Figure A-39 shows that the set of concentration predictions from CALPUFF are very similar to the corresponding ASPEN predictions from the 1996 NATA national-scale assessment.

5.3.9 Primary Formaldehyde

As noted above ambient formaldehyde is comprised of both primary and secondary components. Due to limitations of the CALPUFF model only the primary components were simulated in this study.

Although it is not possible to determine the secondary fraction of ambient acetaldehyde concentrations directly from monitoring data some estimates are available from previous modeling studies. The UAM-Tox study of Baltimore-Washington mentioned above suggest that the secondary fraction of formaldehyde in that area was about 20%-30% in winter and 75%-80% in summer, or about 65%-70% of the annual average. These values include much of the background formaldehyde concentration included in this study, which is largely of secondary origin. The 1996 NATA national-scale assessment found the average fraction ambient formaldehyde that was secondary according to ASPEN predictions was 23%, not including background formaldehyde. The sum of the secondary fraction and the background fraction was 43%. Given these findings it is likely that total formaldehyde concentrations in Portland are substantially higher than the concentration predictions for the primary and background components alone.

Figure A-40 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of primary and background formaldehyde. The total boxplot indicates that the average prediction is about $1.3 \mu\text{g}/\text{m}^3$, the 95th percentile value about $2.2 \mu\text{g}/\text{m}^3$, and about half of the model predictions exceed the 1 per million risk level of $0.077 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to about $5.0 \mu\text{g}/\text{m}^3$.

The figure suggests that the total concentration prediction is dominated by the contribution from onroad mobile emission sources, with a smaller but substantial contributions from nonroad mobile sources (about 60% from construction equipment) and special nonroad mobile sources (about half from railroads, 25% from RMV, and 25% from airports). Note, however, that even the background contribution exceeds the 1 per million risk concentration.

Consistent with the boxplots, the isopleths in Figure A-41 shows elevated concentrations near throughout the urbanized area, with an extreme “hot spot” in the downtown area.

In Figure A-42 a comparison of annual average model predictions with measured values shows a general underprediction, as expected, since the predictions include only the primary and background components of total acetaldehyde, while the measured values also include secondary components. Table 5 shows that for all the monitor locations, the ratio of the mean primary formaldehyde concentration within 4 km to the mean measured total acetaldehyde concentration ranged from 0.52 to 0.95.

Figure A-43 shows that at the monitor locations about half of the total concentration predictions are contributed by onroad mobile sources, about 10% to 25% from nonroad mobile sources, and about 2% to 20% from special nonroad sources. The background concentration estimate contributes about 5% to 20%.

Figure A-44 shows that the set of concentration predictions from CALPUFF are consistently about 30% lower than the corresponding ASPEN predictions from the 1996 NATA national-scale assessment. This discrepancy is expected since the ASPEN predictions include secondary formaldehyde as well as primary and background.

5.3.10 Nickel

Figure A-45 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of nickel. The total boxplot indicates that the average prediction is about $0.0009 \mu\text{g}/\text{m}^3$, the 95th percentile value about $0.0020 \mu\text{g}/\text{m}^3$, and less than 5% of the model predictions exceed the 1 per million risk level of $0.0021 \mu\text{g}/\text{m}^3$. "Hot spot" concentration predictions range up to about $0.0030 \mu\text{g}/\text{m}^3$.

The figure shows that the total concentration prediction is dominated by area sources (primarily combustion of residual oil and natural gas).

The isopleths in Figure A-46 show elevated concentrations only in a few small locations, including the downtown area and the industrial/commercial portion of Washington County not far from the Beaverton monitor.

The monitoring data presented in Figure A-17 is for nickel as $\text{PM}_{2.5}$, which was the particle size fraction collected by ODEQ during the modeling time frame. The size fraction of the nickel model predictions depends on the size fraction of the nickel emissions in the PATA inventory. This was unspecified. The emissions, and thus the model predictions, are likely to include particles above the 2.5 micron size range that were omitted from the measurement data. The largest emission sources of nickel in the PATA inventory were combustion of residual oil and natural gas. The 1996 NATA national-scale assessment adopted particle size fractions from the earlier Cumulative Exposure Project national emission inventory. In that inventory nickel from industrial area sources was assumed to be comprised of 62% particles of size 2.5 microns or less. Therefore, the model predictions should be somewhat higher than the measured values.

In Figure A-47 the extremely large 95% confidence intervals around the annual averages of the monitoring data indicate that many of the measured nickel concentrations were below the MQL at all monitors, ranging from 26% to 93%. The figure shows that the annual average model predictions are consistent with the measured values, with the sets of receptor concentrations within 4 km of each monitor substantially overlapping the wide 95% confidence intervals for the average of the measured values in all cases. Table 5 shows that the ratios of the mean concentration within 4 km to the mean measured

concentration ranged from 0.39 to 1.9. However, given the uncertainties of the measured values, the true ratios may be somewhat higher or lower.

Figure A-48 shows that at the monitor locations about 70% to 95% of the total concentration predictions are contributed by area sources. The remainder comes from a combination of onroad mobile, nonroad mobile, and point sources.

Figure A-49 shows that the set of concentration predictions from CALPUFF are much lower than the corresponding ASPEN predictions from the 1996 NATA national-scale assessment, due to much smaller contributions from area and nonroad sources. The smaller nonroad contribution indicates a change in the NONROAD model since the 1996 NATA national-scale assessment.

5.3.11 Polycyclic Organic Matter (POM) as 16-PAH

Figure A-50 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of POM as 16-PAH. The total boxplot indicates that the average prediction is about $0.3 \mu\text{g}/\text{m}^3$, the 95th percentile value about $0.6 \mu\text{g}/\text{m}^3$, and all the model predictions exceed the 1 per million risk level of $0.018 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to about $1.0 \mu\text{g}/\text{m}^3$.

The figure suggests that the concentrations are dominated by area sources (primarily residential wood combustion).

The isopleths in Figure A-51 show a pattern of elevated concentrations that appear to be correlated with residential land use.

The model-to-monitor comparison in Figure A-52 shows a consistent extreme overprediction, suggesting that the POM emissions in the PATA inventory may be overestimated. Table 5 shows that for all the monitor locations, the ratio of the annual average concentration predictions within 4 km to the mean measured concentration ranged from 6.0 to almost 21.

Figure A-53 shows that at all monitors except downtown the area source contribution is more than 95%, with about 90% of that coming from residential wood combustion. The area source contribution at the downtown monitor is about 65% with another 30% from special nonroad (primarily RMV).

In order to assess why the POM concentrations appear to be overestimated we examined the largest contributor to the concentration predictions: residential wood combustion. Since no residential wood combustion emissions were temporally allocated to the third quarter (June-August), we were able to examine the model performance for POM in the absence of residential wood combustion contributions by limiting our model-to-monitor comparison to the third quarter, as we did with benzene. (See Figure A-54.) The third quarter comparison shows much improved model performance, with the concentration predictions within 4 km of each monitor overlapping the 95% confidence intervals for the

monitored values in all cases. Note the relatively higher measured concentrations at the downtown and NW Post Office monitors are reflected in the model predictions. Table 5 shows that for the third quarter the ratios of the mean concentration within 4 km to the mean measured concentration ranged from 0.33 to 1.0. These findings suggest that POM emissions from residential wood combustion are likely to be overestimated in the PATA inventory.

Figure A-55 shows that the set of concentration predictions from CALPUFF are higher than the corresponding ASPEN predictions from the 1996 NATA national-scale assessment in the upper half of the distribution by a factor of 2 to 3. This discrepancy is due to the higher emission estimates for area sources (i.e., residential wood combustion) in the PATA inventory, in spite of lower point source emission estimates.

5.3.12 Tetrachloroethylene

Figure A-56 presents boxplots summarizing the CALPUFF predictions of annual average concentrations of tetrachloroethylene. The total boxplot indicates that the average prediction is about $0.20 \mu\text{g}/\text{m}^3$, the 95th percentile value about $0.25 \mu\text{g}/\text{m}^3$, and about half of the model predictions exceed the 1 per million risk level of $0.18 \mu\text{g}/\text{m}^3$. “Hot spot” concentration predictions range up to about $0.80 \mu\text{g}/\text{m}^3$.

The figure shows that the total concentration prediction is dominated by background concentrations, with additional contributions from point sources (primarily dry cleaners) and area sources (primarily consumer auto after-market products).

The isopleths in Figure A-57 show concentrations just over the 1 per million risk level broadly over the urbanized part of Multnomah County, and an elevated “hot spot” in the vicinity of a large dry cleaning operation in Washington County not far from the Beaverton monitor.

In Figure A-58 the large 95% confidence intervals around the annual averages for monitored values indicate a large number of concentrations below the MQL, ranging from 28% at the NW Post Office monitor to more than 90% at the other four monitors. The figure shows that the annual average concentration predictions are consistent with the measured values, with the sets of receptor concentrations within 4 km of each monitor substantially overlapping the 95% confidence intervals for the average of the measured values for all monitors except the NW Post Office. Table 5 shows that, except for the NW Post Office monitor, the ratios of the mean concentration within 4 km to the mean measured concentration ranged from 0.40 to 0.63. However, given the uncertainty of the measured values the true ratios may be somewhat higher or lower.

The ratio at the NW Post Office is 0.09. ODEQ has indicated that the NW Post Office monitor is located very near a dry cleaning facility, and therefore would qualify as a microscale monitor with respect to tetrachloroethylene. The CALPUFF modeling predictions are not designed to detect such microscale effects. Thus, the extreme underprediction of the tetrachloroethylene concentration at this monitor is expected.

Figure A-59 shows that at the monitor locations about 50% to 70% of the total concentration predictions are contributed by background. Point sources (primarily dry cleaners) make a substantial contribution only at the NW Post Office monitor. From about 10% to 30% is contributed by area sources.

Figure A-60 shows that the set of concentration predictions from CALPUFF are only about half as high as the corresponding ASPEN predictions from the 1996 NATA national-scale assessment, due to smaller contributions from area sources. Some of the difference in area source contributions reflects the shift of dry cleaners from the areas source category in NATA to the point source category in PATA. Another important difference is a substantially smaller estimate of tetrachloroethylene emissions from degreasing in PATA.

6. Summary and Recommendations

6.1 Model Performance

Model-to-monitor comparisons were made for 10 of the 12 target HAPs. Model predictions for six of these HAPs were consistent with measured values for all or nearly all monitors: 1,3-butadiene, arsenic, chloroform, chromium (4 out of 5 monitors), nickel, and tetrachloroethylene (4 out of 5 monitors). One chromium prediction overestimated the measured value, indicating a likely problem with chromium emissions estimates for surface coating of plastic parts. One tetrachloroethylene predictions underestimated the measured value, indicating a likely problem with the monitor placement.

Predictions for two HAPs, primary acetaldehyde and primary formaldehyde, were correctly found to be generally lower than monitored values that included both primary and secondary components.

Annual average predictions of both benzene and POM were substantially higher than measured values. Both has large contributions from residential wood combustion. Because predictions of both HAPs were in good agreement with measured values for the third quarter (June –August), and residential wood combustion is absent from the inventory during that time period, it suggests that emissions for residential wood combustion are likely to be overestimated in the PATA inventory.

6.2 Concentration Predictions Compared to Risk Levels

Concentration predictions were compared to risk levels provided by ODEQ, as explained in Section 5.2.1. Table 6 summarizes the results.

As the table shows concentration predictions for 6 of the target HAPs - primary acrolein, benzene, chloroform, chromium, diesel PM, and POM - exceed ODEQ's risk level at all model receptors.

Concentration predictions for 1,3-butadiene exceed ODEQ's risk level at almost all model receptors.

Concentration predictions for 3 other target HAPs - primary acetaldehyde, primary formaldehyde, and tetrachloroethylene - exceed ODEQ's risk levels at about half the model receptors.

Only about 20% of the receptors have concentration predictions exceeding ODEQ's risk level for arsenic, and fewer than 5% for nickel.

Table 6. Fraction of receptor concentration predictions exceeding risk concentrations.

Pollutant	Fraction of receptors exceeding risk level	Important Source Categories
1,3-Butadiene	95%	Onroad mobile, lawn and garden equip, RMV
Primary Acetaldehyde	50%*	Onroad mobile, construction equip
Primary Acrolein	100%*	Structural fires, onroad mobile, nonroad mobile
Arsenic	20%	Distillate oil combustion, natural gas combustion
Benzene	100%**	Onroad mobile, residential wood combustion
Chloroform	100%	Background
Chromium	100%	Surface coating plastic parts
Diesel PM	100%	Construction equip, onroad mobile, RMV
Primary Formaldehyde	50%*	Onroad mobile, construction equip, RR, RMV, airports
Nickel	<5%	Residual oil combustion, natural gas combustion
POM	100%**	Residential wood combustion
Tetrachloroethylene	50%	Background, dry cleaners, consumer products

* Model predictions address only the primary component of this pollutant. Total concentrations are expected to be substantially higher.

** Annual average model predictions are higher than measured values, suggesting that actual concentrations are likely to be lower than the predictions. However, all measured values also exceeded the risk concentrations.

6.3 Important Emission Sources

Table 6 also summarizes which emission sources have the most influence on model concentration predictions.

As the table shows onroad mobile sources are the largest contributors to 1,3-butadiene, primary acetaldehyde, benzene, and primary formaldehyde concentration predictions. They are also important contributors the primary acrolein and diesel PM concentration predictions.

Construction equipment was the largest contributor to concentration predictions of diesel PM, and an important contributor to concentration predictions of primary acetaldehyde and primary formaldehyde.

RMVs are important contributors to concentration predictions of 1,3-butadiene, diesel PM, and primary formaldehyde.

Structural fires are the largest contributors to primary acrolein concentration predictions.

Background concentrations were the largest contributors to chloroform and tetrachloroethylene concentration predictions.

Other important contributors to concentration predictions are lawn and garden equipment (1,3-butadiene), railroads (primary formaldehyde), airports (primary formaldehyde), dry cleaners (tetrachloroethylene), and consumer automobile after-market products (tetrachloroethylene).

Surface coating of plastic parts was the largest contributor to concentration predictions of chromium. However, the model performance evaluation suggests that emissions from this source category may be overestimated.

Similarly, residential wood combustion was the largest contributor to POM concentration predictions and an important contributor to benzene concentration predictions; but the model performance evaluation suggests that emissions from this source category may be overestimated.

Oil combustion and natural gas combustion are the largest contributors to arsenic and nickel concentrations predictions.

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