The Emissions Inventories and SMOKE modeling efforts used to support the BRAVO study

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ABSTRACT

The Big Bend Regional Aerosol and Visibility Observational (BRAVO) study was commissioned to investigate the sources of haze at Big Bend National Park in South West Texas. Mexican and United States emissions inventories have been assembled and processed through the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling to support the BRAVO study. The domain of the inventory includes the U.S. states of Texas, New Mexico, Colorado, Kansas, Oklahoma, Louisiana, and Arkansas; the Mexican States of Chihuahua, Durango, Sinaloa, Zacatecas, Tamaulipas, Coahuila De Zaragoza, San Luis Potosi, and Nuevo Leon; and offshore activities in the Gulf of Mexico. The emissions inventory for Mexico is the first regional scale inventory for this area. Emissions data have been compiled from numerous sources including U.S. Environmental Protectional Agency, the Texas Natural Resources Conservation Commission, the Eastern Research Group, the Minerals Management Service, the Instituto Nacional de Ecologia, and the Instituto Nacional de Estadistica Geografia y Informatica. The inventory includes the species ammonia (NH_3), carbon monoxide (CO), nitrogen oxides (NOx), sulfur dioxide (SO_2), volatile organic compounds (VOC), particulate matter less than 10 microns (PM_{10}), and particulate matter less than 2.5 microns ($PM_{2.5}$). These inventories consisted of point, area, non-road, mobile, and biogenic sources. Omissions include wind blown dust and forest fires. The SMOKE modeling system was used to generate 4-kilometer, 12-kilometer and 36-kilometer gridded emissions estimates for use in the Community Multi-scale Air Quality (CMAQ) and the Regional Modeling System for Aerosols and Deposition (REMSAD) models.

INTRODUCTION

In West Texas, sulfate, organic material, and elemental carbon account for 41%, 30%, and 3.5% of the fine mass budget on an annual basis. Moreover, sulfate, organics, and light absorbing aerosol are responsible for 80% of the total visible light extinction in the area. Although the predominant sources of these species are generally known to be coal combustion, motor vehicles, biogenics, and biomass burning, an integrated emissions inventory is needed to evaluate where the major sources of the regional haze at Big Bend National Park (BBNP) originate.

The Big Bend Regional Aerosol and Visibility Observational (BRAVO) Study was commissioned to investigate the causes of visibility reducing hazes at Big Bend National Park (BBNP) and was funded by both the U.S. Environmental Protection Agency (USEPA) and the National Park Service. The overall study integrates the results of various measurement and modeling efforts. The field study portion of the BRAVO Study occurred during July through October 1999 in the region surrounding BBNP in west Texas. The study involved speciated air quality monitoring at more than 30 sites in Texas as well as measurements of upper-air meteorology. Also, an artificial tracer was released from four different sites in Texas (Big Brown Power Plant, Parish Power Plant, Eagle Pass, and San Antonio) and monitored at many of the air quality sites. Air quality transport, chemical, and dispersion models are currently being applied to the region to assess the impacts of major sources on visibility at BBNP. The field measurement data from the study is being used, in part, to validate the accuracy of the air quality models.

The BRAVO Study Emissions Inventory (BRAVO-EI)[1] was used as input into the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system[2]. The BRAVO-EI was compiled and assembled from existing emissions inventories in the United States, the Gulf of Mexico, and Mexico. The inventory was processed through the SMOKE modeling system to support two different air quality modeling systems. SMOKE modeling supported Regional Modeling System for Aerosols and Deposition (REMSAD)[3] modeling for the entire United States and most of Mexico to simulate air quality for the period of July through October 1999. SMOKE was also used to support Community Multiscale Air Quality (CMAQ)[4] modeling applications over a more limited domain and for a few episodes, to investigate specific episodes of poor air quality at BBNP. SMOKE version 1.4 beta was used for this effort.

This paper focuses on the tasks completed to generate the emissions input data for these air quality models and documents the modeling domains, the input data used in the SMOKE modeling tasks, and a summary of the SMOKE processing tasks completed to support the BRAVO modeling effort.

BODY

Inventory Domain

The BRAVO-EI covers 14 states in the U.S. (Texas, Arkansas, Louisiana, Oklahoma, New Mexico, Colorado, Utah, Arizona, Kansas, Missouri, Illinois, Kentucky, Tennessee, and Mississippi), 10 states in Mexico (San Luis Potosi, Baja California Norte, Sonora, Chihuahua, Coahuila de Zaragoza, Nuevo Leon, Tamaulipas, Sinaloa, Durango, and Zacatecas) and offshore platforms in the Gulf of Mexico.

Inventory Methodology

United States

The National Emissions Inventory for base year 1999 version 100 (NEI99) was used as a starting point for the U.S. emissions inventory.[5] The database of annual and ozone season day (OSD) emissions was reduced to contain only the emissions from the 14 BRAVO states. The Texas Natural Resources Conservation Commission provided improved emissions data for onroad mobile sources, commercial ships, construction equipment, and oil field equipment in the state of Texas. The NEI emissions inventory was updated with these locally produced emissions datasets.

Hourly emissions data from Continuous Emissions Monitors (CEM's) on power plants were obtained from the U.S. E.P.A.'s Clean Air Market Program[6]. These SO_2 and NO_x emissions data were reconciled with the NEI datasets by matching facility process emissions in the NEI to stack emissions from the CEM's. The matched emissions account for 89% of all SO_2 and 86% of all NO_x emitted from external combustion power generators in the14 BRAVO states.

Mexico

A national emissions inventory for criteria pollutants does not currently exist for the country of Mexico. Data was assembled from a variety of sources in order produce the BRAVO EI. Urban scale emissions inventories have been assembled for the cities of Tijuana, Mexicali, Juarez, and Monterrey as part of Mexico's Program to Improve Air Quality.[7] Area and mobile emissions factors were calculated for these cities based on five activity indicators: population, number of households, total number of registered vehicles, agricultural acreage, and number of head of cattle.[8] Activity data obtained from the Mexican Census Borough (INEGI) was used to estimate emissions for the uninventoried areas of Mexico within the BRAVO domain.

Emissions from power plants were estimated from fuel usage and facility type data obtained as part of the Center for Environmental Cooperation's "Taking Stock" program.[9] These data were generated as part of an ongoing hazardous air pollutant emission inventory for North America. Emissions for these facilities were calculated using AP-42 emissions factors. Emissions for manufacturing facilities were calculated using emissions factors based on manufacturing sector employment from the Sistema Nacional de Informacion de Fuentes Fijas (SNIF) database maintained by the Mexican Instituto Nacional de Ecologia (INE). Employment data was obtained from INEGI for the top 4 manufacturing sectors for each Mexican state.

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 3000-5000 tons per day.[10] 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 approximations of the true emissions. Aggregate emissions from Mexico City and the industrialized area of Tula-Vitro-Apaxco were included into the inventory as point sources. No source classification was given to these cities.

All Mexican emissions data were integrated into a unified database of both area and point emissions. Precautions were taken to prevent double counting of emissions obtained from separate data sources.

Offshore

The Minerals Management Service Outer Continental Shelf Activity Database (MOAD3) inventories emissions for the development of outer continental shelf petroleum resources in the Gulf of Mexico.[11,12] The MOAD3 catalogs emissions from the development of petroleum resources in the Gulf of Mexico for base year 1992. Sources are based activities occurring on 1857 platforms. Emissions of CO, SO_x, NO_x, PM, and VOC's are reported for several activities in the gulf. These data consisted of emissions from processes occurring on platforms, commercial shipping and helicopter traffic. Only VOC emissions are reported for the majority of flaring emissions. As a result, the inventory may grossly underestimate CO, SO_2, NO_x, and PM emissions from flaring. The database has been recently updated to correct an original inclusion of methane in the tabulation of VOC emissions from flaring[13]. The revised database now includes only non-methane hydrocarbons in its flaring emissions.

Inventory Summary and Results

Detailed summaries of emissions by state for all domains are available in an associated technical report[14]. The top three major source categories and their percentage of total emissions are shown in Table 1 for each of the three regions in the BRAVO inventory domain: U.S. BRAVO states, Mexican BRAVO states, and Offshore. Emissions from forest fires, biogenic sources, and windblown dust are not considered in the following summary.

Figure 1 show the emissions density of SO_2 over the BRAVO EI domain. Emissions were summarized for all BRAVO EI counties in the U.S. and BRAVO EI municipios in Mexico for all inventoried sources. The figure shows annual emissions gridded at 0.5 degree by 0.5 degree resolution. Emissions of offshore platforms are not shown in this figure, but are negligible since SO_2 emissions from flaring were not reported. The largest single source of SO_2 on the map is the Popocatepetl Volcano in Mexico that emits approximately 1.4 million tons of SO_2 per year.

SMOKE Inventory Processing

Modeling Domains

The air quality modeling domains used in this effort included several different regional- and urban-scale domains. The CMAQ modeling effort used 12-km and 4-km horizontal resolution grids (Figure 2). The 4-km CMAQ grid includes southwestern Texas and portions of northeastern Mexico. The 12-km CMAQ grid includes all of Texas and its surrounding states and most of northern Mexico.

The REMSAD modeling effort included a regional 36-km horizontal resolution grid that covered most of the continental United States and Mexico (Figure 3). The REMSAD 4-km horizontal resolution grid covered approximately the same area as the CMAQ 4-km grid. The REMSAD 12-km grid covered the same area as the CMAQ 12-km grid plus a few other states and regions.

Input Data

The anthropogenic BRAVO-EI consisted of the point-, mobile- and area/nonroad source inventory data as described in the previous section. The emissions inventory was assembled in the Inventory Data Analysis (IDA) format, which is compatible with the SMOKE modeling system. Based on their regional coverage, emissions data sources were divided into three groups: (1) United States, (2) Mexico, and (3) Offshore. The emissions inventory for Mexico is the first regional scale inventory for this area. Inventory pollutants for all regions included CO, NH_3, NO_x, PM_{10}, $PM_{2.5}$, SO_2, and VOC.

The Penn State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Modeling System (MM5)[15] was used to generate meteorological input data for the air quality and emissions modeling systems. The MM5 output data were then processed using the Meteorology/Chemistry Interface Processor (MCIP)[16] and other meteorological preprocessors so they could be used as input into the air quality models. These MCIP data were then used in the SMOKE processing to support the domains shown in Figure 2 and Figure 3. The meteorological data were used for biogenic emissions processing as input into SMOKE-Biogenic Emissions Inventory System version 2 (BEIS2)[17] to support both REMSAD and CMAQ applications. The meteorological data were also used for plume rise calculation and vertical allocation of point-source emissions in SMOKE to support CMAQ applications.

Additional SMOKE input files were generated to support the BRAVO modeling effort. These included spatial surrogate data and gridded land use data. The surrogate data were created for all modeling domains shown in Figures 1 and 2. The surrogates were generated using the MIMS Spatial Allocation Tool[18,19]. 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 3.

The land use data were generated using the Biogenic Emissions Landcover Database version 3 (BELD3)[20]. 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.

Point Sources

The point source inventories were processed through the SMOKE modeling system in three separate pieces: United States sources, Mexican sources, and offshore sources. The CEM data was implemented as hour-specific emissions for two episodes (Aug. 15-25 and Oct. 5-15) and as day-specific for the other time periods encompassing the four-month episode (July-Oct 1999). The modeling days of July 4 and September 6 (Labor Day) were treated as holidays by applying a Sunday temporal profile to each source. It was assumed there were no Mexican holidays during the four-month period. Latitude and longitude coordinates were used in spatial allocation of each source. The offshore sources are included in every modeling domain except the 4-km horizontal resolution domains.

To support CMAQ modeling efforts, 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)21 chemistry mechanism within the CMAQ model. The RADM2 emitting species generated by SMOKE are listed in

Table 4.

The 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. The program laypoint was run for all U.S., Mexican, and offshore sources to support the CMAQ modeling effort.

To support REMSAD modeling efforts, speciation profiles and cross-reference data were used to create emissions to support the micro-Carbon Bond IV (CB-IV)[3] with PM chemistry mechanism within REMSAD. The CB-IV with PM emitting species generated by SMOKE are listed in

Table 5.

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. We used the Emissions Preprocessor System version 2 (EPS2)[22] program called ptsrce to convert the elevated-point-source file output by SMOKE into REMSAD-ready format.

Area/Nonroad and On-Road Sources

As with the point-source data, we processed the area, nonroad, and on-road mobile-source inventories through the SMOKE modeling system in three separate pieces: United States sources, Mexican sources, and offshore sources. The modeling days of July 4 and September 6 (Labor Day) were treated as holidays by applying a Sunday temporal profile to each source. It was assumed there were no Mexican holidays during the four-month period.

The surrogate data generated for each modeling domain were applied to each of these inventories to spatially allocate the emissions. Cross-reference files were used to allocate emissions by source category to the 18 surrogate types listed in

Table 3. No meteorological data were used in processing these inventory data. The same speciation of emissions as listed in

Table 4 and
Table 5 were used to support CMAQ and REMSAD models.

Geogenic and Biogenic Sources

The geogenic and 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). The Popocatepetl 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[23] into a three-dimensional model.

BEIS2

The land use data generated for each modeling domain briefly described earlier were used as input into SMOKE-BEIS2. There are two major steps to the SMOKE-BEIS2 modeling system. The first program, *rawbio,* used the land use data and BEIS2 emissions factors[17] to generate normalized emissions. The emissions factors are the flux rate that each species emits under standard environmental conditions (i.e., 30ºC and 1000 $\mu mol \cdot m^{-2} \cdot s^{-1}$ PAR for isoprene, and 30ºC for monoterpenes, other VOCs, and NO). BEIS2 has both a summer and a winter table of emissions factors. Only the summer emissions factors were used for the BRAVO modeling effort. The second program, *tmpbio*, environmentally corrected the normalized emissions based on the meteorological data. The basic equation used for computing biogenic emissions is shown as:

Equation (1)
$$E = \sum \left(F_i \times A_i \times M \right)$$

where E is the emission rate [g/h] for each grid cell, F is a standardized emission flux [$\mu g/m^2$-h] for each land use type i, A is the area [m^2] of each land use type i in a grid cell, and M is the environmental correction factor. The meteorological variables used were temperature at 10 meters and solar radiation reaching the ground. Biogenic VOC and NO emissions in the model respond to changes in temperature. Isoprene emissions also respond to the amount of solar radiation that reaches the vegetation and are negligible when sunlight is not present. Other documentation outlines the algorithms used to apply the environmental corrections[24,25]. Speciation profiles are used to allocate other VOC and monoterpene emissions to species recognized by the chemistry mechanism in the desired air quality model. SMOKE-BEIS2 outputs only NO and ISOP emissions to support REMSAD applications; to support CMAQ applications, it outputs NO, ISO, OLI, and HC3 emissions. The output from *tmpbio* is gridded, speciated, and temporally allocated emissions in gram-moles per hour. SMOKE also has a conversion program called *smk2emis* that was used to convert the netCDF BEIS2 output files into the binary format recognized by REMSAD.

<u>Sea-salt emissions</u>

Sea-salt particles are directly produced by spume drops resulting from the mechanical disruption of wave crests by the wind, and indirectly produced by the bursting of air bubbles resulting from the entrainment of air induced by wind stress. While spume drop formation contributes significantly to large spray droplets (>10 µm in radius), other drops produced from bubbles contribute to sea-salt particles with radii <10 µm. Sea-salt particles provide a significant source of sodium (Na^+), chlorine (Cl^-), and sea-salt sulfate (s.s. SO_4^{2-}). The production rate of sea-salt particles through both direct and indirect mechanisms has been studied by a number of researchers[26,27,28]. These studies show that the production rate of sea-salt particles is strongly dependent on meteorological conditions, especially on surface wind speed.

To support the CMAQ modeling effort a one-dimensional sea salt module[23] was converted into a three-dimensional module. The one-dimensional module calculates the surface fluxes of sea-salt particle and sea-salt species (i.e. Na^+, Cl^-, and s.s.SO_4^{2-}) as a function of meteorological conditions (i.e. wind speeds, temperature, and relative humidity). The surface flux of sea-salt particles is calculated based on previous works[24,25]. The one-dimensional module was converted from FORTRAN 77 to FORTRAN 90 and implemented the Input/Output Applications Programming Interface (I/O API)[2329] to read in the three-dimensional meteorological MCIP fields. Other software changes included reading in the necessary meteorological data and calculating other needed variables (e.g., relative humidity). An additional input file had to be created that indicates which grid cells contain salt water and how much of each of those grid cells is over salt water (e.g., 50% salt-water). It was assumed that there were no grid cells in the 4-km CMAQ grid that contained salt water. The 12-km CMAQ grid did include many grid cells that contained salt water in the southeastern part of the domain (Gulf of Mexico). There were also a few grid cells in the southwestern corner (Pacific Ocean) that contained salt water. Figure 3 illustrates the salt-water file for the CMAQ 12-km domain. The output data from the three-dimensional sea-salt module are emissions for six species, including fine and coarse Na^+, Cl^-, s.s.SO_4^{2-} in grams per second.

CONCLUSION

A regional emission inventory was assembled for 10 northern Mexican states, 14 U.S. states, and offshore activity in the Gulf of Mexico. The inventory documents the emissions of CO, NO_x, SO_2, VOC, PM_{10}, $PM_{2.5}$, and NH_3. Annual emissions data have been processed through the SMOKE emissions processing model to support the Big Bend Regional Aerosol and Visibility Observational (BRAVO) study. This study was one of the first studies to include emissions from major portions of Mexico in a regional modeling study. These inventories consisted of point, area, non-road, mobile and biogenic sources. The biogenic sources included emissions from a volcano in Mexico, vegetation, soils and bodies of salt water. Other data was generated to support spatial allocation of anthropogenic, biogenic, and geogenic sources. A one-dimensional sea salt emissions module was converted into a three-dimensional module to make use of the meteorological data available. The SMOKE modeling system was used to generate 4-kilometer, 12-kilometer and 36-kilometer gridded emissions estimates for use in the CMAQ and the REMSAD models. The modeling included processing inventories for various periods throughout the period of July through October 1999. Further application of these emissions modeling inventories is needed to evaluate the possible impacts of trans-boundary issues between the United States and Mexico and also to begin to quantify the uncertainty of the emissions estimates.

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KEY WORDS

Mexican Emissions, Emissions Processor, SMOKE, BRAVO, Emission Inventory

TABLES

Table 1. Major source types and emissions from U.S. and Mexican BRAVO States and Offshore Platforms. Total emissions have units of 1 million U.S. tons per year.

Region	CO	NH_3	NO_x	PM_{10}	$PM_{2.5}$	SO_2	VOC
U.S. BRAVO EI States Major Sources	Highway light duty gasoline vehicles (30%) Highway light duty gasoline trucks (12%) 4-Stroke Lawn and garden equipment (9%)	Cattle and Calves (58%) Fertilizer Application (15%) Hogs and Pigs (8%)	Electric Generation Bituminous/Subbituminous Coal (18%) Highway heavy duty diesel vehicles (12%) Highway light duty gasoline vehicles (10%)	Unpaved roads (47%) Agriculture crop tilling (19%) All paved roads (8%)	Unpaved roads (29%) Agriculture crop tilling (15%) All paved roads (8%)	Electric Generation Bituminous/Subbituminous Coal (53%) Electric Generation Lignite Coal (7%) Industrial Bituminous /Subbituminous Coal (4%)	Highway light duty gasoline vehicles (17%) Highway light duty gasoline trucks (7%) Gasoline service stations (5%)
U.S. BRAVO EI States Total	28.8	2.1	9.4	9.9	2.4	5.8	5.8
Mexican BRAVO EI States Major Sources	Highway light duty gasoline vehicles (60%) Highway light duty gasoline trucks (22%) Agricultural field burning (9%)	All livestock (55%) Fertilizer Application (37%) Domestic ammonia (8%)	Highway light duty gasoline vehicles (34%) Electric Generation Lignite Coal (15%) Highway heavy duty diesel vehicles (12%)	Unpaved roads (58%) Agriculture crops field burning (10%) All paved roads (7%)	Unpaved roads (34%) Agriculture crops field burning (27%) All paved roads (9%)	Popocatepl Volcano (65%) Electric Generation Residual Oil (12%) Electric Generation Lignite Coal (10%)	Highway light duty gasoline vehicles (35%) Highway light duty gasoline trucks (13%) Petroleum Storage and Transport (10%)
Mexican BRAVO EI States Total	7.2	0.3	0.6	0.9	0.3	2.6	1.4
Offshore Major Sources	Reciprocating engines natural gas (81%) Turbine engines natural gas (12%) Flaring (3%)		Reciprocating engines natural gas (87%) Turbine engines natural gas (6%) Natural gas Boilers (4%)	Reciprocating engines natural gas (58%) Turbine engines natural gas (30%) Reciprocating engines diesel (9%)	Reciprocating engines natural gas (58%) Turbine engines natural gas (30%) Reciprocating engines diesel (9%)	Reciprocating diesel engine (79%) Large bore diesel engine (10%) Reciprocating engines natural gas (5%)	Flaring (82%) Reciprocating engines natural gas (13%) Crude oil tank breathing (4%)
Offshore Total	0.022	0.000	0.093	0.002	0.002	0.000	0.278

Table 2. List of States in BRAVO Northern Mexico Emission Inventory Database

State	**MX State ID**
Baja California Norte	2
Chihuahua	8
Coahuila De Zaragoza	5
Durango	10
Nuevo Leon	19
San Luis Potosi	24
Sinaloa	25
Sonora	26
Tamaulipas	28
Zacatecas	32

Table 3. Surrogate types for the BRAVO modeling domains.

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

Table 4. Emissions species for input into the RADM2 chemistry mechanism.

SMOKE-RADM2 Species	Description	SMOKE-RADM2 Species	Description
NO	Nitrogen oxide	ALD	Acetaldehyde
NO2	Nitrogen dioxide	ISO	Isoprene
CO	Carbon monoxide	TOL	Toluene
SO2	Sulfur dioxide	XYL	Xylene
SULF	Sulfuric acid	ETH	Ethane
NH3	Ammonia	HC3	Slow-reacting alkanes
PMFINE	Other fine particulates	HC5	Medium-reacting alkanes
PMCOARS	Particulates <10 µm	HC8	Fast-reacting alkanes
PSO4	Particulate sulfate	OLT	Terminal alkenes
PNO3	Particulate nitrate	OLI	Internal alkenes
POA	Other aerosols	CSL	Cresol
PEC	Elemental carbon	KET	Ketones
OL2	Ethene	ORA2	Acetic acid
HCHO	Formaldehyde		

Table 5. Emitting species for input into the CB-IV with PM chemistry mechanism.

SMOKE-CB-IV with PM Species	Description	SMOKE-CB-IV with PM Species	Description

NO	Nitrogen oxide	PNO3	Particulate nitrate
NO2	Nitrogen dioxide	POA	Primary organic aerosols
CO	Carbon monoxide	PEC	Primary elemental carbon
SO2	Sulfur dioxide	GSO4	Gaseous pathway sulfate particles
NH3	Ammonia	VOC	Volatile organic compounds
PMFINE	Other fine particulates	ISOP	Isoprene
PMCOARS	Coarse particulates		

FIGURES

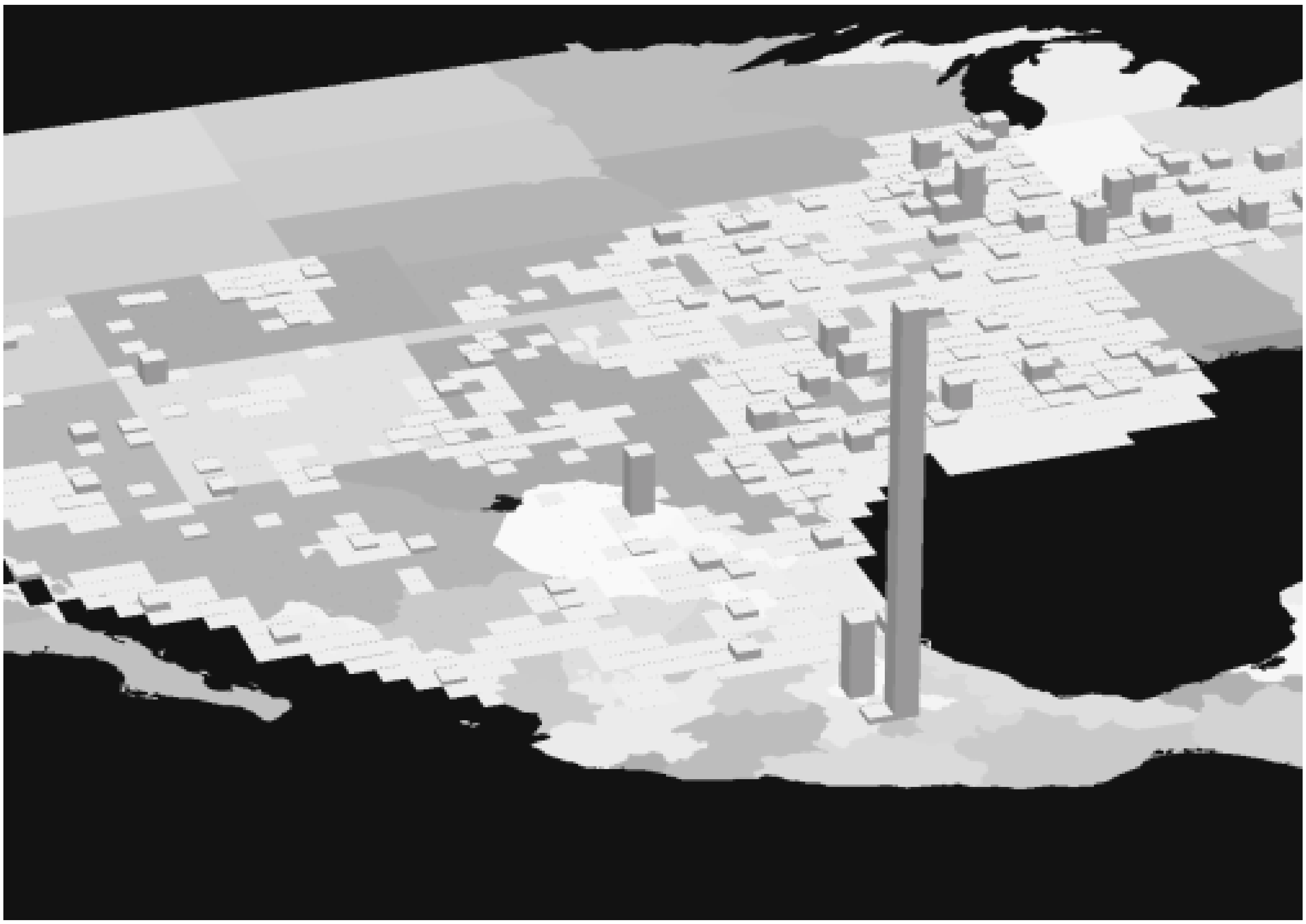

Figure 1. Gridded SO_2 emissions inventory from BRAVO study. The largest data point in Southern Mexico is the Popocatepetl Volcano emitting an estimated 1.3 million tons of SO_2 annually.

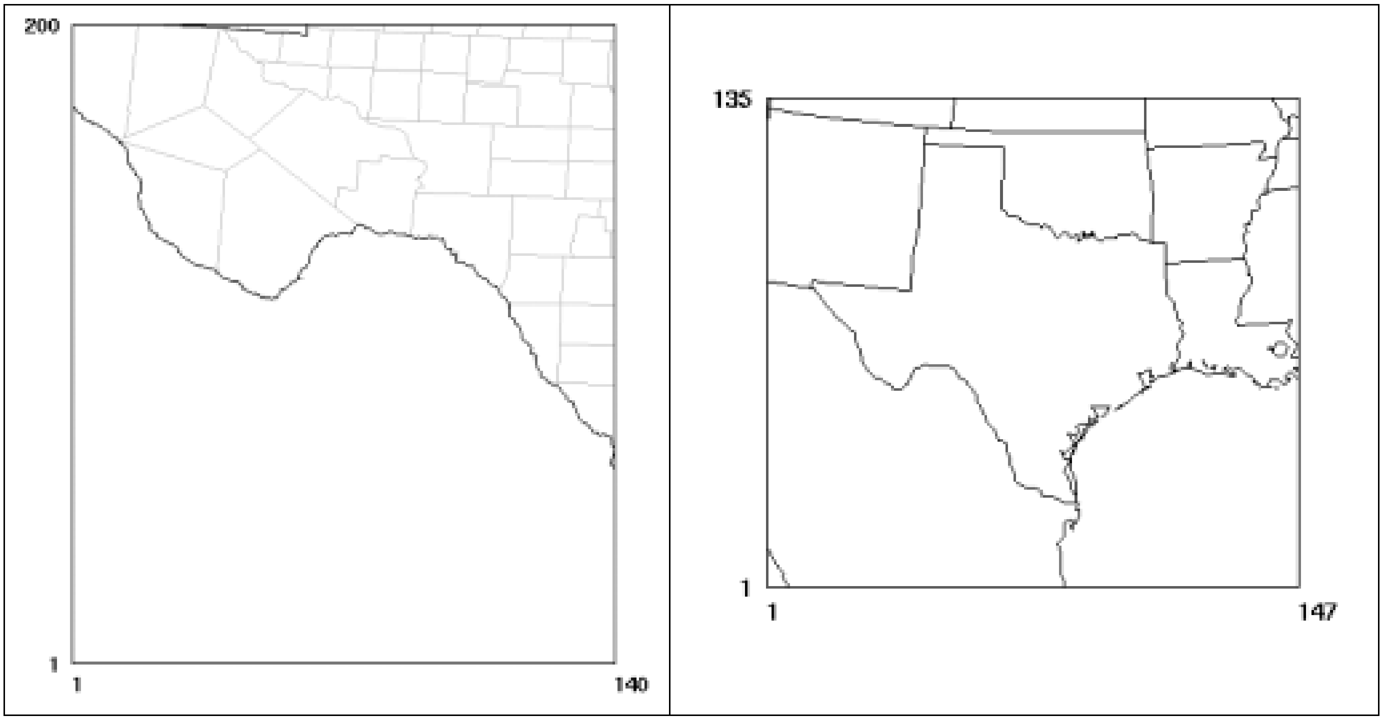

Figure 2. CMAQ 4-km (left) and 12-km (right) modeling domains.

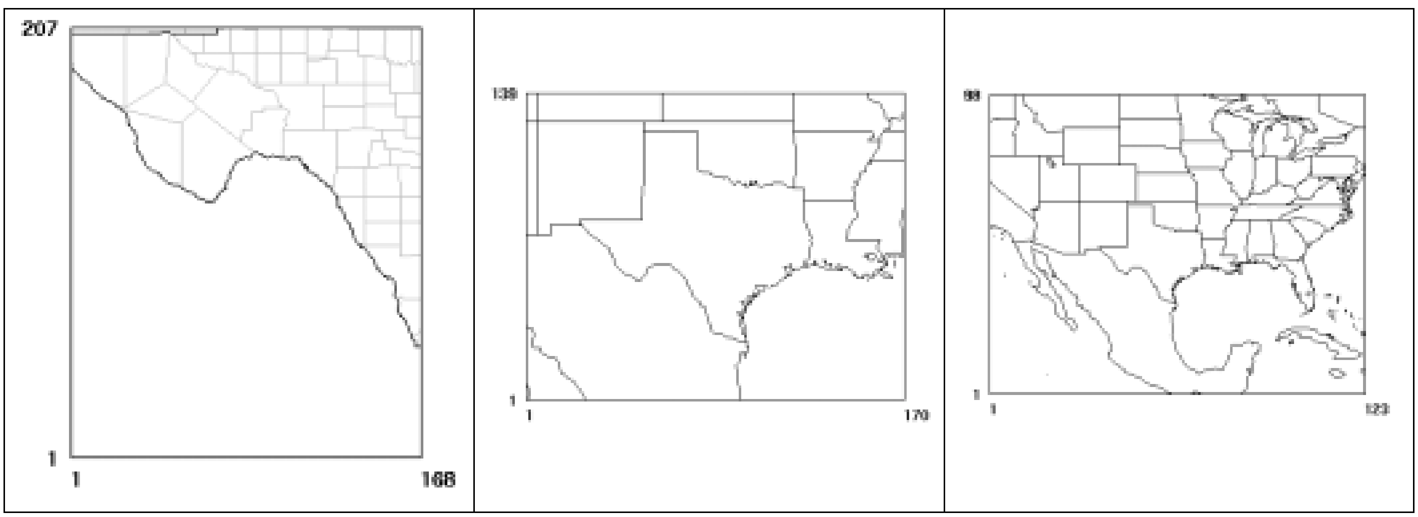

Figure 3. REMSAD 4-km (left), 12-km (middle), and 36-km (right) modeling domains.

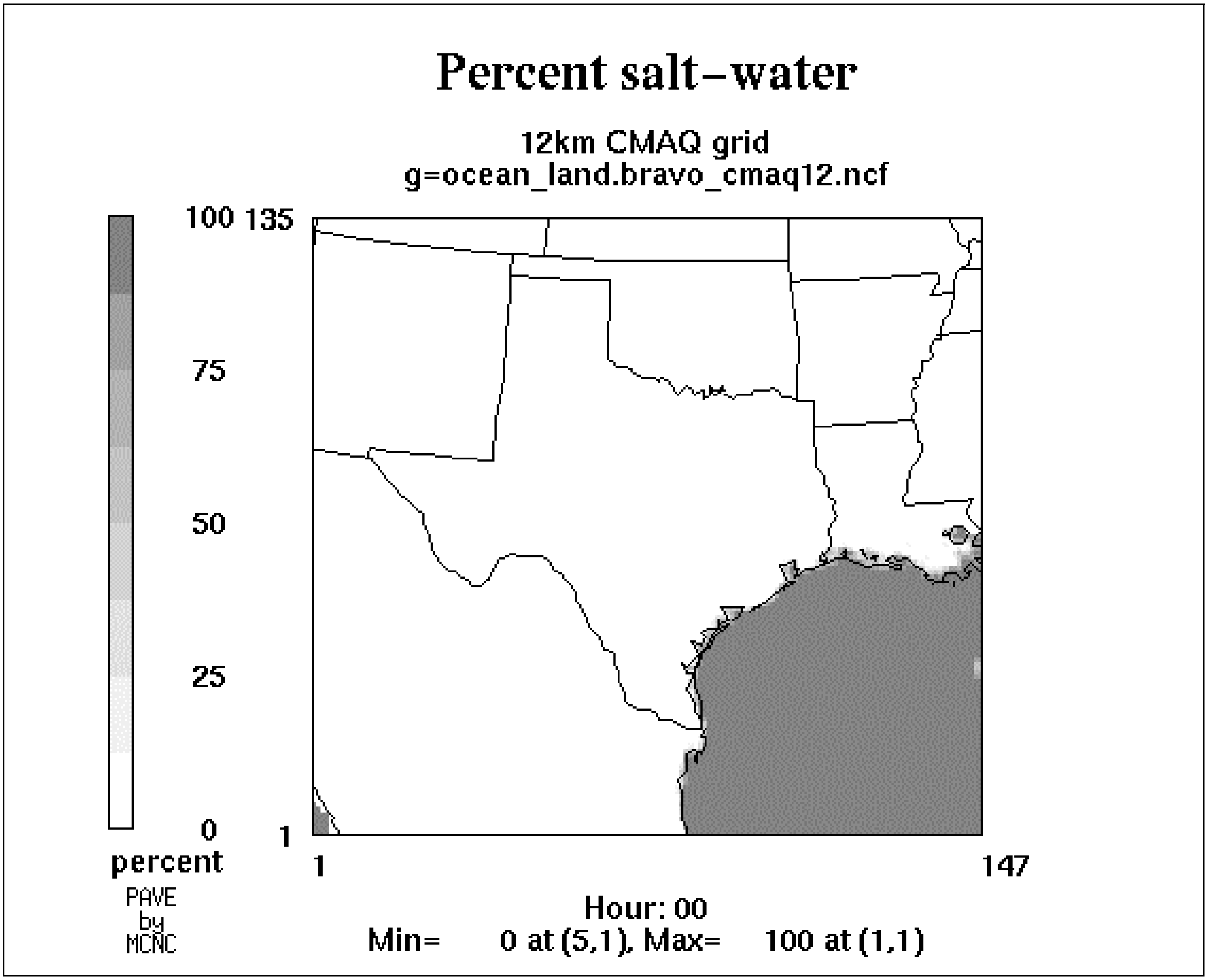

Figure 4. The percent salt water for the CMAQ 12-km horizontal resolution domain.