

# **Compilation and Evaluation of a Paso del Norte Emission Inventory for Use in Photochemical Dispersion Modeling**

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## **ABSTRACT**

Emission inventories are now routinely used for planning purposes and as input to comprehensive photochemical air quality models. Photochemical model performance and the development of effective air pollution control strategies is predicated on the accuracy of an underlying emission inventory. The purpose of this study is to compile all existing air pollution emission inventory information for the El Paso / Ciudad Juarez / Southern Dona Ana region; generate a gridded, speciated emission inventory; and evaluate the accuracy and representativeness of the inventory. Existing point, area, and mobile source emissions data were obtained from local government agencies. Emissions were spatially and temporally allocated to a gridded domain using region-specific demographic and land cover information. The inventory was processed using the U.S. Environmental Protection Agency (EPA) recommended Urban Airshed Model Emissions Preprocessor System 2.0 (UAM-EPS 2.0) which generates emissions files that can be directly used as input to the Urban Airshed Model. An evaluation of the emission inventory was then performed by comparing inventory non-methane hydrocarbon (NMHC)/NO<sub>x</sub> and CO/NO<sub>x</sub> ratios to ambient ratios using air quality data collected during the 1996 Paso del Norte Ozone Study. Detailed NMHC species comparisons were also made in order to investigate the relative composition of individual hydrocarbon species in the emission inventory and in the ambient data.

## **BACKGROUND**

In 1991, an agreement between the U.S. Environmental Protection Agency (EPA) and the Texas Air Control Board (predecessor to the Texas Natural Resource Conservation Commission, TNRCC) established 1999 as the target year to complete the data collection and air quality modeling activities required under Annex V. To provide the data necessary to conduct ozone air quality modeling, the EPA, TNRCC, and Mexico's Secretariat of Natural Resources and Fisheries (SEMARNAP) participated in the 1996 and 1997 Paso del Norte Ozone Studies (PDNOS).<sup>1,2</sup> Additionally, the EPA sponsored analyses of the 1996-1997 PDNOS data in order to support the formulation of meteorological and air quality modeling protocols. The next step required before airshed modeling may commence is the compilation of an accurate emission inventory. Previously, no unified, gridded emission inventory existed for the El Paso/Ciudad Juarez modeling domain. Thus, the purpose of this work effort is to compile a "first-cut" gridded emission inventory for the Paso del Norte region.

The objectives of this study were three-fold: (1) acquire existing emissions data from El Paso, Hudspeth, Dona Ana, and Otero counties in the United States and from Ciudad Juarez and its surroundings in Chihuahua, Mexico; (2) compile a gridded emission inventory for the El Paso/Ciudad Juarez modeling domain using the acquired data; and (3) evaluate this inventory and recommend methods for its improvement. This inventory represents a “first-cut” effort that should be modified and updated as new data become available.

## **EMISSION INVENTORY COMPILATION – TECHNICAL APPROACH**

### **Data Acquisition, Quality Assurance, and Spatial Allocation of Emissions Data**

Emissions and surrogate data were obtained for point, area, and mobile sources throughout the modeling domain. The following local agencies and institutions provided emissions, demographic, and land use/land cover data: TNRCC, Texas Department of Transportation (TxDOT), University of Texas at El Paso (UTEP), New Mexico Environment Department (NMED), SEMARNAP, State of Chihuahua Ciudad Juarez, Instituto Municipal de Investigacion y Planeacion (IMIP), and the EPA. The EPA’s Biogenic Emissions Inventory System-2 (BEIS-2) model was used to estimate biogenic emissions for the entire domain. When data were obtained, an assessment was performed to ensure that the reported emissions were within a reasonable range or limit. Quality assurance guidelines were followed as outlined in the Emissions Inventory Improvement Program, 1996.<sup>3</sup>

In the absence of emissions source locations, emissions are spatially allocated using surrogates. Surrogates are spatially resolved demographic and/or socioeconomic data, such as population and employment, that are often used to allocate emissions within a region. When surrogates are used, the emissions are distributed over the modeling domain proportionally to a directly related surrogate category.

When available, reported facility coordinates were used to spatially allocate emissions from large point sources. For a few facilities without reported coordinates, point source emissions were allocated on the basis of employment data. For El Paso County and Juarez, area sources were spatially distributed using a combination of land use data obtained from the United States Geologic Survey (USGS) and UTEP. In the outlying counties of Hudspeth, Otero, and Dona Ana, area sources were spatially allocated according to land use data obtained from the USGS. In the case of mobile sources, road type, position, and length were used to distribute emissions.

### **Compilation of the Gridded, Speciated Emission Inventory**

The modeling grid defined for this study covers a 144-km x 168-km geographic region including all of El Paso County, Texas; parts of Dona Ana and Otero Counties, New Mexico; part of Hudspeth County, Texas; and Ciudad Juarez and its surroundings in Chihuahua, Mexico. The grid resolution is 2 km x 2 km and the position of the domain’s southwest corner is (300 km easting, 3432 km northing) in Universal Transverse Mercator (UTM) zone 13. Emissions files were compiled using version 2.0 of the Emissions Processing System (EPS 2.0), the EPA’s recommended emissions processing software. EPS 2.0 consists of a set of FORTRAN modules that perform basic data manipulations and produce UAM-IV ready files. These modules are discussed further in the EPS 2.0 User’s Guide.<sup>4</sup> EPS 2.0 requires a variety of input data, including emissions data, speciation data, temporal and spatial data, and region-specific data.

The compiled inventory contains gridded emission estimates for average summer weekday NMHC, CO, and NO<sub>x</sub> emission totals as well as speciated hydrocarbon emissions. The major source categories of the emission inventory include: area, point, mobile, and biogenic emissions.

## **Overview of the Compiled Emission Inventory**

Total combined volatile organic compounds (VOC), NO<sub>x</sub>, and CO emissions for the entire modeling domain are illustrated in Figures 1 through 3. Note that NMHC and VOC are used interchangeably for the remainder of the inventory discussion. El Paso and Ciudad Juarez together are responsible for about 70 percent of the total VOC and 85 percent of total NO<sub>x</sub> and CO emissions in the domain. About 60 percent of the biogenic VOC emissions in the domain are from Otero County located in the rural, northeastern portion of the domain. The remaining 40 percent are distributed throughout the domain. On-road mobile sources are the greatest contributor to total emissions in the domain. Area sources contribute about 15 percent of total NO<sub>x</sub> and CO emissions, while point sources contribute approximately 40 percent of NO<sub>x</sub> and 5 percent of CO emissions. Biogenic VOC emissions are responsible for 27 percent of VOC emissions for the entire domain. In addition to considering the whole domain, it is also important to focus attention on the populated areas. In the urban region of El Paso and Ciudad Juarez, emission densities are highly concentrated. Of the whole domain, 66 percent of the VOC, 84 percent of the NO<sub>x</sub>, and 85 percent of the CO are emitted within the central urban region of the domain.

## **EMISSION INVENTORY EVALUATION – TECHNICAL APPROACH**

The El Paso/Juarez gridded emission inventory compiled in this study is intended for use as input to the UAM-IV. Because of the complexities involved in developing and compiling emission inventories, it is important to evaluate the accuracy and representativeness of the inventory in order to improve future inventory development. One way to assess regional emission inventories is to perform a top-down evaluation by comparing emission estimates to ambient air quality data using emission inventory ratio comparisons of NMHC/NO<sub>x</sub> and CO/NO<sub>x</sub>. Ambient/emission inventory comparisons are useful for examining the relative composition of emission inventories. However, they are not useful for examining the relative composition of emission inventories unless they are combined with bottom-up evaluations.

Top-down emission inventory evaluations are based on the premise that ambient NMHC, CO, and NO<sub>x</sub> pollutant concentrations are primarily influenced by fresh emissions emitted in the vicinity of the ambient monitor; however, precursor transport, carryover effects, and chemical reactions can also influence ambient concentrations. The influence of these confounding effects on the comparison can be minimized (but not eliminated) by selecting monitoring sites located in areas with high emission rates, and by examining data collected when photochemical reaction rates are low. To effectively minimize the effects of upwind transport and photochemistry, early morning sampling periods are the most appropriate to use when making emission comparisons. This is because, typically, emissions are high and wind speed, atmospheric mixing height, temperature, and chemical reactivity are low. Comparisons of ambient data and emission estimates are commonly based on the assumption that emission inventory NO<sub>x</sub> estimates are more accurate than emission inventory hydrocarbon estimates.<sup>5</sup>

Comparisons of ambient data and emission estimates for NMHC, CO, and NO<sub>x</sub> were made at two urban monitoring sites: the 20/30 Club in Juarez, Mexico and Campbell in El Paso, Texas during the early morning hours (0600-1000 MDT). Ambient data were collected during the Paso del Norte Ozone Study conducted during the summer of 1996. In order to compare and evaluate the spatial distribution and resolution of an emission inventory, it is important to select ambient monitoring sites

that are representative of a diverse mix of emission sources. The 20/30 Club is located in downtown Juarez and Campbell is located in downtown El Paso near Interstate 10. The 20/30 Club and Campbell are located near major roadways and are likely to be influenced by a mix of urban and mobile source emissions.

In order to investigate how sensitive the ambient- to emission inventory-derived ratios are to transport, wind analyses were performed to calculate air parcel travel distances during the early morning time period. The results of the wind analyses showed spatial variability of wind direction and wind speed throughout the El Paso region. This means that as an air parcel is transported, its direction will change in space. Thus, the vector average wind speed and transport distances calculated are not indicative of the actual transport path of the parcel and the actual transport distance is likely much shorter. For the purposes of the inventory evaluation, it was assumed that the ambient monitor could potentially detect emissions that emanated from 6 km to 10 km (3 to 5 grid cells) away from the ambient monitor.

Because of the various factors that could affect differences between ambient- and emission-derived ratios and compositions, several different comparisons were considered, each representing a different spatial configuration of grid cells surrounding the ambient monitoring site. Comparisons between ambient- and emission-derived NMHC/NO<sub>x</sub> and CO/NO<sub>x</sub> ratios were calculated for a 4-km<sup>2</sup> (grid cell containing the ambient monitor) area immediately surrounding a monitoring site, a 36-km<sup>2</sup> (3 x 3 grid cells) area, and an extended 100-km<sup>2</sup> (5 x 5 grid cells) area surrounding the site. The dimensions of the gridded areas surrounding each ambient monitoring site correspond to the 2-km El Paso/Juarez grid resolution. Comparisons of ambient- and emission inventory-derived NMHC/NO<sub>x</sub> and CO/NO<sub>x</sub> ratios were made to evaluate the relative amounts of emissions in and around El Paso and Ciudad Juarez. Comparisons of the relative amounts of individual organic species in the ambient data and the inventory were made to evaluate the hydrocarbon speciation of the inventory.

## **Uncertainty Issues**

The uncertainties associated with comparisons of emission inventory-derived and ambient-derived NMHC/NO<sub>x</sub> and CO/NO<sub>x</sub> ratios include the spatial and temporal allocation of emissions, speciation profiles used to speciate the inventory, and the assignment of the correct profiles to source categories. Issues pertaining to ambient measurements and data quality include the influence of instrument detection limits and precision; the identification, misidentification, or lack of identification of species; potential sampling or handling losses of total mass or individual species; and the overall uncertainties associated with the ambient measurements. Comparison-related uncertainties include the matching of hydrocarbon species in the emission inventory and ambient hydrocarbon species; the temporal matching of the emissions and ambient data; and meteorological factors such as inversion height, wind speed, and wind direction which influence the emissions sampled in the ambient air. In this study, the uncertainties associated with the ratio comparisons were minimized by selecting ambient monitoring sites located in areas with high emission rates, and by examining data collected during early morning hours when emission rates are typically high and reaction rates, wind speeds, mixing heights, and temperatures are low.

## **Emission Inventory Data**

The compiled point, area, and mobile source gridded emission inventory for the Paso del Norte region was evaluated. Individual source category emissions were examined to determine the major source contributions to NMHC, CO, and NO<sub>x</sub> in the emission inventory during the 0600-1000 MDT time period at the 20/30 Club and Campbell. Based on the inventory, mobile sources contribute more

than 50 percent of total  $\text{NO}_x$ , NMHC, and CO emissions at both sites. Area sources are responsible for 30 to 40 percent of NMHC emissions and very little  $\text{NO}_x$  and CO at the 20/30 Club and Campbell. Point sources are responsible for about 20 percent of total  $\text{NO}_x$  emissions at Campbell, but are not a significant contributor of emissions at the 20/30 Club. In order to place the emission inventory data and the ambient data on a common basis, the speciated emission inventory was converted to a molar basis and the output files were modified to include only the chemical species that were measured at the ambient sites.

## RESULTS

### NMHC/ $\text{NO}_x$ and CO/ $\text{NO}_x$ Ratio Comparisons

The relative amounts of NMHC, CO, and  $\text{NO}_x$  in the emission inventory and in ambient air were examined by comparing NMHC/ $\text{NO}_x$  and CO/ $\text{NO}_x$  ratios. Ratios were calculated for the area immediately surrounding each ambient monitoring site, for the four quadrants surrounding the site (northeast, northwest, southeast, and southwest), for the 6-km x 6-km region surrounding the ambient monitor, and for the 10-km x 10-km region surrounding the monitor. The remainder of this paper will focus on comparisons made for the 6-km x 6-km area surrounding each site.

Comparisons between the 0600-1000 MDT average ambient and average emission inventory NMHC/ $\text{NO}_x$  and CO/ $\text{NO}_x$  ratios for the 6-km x 6-km area surrounding the 20/30 Club and Campbell are shown in Figure 4. The results of the NMHC/ $\text{NO}_x$  and CO/ $\text{NO}_x$  ratio comparisons indicate that the ambient NMHC/ $\text{NO}_x$  ratio at the 20/30 Club is three times higher than the emission inventory ratio, while the ambient CO/ $\text{NO}_x$  ratio is 1.3 times lower than the inventory ratio. At Campbell, the ambient NMHC/ $\text{NO}_x$  and CO/ $\text{NO}_x$  ratios are both higher than the inventory ratios, but agree within 25 percent. The differences in ambient- and emissions-derived ratios at the 20/30 Club warrant further investigation.

### Detailed NMHC Composition

Comparisons of average weight percent composition of ambient hydrocarbon data collected during the 1996 PDNOS from 0600-1000 MDT and emission inventory weight percent composition of individual species for all source categories combined at the 20/30 Club and Campbell are shown in Figures 5 and 6. All of the fingerprint plots list the species in the same order. There were 104 hydrocarbon species reported at the 20/30 Club and Campbell. However, only the 63 most abundant species are shown in the plots.

### Area and On-Road Mobile Source NMHC Compositions

Significant differences exist between ambient NMHC species compositions and the inventory NMHC species compositions as shown in Figures 5 and 6. Because area and mobile sources are the largest contributors to total emissions in the El Paso/Juarez region, the detailed NMHC composition of area and mobile source emissions were plotted independently against the ambient NMHC data. Figures 7 and 8 show comparisons of average weight percent composition of ambient hydrocarbon data collected during the 1996 PDNOS from 0600-1000 MDT and emission inventory weight percent composition of individual species for area and mobile source emissions at Campbell. The following observations summarize the weight percent plots for area and mobile sources:

- For area and mobile sources in general, the emission-derived compositions of n-heptane, methylcyclohexane, toluene, o-xylene, n-nonane, and n-undecane are significantly higher than the ambient-derived compositions. All of these compounds are commonly used for industrial

coating and degreasing processes and/or are emitted from petroleum product storage. Toluene and o-xylene are also emitted in fuel exhaust and evaporation. N-nonane is emitted by dry cleaning facilities.

- For area sources in general, the emission-derived compositions of acetylene, ethene, ethane, propane, isopentane, n-pentane, and m/p-xylenes are significantly lower than the ambient-derived compositions. Acetylene and ethene are both emitted during various combustion processes. Ethane and propane, both emitted by a variety of sources, react slowly in the atmosphere and tend to accumulate. Isopentane and m/p-xylenes are major components of mobile source exhaust. N-pentane is emitted during petroleum transport and storage.
- For mobile sources in general, the emission-derived compositions of n-butane, benzene, 2,2,4-trimethylpentane, 2,3,4-trimethylpentane, toluene, and m/p-xylenes are higher than ambient-derived compositions. All of these compounds are products of mobile source evaporative and exhaust emissions.
- For mobile sources in general, the emissions-derived compositions of ethane, propane, and dimethylpentanes are lower than the ambient-derived compositions. All of these chemical species are emitted during combustion processes including mobile source exhaust.

## **CONCLUSIONS AND RECOMMENDATIONS**

### **Emissions Issues – United States**

Emissions data for El Paso, Hudspeth, Dona Ana, and Otero counties were obtained from published sources compiled by the EPA and local air districts. Prior to compiling the El Paso/Juarez gridded emission inventory, standard guidelines were followed to assess the overall reasonableness of the inventory data for the United States portion of the domain. None of the United States emission inventory data were altered or changed. It is recommended that in future inventory development, the existing emission inventory data be evaluated by local agencies and updated as necessary. In particular, area and mobile source emission estimates should be assessed since they are the largest contributors to total emissions in the modeling domain.

### **Emissions Issues – Ciudad Juarez**

Because the overall Ciudad Juarez air emissions data set appears to be reasonable, the current inventory is recommended for use to develop a preliminary ozone air quality model for the Ciudad Juarez region and surrounding airshed. In order to improve the inventory, additional data would be useful for each of the sources with suspect QA/QC flags and for the largest point sources. If possible, consistent data elements should be gathered for all other point sources. The inclusion of these additional data will help to refine the model analyses and will increase confidence in the model's results. A review of the El Paso air emissions data suggests that the data set does not include emission estimates for non-road emissions sources including: aircraft, trains, off-road recreational vehicles, commercial and industrial mobile equipment, and farm equipment. Emissions from heavy-duty diesel trucks appears to be underestimated in the on-road mobile inventory, and the inventory should also include emissions from urban buses.

### **Emission Inventory Evaluation**

On a source category basis, on-road mobile source contributions were dominant at both the 20/30 Club and Campbell contributing more than 50 percent of total NMHC emissions. Area sources were the second most contributing source category and point source contributions to NMHC were

negligible. Future inventory modifications and evaluations should focus on mobile and area source categories.

Ambient NMHC/NO<sub>x</sub> ratios at the 20/30 Club are three times higher than the emission inventory ratios. The large difference at the 20/30 Club suggests that NMHC emissions in the inventory are underestimated, NO<sub>x</sub> emissions are overestimated, or both. In addition, it is possible that the early morning ambient measurements may include some aged emissions (due to transport and/or carryover). At Campbell, ambient NMHC/NO<sub>x</sub> ratios are within 25 percent agreement with inventory ratios. The ambient CO/NO<sub>x</sub> ratio at the 20/30 Club is about 1.3 times lower than the emission inventory CO/NO<sub>x</sub> ratio, and at Campbell, the ambient- and emission inventory-derived ratios are within 25 percent agreement. The differences in CO/NO<sub>x</sub> ratios are relatively small and suggest that CO emissions in the inventory may be reasonable, assuming NO<sub>x</sub> emissions are reasonable.

On a speciated basis, the chemical composition of the ambient NMHC data at both sites is consistent with the motor vehicle exhaust signature. Since point source emissions do not appear to significantly impact the ambient monitoring sites, and assuming NO<sub>x</sub> emissions are reasonable, it is likely that the absolute amount of on-road mobile source hydrocarbon and/or area source hydrocarbon emissions may be underestimated in the inventory. Differences between ambient and emission inventory n-butane compositions at each of the sites may be indicative of the emission inventory containing too much mobile source evaporative emissions from 0600-1000 MDT, and/or the mobile source speciation profiles may not reflect properties of the fuel used in the region.

At both sites, the emission-derived composition of toluene is significantly higher than ambient compositions. Because the speciation plots for area sources show the largest differences in toluene compositions, it is likely that the area source speciation profiles and/or temporal profiles may not be representative of industrial toluene use in the region. The fact that the area source speciation plots show the largest differences between ambient and emission inventory acetylene and ethane compositions suggests that the inventory may not be representative of area source combustion processes and natural gas emissions. Significant differences between ambient and emission inventory propane (and ethane) compositions for both area and mobile sources are indicative of the inventory under-representing propane compositions in the El Paso/Juarez region. Further investigation should be done to determine the extent of propane use and area and mobile source emission inventories should be adjusted accordingly.

Possible biases in the NMHC and NO<sub>x</sub> emission inventories should be investigated. Source categories should be reviewed for these species, including spatial and temporal allocation of on-road motor vehicles and area sources. After review of bottom-up evaluations, further top-down evaluations should be performed. The NMHC speciation profiles used in compiling the inventory should be reviewed. In particular, speciation profiles used for motor vehicle source emissions and other profiles with aromatic hydrocarbons should be reviewed. Three principal areas of concern should be addressed: 1) the representativeness of the speciation profile to the actual species emitted by each source category, 2) the proper assignment of profiles to source categories, and 3) the fuel composition characteristics for the El Paso/Juarez region. The speciation profiles in the EPA speciation database, SPECIATE, were developed based on emissions processes in the United States, which may be different than those in Juarez, Mexico. More representative speciation profiles for mobile and area sources should be obtained and used for Juarez.

The speciation profiles used for compiling the El Paso/Juarez emission inventory are default profiles built in to EPS 2.0. Although the profiles are standard and widely accepted, several appear to be out of date, and/or may not reflect the chemical speciation of current emissions processes. Also, there

are several mobile source speciation profiles, each representing a different fuel composition. It is important that the correct evaporative and exhaust speciation profiles are used for mobile sources based on the type of fuel that is consumed in the study region (i.e., reformulated versus non-reformulated). For example, in the El Paso region in 1995 non-reformulated fuel was being sold.<sup>6</sup> Prior to compiling the gridded emission inventory, the mobile source speciation profiles were assigned based on the fuel being used in the region. Although the correct profiles were assigned, the profiles themselves are not necessarily correct. A major recommendation of this study is that the speciation profiles for major emissions source categories be reviewed and updated or corrected as necessary.

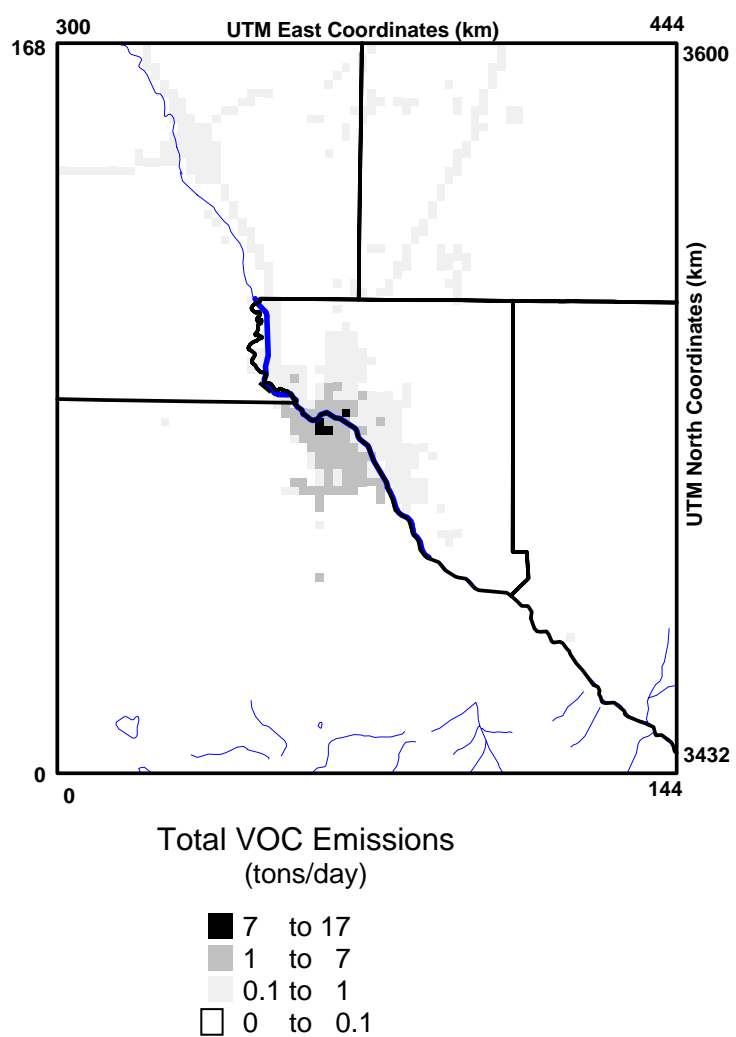
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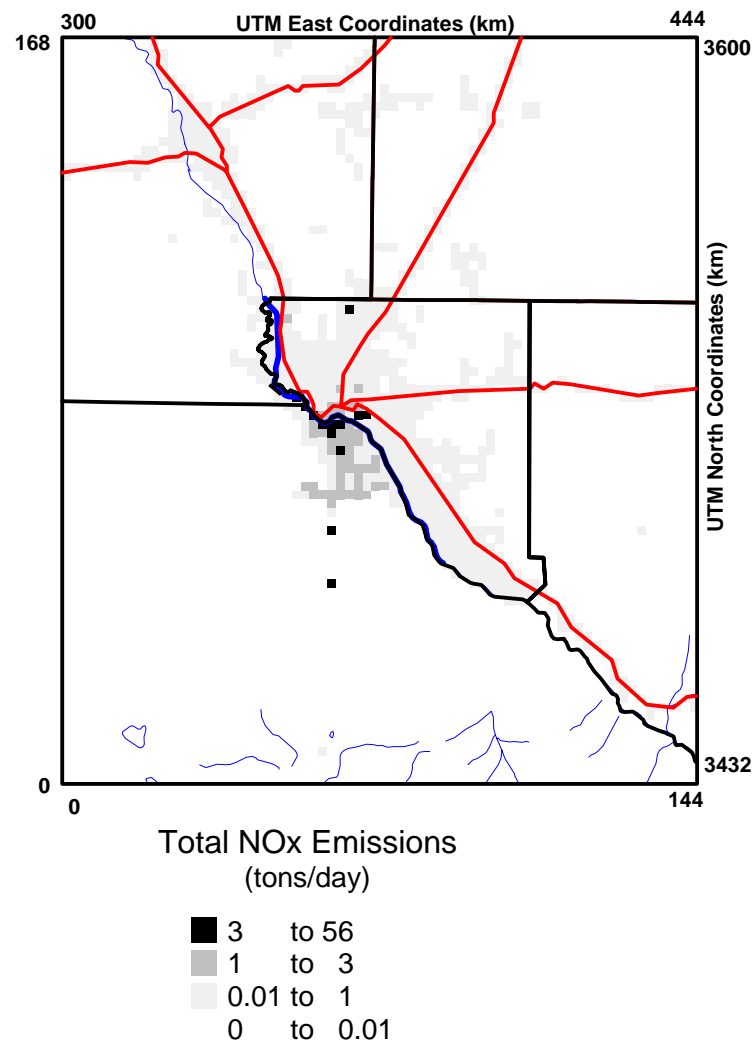
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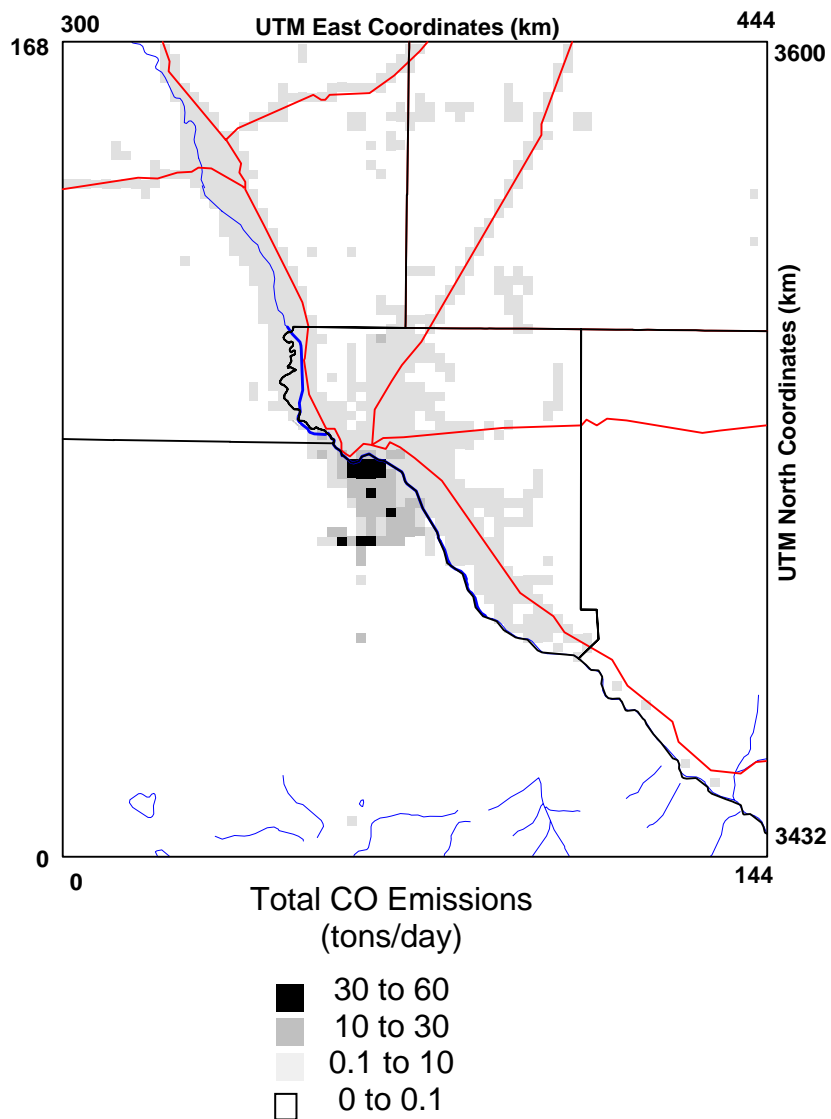
**Figure 1.** Total daily anthropogenic and biogenic VOC emissions in the Paso del Norte domain.



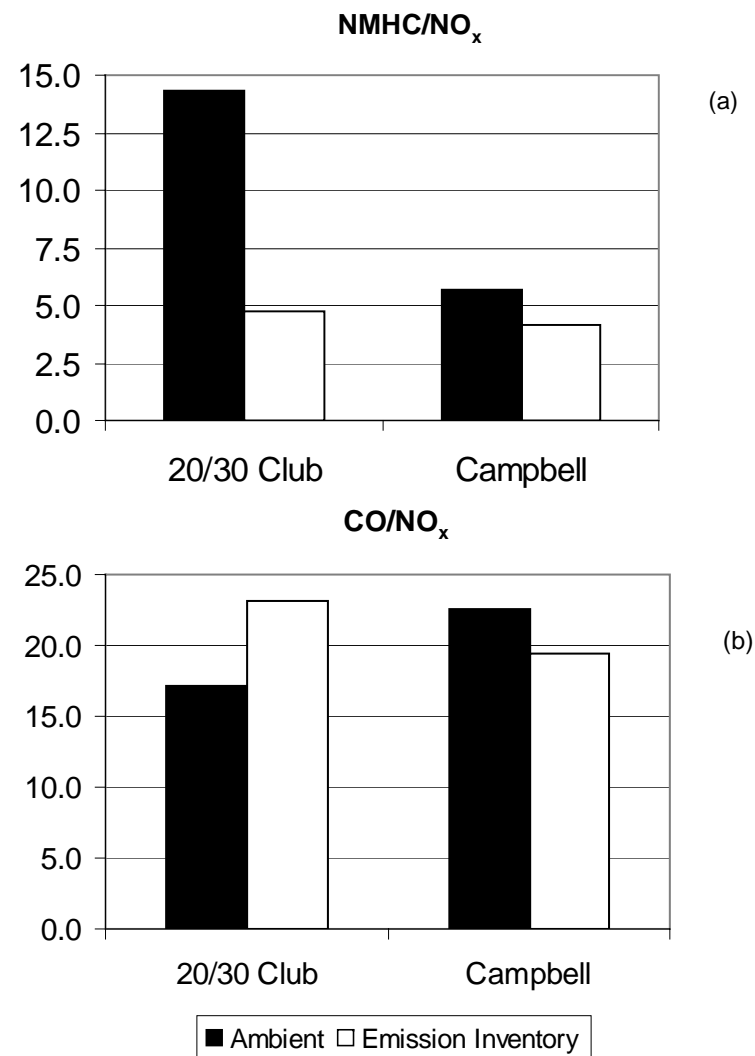
**Figure 2.** Total daily anthropogenic and biogenic NO<sub>x</sub> emissions in the Paso del Norte domain.

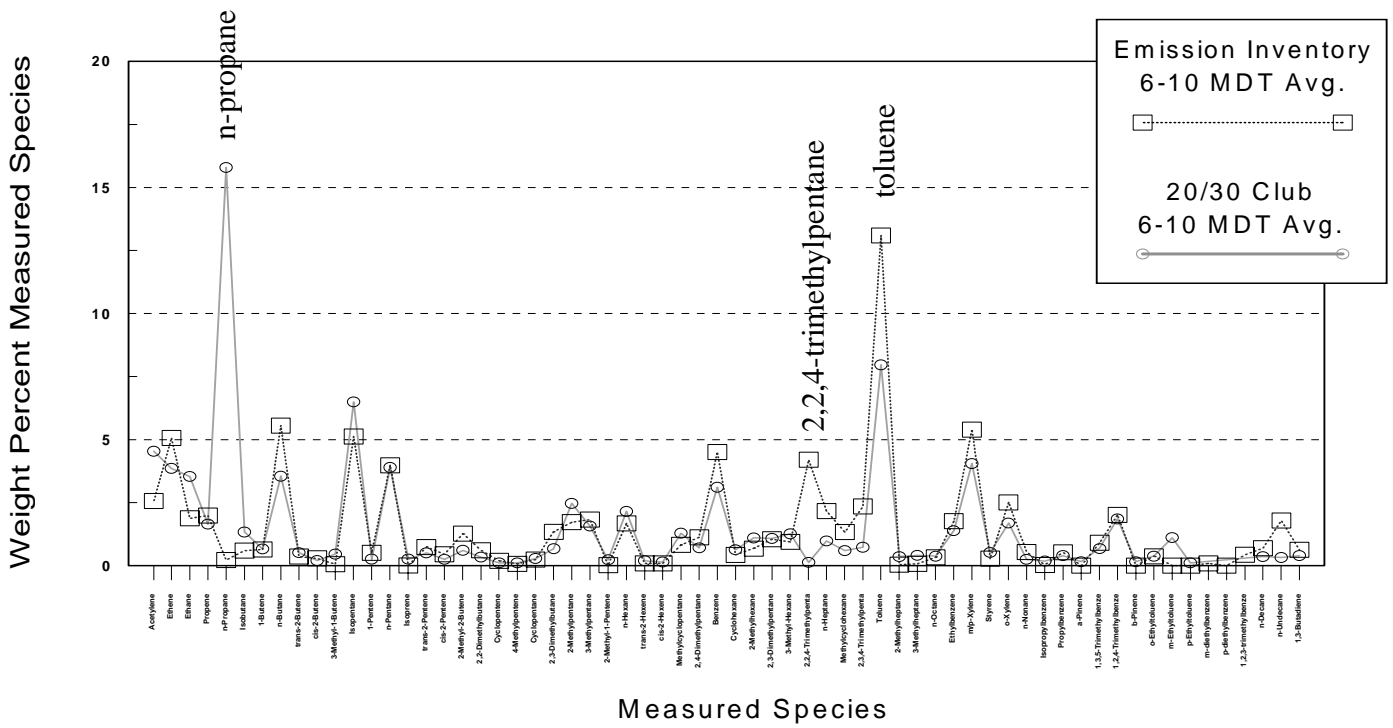


**Figure 3.** Total daily anthropogenic and biogenic CO emissions in the Paso del Norte domain.

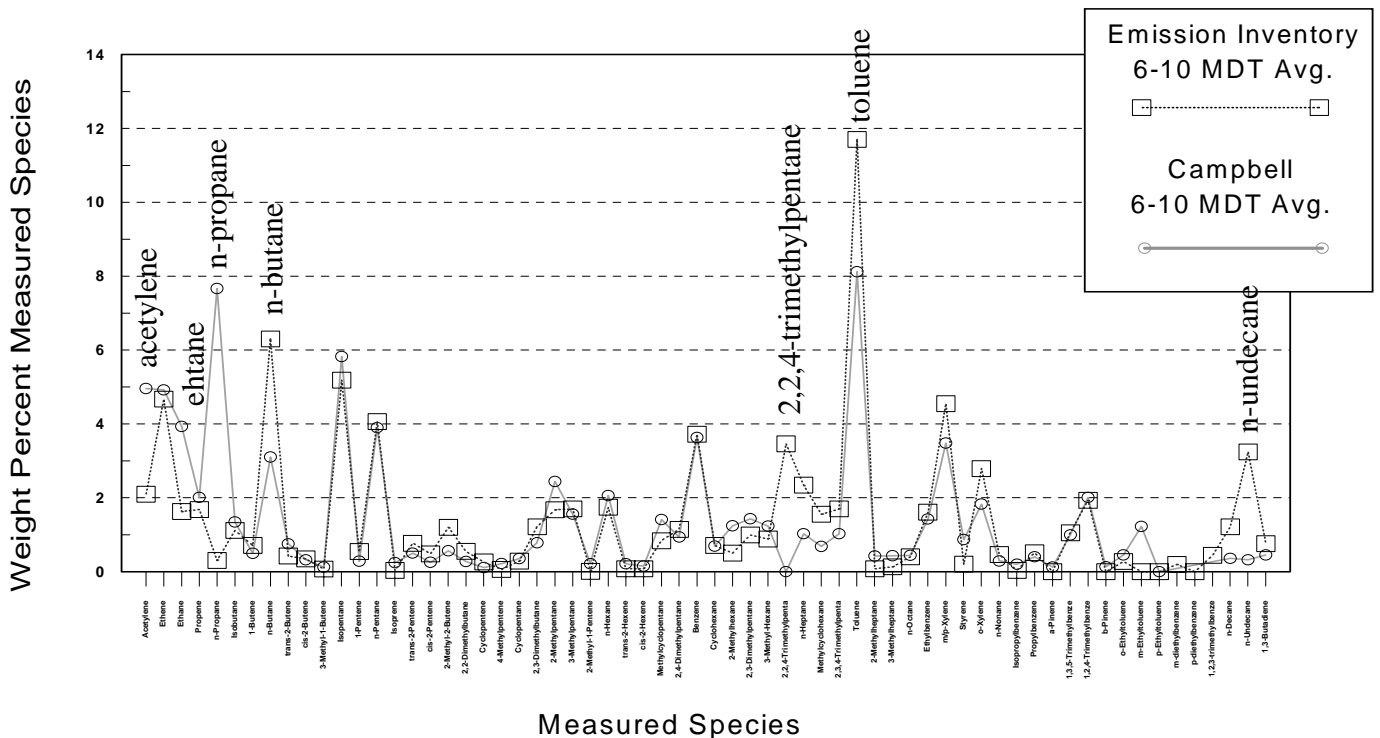


**Figure 4.** Average-ambient and emission inventory-derived (a) NMHC/NO<sub>x</sub> and (b) CO/NO<sub>x</sub> ratios at the 20/30 Club and Campbell.

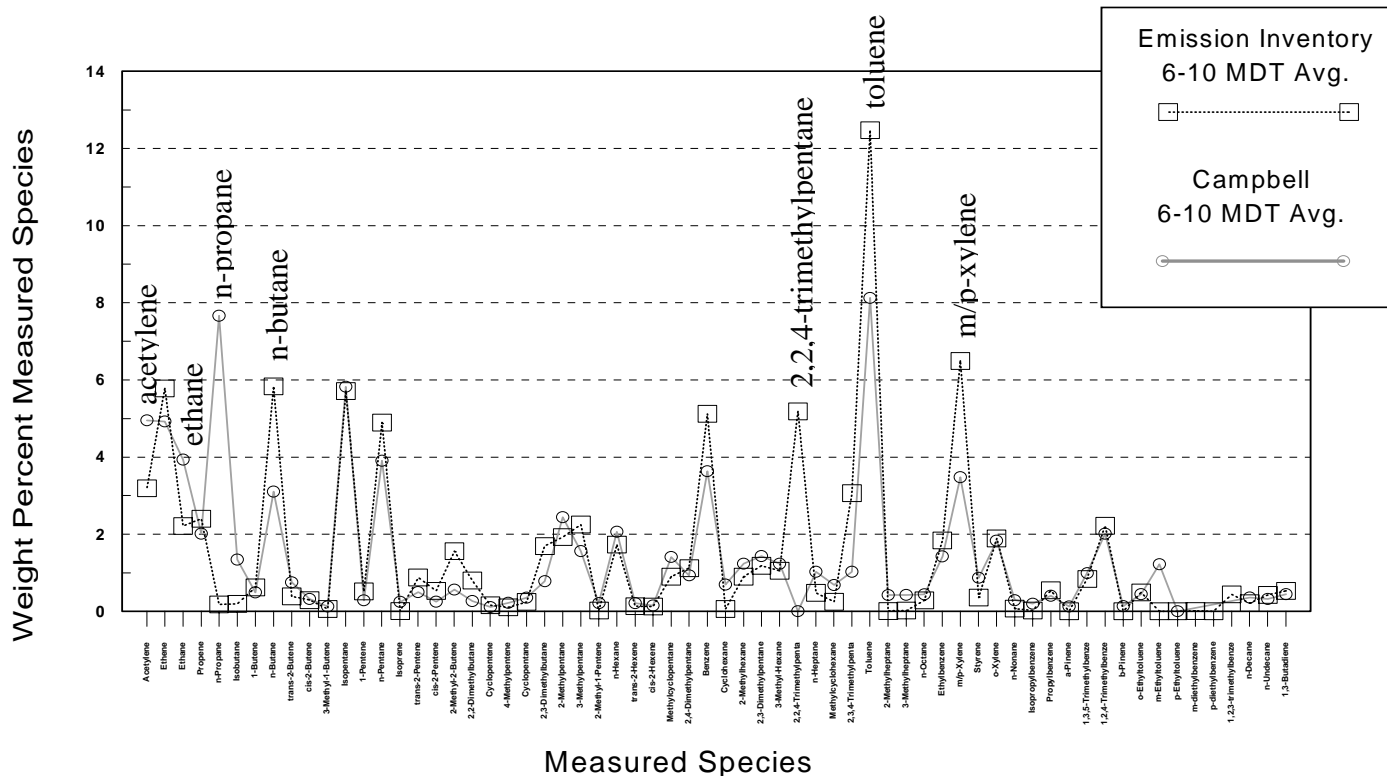




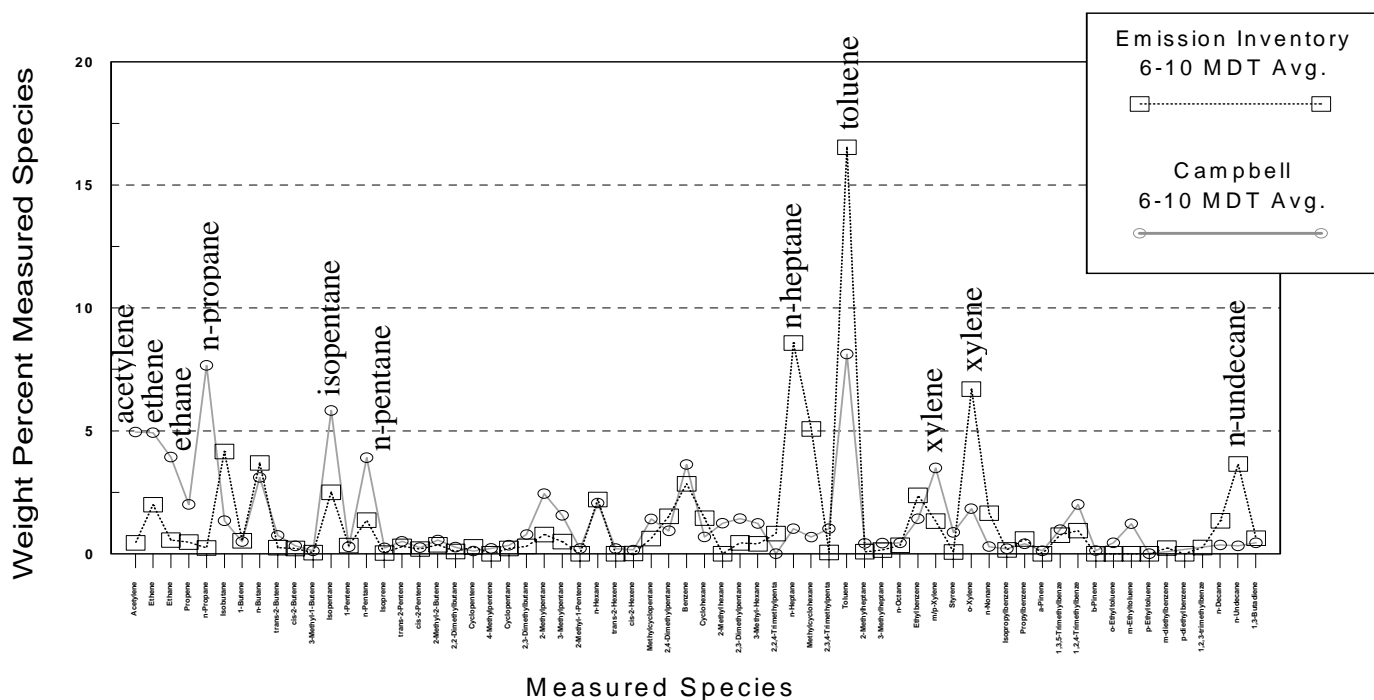
**Figure 5.** Comparison of average weight percent composition of ambient hydrocarbon data collected during the 1996 PDNOS from 0600-1000 MDT and emission inventory weight percent composition of individual species for all source categories combined at the 20/30 Club. Species with large discrepancies are labeled.



**Figure 6.** Comparison of average weight percent composition of ambient hydrocarbon data collected during the 1996 PDNOS from 0600-1000 MDT and emission inventory weight percent composition of individual species for all source categories combined at Campbell. Species with large discrepancies are labeled.



**Figure 7.** Comparison of average weight percent composition of ambient hydrocarbon data collected during the 1996 PDNOS from 0600-1000 MDT and emission inventory weight percent composition of individual species for mobile sources at Campbell. Species with large discrepancies are labeled.



**Figure 8.** Comparison of average weight percent composition of ambient hydrocarbon data collected during the 1996 PDNOS from 0600-1000 MDT and emission inventory weight percent composition of individual species for area sources at Campbell. Species with large discrepancies are labeled.

## **Keywords and Phrases**

Emission Inventory

Nitrogen Oxides (NO<sub>x</sub>)

Non-Methane Hydrocarbon Compounds (NMHC)

Emission Inventory Evaluation

1996 Paso del Norte Ozone Study

Speciation profile