4. EMISSIONS INFORMATION

With the BRAVO Study's emphasis on particulate sulfate contributions to Big Bend haze, a general knowledge the SO_2 emission source types and locations in the region was a factor in designing the study. In Texas the primary sulfur sources are power plants in east and southeast Texas, and refineries and industrial plants along the Gulf Coast. A coal deposit, known as the Lignite Belt, extends from northeast of Dallas-Ft. Worth to the border area south of San Antonio. There are about 20 power plants in this region, located near mines, which use coal from this deposit as their primary fuel. Oil refineries and chemical operations along the Gulf Coast, primarily in the Houston area, are potential sources of sulfur that could potentially find their way to Big Bend. More distant regions of high SO_2 emissions include the coal-fired power plants and other industry in the eastern U.S., especially in high density emission regions such as the Ohio River and the Tennessee valleys.

Regional sulfur sources in Mexico that may contribute to the haze at Big Bend are coal-fired power plants, oil refining, oil-fired power production, steel production, and other industrial operations. *Carbón* I and II are power plants with 1200 and 1400 megawatt capacities located approximately 32 km south of the U.S.-Mexico border near the town of Eagle Pass, Texas, which is only about 225 km southeast of Big Bend. The Tampico region on the Gulf of Mexico is sulfur source that potentially impacts Big Bend. It is a center of oil refining and oil-fired power generation. Other, more distant, industrial areas on the Pacific Coast and to the north and south of Mexico City are also potential sources of the sulfate seen in the park. The largest SO_2 emissions source in North America during the BRAVO Study was the Popocatepetl Volcano just south of Mexico City.

4.1 Emission Inventory

A comprehensive emissions inventory was compiled for air pollution sources within the BRAVO study domain[1], which includes fourteen states and northern Mexico as shown in Figure 4-1. Within the database, all emissions data were linked to the data provider so that the information can be traced back to its origin. The sources of data used to compile the emission inventory organized by source type and country are shown in Table 4-1.

[1] The original Community Multi-Scale Air Quality (CMAQ) modeling domain (see Section 8.4.3) for the BRAVO Study is shown on the map in Figure 4-1 as the box that includes Texas and surrounding states. After the emissions inventory was completed, the decision was made to include Regional Modeling System for Aerosols and Deposition (REMSAD) modeling with a much larger domain. U.S. emissions for the larger domain were compiled from the National Emissions Inventory as part of the emissions modeling step (Section 4.2).

Figure 4-1. *The BRAVO Study emission inventory was compiled for the shaded areas of the U.S. and Mexico shown here.*

Table 4-1. BRAVO Study emissions inventory data sources.

	United States	Mexico	Off Shore
Area	• NEI database for 14 BRAVO States. • Replace TX sources for Construction and Oil and Gas using NONROAD model with TCEQ Activity.	• ERG Emissions Factors from TJ, CJ, and Mexicali supplemented with Monterrey emissions. • Extrapolate emissions across non-inventoried areas based on activity from MX Census.	• N/A
Mobile	• NEI county level database for 14 BRAVO States. • Replace TX onroad mobile with 1996 base year emissions from TTI.	• ERG Emissions Factors from TJ, CJ, and Mexicali supplemented with Monterrey emissions. • Extrapolate emissions across non-inventoried areas based on activity from MX Census.	• N/A
Point	• CEM database for point sources in 14 BRAVO states. • NEI Point sources from 14 BRAVO states.	• Acosta y Associados–42 Power plants based on fuel use and type. • ERG-Carbon I/II and Nacozari. • Watson/Profepa–20 SO_2 sources. • CENAPRED–Popocatepetl Volcano. • INEGI–Mexico City and Tula.	• MMS MOAD3 database
Biogenic	• Calculated by MCNC in SMOKE.	• Calculated by MCNC in SMOKE.	• N/A

The U.S. emissions inventory is taken from the 1999 base year National Emissions Inventory (NEI) version 100. It includes annual area and mobile sources resolved at the county level, point sources resolved at the process level and reports CO, NH_3, NO_x, PM_{10}, $PM_{2.5}$ and VOC emissions. Continuous Emissions Monitors (CEM) provided hourly resolution data for NO_x, SO_2, and CO emissions from the large power plants. CEM data were reconciled with the NEI for 477 unique systems in the 14 state BRAVO Study region. The CO, NH_3, PM_{10}, $PM_{2.5}$ and VOC emissions were scaled to NO_x emissions based on annual NEI profiles.

The Mexico emissions inventory for area and mobile sources was based on the Eastern Research Group's WRAP (Western Regional Air Partnership) emission inventory for NW Mexico. Emissions factors averaged from inventories in Tijuana, Mexicali, Ciudad Juarez, and Monterrey were use to estimate emissions elsewhere in northern Mexico. This was done by applying the average emission factors to census data for population, households, agricultural acreage, head of cattle and registered vehicles by *Municipios*. Point source emissions were obtained from a number of sources as shown in Table 4-2.

Table 4-2. Point source emissions data for Mexico.

Point Source	Data Source	SO_2 Emissions (tpy)
Popocatepetl Volcano	CENEPRED	1,400,000
Tula-Vito-Apaxco	INEGI	355,000
42 power plants in northern Mexico	Acosta y Associados	316,000
Carbón I/II	Yarbrough / EPA	241,000
Other industrial sources	Watson / PROFEPA	73,000

Offshore emissions information was obtained from the Minerals Management Service (MMS) Outer Continental Activity Database (MOAD). Emissions for offshore platforms as shown in on the map in Figure 4-2 include boiler, diesel generators, tank breathing, and gas flaring. The base year for the inventory is 1992. Approximately 20% of the Texas total VOC but less than 5% of other emissions are from these sources. Particle emissions from flaring were not reported.

Figure 4-3 shows the SO_2 emissions as a bar plot over a map of the study region. Similar maps of the other inventoried emissions are shown in Kuhns et al. (2003) (in the Appendix). The largest emissions shown on the map are from the Popocatepetl volcano that is just south of Mexico City.

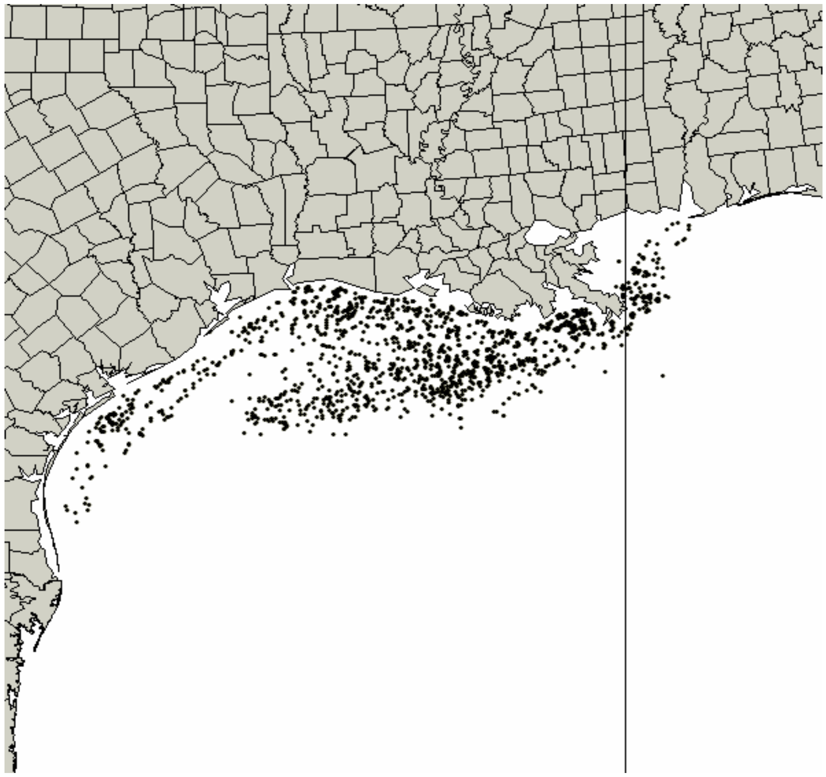

Figure 4-2. *Locations of offshore platforms included in the BRAVO Study emissions inventory.*

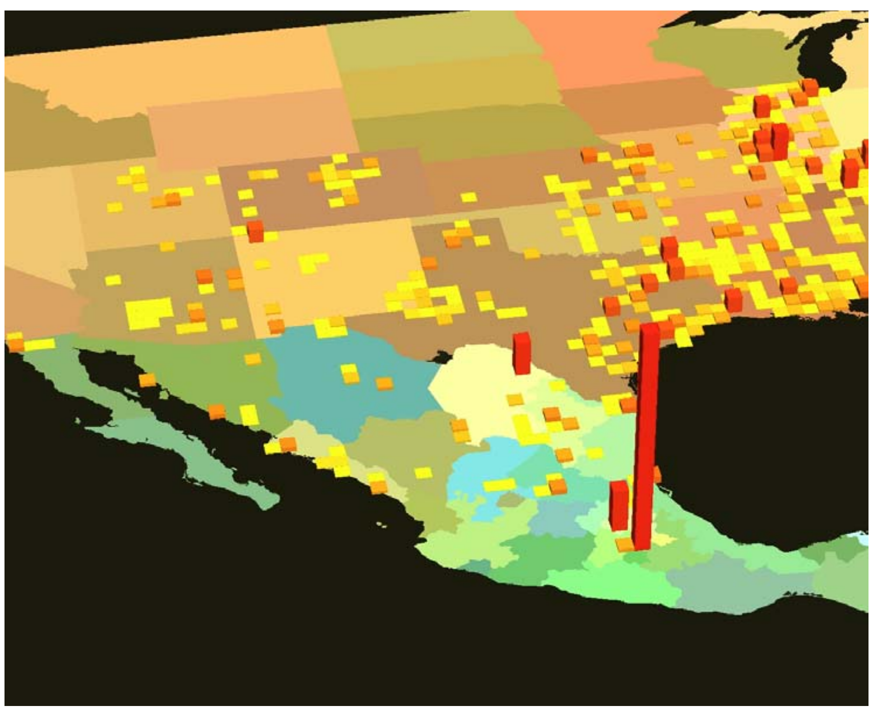

Figure 4-3. *SO_2 emissions rates from the BRAVO Study emissions inventory are shown as proportional to the bar heights on the map. The largest bar is in central Mexico at the Popocatepetl Volcano.*

4.2 Emissions Modeling

The BRAVO Study emissions inventory was processed using the Sparse Matrix Operator Kernel Emissions (SMOKE) model in order to prepare it for use in the regional air quality models used in the study (MCNC, 2002). Emissions models are a necessary intermediate step prior to using emissions inventory data in a regional scale model. Such models perform the following tasks: distributes emissions into the spatial grid cells used by the regional air quality model, adds time of day and day of the week modulation to annual or other time/averaged emissions, estimates emissions from certain types of sources not included in the emissions inventory, estimates plume heights for air quality models that require such processing, and provides detailed chemical species emission profiles by source type as required by the air quality models.

To accomplish these tasks SMOKE requires additional information including meteorological fields supplied by the Mesoscale Modeling System (MM5) (Grell et al., 1994), spatial surrogate data (e.g., census data), speciation cross-reference data by emission process, NEI emissions for states within the 36-km grid domain not included by the BRAVO emissions inventory, and gridded land use data. MM5, was run for the BRAVO Study by the Penn State University/National Center for Atmospheric Research for use by the regional air quality models and SMOKE, and is described in a subsequent section and by Seaman and Stauffer (2003) (in the Appendix). The surrogate data were created for all modeling domains. The surrogates were generated using the MIMS Spatial Allocation Tool (Fine et al., 2002; USEPA, 2002). The tool calculates the surrogates by using shape-files and grid information to overlay the desired grids on the geographic data layers. The shape-files were obtained from multiple sources, including the U.S. Census Bureau, Environmental Systems Research Institute (ESRI), and the Center for International Earth Science Information Network - Socioeconomic Data and Applications Center. The surrogate data types generated for this modeling effort are listed in Table 4-3.

Table 4-3. Surrogate types for the BRAVO modeling domains.

1. Agriculture	7. Ports	13. Urban Primary Roads
2. Airports	8. Railroads	14. Rural Primary Roads
3. Land Area	9. Water Area	15. Urban Secondary Roads
4. Housing	10. Rural Area	16. Rural Secondary Roads
5. Major Highways	11. Urban Area	17. Urban Population
6. Population	12. Forest Area	18. Rural Population

The land use data were generated using the Biogenic Emissions Landcover Database version 3 (BELD3) (Pierce et al., 1998). The BELD3 consists of 1-km horizontal resolution for 230 different land use types. The previous version, BELD2, was used in most BEIS2 applications and consisted primarily of county-level land use based on 156 different land use types. BELD3 combines the spatial resolution available from the U.S. Geological Survey (USGS) 1-km data with the detailed tree and crop species information available in county-level forest and agricultural datasets. The BELD3 was aggregated and interpolated to the desired modeling domain and resolution and the land use data input into SMOKE-BEIS2.

To support Regional Modeling System for Aerosols and Deposition (REMSAD) modeling efforts (see Section 8.4.2), speciation profiles and cross-reference data were used to create emissions to support the micro-Carbon Bond IV (CB-IV) (SAI, 2002) with PM chemistry mechanism within REMSAD. This requires SMOKE to generate four particulate and two gaseous species that are not explicitly provided in the original seven-component emissions inventory.

To support Community Multi-Scale Air Quality (CMAQ) modeling efforts (see Section 8.4.3), speciation profiles and cross-reference data were used to create emissions to support the Regional Acid Deposition Model version 2 (RADM2) with Particulate Matter (PM) (USEPA, 2000) chemistry mechanism within the CMAQ model. This requires SMOKE to generate five particulate species plus one inorganic and 16 organic species not in the original seven-component emissions inventory.

The Meteorology-Chemistry Interface Processor (MCIP) data were used in the SMOKE program called *laypoint* to calculate the plume rise of each point source and allocate them vertically for each hour of each episode. *Laypoint* was executed for all U.S., Mexican, and offshore sources to support the CMAQ modeling effort.

No meteorological data were used in SMOKE to compute plume rise before the REMSAD simulations. However, a stack height cutoff of 30 m was used to differentiate between elevated and low-level point sources. Two emissions files are input into REMSAD: an elevated-point-source file and a file that contains all low-level emissions sources (low-point, area, nonroad, mobile, and biogenic). REMSAD performs a plume rise calculation on the elevated sources only during model execution. All sources that have a stack height ≥30 m were written to the SMOKE elevated-point-source file, while all other sources were written to the SMOKE low-level point source file. The elevated-point-source file output from SMOKE required additional processing before input into REMSAD. The Emissions Preprocessor System version 2 (EPS2) (USEPA, 1992) program called *ptsrce* was used to convert the elevated-point-source file output by SMOKE into REMSAD-ready format.

The biogenic emissions sources that were estimated to support the BRAVO modeling effort were emissions from a volcano, vegetation, soils, and large bodies of salt water (e.g., the Gulf of Mexico). Average annual emissions from the active Popocatepetl Volcano for 1999 were acquired from scientists at the Centro Nacional de Prevencion de Desastres (CENAPRED) in Mexico. SO_2 emissions from the volcano are measured with a correlation spectrometer (COSPEC) two to three times per week. The highest measured SO_2 emissions from the crater since 1994 were 50,000 tons per day while typical emissions are approximately 3,000-5,000 tons per day (Galindo et al., 1998). Annual volcanic emissions were estimated for PM_{10}, $PM_{2.5}$, and SO_2 only. These estimates are highly uncertain and should be considered as order of magnitude approximates of the true emissions. This volcano was given estimated stack parameters and was treated as a point source in the SMOKE processing tasks. SMOKE-BEIS2 was used to approximate emissions from vegetation and soils. The sea-salt emissions were estimated by converting a one-dimensional box model acquired from previous work (Zhang, 2001) into a three-dimensional model.

4.3 Emissions Inventory Assessment

REMSAD and CMAQ modeling using the BRAVO Study emissions inventory (BRAVO EI) began in late 2002, with results available by mid-2003. Model-estimated particulate sulfate at Big Bend during periods with airflow from Mexico had a tendency to be significantly lower than measured particulate sulfate. During periods of air flow from the U.S., the estimated particulate sulfate was not biased to the same degree. The first draft of the *Mexican National Emissions Inventory, 1999* developed for the Mexican Secretariat of the Environment and Natural Resources (*Secretaría de Medio Ambiente y Recursos Naturales – SEMARNAT*) and the National Institute of Ecology (*Instituto Nacional de Ecología – INE*) was released for public review on July 21, 2003. The availability of this draft inventory, which contains emissions estimates for point, area, and on-road mobile sources during 1999 for the six northernmost states of Mexico, and the concerns for model under-estimation of particulate sulfate when flow was from Mexico motivated an assessment of the BRAVO EI late in 2003. Due to scheduling constraints, the insights from this assessment could not affect any changes to the BRAVO Study EI. However, the air quality modeling conducted for the Study employed a number of methods to test the sensitivity and work around possible bias in the input emissions information. (Chapters 9, 11, and 12 contain additional information of the model performance.) The material below summarizes that assessment. (More information is available in Pun et al. [2004] in the Appendix.)

The assessment was limited to a reassessment of the *Carbón* power plant SO_2 emissions based upon new information, comparisons of the BRAVO EI to the draft Mexican National Emissions Inventory (hereafter referred to as N MX NEI), as well as a comparison to the EDGAR 3: *Emissions Database for Global Atmospheric Research.* The EDGAR dataset, which represents 1995 emissions, is a part of the *Global Emissions Inventory Activity (GEIA)* and has been used in Intergovernmental Panel on Climate Change (IPCC) Assessments. The purpose of the comparison of the BRAVO EI to the draft N MX NEI is to assess the emissions from northern Mexico in the BRAVO EI, while the purpose of the comparison of the BRAVO EI to EDGAR EI is to assess the relative magnitude of emissions in the larger REMSAD modeling domain that were not included in the BRAVO EI (i.e., those in southern Mexico, western Caribbean, southern Ontario and Quebec Canada, and the Atlantic and Gulf shipping lanes).

Emissions information for the *Carbón* power plant facility in the state of Coahuila, Mexico about 225km from Big Bend National Park is of particular interest to the BRAVO Study because it is the largest SO_2 emissions source within 500km of the park. The BRAVO EI used an emission rate of 241,000 tons per year based on an assessment using operational and coal characteristics data provided by Southern California Edison and the U.S. EPA. Subsequently, BRAVO Study data analysts suggested that this emission rate may be as much as a factor of two too high based upon their application of Eagle Pass tracer-determined dispersion factors to estimate the *Carbón* power plant sulfur impacts at Big Bend and comparing these to the measured SO_2 and particulate sulfate (Green, et al., 2003). In January of 2002, Dr. Barnes de Castro, the Undersecretary of Energy Policy and Technology in the

Secretariat of Energy in Mexico, made a presentation in Cancun, Mexico that showed the *Carbón* power plant SO_2 emissions to be 152,000 tons per year. The decision was made to maintain the original estimate of 241,000 tons per year in the BRAVO EI, but to use both power plant emissions estimates in BRAVO Study air quality modeling (by modifying the SMOKE output file) and referring to them as the high and low *Carbón* emissions rates.

The comparison of SO_2 emissions in the BRAVO EI and the Draft N MX NEI for the six northern Mexico states common to both inventories resulted in BRAVO EI having greater estimated point source and total SO_2 emissions than the draft N MX NEI in only one state, Coahuila, in which the *Carbón* power plant is located. Substituting the low *Carbón* SO_2 emissions rate for the high rate that is used in the BRAVO EI would largely eliminate the discrepancy for Coahuila. With this modification the ratio of N MX NEI SO_2 emissions to BRAVO EI SO_2 emissions for the six-state region of northern Mexico is about 1.3. It is uncertain how similar the final Mexico National Emissions Inventory (to be completed in June 2004) will be to the draft inventory for these northern states. For example, the Draft N MX NEI did not include off-road mobile sources, thus the SO_2 emissions will increase due to inclusion of this source group. However, the SO_2 emissions may also decrease during quality assurance checks. In summary, this preliminary assessment suggests that the BRAVO EI could underestimate Mexico's SO_2 emissions by 30% or more by comparison to the draft N MX NEI.

The comparison of SO_2 emissions in the 1995 EDGAR EI (updated using data for the *Carbón* power plants and the Ciudad Madero petroleum refining facilities) with the BRAVO EI for the ten northern Mexico states in common show the modified EDGAR EI is a factor of 1.9 greater than the BRAVO emissions (1,914,000 tonnes/year compared to 1,027,000 tonnes/year). The modified 1995 EDGAR emissions provide another indication of a potential underestimate in the BRAVO Mexican SO_2 emissions, but the values may be outdated and are as inherently uncertain as the two more recent emissions inventories. However, because it includes emissions estimates for all of Mexico, the modified EDGAR EI affords an opportunity to examine the relative amount of emission from locations not included in the BRAVO EI. Based upon the modified EDGAR EI, 20% of the total Mexico SO_2 emissions are from the regions of southern Mexico not included in the BRAVO EI (881,000 tonnes/year compared to 4,340,000 tonnes/year). Using the same approach for the entire REMSAD domain not including the U.S., 20% (996,000 tonnes/year compared to 5,336,000 tonnes/year) of the total non-U.S. SO_2 emissions are from non-Mexican source areas not covered by the BRAVO EI (Canada, western Caribbean, and shipping lanes). Including the U.S. emissions, the relative amount of SO_2 emissions within the REMSAD domain not included in the BRAVO EI are about 9% of the total SO_2 emissions (1,877,000 tonnes/year compared to 21,837,000 tonnes/year); and presuming that the modified EDGAR SO_2 emissions for northern Mexico is correct the total missing plus Mexican underestimated SO_2 emissions by the BRAVO EI is about 13% (2,765,000 tonnes/year compared to 21,837,000 tonnes/year).

The uncertainty of air quality model estimates of particulate sulfate that results from uncertain SO_2 emissions input information depends on the locations of emissions as well as the magnitude of the discrepancies. Figure 4-4 contains maps of the SO_2 emissions from the BRAVO EI and the EDGAR EI excluding emissions from the U.S. During the late summer and fall months of the BRAVO Study period, airflow to Big Bend is most often from the southeast to due east over northern Mexico and Texas where the BRAVO EI has coverage, but may be somewhat under-estimating emissions for Mexico. The BRAVO EI has no emissions for the Yucatan Peninsula and the western Caribbean, which may be a modest factor under predominate wind patterns for this time of year.

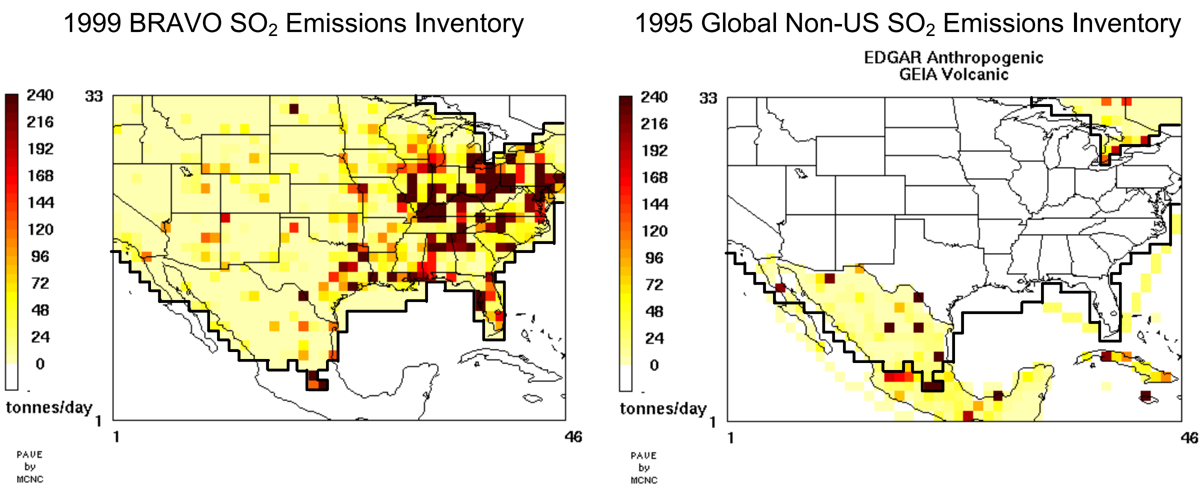

Figure 4-4. *(Left) SO_2 emissions based on the 1999 BRAVO emissions inventory used in the REMSAD and CMAQ-MADRID modeling. No emissions were included beyond the black outline shown in the figure. (Right) SO_2 emissions outside of the United States based on 1995 EDGAR global emission inventories used by climate models.*