A COMPARATIVE STUDY OF US EPA NET96 AND NEI99 EMISSION INVENTORIES IN WEST GULF OF MEXICO COAST REGION

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1. INTRODUCTION

Emission inventory input has long been recognized as the most predominant factor for air quality problems including ground-level O_3 formation aside from meteorological parameters. Numerous studies have emphasized the importance of the accuracy of emission inventory data, since one of the major uncertainties involved in air quality models arises from the deficiency in emission inventories (Jiang *et al*., 1997; Hanna *et al*., 1998; Bergin *et al*., 1999; Seigneur *et al*., 1999; Mukherjee *et al*., 2000; Placet *et al*., 2000 and the references cited therein). These studies indicated that air pollutant concentrations are very sensitive to the emission quantity, speciation distribution (e.g., NO_x/VOC ratio) and other site-specific conditions such as meteorological factors.

In December 2002, EPA released the data sets of 1999 NEI estimates. This represents the newest national emission data in the US to date. However, the emission inventory files are provided in the formats of reported records and cannot be used directly in emission inventory and air quality models. Furthermore, it is of special interest to compare the new NEI99 data to the widely employed NET96 data for regional air quality modeling assessments. One objective of this study is to convert the NEI 99 raw emission inventory data into the model-ready input format for the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system, which can be used to generate gridded emission inventory inputs for supporting a wide variety of air quality models, including the CMAQ, MAQSIP, UAM-IV, UAM-V, and CAMx. Comparative study using the NEI99 and NET96 data sets is also performed using SMOKE. This model domain covers the West Gulf Coast Region of the US. The spatial and temporal emission characteristics of different pollutants from various sources are assessed.

2. METHODS

2.1 Domain Grids and Episode

The domain is comprised of 87 x 87 Lambert Conformal grids encompassing an area of 1,089,936 km^2 with a 12-km resolution centered at 31.1N and 94.5W. The horizontal grid specification of the domain follows that of the 12-km MM5 meteorological grids, except that the outer five horizontal layers were removed to reduce the boundary effects. The selected simulation period is from August 22 to August 26, 2000.

2.2 Input Data

The meteorological fields for the gridded emission processing and chemical transport simulations were generated during Texas Air Quality Study 2000 (TexAQS 2000) by Nielsen-Gammon (2002) using MM5 Release 3.4. The MM5 output files for the study domain were post-processed by EPA's Models-3 Meteorology-Chemistry Interface Processor Version 2.2 (MCIP2). During the processing, we performed a vertical layer collapsing to reduce the vertical layers from 43 sigma levels (42 vertical layers) to 22 sigma levels (21 vertical layers) for alleviating the computational costs associated with using a larger number of vertical layers.

Two emission inventory data sets, National Emission Trend 1996 (NET96) and National Emission Inventory 1999 (NEI99) Final Version 2, are compared with each other in this study. The NET96 were obtained from MCNC at http://www.emc.mcnc.org/emcenter. The NET96 data, which have been updated and revised by taking into the considerations of state-level and off-road emission data, are stored in by Inventory Data Analyzer (IDA) format and can be directly used as the inputs for SMOKE processing. The NEI99 data for criterion pollutants and precursors were obtained from USEPA's ftp site at ftp://ftp.epa.gov/EmisInventory. This version includes the estimate of 1999 anthropogenic emissions submitted by state/local/tribal agencies by February 2002. Other NEI99 versions are also available on the EPA's ftp site. Version 1 of NEI99 represents the emission data estimated from 1996 NET data for criterion pollutants considering economic growth factors, while the draft of Version 3 of NEI99 includes the emission data submitted by June 2002.

The downloaded NEI99 data are not in model-ready input formats for SMOKE modeling (i.e., IDA or EMS95 formats). Furthermore, the fields required for SMOKE input are located in different NEI99 data files for each emission source. Therefore, particular codes were developed to rearrange the emission data into IDA format for point, mobile, area and non-road sources. To

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achieve this, the raw 1999 NEI data were sorted according to the state and county codes (FIPS), source classification codes (SCC), and pollutant codes for all the emission sources (point, mobile, area, an non-road). For point source, additional sorting was also conducted based on emission unit ID and emission release point ID to obtain the required data such as site location and plume characteristics for each emission facility unit. After the sorting, the required fields from the respective files associated with each emission source were retrieved and rearranged into IDA format. After the data retrieval was performed, the area and non-road sources data were then combined into a single, unified file for area source processing. The biogenic emission was calculated by the biogenic emission processor (BEIS3) with input data of landuse, surface temperature and solar intensity from the meteorological fields.

Since IDA format requires total annual emission quantity and part of the NEI99 data are reported as daily and/or weekly averages for a given period (e.g., for several months or a season) only, additional codes were developed to calculate their respective total annual emissions and ozone season averages. For all the emission sources, this was achieved by multiplying the reported emission quantities to an emission factor calculated from the temporal allocation profiles for the respective SCC codes listed by EPA's CHIEF site (http://www.epa.gov/ttn/chief). A quality assurance routine was also written to eliminate repeated emission records and to correct typographical errors or erroneous data in the raw emission files. For examples, some of the emission records report a smaller $PM_{2.5}$ than PM_{10}; some records only report $PM_{2.5}$; and some records only report condensable PM (PM-CON) or filterable PM (PM-FIL), etc. Whenever such data discrepancies were detected, necessary adjustments of the emission values were then made. In addition, the point source emissions with the same SCC categories and locations, but different process ID were summed up to represent the total emission quantity. Finally, some point source emission records being reported in UTM coordinates were converted into the latitude-longitude pairs required for SMOKE processing. A total of more than nineteen (19) million emission inventory records in numerous files were sorted and rearranged into three emission files in IDA format. After having performed the overall data format conversions, the completed database is made of 795348, 291308 and 448675 emission records for the area (including non-road), mobile and point sources, respectively. For its counterparts in NET96, however, there are only 327883, 298181 and 397546 emission records associated with area (including non-road), mobile and point sources.

2.3 Emission Inventory Model

In this study, SMOKE Version 1.4β was compiled on a Linux platform to generate the gridded emission inventories. The temporal allocation of the emissions follow the temporal profiles listed at EPA's Clearinghouse for Inventories and Emission Factors (CHIEF) website (http://www.epa.gov/ttn/chief). The spatial allocation factors were prepared using SMOKE Tool. The national emission inventory data obtained from MCNC and EPA were speciated to follow the Carbon Bond IV chemical mechanism (Grey *et al.*, 1989). In SMOKE Version 1.4, MOBILE 5b and BEIS3 are used for mobile and biogenic emission processing, respectively. A total of 22 gaseous and PM species were included in the emission processing.

3. RESULTS AND DISCUSSIONS

3.1 Source Contribution for Criterion Pollutants and Precursors

As a general temporal emission trend, the peak emission usually occurs in the afternoon due to higher temperature (thus greater evaporation of VOC, for instance) and greater degree of human activities, while the minimum emission usually occurs in the early morning. Therefore the emission contribution from various sources is shown at two different local times (2:00 am and 2:00 pm) reflecting the typical maximum and minimum emissions during a day. The date selected for displaying the emission data is August 25, 2000, when an ozone episode took place in the southeast Texas airshed.

Table 1 shows the source contribution with respect to the criterion pollutants and precursors in NEI99 and NET96 at two different times representing the typical nighttime and daytime emissions. The source emission in NEI99 and NET 96 data are comparable. During daytime, CO emission is dominated by mobile emission due to heavier traffic in the metropolitan areas (e.g., Houston, Dallas and Baton Rouge) and on major roadways within the model domain. Emissions of the oxides of nitrogen (NO_x) are mainly from point, area and mobile sources, although the mobile contribution decreases significantly during nighttime due to reduced traffic (e.g., from 32.7 % to 10.3 % for NEI99 and from 27.6 % to 10.7 % for NET96). Sulfur dioxide (SO_2) emission is dominated by point source because of combustion of fossil fuels and industrial production of acids. Gaseous ammonia (NH_3) emission is dominated by area sources due to agricultural application of fertilizers. Emission of $PM_{2.5}$ is dominated by area sources. The emission of VOC for the entire domain is dominated by biogenic emission (over 80 % for both NET99 and NET96). This is due to the large area of vegetations in the northern and eastern sides of the domain, which emit great quantity of isoprene and paraffin. However, in the metropolitan areas where ozone non-attainments are documented, the VOC emission is dominated by area and non-road sources that emit large amount of paraffin. Mobile source also contributes the daytime VOC emission in non-attainment areas, mainly consisted of paraffin.

Table 1. Emission contribution for various pollutants from each emission source

Emission Sources	NEI99						NET96					
	CO	NH_3	NO_x	SO_2	$PM_{2.5}$	VOC	CO	NH_3	NO_x	SO_2	$PM_{2.5}$	VOC
Emissions at 2:00 am local time (%)												
Mobile	43.8	2.1	10.3	0.7	0.2	2.0	41.3	2.0	10.7	0.7	0.3	2.2
Area	42.8	91.5	24.4	9.4	84.5	9.0	41.5	83.6	31.3	14.5	78.2	12.1
Point	13.4	6.4	49.6	89.9	15.3	3.5	17.2	14.4	43.7	84.8	21.5	3.3
Biogenic	0	0	15.7	0	0	85.5	0	0	14.3	0	0	82.4
Emissions at 2:00 pm local time (%)												
Mobile	61.3	4.9	32.7	2.9	0.4	5.0	57.9	4.1	27.6	2.5	0.7	4.7
Area	32.8	89.6	25.1	13.5	85.3	3.4	35.7	90.0	32.8	19.4	78.1	12.7
Point	5.9	5.5	35.9	83.6	14.3	9.8	6.4	5.9	33.7	78.1	21.2	3.1
Biogenic	0	0	6.3	0	0	81.8	0	0	5.9	0	0	79.5

3.2 Comparison between NEI99 and NET96

Compared to NET96, NEI99 generally reports larger emissions from mobile and point sources, but smaller emissions from area sources. Emissions from biogenic sources remain unchanged since they are affected by the GIS and meteorological data only. After combining the emissions from all sources for different pollutants (merging), it is known that NEI99 data report larger emission quantities in CO, $PM_{2.5}$, SO_2 and NO_x, but smaller quantity in NH_3 and VOC as compared to those NET96 counterparts in the model domain.

The spatial difference between the NEI99 and NET96 data with respect to all the inventoried pollutants were summarized. Data shown in Figure 1 are the merged gridded NEI99 emission estimates based on all the emission sources with respect to the inventoried pollutants, while Figure 2 shows the spatial emission difference between the NEI99 and NET96 data at 2:00 pm local time. In Figure 1, it can be seen that NO_x and CO emissions bear the mobile source signature (Figure 1a & 1c); NH_3 emissions scatter over the agricultural and industrial areas (Figure 1b); $PM_{2.5}$ emissions are mainly from area sources (Figure 1d); SO_2 emissions are clearly contributed primarily by the point sources (Figure 1e); and VOC emissions are dominated by biogenic emissions in the north and east of the domain with additional "hot zones" in the metropolitan areas (Figure 1f). After subtracting the gridded NET96 emissions from the NEI99 emissions (Figure 2), it can be seen that the primary sources causing the emission difference in CO between NEI99 and NET96 data are mobile sources (i.e., the difference bears mobile source signature, Figure 2a); the sources producing the difference in NH_3 emissions are area and point sources (Figure 2b); the sources generating the difference in NO_x emissions are area, mobile and point sources (Figure 2c); the sources resulting in the difference in $PM_{2.5}$ emissions are area sources (Figure 2d); the sources making the difference in SO_2 emissions are point sources (Figure 2e); and the sources leading to the difference in VOC are point (higher) and area (lower) sources (Figure 2f).

Figure 2 characterizes some interesting distinctions between the NEI99 and NEI96 data. For example, as for $PM_{2.5}$ emission difference in Figure 2d, there is a clear "hot" and "cold" zone boundary following the state border of Texas. This indicates that in the NEI99 data, the state of Texas has a lower $PM_{2.5}$ emission inventories when compared that to NET96 data; while other adjacent states (Oklahoma, Arkansas, Louisiana and Mississippi) have larger $PM_{2.5}$ inventories. NEI99 data should better represent the actual PM emissions in these states since the $PM_{2.5}$ emission is abnormally "cold" in major areas of these states in NEI96. Furthermore, the situation of much lower area source emission quantities of $PM_{2.5}$ and VOC in the state Texas data may be due to a data discrepancy in the NEI99 estimates that requires further verification with more updated data in the future NEI releases (Figure 2d).

4. ACKNOWLEDGEMENT

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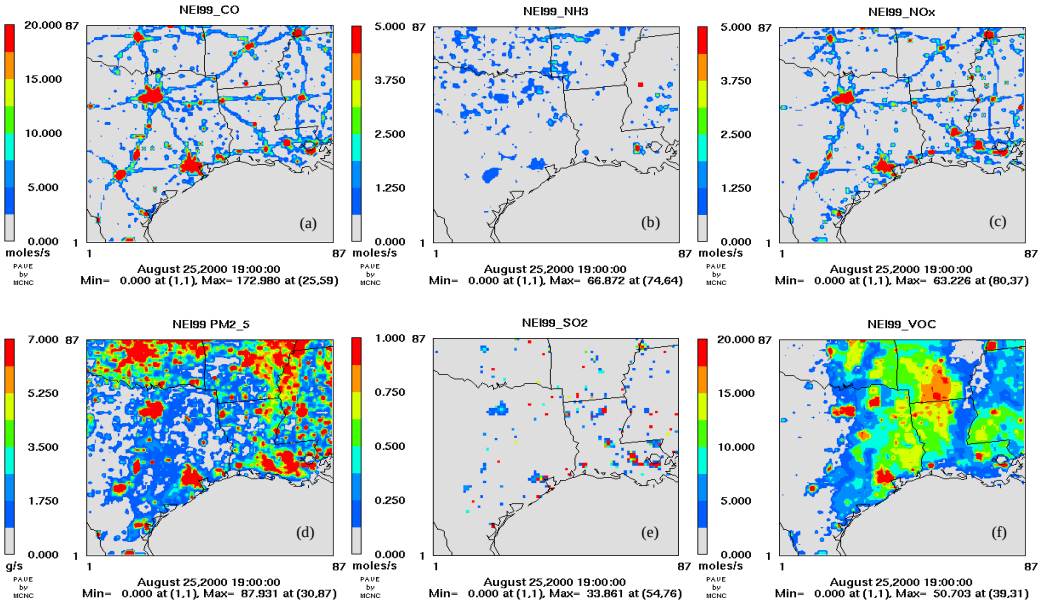

Figure 1. The gridded, merged NEI99 emissions from all the emission sources for the inventoried pollutants. The source contribution for each pollutant can be seen from these plots.

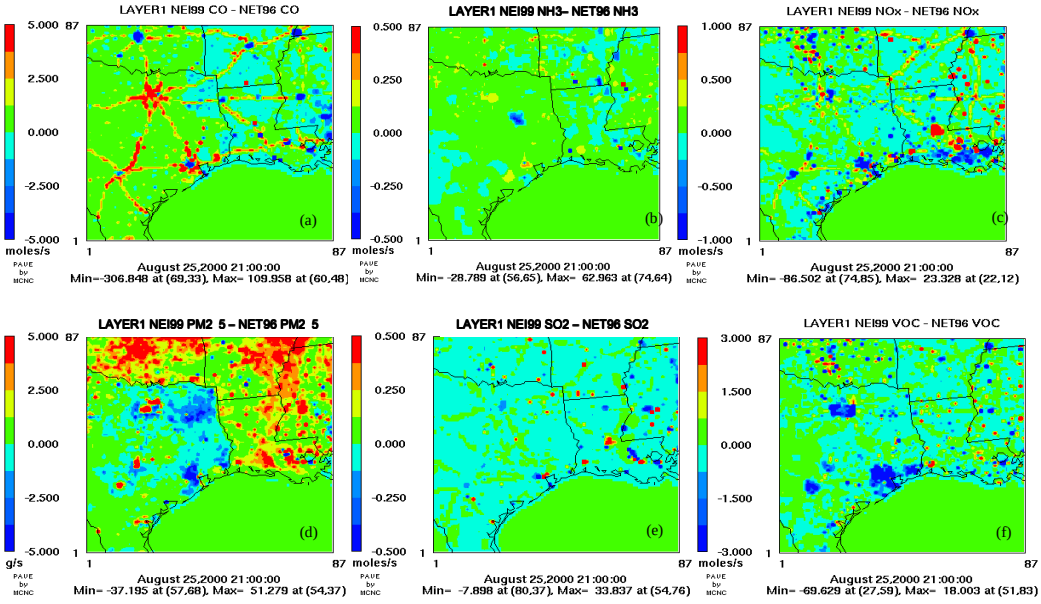

Figure 2. The spatial emission differences between the NEI99 and NET96 data. The emission sources contributing to the difference in each pollutant can be seen from these plots.