Preparation of the First National Emissions Inventory for Modeling at a national level in Mexico

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ABSTRACT

The first Mexico's National Emissions Inventory (MNEI), was developed for base year 1999 and includes emission estimates for seven pollutants (VOC, CO, NO_x, SO_2, PM_{10}, $PM_{2.5}$, and NH_3) for point, area, on-road mobile, nonroad and natural sources. These emission estimates are available for each one of the 2,443 municipalities of Mexico.

The MNEI represents a significant effort of diverse public and private entities in México, U.S. and Canada. The data and report of the first national emissions inventory for México were published in September, 2006 and are now available for use in air quality modeling.

This paper focuses on the progress to date in the development of the first MNEI for air quality modeling at a national level with the Comprehensive Air Quality Model with Extensions (CAMx) modeling system. The information of point, area, on-road mobile, nonroad and natural sources are temporally and spatially allocated with the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system for a modeling domain over the whole country with a grid cell resolution of 24 km. This paper emphasizes the main considerations, assumptions and limitations to develop the spatial emission allocation.

This work represents the first attempt to develop an emission inventory for modeling at national level in Mexico and its objective is to promote the use of the NEI for modeling at INE and in other institutions. Hence, there are several areas of opportunity to enhance the results, basically by improving the assumptions used in this work.

INTRODUCTION

The first National Emissions Inventory of Mexico, 1999 (1) was published on September 2006. The scope of the Mexico NEI is defined by its geographic domain, base year, pollutants, and source types. The geographic domain is the country of Mexico. The base year of 1999 was chosen because most governmental agencies possessed complete sets of the types of data needed to estimate emissions for that year. Also, the year of 1999 corresponds with U.S. EPA's National Emissions Inventory triennial reporting cycle.

The Mexico NEI contains estimates of nitrogen oxides (NOx), sulfur oxides (SOx), volatile organic compounds (VOC), carbon monoxide (CO), particulate matter (PM) less than 10 micrometers (µm) in aerodynamic diameter (PM10) and less than 2.5 µm in aerodynamic diameter (PM2.5), and ammonia (NH3) emissions for the year of 1999. The final report of this MNEI contains emissions estimates for the entire country at the state and municipality levels.

The Mexico NEI includes emissions for five specific types of sources including:

- Point sources – Stationary industrial facilities that are regulated by SEMARNAT, state, or municipal environmental agencies. Emission thresholds were established to determine whether emissions for a given facility would be considered within the point source inventory (i.e., emissions greater than the threshold) or within the area source inventory (i.e., emissions less than the threshold)

- Area sources – Small industrial facilities that are not classified as point sources; disperse activities such as dry cleaners, consumer solvents; and fugitive sources of particulate matter such as agricultural tilling, vehicle travel on unpaved roads, and windblown dust. Also included as area sources are locomotives, aircraft, and commercial marine vessels.

- Motor vehicle sources – Exhaust emissions from vehicles that travel on roadways, including private automobiles, motorcycles, taxis, buses, and heavy-duty diesel trucks.

- Nonroad mobile sources – Exhaust emissions from agricultural and construction equipment.

- Natural sources – Natural occurring emissions of VOC from vegetation, NOx from soils, and SO2 and PM from volcanoes.

A summary of the 1999 Mexico NEI for the entire country is shown in Table 1. The following are the main findings regarding this summary:

- Nearly half of the national NOx emissions are from biogenic sources. Of the anthropogenic sources, on-road motor vehicles are the most significant contributor of NOx, followed by nonroad mobile sources and power plants. On-road motor vehicles, power plants, and nonroad mobile sources emit approximately over 67 percent of the anthropogenic NOx emissions (i.e., approximately 959,000 Mg/year), or approximately 39 percent of the total (i.e., anthropogenic plus natural sources) NOx inventory.

- After geogenic/volcanic sources, power plants are the next major contributors of SOx, followed by manufacturing and other industrial processes, petroleum and coal product manufacturing (i.e., refineries), and industrial fuel combustion (an area source). These sources emit over 93 percent of the anthropogenic SOx emissions (i.e., approximately 2,676,000 Mg/year), or approximately 49 percent of the total (i.e., anthropogenic plus natural sources) SOx inventory.

- Of the anthropogenic sources, solvent utilization, on-road motor vehicles, fuel distribution (i.e., gasoline and liquefied petroleum gas [LPG]), and other fuel combustion (i.e., mainly residential wood combustion) are the most significant VOC emitters. These four categories emit over 84 percent of the anthropogenic VOC emissions (i.e., approximately 2,192,000 Mg/year), or nearly 11 percent of the total (i.e., anthropogenic plus natural sources) VOC inventory.

Details about emissions by state and pollutant can be found at INE's website http://www.ine.gob.mx/dgicurg/calaire/inem.html (Spanish) or http://www.epa.gov/ttn/chief/net/mexico/1999_mexico_nei_final_report.pdf (English).

Mexican federal environmental authorities will use the Mexico NEI as the primary basis for initiating air quality management plans and programs in areas not currently covered by the existing local air quality management programs. It will also be used to reformulate or otherwise validate current air quality improvement policies and to develop better regulations. Overall, it represents an opportunity to invite all stakeholders with an impact on air quality issues to become involved in this assessment. In particular, for Mexican municipal and state authorities participating in the NEI, this effort has provided a unique opportunity for capacity building and technical training.

Table 1. 1999 Mexico National Emissions Inventory – Summary by Source Category and Pollutant.

Source category	Emissions (Mg/year)						
	NO_x	SO_x	COV	CO	PM_{10}	$PM_{2.5}$	NH_3
Mining	30,323.7	147,108.2	27,977.6	45,983.7	32,427.6	15,538.0	
Utilities – Electricity Generation	259,833.8	1,604,849.2	11,394.4	25,310.8	79,508.3	62,884.7	
Petroleum and Coal Products Manufacturing	39,078.3	389,056.5	55,074.0	19,765.9	18,516.8	13,043.7	
Manufacturing and Other Industrial Processes	119,537.0	492,580.8	105,981.4	76,433.7	166,802.8	107,560.5	
Other services	50.9	276.1	80.4	8.4	20.9	14.7	
Merchant Wholesalers, Nondurable Goods	50.7	64.3	47,347.2	109.1	11.8	8.6	
Industrial Fuel Combustion	53,286.9	189,420.7	8,953.0	48,233.5	14,438.3	11,231.4	
Other Fuel Combustion	89,276.8	3,051.3	421,282.5	1,993,769.1	227,681.5	219,218.1	
Fuel Distribution			423,658.5				
Solvent Utilization			773,944.0				
Fires/Burning	9,174.4	537.5	54,943.7	402,537.2	58,689.1	53,627.7	
Fugitive Dust					127,703.9	27,279.1	
Ammonia Sources							1,297,832.5
Other Area Sources	124,582.5	1,632.2	60,805.6	56,312.2	10,740.4	9,012.9	
On-Road Motor Vehicles	435,664.7	24,452.8	573,042.4	4,671,841.8	20,567.5	18,844.9	7,609.4
Non-Road Mobile Sources	263,767.8	3,485.9	35,169.1	153,603.5	37,240.1	36,122.9	
Biogenic Sources	1,018,613.2		17,443,902.4				
Geogenic Sources		2,606,550.0			1,954,913.0	390,983.0	
Total	**2,443,240.7**	**5,463,065.5**	**20,043,556.2**	**7,493,908.9**	**2,749,262.0**	**965,370.2**	**1,305,441.9**
Source Category	**Emissions (percent)**						
	NO_x	SO_x	COV	CO	PM_{10}	$PM_{2.5}$	NH_3
Mining	1.24	2.69	0.14	0.61	1.18	1.61	
Utilities – Electricity Generation	10.63	29.38	0.06	0.34	2.89	6.51	
Petroleum and Coal Products Manufacturing	1.60	7.12	0.27	0.26	0.67	1.35	
Manufacturing and Other Industrial Processes	4.89	9.02	0.53	1.02	6.07	11.14	
Other services	0.00	0.01	0.00	0.00	0.00	0.00	
Merchant Wholesalers, Nondurable Goods	0.00	0.00	0.24	0.00	0.00	0.00	
Industrial Fuel Combustion	2.18	3.47	0.04	0.64	0.53	1.16	
Other Fuel Combustion	3.65	0.06	2.10	26.61	8.28	22.71	
Fuel Distribution			2.11				
Solvent Utilization			3.86				
Fires/Burning	0.38	0.01	0.27	5.37	2.13	5.56	
Fugitive Dust					4.65	2.83	
Ammonia Sources							99.42
Other Area Sources	5.10	0.03	0.30	0.75	0.39	0.93	
On-Road Motor Vehicles	17.83	0.45	2.86	62.34	0.75	1.95	0.58
Non-Road Mobile Sources	10.80	0.06	0.18	2.05	1.35	3.74	
Biogenic Sources	41.69		87.03				
Geogenic Sources		47.71			71.11	40.50	
Total	**100**	**100**	**100**	**100**	**100**	**100**	**100**

Some specific end uses for the Mexico NEI are to provide the technical data needed for national-level analyses of air emission sources affecting air quality and public health in Mexico, and to provide the input data needed to conduct air quality modeling of criteria and visibility pollutants.

Currently, the National Institute of Ecology (INE) is adapting the CAMx (2) air quality model to Mexican conditions in order to evaluate emission control measures at a national level in the near future. As part of this work, we are preparing the NEI with the Sparse Matrix Operator Kernel Emissions

(SMOKE) modeling system (3) for a modeling domain over the whole country with a grid cell resolution of 24 km. The main objective of this work is to present our progress to date regarding temporal and spatial emission allocation.

METHOD

Modeling Domain

The air quality modeling domains used in this effort include a regional domain and several different urban-scale domains, using 24-km and 8-km horizontal resolution grids (Figure 1). The 24-km CAMx grid includes the whole of Mexico (32 states and 2443 municipalities) and part of southern states of the U.S. (16 states and 895 counties) (Figure 1). The 8-km CAMx grid covers four nesting domains, each one over a metropolitan area with air quality problems, such as the Metropolitan Area of Mexico City, the Metropolitan Area of Guadalajara, the Metropolitan Area of Monterrey; Tijuana and Mexicali (Table 2).

Figure 1. Geographical coverage of Domain 1

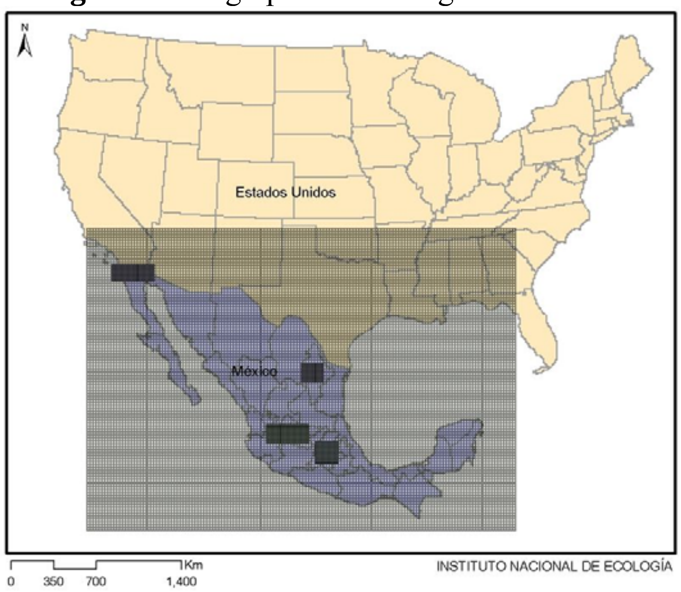


Table 2. Emission modeling domains

Domain	CAMx		Spatial Resolution	Description
	Cells in X	Cells in Y		
1	147	104	24 km	Whole country
2	23	23	8 km	Metropolitan Area of Mexico City
3	44	20	8 km	Metropolitan Area of Guadalajara
4	23	20	8 km	Metropolitan Area of Monterrey
5	44	17	8 km	Tijuana and Mexicali

Modeling periods

Due to future plans to evaluate control scenarios on an annual basis, we will model the air quality for a complete year through a "synthetic year" that comprises several episodes that characterize the air quality problem. According to Cohn et al (4) and EPA guidance (5) we will construct our "synthetic year" by modeling several days (a minimum of 15) per quarter in order to obtain "stable" values of relative reduction factors for use in evaluations. We prepared the emission inventory for four months of the year

1999: February, May, August and November of 1999. Each one was assumed to be representative of each quarter.

SMOKE Input Data

The Sparce Operator Kernel Emission (SMOKE) modeling system is being applied to convert the annual aggregated data of the MNEI to the resolution needed by the CAMx air quality model. The Mexico NEI comprises total annual emissions for area, mobile, point sources, non-road and biogenic emissions by state and municipality. The CAMx model requires emissions data on an hourly basis, for each model grid cell, and for each model species of the CB-IV photochemical mechanism. To comply with CAMx input requirements, we followed a four steps process, namely: temporal allocation, chemical speciation, spatial allocation, and merging of the MNEI. The following paragraphs will highlight the main features of the method used to develop the spatial allocation of Mexican sources.

Anthropogenic Inventory Data

Based on their regional coverage, emission data sources were divided into two groups: (1) Mexico and (2) United States. A deliverable from the Mexico NEI process were the Inventory Data Analysis (IDA) format files assembled by Eastern Research Group (ERG) for point, mobile area/nonroad and biogenic source emissions. Point, mobile and area/nonroad source inventory data from the U.S. in IDA format were taken from the EPA web page. IDA format is compatible with the SMOKE modeling system.

Meteorological Data

The Penn State University/National Center for Atmospheric Research (PSU/NCAR) Mesoscale Modeling System (MM5) (6) was used to generate meteorological input data for the air quality and emissions modeling systems. The meteorological data will be used for biogenic emissions processing as input into SMOKE-Biogenic Emissions Inventory System version 3 (BEIS3) (7) to support CAMx applications. The meteorological data are being also used for vertical allocation of point source emissions in SMOKE to support CAMx applications.

Other Data

Additional SMOKE input files to support the CAMx modeling setup are: gridded land use data an spatial surrogate data. We generated the land use data through the use of the Biogenic Emissions Landcover Database version 3 (BELD3) (7). The BELD3 consists of 1-km horizontal resolution for 230 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. We interpolated the BELD3 data to the desired modeling domain and resolution and the land use data input into SMOKE-BEIS3.

The construction of surrogate data for Mexico and the US is described in the following sections.

Emission processing

Point Sources

Mexican and United States emissions from point sources were processed separately with SMOKE. In general, point sources were assigned to grid cells using the geographic coordinates that are stored in each point-source record. To ensure consistency with the CAMx modeling system, we used the default speciation profiles and cross-reference data to create emissions profiles to support the Carbon Bond IV (CB-IV) with PM chemistry mechanism within CAMx model.

No meteorological data was used in SMOKE to compute plume rise prior to the CAMx simulations. However, a stack height cutoff of 40 m was used to differentiate between elevated and low-level point sources. Two emissions files are currently being created: an elevated-point source file and a file that contains all low-level emissions sources (low-point, area, nonroad, mobile, and biogenic). CAMx performs a plume rise calculation on the elevated sources only during model execution. All sources that have a stack height ≥40 m were written to the SMOKE elevated-point-source file, while all other sources were written to the SMOKE low-level point sources file.

Area/Nonroad and On-road Mobile Sources

As with the point-source data, Mexican and United States emissions from area/non-road and on-road sources sources were processed separately with SMOKE. The U.S. inventory included the 1999 NEI data obtained from EPA. The Mexican inventory included 32 states.

We used surrogates to spatially allocate emissions from area/nonroad and on-road mobile sources. Surrogates are human activities or land use information that are used to represent a more precise location of emission source category groups. A gridded surrogate ratio is the ratio of the amount of a surrogate in a modeling grid cell to the total amount of that surrogate in a county. Grid cell emissions are calculated by multiplying the cell's gridded surrogate ratio by the county emissions. Hence, in this phase, we aimed at identifying data sources that could be used as surrogates, gridding the surrogates to a 24 km grid, and creating surrogate cross-references and spatial surrogate ratios that could be used with the SMOKE emissions processing system for the specified 24 km and 8 km grid. The files belonging to the U.S. were also processed with SMOKE, however, this document will only describe the construction of the surrogates for Mexico.

To create the surrogates for Mexico, the following activities were developed:

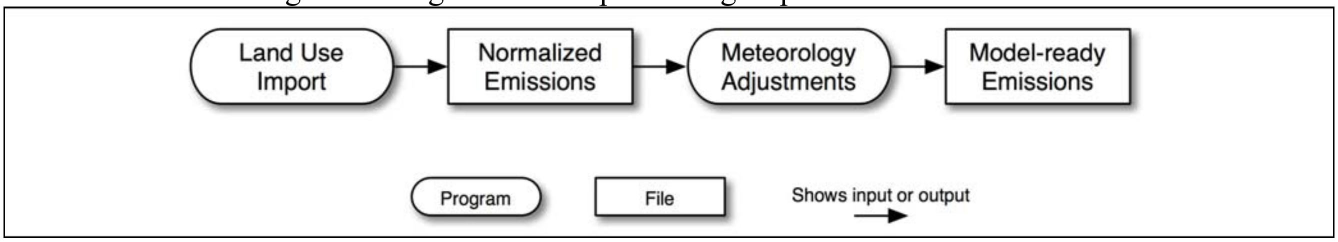
- For each Mexican emission source category we identified the corresponding Source Classification Code (SCC), and through the comparison between these SCC and the surrogate reference file (Amgref_us_051704) included in SMOKE we identified the surrogate assigned to each SCC. 52 different surrogates were identified to allocate Mexican emissions (see Table 3).
- We collected and processed the best available information in Mexico to create surrogates according to the EPA document "Process for Developing SMOKE Ready Surrogates Files" (8).
- We created the corresponding shape files with ArcGis® tools for each identified surrogate and emission source.
- We created the SMOKE-ready gridded surrogates files with the Emission Modeling Framework Surrogate Tool (9). 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 to Mexico were created basically with information from the XII Mexican population and housing census for 2000, the economic census for 1999 and vectorial files for land use available directly form INEGI's web page (http://www.inegi.gob.mx/). The surrogate data created for each modeling domain were applied to the U.S. and Mexican inventories to spatially allocate the emissions. Cross-reference files were used to allocate emissions by source category. To ensure consistency with the CAMx modeling system, we used the default speciation profiles and cross-reference data to create emissions profiles to support the Carbon Bond IV (CB-IV) with PM chemistry mechanism within CAMx model.

Biogenic Sources

We used the SMOKE- BEIS3 model for computation of hour-specific, meteorology-based biogenic emissions from vegetation and soils. SMOKE biogenic emissions modeling was accomplished with an approach that uses version 3.09 of BEIS, which was developed as part of the SMOKE system and is therefore the original version of BEIS3. Figure 2 shows the general processing scheme. The raw land use inventory data are imported and output as normalized emissions. Meteorology adjustments are then applied to the normalized emissions to create hourly model-ready emissions estimates.

Figure 2. Biogenic-source processing steps and intermediate files



RESULTS AND DISCUSSION

From the comparison between SCC for Mexican source emissions and the surrogate reference file (Amgref_us_051704) included in SMOKE we identified 55 common SCC and 27 possible surrogates to develop the spatial allocation of Mexican emissions. Table 3 shows the list of these SCC and surrogates. However, information was only available at the municipal level for 20 of them. Table 4 shows the 20 surrogates created for Mexico. Note that the spatial allocation factors and emissions category assignments vary by municipality, depending on the data available for each municipality. We did not develop gap-fill surrogates as is usually done in the U.S. Gap-fill surrogates are developed when it is possible to find that inventory emission exist for a particular county but there is not data, for that county, for the surrogate assigned. In this case it is usual to incorporate, within the assigned surrogate, a different source of data (a different surrogate) for a particular county. As part of a quality assurance procedure, we made sure that surrogates developed guaranteed to us the emissions allocation from all sources in all municipalities. To guarantee this we used surrogate tools' attributes, which allow us to check that the surrogate ratios for each county sum approximately 1.00.

Regarding the 20 Mexican surrogates created as part of this project it is important to say that they were created with the best available information at municipality level for the years 1999 and 2000 at the National Institute of Statistic, Geography and Computer Science (INEGI), which includes data for population, housing, residential heating, commercial, industrial, residential and agricultural land use, roads, etc.

One important observation about the assignment of these surrogates to each SCC is that we did not carry out a specific analysis to verify the spatial representativeness of these surrogates in Mexico. Instead, we used the default surrogates assigned in SMOKE to different SCCs included in the U.S. emission inventory, and those surrogates used previously in some US air quality modeling studies such as the BRAVO (10) and the VISTAS studies (11). A necessary next step to reduce uncertainty in the spatial allocation of emissions in Mexico is to assess the representativeness of the spatial distribution of emissions activities in Mexico and improve the available information for this purpose.

Table 3. 30 original possible surrogates for MNEI spatial allocation

No.	Surrogate assigned	Surrogate description
1	21	LPG Distribution, Mexico
2	22	Brick Kilns, Mexico
3	23	Domestic Ammonia, Mexico
4	24	Mobile sources. Border Crossing, Mexico
5	100	Population

6	140	Housing Change and Population
7	160	Residential Heating – Wood
8	170	Residential Heating - Destilate Oil
9	180	Residential Heating – Coal
10	190	Residential Heating - LP Gas
11	240	Total Road Miles
12	255	3/4 Roadway Miles plus 1/4 population)
13	260	Total Railroad Miles
14	310	Total Agriculture
15	311	Total Agriculture without Orchards/Vineyards
16	312	Orchards/Vineyards
17	320	Forest Land
18	500	Commercial Land
19	505	Industrial Land
20	510	Commercial plus Industrial
21	515	Commercial plus Institutional Land
22	535	Residential + Commercial + Industrial + Institutional + Government
23	545	Personal Repair
24	600	Gas Stations
25	700	Airport Areas
26	800	Marine Ports
27	880	Drycleaners

In the VISTAS study some preliminary surrogates were prepared to develop the spatial allocation of Mexican emission for the area included in its modeling domain. However, in this study the surrogates were created with geographical and land use information obtained from the XI Mexican population and housing census developed in 1990. Since we used more recent data, we improved the available information in terms of its updating and coverage because we created the new surrogates with geographical information closer to the emission inventory base year and for the whole country. So, we assume these surrogates to be the best approximation for spatial allocation of the Mexican emissions at this moment.

The SMOKE spatial surrogate files for Mexican and US emission sources have been concluded, while other activities as the emission processing with SMOKE are in progress. In this sense, one of the most important activities in progress at this moment is the verification of the stack parameter data to ensure that point source emissions are properly allocated both horizontally and vertically on the modeling grid. Other quality assurance activities were considered during the processing of the point, area, nonroad and on road mobiles sources datasets, including:

- Comparing inventory totals versus emission totals after import into SMOKE
- Comparing emission totals after import into SMOKE versus emission totals after application of a grid (e.g., CAMx 24 and 8 km)
- Comparing emission totals after import into SMOKE versus emissions totals after application of speciation profiles
- Comparing emission totals after import into SMOKE versus emission totals after application of temporal profiles
- Compared emission totals after import into SMOKE versus emission totals for each month

Table 4. Surrogates for MNEI spatial allocation

No.	Surrogate	Surrogate Code	Data Source
1	Brick Kilns; Mexico	22	Censo económico del 2000

2	Mobile sources. Border Crossing, Mexico	24	Board of statistical transport
3	Population	100	XII. Censo de población y vivienda 2000
4	Housing	110	XII. Censo de población y vivienda 2000
5	Residential Heating – Wood	160	XII. Censo de población y vivienda 2000
6	Residential Heating - Distillate Oil	170	XII. Censo de población y vivienda 2000
7	Residential Heating – Coal	180	XII. Censo de población y vivienda 2000
8	Residential Heating - LP Gas	190	XII. Censo de población y vivienda 2000
9	Total Road Miles	240	INEGI
10	Total Railroads Miles	260	Provided by UNC
11	Total Agriculture	310	Agriculture hectares
12	Forest Land	320	INEGI
13	Commercial Land	500	Censo económico del 2000
14	Industrial Land	505	Censo económico del 2000
15	Commercial plus Industrial Land	510	Censo económico del 2000
16	Commercial plus Institutional Land	515	Censo económico del 2000
17	Residential/RES1-4)+Commercial + Industrial +Institutional + Government	535	Censo económico del 2000
18	Personal Repair (COM3)	545	Censo económico del 2000
19	Airport Point	700	Provided by UNC
20	Marine Ports	800	Provided by UNC

CONCLUSIONS

Although at the moment we have very preliminary results, these are crucial to achieve our objective to set up the first ever air quality model in Mexico at a national level. It is also the first time in Mexico that the SMOKE model system is applied. In this sense, this work has been useful not only for our air quality modeling effort but also to develop the institutional capacity at INE for emission processing and to apply air quality models. Additionally, the surrogates created as part of this project will be also useful for other national and international institutions interested in applying air quality models for Mexico.

This first effort to process an emission inventory for modeling in Mexico has allowed us to get familiar with the SMOKE modeling tool and create very preliminary spatial surrogates for area/nonroad and on-road mobile sources. Hence, there are several areas of opportunity to improve this work such as increase the number of spatial surrogates and the cross reference file to link these surrogates with the appropriate emission source. Regarding temporal allocation, local information should also be included in this process to make a more realistic temporal allocation of our emissions. This is also the case for chemical speciation. There is little information available on hydrocarbons profiles for Mexican emission sources; however, this information could allow for improved chemical characterization of Mexican emission sources than the default values.

Pursuing these improvements will not only enhance the air quality model, but will also promote better interactions with our colleagues in charge of developing and updating the national emission inventory.

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KEY WORDS

Emission Inventory
Mexico National Emission Inventory
Mexican Surrogates