

Steps in Conducting an Urban Air Toxics Assessment: Methodology for Converting Emission Inventories into Model-Ready Input Files

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ABSTRACT

The Clean Air Act Amendments of 1990 define two classes of pollutants: criteria pollutants and hazardous air pollutants (HAPs, otherwise known as air toxics). Criteria pollutants are regulated with standards that govern their ambient levels. An extensive amount of health and welfare information relating to criteria pollutants has been compiled and monitoring networks have been in place for decades.

In contrast, little information is available on ambient concentrations of air toxics. There are 188 listed air toxics, and they come from both natural and man-made sources. EPA has classified many of these pollutants as known, probable or possible human carcinogens, and many are associated with other adverse health effects such as reproductive effects, developmental defects and neurological effects¹.

In the fall of 1999, the Environmental Protection Division (EPD) of the Denver Department of Environmental Health began conducting an urban air toxics assessment for the Denver area. The assessment was designed to include air dispersion modeling, historical monitoring data, and emission inventory data for various categories of sources, including stationary, mobile and area sources.

Emissions for mobile and area sources were obtained from the 1996 National Toxics Inventory (NTI). Stationary source emissions were obtained from the Colorado Department of Health and Environment (CDPHE). A significant amount of processing is required to convert these inventories into model-ready input files. The results presented here show how different methodologies can affect the modeled concentrations.

INTRODUCTION

EPD's need to complete an air toxics assessment is due to 1990 amendments to the zoning provisions of the Denver Revised Municipal Code. The changes apply to new or expanding industrial facilities and established criteria under which city agencies must complete reviews. Specifically, all proposed conditional uses must be reviewed on the basis of potential environmental problems and/or detrimental effects for numerous issues that include:

- Air pollution caused by a stationary source;
- An evaluation of undue concentration of uses that create environmental problems and external effects listed in the ordinance is required.

To adequately address the issue of undue concentrations of air pollution, EPD needed to establish existing baseline concentrations in the Denver area. Air toxics monitors are scarce and are not usually located near major industries. Through the use of air dispersion models, an understanding of how a facility's emissions impact certain receptors can be estimated. In urban areas, similar pollutants are emitted from a variety of sources so in order to fully estimate the impact from a new or expanding facility's emissions, the existing concentrations have to be taken into account. By understanding the existing concentrations, estimates of the risks associated with the existing concentrations can be inferred; then the additional risk from the emissions of new or expanding facilities can be evaluated.

This assessment began at about the same time as the U.S. Environmental Protection Agency's (USEPA) National Air Toxics Assessment (NATA). In fact, the Nation Toxics Inventory (NTI) was developed by the USEPA in order to conduct national scale air dispersion modeling. The mobile and area source air toxics emission inventories developed for the NATA were also used in EPD's

assessment. Whereas the USEPA recommends ambient concentrations and estimated risks from the NATA not be evaluated below the county level, EPD's intent was to perform a more refined assessment with locally available data.

Significant use of a Geographic Information System (GIS) was required to perform this assessment. The GIS greatly simplifies tasks associated with allocating emissions and evaluating model predictions. In addition, tasks such as geocoding and assigning elevation data to emission sources and receptors are made much easier with the use of a GIS. To the end user, the data made available in a GIS is more easily understood when viewed against output from conventional plotting packages. GIS data can be overlaid with themes such as highways, county boundaries, and landmarks. ESRI's ArcVIEW was the GIS used for this assessment.

The air dispersion modeling portion of the assessment was performed using the Industrial Source Complex model (ISCST3; version 99155). An excellent reference titled, *Air Dispersion Modeling of Toxic Pollutants in Urban Areas: Guidance, Methodology and Example Applications*, is available from the USEPA². This document details the data that are needed to conduct an urban air toxics assessment.

BODY

Emissions Processing

Each source category database requires a significant amount of processing. The methods presented below cover the major issues associated with performing an urban air toxics analysis that are not explained in the literature. It is assumed that the reader is an advanced or expert user of spreadsheet, database and word processing software.

Stationary Source Database

CDPHE provided stationary (i.e. point) source information in a Microsoft Access database. Information pertaining to emissions of individual pollutants, stack parameters, and hours of operation were included in the database. For stationary sources, emissions of individual air toxics were provided with totals as low as 50 pounds per year. Most of the HAP sources in the stationary source database are not major sources, that is they do not emit more than 10 tons per year (TPY) of any individual HAP or more than 25 TPY of a combination of HAPs.

At a minimum, emissions and stack parameters are needed to run an air dispersion model. When stack parameters such as stack height, stack diameter, stack gas exit temperature, and stack gas exit velocity are not included, default values are available based on source classification code (SCC). The default values used in this assessment were obtained from the USEPA's urban air toxics modeling guidance². Where default values were not provided for a specific SCC, the Aerometric Information Retrieval System (AIRS) was searched for additional data. As of February 2001, stack parameters are no longer available through the AIRSData web site; this data will have to be obtained from the state agency responsible for maintaining the database. In cases where no stack data were available, professional judgement was utilized.

The stationary source database also contained information pertaining to facility location in both the universal transverse mercator (UTM) and latitude/longitude coordinate systems. As a check, EPD used the GIS to geocode the location of each facility based on the facility address. Using spreadsheet software, EPD's geocoded locations were then compared with the coordinates provided in the database. Where the differences exceeded 100 feet (30.5m), the coordinates were further verified using the GIS and high-resolution street maps. Geocoding has errors associated with it, and is dependent on the quality of the road theme that is utilized to match addresses. EPD's geocoding often had errors associated with it, but in about 20 percent of the cases the coordinates provided in the database were found to be in error. It is assumed that geocoding was also used to obtain the coordinates provided in the stationary source database. While this was a time consuming process, it resulted in increased confidence in predicted model impacts.

Unfortunately, location data is not available for each individual point or stack at a facility. It is therefore necessary to model each facility's emissions as emanating from a single point. This introduces

a degree of uncertainty into the modeling that cannot realistically be eliminated, especially when modeling over an entire urban area. For facilities where multiple stacks are spread across the property, modeling the facility emissions as an area or volume source is an option. However, the amount of work necessary to obtain property boundaries and coordinates is prohibitive for an urban scale assessment. It is expected that by modeling each facility's emissions from a single point, any significant impacts would be observed in the results. If the results warrant, a more refined microscale analysis could be performed in predicted "hot spot" areas. In these cases, more detailed data could be obtained from GIS coverages or aerial photography.

Since emissions from each facility were modeled from a single point, appropriate stack parameters should be utilized. For EPD's assessment, weighted stack parameters were developed. First, the total facility emissions were calculated. Then, the total emissions from each stack were calculated. The fraction of each stack's emissions to the facility emissions was then calculated. Each stack's parameters were then multiplied by this fraction and the resulting multiples were then summed for each stack parameter to obtain the weighted stack parameters. For example, assume that a facility has two stacks. Stack 1 has a height of 100 m and stack 2 has a height of 50 m. If 75 percent of the facility's emissions are emitted from stack 1, then the weighted stack height is calculated as shown in Equation 1. The same process is applied when calculating the other stack parameters.

$$\text{Equation (1) Weighted Stack Height} = 100\text{m} \times 0.75 + 50\text{m} \times 0.25 = 87.5\text{m}$$

Many stationary sources do not operate on a continuous basis. Facilities such as dry cleaners and autobody repair shops usually operate 8-10 hours per day. Emissions from these facilities generally occur when meteorological conditions for dispersion are more favorable (i.e. daytime hours). Emission factors should be developed so as to simulate conditions that are as representative of the real world as possible. The stationary source database contained operating schedule information such as percent operation by season, number of days per week, and the number of hours per day and/or year for each stack/point. Based on this information, emission factors were developed for each facility. The emission factors developed for EPD's assessment were by season and hour-of-day. At the time when the emission factors were being developed, the option by season, hour-of-day, and day-of-week was not available in ISCST3. Common spreadsheet software can be used to calculate the emission factors.

The process used to develop the seasonal emission factors is summarized below:

- 1) Calculate the weighted seasonal operating load (WSOL) for each facility. This process is identical to that for which weighted stack parameters were developed, namely the ratio of each stack's emissions to the total facility emissions is multiplied by the seasonal operating percentage of each stack. These values are then summed to obtain the facility weighted seasonal operating load; this value can be expressed as a fraction or percentage.
- 2) Divide the weighted seasonal operating load by 25 percent (or 0.25); four seasons per year.
- 3) Divide the number of days per season (90 for winter, 92 for spring and summer, 91 for fall) by 365 (or 366 for leap year), then divide again by 0.25. This value should be close to 1.
- 4) Divide the value obtained in step 2 by the value obtained in step 3. This is the seasonal emission factor.

Emission factors for each hour of the day must also be calculated. This is done using the number of operating hours per day for each facility. Since the actual hours are not specified (i.e. 8 am – 5 pm), the modeler must make some assumptions. EPD assumed the following: an 8-hour workday began at 9 am, any workday longer than 12 hours began at 6 am. For any time frame less than 8 hours, operating hours were usually centered on the noon hour. The process used to develop the emission factors by season and hour of day is summarized below:

- 1) In the same spreadsheet used to calculate the seasonal emission factors, paste the number of hours of operation for each facility. In an immediately adjacent blank column, divide 24 hours by the number of hours each facility operates per day. This value is the hourly emission factor.

- 2) Setup 24 columns, one for each hour of the day, to be populated with the flag values 1 or 0. In the first row of each of these columns, enter formulas or logic statements to populate the cells with a 1 or 0, meaning the facility is emitting at that hour (1) or is not emitting at that hour (0). Base this on the number of hours that the facility operates per day. For example, if a facility operates 8 hours per day (9 am – 5 pm), then in the columns for hours 1 through 9, a logic statement would be entered that sets the cell value to 0 if operating hours per day is less than 8.
- 3) Setup 96 additional columns that will contain the emission factors by season AND hour of day (24 hours/day * 4 seasons). In each column, enter a formula to calculate the emission factor. The formula should be a product of the seasonal emission factor (see Step 4 from calculating the seasonal emission factor), the hourly emission factor (see Step 1 above), and the flag value of 1 or 0 for the corresponding hour of the day.

The emission factors can then be rearranged in a separate spreadsheet to put them into a model-ready format.

In many cases, EPD rearranged values calculated in spreadsheets to fit the format the model requires. EPD also added the appropriate model cards or commands such as the SO and RE commands that the ISC3ST model needs to run. These spreadsheets were then saved in a format in which they could be opened with word processing software and pasted into the model input file with little additional work. It is recommended that spreadsheet files created for this purpose be saved as comma-delimited files. Doing so allows the modeler to open each file in the word processor, then search for and replace all commas with a single space, then copy and paste that portion of the input file into the full model input file.

Mobile and Area Sources

The mobile and area source inventories obtained from the NTI have similar formats, with emissions of individual HAPs provided at the county level. However, emissions within a county are not uniform. To allocate county-level emissions to smaller areas such as census tracts or grid cells, activity data or other surrogates are needed. Population, population density, and vehicle miles traveled (VMT) are all examples of emissions surrogates. In addition to providing emissions at the county level, emissions are also broken down by source category. For mobile source emissions, source categories include light-duty gasoline vehicles, heavy-duty diesel vehicles, railroads, etc. Area source categories include wood burning, consumer products usage, and architectural surface coatings to name a few. Source category information is helpful in choosing the appropriate surrogate to allocate emissions to the sub-county level.

EPD had to decide what geographic sub-unit it would allocate county level emissions to. Previous modeling studies have used uniform grid cells of 1, 2, or 4 km². The main drawback to using this method is that you will inevitably have overlap with the county boundaries, especially with irregularly shaped counties such as Denver.

With the emergence of GIS, it was decided that emissions should be allocated to either census tracts or census block groups. One advantage to this is that census polygons are contained within the county boundary, i.e. there is no overlap. Another advantage is that census polygons are smaller in densely populated areas, which eliminates the need for nested grids to better define emissions and/or concentrations in these areas. In addition, important statistics related to population and demographics are contained in the census coverages, which become important when evaluating pollution impacts on various socioeconomic classes. The main disadvantage to using census polygons is that significantly more processing is required to obtain and perform QA/QC on the polygon vertices.

There are 556 census tracts in Metro Denver, 181 of which are in Denver County. There are 1800 census block groups in Metro Denver, 637 of which are in Denver County. Of the 181 census tracts in Denver County, 75 (41 percent) have an area of less than 1 km². Of the 637 census block groups in Denver County, 596 (93 percent) have an area less than 1 km². It was decided that emissions would be allocated to census block groups to achieve the highest resolution possible.

Mobile source emissions were summed for similar source categories. For instance, emissions for on-road vehicles were summed together independent of which fuel they used. The same was done for off-road vehicles, two and four stroke gasoline engines, railroads, and airport emissions. Different surrogates will be utilized to allocate county level emissions from these source categories.

For on-road mobile sources, emissions were allocated using vehicle miles traveled (VMT) data developed by the Denver Regional Council of Governments (DRCOG). This data consists of a network of road links with vehicle volume and VMT data broken down by morning peak, afternoon peak, and non-peak commute hours. Data such as link length and road class are also included. Most metropolitan areas have a Regional Council of Governments who are most likely responsible for creating travel demand models. Without specific VMT data, one could allocate emissions based on road types such as freeway, principal arterial, or local. Allocating emissions in this way will likely require that several additional assumptions be made.

To allocate on-road mobile source emissions using VMT data, the census block group theme and the VMT coverage were overlaid in the GIS. An intersect operation was then performed on the VMT line coverage using the census block group polygon borders. This operation eliminates overshoots and undershoots of the VMT line coverage and allows the modeler to calculate the exact VMT in each census polygon. The length of each link was then re-calculated to account for changes made by the intersect operation. Next, the total daily VMT was calculated for each census block group by multiplying the road link length and total daily volume. Ratios of block group VMT to county VMT were then calculated. The VMT ratio acts as the surrogate used to allocate county level emissions to each census block group.

One concern was that if the emissions grid resolution becomes too fine, there is a chance that many of the grid cells will not intersect with the VMT coverage and therefore have “zero” emissions allocated to them. However, at the census block group level of resolution, only 15 out of 637 census block groups (2.4 percent) did not have VMT data assigned to them. Most of the block groups with no data were sliver polygons, encompassing very little area.

Another concern stems from the fact that the VMT coverage did not completely cover all counties in the modeling domain, just the metropolitan portion of each county. Here, estimates had to be made regarding the percentage of emissions that occurred inside and outside the VMT coverage area in each county. Complete coverage exists for Denver County, but for the other counties 88-99 percent of the on-road mobile emissions were assumed to occur within the VMT coverage area. The emissions allocation procedures were calculated using spreadsheets. This allows the user to change assumptions on the fly with automatic updates to all of the necessary cells.

Off-road mobile source emissions were allocated using population, inverse population density, or a combination of VMT data and inverse population density. It is assumed that in Denver County the majority of off-road diesel emissions are produced by construction equipment. It is also assumed that the majority of the construction occurs on or near roadways and the more traveled roadways have more frequent construction activity. The remaining off-road diesel emissions are attributable to agricultural equipment, which is assumed to occur in areas with low population densities. The percentage of off-road emissions attributable to construction and agricultural equipment varies between counties. For this assessment, it was assumed that 90 percent of off-road emissions in Denver County were attributable to construction equipment; for the other counties, which have more rural land, it was assumed 75 percent of emissions were attributable to construction equipment. Taking into account the fact the VMT coverage did not completely cover all counties other than Denver, it was assumed that 80-99 percent of the off-road emissions occurred within the VMT coverage area.

For construction equipment emissions, a surrogate was developed that was weighted 2/3 by VMT data and the remaining 1/3 by inverse population density. The portion for inverse population density takes into account the fact that construction activity also occurs in areas with low population density. For agricultural emissions, only inverse population density was used as a surrogate. It is assumed that all off-road diesel emissions originate from construction and agricultural equipment.

Two and four stroke gasoline engines also contribute to off-road mobile source emissions. The fraction of off-road emissions attributed to gasoline or diesel engines can be calculated for each HAP in

each county. The fractions were derived by summing the county-level emissions from gasoline or diesel engines, then dividing by the county-level emissions from all off-road mobile sources. For example, 89 percent of off-road emissions of 1,3-Butadiene in Denver County emanate from gasoline engines, whereas 84 percent of off-road formaldehyde emissions emanate from diesel engines. For off-road emissions from gasoline engines, the ratio of the census block group population to the county population is the surrogate used to spatially allocate the county-level emissions. This is based on the assumption that the majority of off-road gasoline engine emissions emanate from landscaping equipment such as lawnmowers, weed-trimmers and leaf blowers and tend to be used mostly at private residences.

Once the various surrogate ratios have been calculated and tabulated in the spreadsheet, the off-road emission rates for each census block group can be calculated as follows:

- 1) Multiply the ratio of the block group-to-county population by the emission rate of each HAP from gasoline engine emissions.
- 2) Add to that the product of the ratio of the block group-to-county inverse population density and the emission rate of each HAP from agricultural diesel engines.
- 3) Add the product of the ratio of the combination VMT/inverse population density surrogate for each block group and the emission rate of each HAP from diesel construction activity.

Off-road emissions from railroads are also estimated in the NTI. The process for allocating railroad emissions is much like the process used to allocate on-road mobile source emissions. Using the GIS, the length of rail line in each census block group was calculated using the intersect method previously mentioned. Sum the length of rail lines in each county and calculate the block group-to-county ratio. Multiply the ratio for each block group by the county average emission rate to spatially allocate the county level railroad emissions.

Off-road emissions from airports are also estimated for each county. In Metro Denver, Jefferson and Arapahoe Counties have busy, general aviation type airports. However, airport emissions estimates were only provided for Denver County which is home to Denver International Airport (DIA), the region's commercial airport. Airport emissions were not allocated to the census block groups; they were contained within the airport property boundary obtained using the GIS.

When emission rates have been calculated for each block group for each source category (i.e. area, on-road mobile, off-road mobile and railroad), sum the totals and calculate the emission flux by dividing by the block group area (m^2). The ISC3ST model requires that the emission flux be in units of grams per second per square meter ($g/[sec*m^2]$).

As with stationary source emissions, most area and mobile source emissions are not evenly distributed throughout the day and emission factors can be developed to temporally allocate emissions. For EPD's urban air toxics assessment, emission factors were developed for season and hour of day. The first step was to gather any data available regarding activity patterns. EPD was able to utilize 1997-1998 survey data of driving habits published by DRCOG³. This data included household surveys and roadside surveys along major roads leading into and out of Metro Denver. Of particular note, the DRCOG survey showed two distinct daily travel peaks, one well-defined peak between 6-9 am and another broader peak between 2-6 pm, corresponding to morning and afternoon "rush hours".

The mobile and area source emission factors were calculated in a spreadsheet. First, information pertaining to seasonal emissions must be calculated. In the absence of specific data, it was assumed that emissions in winter, spring and fall each accounted for 26 percent of the annual total, while only 22 percent of annual emissions occurred during the summer months. The reasons for the lower summer total are 1) school is not in session and 2) increased use of alternative modes of transportation such as bicycling and walking. To calculate the seasonal emission factors, multiply the fraction of emissions that occur during each season by 365 and divide by the number of days per season (90 in winter, 92 in spring and summer and 91 in fall).

To calculate emission factors for the hour of day, some assumptions need to be made unless more specific data is available. EPD estimates that 70 percent of on-road mobile source emissions occur between the hours of 6 am and 8 pm, while 20 percent of emissions occur between 8 pm and 1 am, with the remaining 10 percent occurring between 1 am and 6 am. In addition, of the 6 am to 8 pm emissions 65 percent are assumed to occur during the "rush hour" times previously mentioned.

In the spreadsheet, 24 different columns were setup to calculate hourly emission factors. To calculate the hourly emission factor for hour seven (6-7 am), multiply the fraction of emissions that occur between 6 am and 8 pm by the fraction of emissions that occur during rush hours, then divide by the number of rush hours, which in EPD's assessment constitutes seven total hours. No distinction was made to differentiate between emissions during morning and afternoon rush hours. Check the calculations to confirm that the emission factors during rush hours are higher than daylight non-rush hours, which in turn are higher than late evening emission factors. Finally, multiply each seasonal emission factor by the hourly emission factors and then by 24 (number of hours per day) to obtain the on-road mobile source emission factors by season and hour of day.

Emission factors for off-road mobile and area sources were assumed to be the same, that is most activity from these source categories occurs during hours when people are awake, or during daylight hours in the summer. An exception to this is for residential and commercial heating due to wood burning in the area source inventory. Seasonal emission factors were calculated as follows:

- 1) Specify the seasonal fraction of annual emissions. For EPD's assessment, it was estimated that 14 percent of area and off-road source emissions occur during the winter season, 20 percent occur during spring, 34 percent occur during summer and 32 percent occur during the fall.
- 2) Multiply the seasonal fraction of emissions by 365 and divide by the number of days per season. This is the seasonal emission factor.
- 3) Calculate the hourly emission factor. It was estimated that 90 percent of daily emissions occur between 6 am and 10 pm and the remaining 10 percent occur between 10 pm and 6 am. To calculate the emission factor for hour seven, multiply the fraction of emissions that occur between 6 am and 10 pm (0.9), and divide by the number of hours (16) in that timeframe.
- 4) Multiply the seasonal emission factor by the hourly emission factor then multiply by 24 to obtain the emission factor by season and hour of day.

Emissions of HAPs emitted from heating due to wood burning can be calculated in the same way as other area source emission factors. The modeler must estimate the seasonal fraction of annual emissions and also estimate the fraction of daily emissions that occur during specific time periods. In Metro Denver, wood burning restrictions are in place from November 1st through March 31st below 7500 feet. The western sections of Jefferson and Boulder Counties have populated areas above 7500 feet. Therefore different emission factors were calculated for Jefferson and Boulder Counties to take into account the fact that some areas are not subject to wood burning restrictions.

No emission factors were developed for railroad or airport sources. Emissions were assumed to be constant throughout the day. While this is probably not the case for airport emissions, the emission totals are generally small as compared to the county-level emissions from all non-road source categories and should not significantly affect the model results. If modeling shows elevated concentrations in the vicinity of the airport, a more detailed assessment can be performed.

Once emission factors have been developed for on-road, off-road, area, and railroad sources, composite emission factors can then be determined. The composite emission factors are used to reflect the total emissions in each block group so that the dispersion model need only be run one time. First, calculate the fraction of emissions of each HAP from on-road, off-road, area, and railroad sources in each block group. While composite emission factors can be developed for each block group, EPD decided to develop county average composite emission factors. This minimizes the file size of both the spreadsheet and model input files and is expected to have minimal effects on the model predictions.

Next, calculate the average emissions fraction for each source category across all block groups in each county. In a separate worksheet, designate four columns for each pollutant that corresponds to the number of seasons. Using formulas, calculate the composite emission factor by season and hour of day by referencing the values previously calculated. Equation 2 details an example calculation used to calculate the wintertime composite emission factor for benzene during hour one (12-1 am).

$$\text{Equation (2) } \text{Compos_EF_win_BZ}_{\text{Hour1}} = \text{Avg_Frac_BZ_onroad} * \text{EF_onroad_win}_{\text{Hour1}} + \\ \text{Avg_Frac_BZ_offroad} * \text{EF_offroad_win}_{\text{Hour1}} + \\ \text{Avg_Frac_BZ_area} * \text{EF_area_win}_{\text{Hour1}} + \\ \text{Avg_Frac_BZ_railroad}$$

where

$\text{Compos_EF_win_BZ}_{\text{Hour1}}$ = composite emission factor for benzene in winter during hour one (12-1 am)

Avg_Frac_BZ_ * = county average emission fraction of benzene from each source category

$\text{EF_}\text{*}\text{_win}_{\text{Hour1}}$ = emission factor for winter season during hour one for each source category

Note that an emission factor was not calculated for railroads and is therefore not included as part of the equation. The same procedure must be repeated for each season and each hour of the day for each county.

Additional Model Inputs

In addition to proper spatial and temporal allocation of emissions, a number of other factors should be incorporated into the model input files. For gaseous HAPs, information pertaining to reactivity or half-life can be included as can solubility, liquid scavenging rates, and the Henry's Law coefficient, all of which affect deposition rates. Most of this information can be found on the internet or in the urban air toxics modeling guidance². For particulate HAPs, information pertaining to particle mass fractions and bulk densities should also be included.

Based on the choice to allocate emissions to census block groups, EPD chose to use the census block group centroids as the model receptors. While the modeling could have been performed using fewer receptors, it was felt that using census block group centroids would minimize the chances of missing high concentrations, especially in the vicinity of point sources. QA/QC was performed on each centroid to ensure that no receptor was closer than 100 m to the nearest point source, which is recommended in the ISC3 user's guide⁴. This resulted in about five percent of block group centroids being displaced. There are residences that are closer to emission sources than are the block group centroids, so it is possible that actual concentrations are higher than predicted concentrations in some areas.

With the large number of sources and receptors required for an urban air toxics assessment, model run times can become excessive. The Sampled Chronological Input Model (SCIM) option was introduced with ISC3ST version 99155. The SCIM option gives the model the ability to sample only one hour of meteorological data per day. The SCIM option is only available when calculating annual average concentrations and is recommended only for multi-year model runs⁵. For EPD's assessment, meteorological data was sampled every 25 hours. Using five years of meteorological data results in each hour of the day being sampled almost 1800 times. This should adequately capture diurnal patterns. EPA tests showed that the SCIM option worked better for area sources than for point sources⁵. Using the SCIM option, it takes approximately 12 hours to model one pollutant for Metro Denver on a workstation with a 1-gigahertz processor. Model runs include approximately 1700 polygon area sources, 825 receptors and varying numbers of point sources up to 825 point sources for benzene.

One of the many benefits to using a GIS is that digital elevation models (DEMs) can be imported to obtain terrain elevations. Using the DEMs, elevations can easily be assigned to polygon vertices, point sources and receptors. Most DEMs are available for free from the U.S. Geological Survey (USGS) and other GIS data outlets on the internet. EPD's assessment utilized 7.5 minute (1:24,000 scale) DEMs for the entire modeling domain.

Model Predictions

The surrogate used to allocate mobile source emissions to the census block groups was the factor most expected to influence the modeling results. Before the DRCOG VMT data became available, mobile source emissions were spatially allocated using the number of roadway miles in each census tract (not block group). On-road mobile sources are the predominant source of benzene, with much higher contributions from gasoline versus diesel engines. Figure 1 shows the results using the roadway miles surrogate. Note that emissions from all sources are reflected in the results, but on-road mobile source emissions are the predominant contributor to the overall concentrations. The results show that concentrations tend to be fairly homogeneous across downtown Denver, where there are high road densities. This surrogate appears to fail in north Denver near the two southernmost benzene monitors. Another feature to note is that the highest concentrations do not occur in the immediate vicinity of major interstates passing through Denver.

Figure 1. Predicted benzene concentrations ($\mu\text{g}/\text{m}^3$) using roadway miles in each census tract as a surrogate for mobile source emissions. Monitored annual avg. concentrations are shown in text callouts.

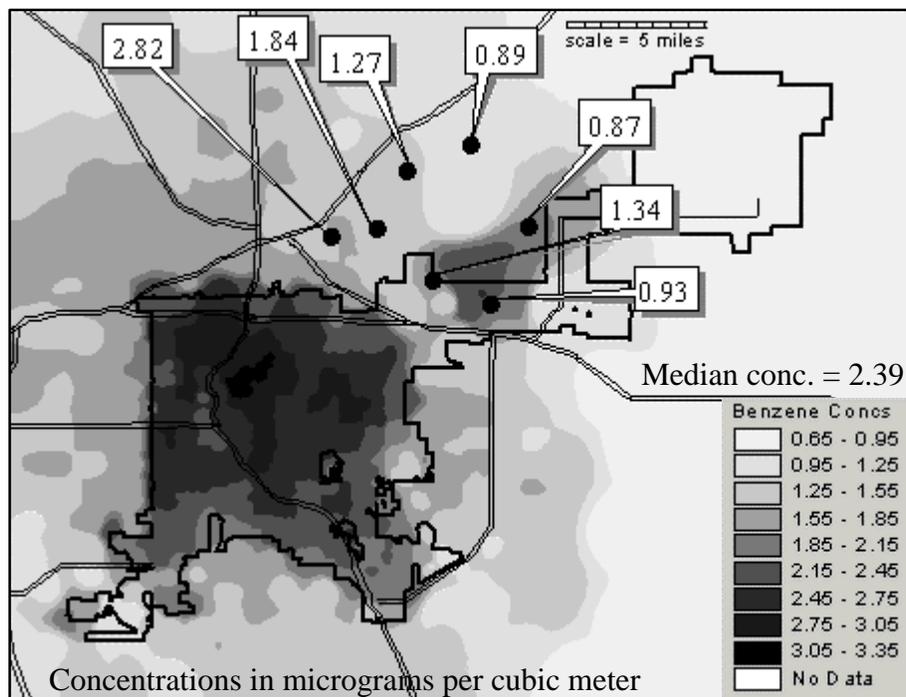
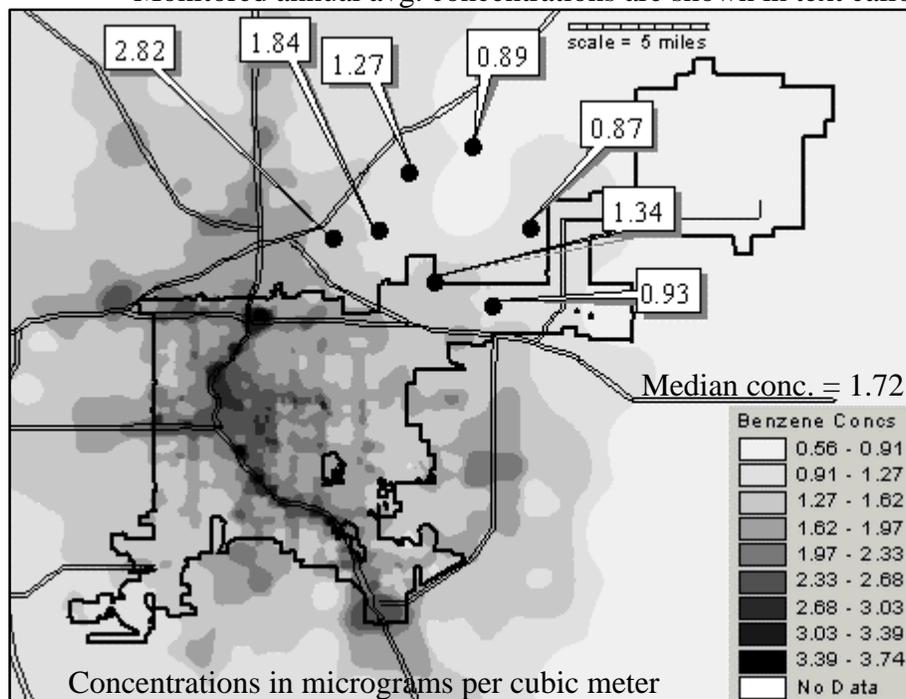


Figure 2 shows the results obtained using the VMT data in each census block group. The spatial distribution of benzene concentrations more closely resembles the distribution of the monitored concentrations. All of the predicted concentrations are within a factor of two of the monitored concentrations. Notice also that the highest concentrations are in the vicinity of major roadways with the highest VMT totals. Several of the major arterials running north-south and east-west through Denver area also evident in Figure 2. The median concentration drops from $2.39 \mu\text{g}/\text{m}^3$ in Figure 1 to $1.72 \mu\text{g}/\text{m}^3$ in Figure 2, however the maximum concentration in Figure 2 increases by roughly 10 percent and the location of the maximum concentration is displaced two miles to the north.

If VMT data are not available, spatially allocating mobile source emissions by lengths of each road class or road type might prove to be more accurate than roadway miles. More weight could be given to class 1 roads (freeways), whereas class 8 (local) roads would be given the least weight. This would introduce additional assumptions but would probably lead to better predictions.

Figure 2. Predicted benzene concentrations ($\mu\text{g}/\text{m}^3$) using VMT in each census block group as a surrogate for mobile source emissions. Monitored annual avg. concentrations are shown in text callouts.



It would be conservative to assume that emissions are evenly distributed throughout the day, hence no emission factors are required. In reality, emissions are not constant and are more heavily emitted during the daytime hours. Meteorological conditions for dispersion such as stability and wind speed are most often favorable during the daytime hours. It is therefore expected that incorporating emission factors into the model will generate lower mean concentrations than if no emission factors are used. Table 1 lists the concentration statistics for model runs for benzene with and without emission factors. The results in Table 1 reflect emissions from all source categories. As expected, predicted mean, median and maximum concentrations are lower by 13 percent whereas predicted minimum concentrations only differ by two percent.

Table 1. Predicted benzene concentration statistics with and without the inclusion of emission factors.

Scenario	Concentrations in micrograms per cubic meter			
	Mean	Median	Maximum	Minimum
With Emission Factors	1.79	1.72	3.74	0.56
Without Emission Factors	2.06	1.98	4.29	0.57

With GIS technology it is possible to model emissions from the roadways themselves instead of from census block groups or any other type of grid cell. This method would initially require an enormous amount of time be spent on obtaining correct vertices that define the polygons. This method would also make model run times prohibitive; as many as 20,000 road links are present in the VMT coverage which in turn would equate to 20,000 polygons being modeled. However, this method might be feasible if modeling “hot spot” areas on a much smaller scale. Figure 3 shows the predicted concentrations for benzene when emissions emanate from roadway polygons instead of from the census block group polygons. Road links in three census block groups are shown and each road segment was modeled as a 20 m wide polygon. The light colored receptor in the center of the figure is 40 m north of a road link that carries approximately 84,000 vehicles per day. The receptor 650 m to the northeast is only 5 m from the nearest road link but carries only 2,200 vehicles per day.

Figure 3. Predicted benzene concentrations ($\mu\text{g}/\text{m}^3$) when emissions are modeled as emanating from the roadway polygons shown. Filled circles indicate location of each model receptor.

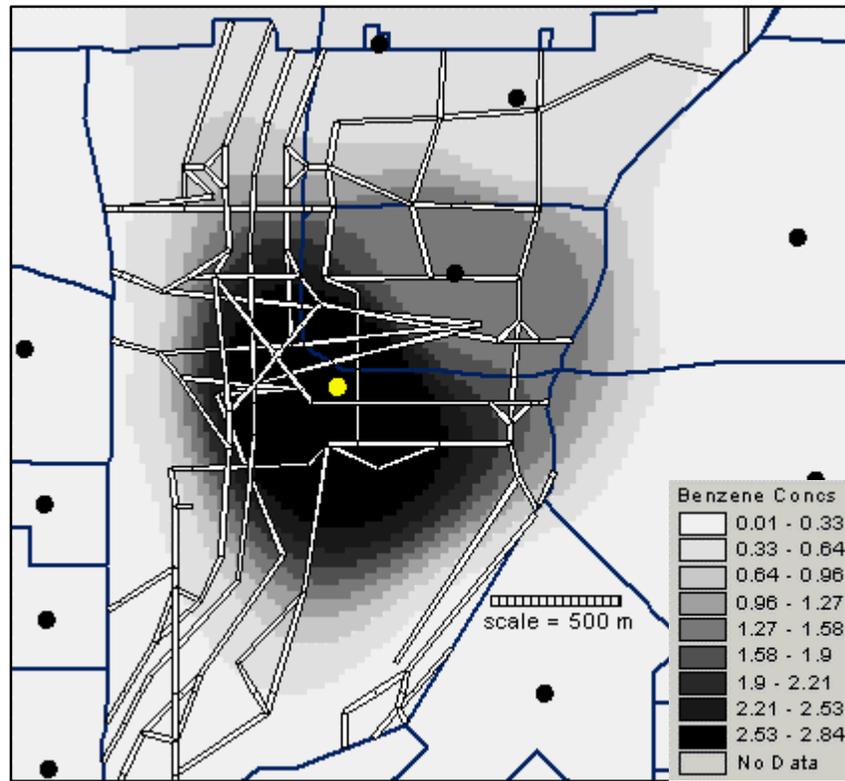


Figure 4. Predicted benzene concentrations ($\mu\text{g}/\text{m}^3$) when emissions are modeled as emanating from the census polygons shown. Filled circles indicate location of each model receptor.

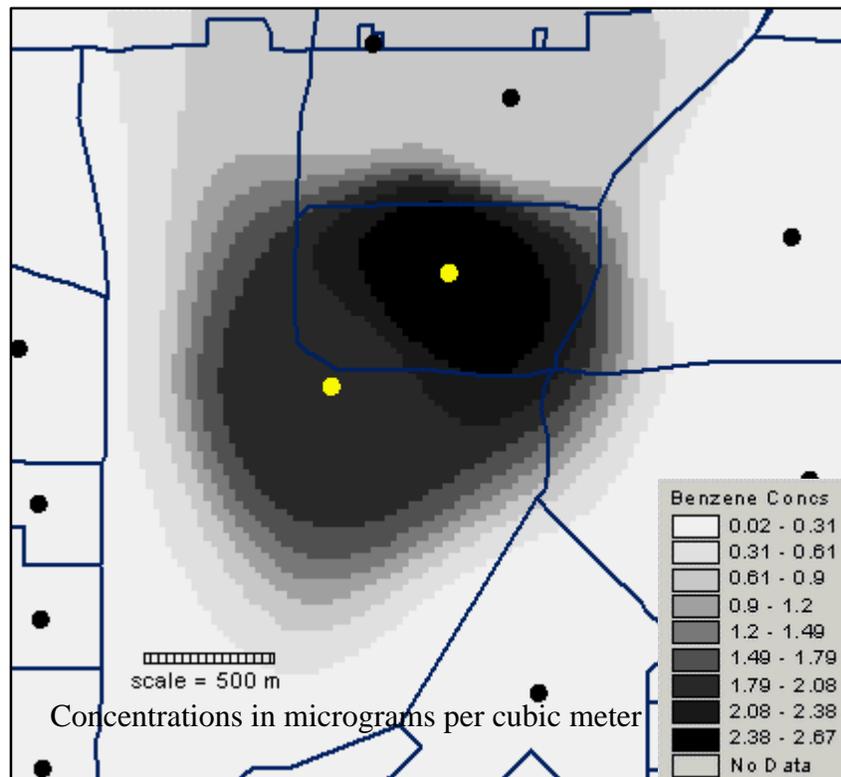


Figure 4 shows the predicted concentrations for benzene when emissions are assumed to emanate over the entire census block group. The location of the predicted maximum concentration is farther northeast and decreases by 6 percent as compared to Figure 3. This is expected as emissions across an entire block group will be more dilute than emissions from roadway polygons. Further analysis shows that the largest block group polygon is 4.8 times larger than the smallest polygon. VMT in the largest polygon is 4.3 times greater than VMT in the smallest polygon. Therefore, the smallest block group polygon will have a higher emission flux that consequently results in the highest predicted concentration at its block group centroid. While higher concentrations are expected closer to the roadway, allocating emissions to the census block groups is meant to capture the approximate exposures of people living within the area. It is important to point out that the VMT coverage used in this assessment is not meant to portray the exact number or location of all roads. In reality, there are many more road links spread throughout the block groups. Therefore, allocating emissions to roadway polygons in the VMT coverage would not necessarily provide a more accurate representation of real world concentrations.

CONCLUSIONS

Through the use of a GIS and commercially available spreadsheet, database, and word processing software, emissions inventories can be processed into a model ready input format for urban air dispersion models. While the processing of these inventories initially requires a significant time investment, future processing of updated inventories can be made much simpler. Local data can be incorporated into the emissions processing which results in increased confidence in air dispersion model results.

The most important component incorporated into the EPD assessment was the use of VMT data as a surrogate to spatially allocate mobile source emissions. The modeling indicates that in Metro Denver, much of the risk associated with certain hazardous air pollutants is due to mobile sources. Accurately allocating these emissions is essential to obtaining an accurate representation of where the potential risks are the greatest. In the absence of VMT data, it is possible to allocate mobile source emissions based on road type or road class. Most metropolitan areas should have VMT data available from their Regional Council of Governments, state government, or local planning agency.

Emission factors are important in capturing the temporal emissions of pollutants. Assuming that emissions from all sources are constant throughout the day will likely lead to an over prediction of concentrations. This is because the majority of pollutants are emitted during daytime hours when meteorological conditions for dispersion are usually more favorable. By excluding emission factors in the model, more pollutants are emitted during the nighttime hours, which leads to higher predicted concentrations at those times. While the development of emission factors requires many assumptions, local knowledge of the area can help to minimize the amount of uncertainty associated with these assumptions.

Incorporating these and additional items into the air dispersion model results in increased confidence in the results. While many of the assumptions introduce a degree of uncertainty, it is likely to be very small when compared to the uncertainty associated with the emissions inventories themselves. Obviously, any long-term monitoring data that is available would go a long way in validating the model and the various methods and assumptions that were introduced into the model.

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KEY WORDS

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