COMPARISON OF EMISSION ESTIMATES FROM SMOKE AND EPS2 USED FOR STUDYING HOUSTON-GALVESTON AIR QUALITY

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1. INTRODUCTION

The Houston-Galveston Area (HGA) is classified as one of the nation's non-attainment areas due to high ground-level ozone and particulate matter concentrations. Several air quality modeling studies are actively being carried out to find cost-effective measures for improving air quality in the region. One essential part of the modeling input data, the emissions inventory (EI), should be processed though emissions modeling systems like SMOKE (Sparse Matrix Operator Kernel for Emissions) and EPS2 (Emissions Preprocessing System version 2) for use in air quality models (AQMs) such as CMAQ (Community Multiscale Air Quality) and CAMx. These emission processing systems may present different AQM-ready emission inputs depending on the use of different cross-reference files, profiles for spatial distribution, temporal allocation methods, and chemical speciations as well as the EIs that are used. Therefore, it is worthwhile to compare one emission modeling system to another by processing the same EI.

To study air quality in HGA, both the national emissions inventories from U.S. EPA such as NET96 (National Emissions Trend for 1996) and NEI99 (National Emissions Inventory for 1999) and the state EI from Texas Commission on Environmental Quality (TCEQ) are currently available. Compared to the national emissions inventories, TCEQ's Texas EI is more specifically prepared for air quality modeling studies in the Houston-Galveston ozone non-attainment area. For example, TCEQ has developed a set of surrogate data and VOC split factors for gridding and chemical speciation in the region (Funk el al., 2002; TNRCC, 2002). Also, TCEQ's Texas EI provides information on the HGA's specific land use land cover (LULC) data and meteorological inputs for biogenic emissions. The biogenics data along with the Texas EI have been processed with the EPS2 system to provide emission inputs for CAMx.

As an alternative modeling tool, EPA's Community Multiscale Air Quality (CMAQ) modeling system, which includes the SMOKE emissions modeling system, is being used to test the emissions scenarios by external organizations or university researchers. However, unlike the EPS2 system, the SMOKE system uses nationwide cross-reference and profile data provided by U.S. EPA.

In this study we compare two emission modeling systems, SMOKE and EPS2, by processing the Texas EI available for the HGA air quality studies, focusing on the effects of differences in spatial surrogates, chemical speciation and temporal allocation data employed in the systems. For each step of the EI processing, EPS2 uses the Texas EI specific cross-reference and profile data developed by TCEQ, and SMOKE uses the U.S. EPA cross-reference and profile data.

2. EMISSIONS MODELING

The TCEQ, Environ, The University of Texas, and others have implemented emissions processing methods for building the Texas EI (ftp://www.tnrcc.state.tx.us/pub/OEPAA/TAD/Modeling/HGAQSE/Modeling/EI/) used for the HGA state implementation plan (SIP) modeling studies. In particular, the inventory data, which includes Houston-Galveston Ship Channel point-source speciated VOC emissions, were processed through the EPS2 system, GloBEIS3, and the U.S. EPA's MOBILE6 modified by the TTI (Texas Transportation Institute).

In this work, the Texas emissions inventory is processed with SMOKE and compared with the EPS2 results. Since the Texas EI has been

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previously processed only with EPS2, we have developed a set of computer codes and quality assurance procedures to enable processing of the Texas EI with SMOKE. The system is called the Texas Emissions Inventory Preparation System (TEIPS). The implementation details of TEIPS can be found in Kim and Byun (2003). The Texas EI was prepared step by step in several subcategories for each geographical location and emission source type, as described in Table 1.

Table 1**.** Summary of the Texas emissions inventory used for the comparison of SMOKE and EPS2.

Source	EI category	Remarks
Area/ Nonroad	Texas area Texas nonroad Louisiana all emissions Off-shore Elevated ship emissions	Peak ozone day emissions (Texas: 2000; Louisiana & offshore: 1999; ship: 1997) [1)]
Point	Texas EGU & NEGU [2)] Louisiana EGU & NEGU Off-shore Texas upset case	Peak ozone day and hourly emissions (1999)
Mobile	MOBILE6 output for HGA 8 counties	Link-based (2000), TTI
Biogenic	BEIS3 / GloBEIS3	BELD3 / Texas LULC data

[1)] Year in parenthesis is the base year of the EI.
[2)] NEGU presents Non-Electric Generating Utilities.

In addition to the anthropogenic Texas EI, results of BEIS3 in the SMOKE system and GloBEIS3 used by TCEQ were examined to compare the biogenic emissions. BELD3 (Biogenic Emission Land use Data) from the U.S. EPA (ftp://ftp.epa.gov/amd/asmd/beld3/) and the MCIP output from MM5 were used in SMOKE to estimate biogenic emissions. GloBEIS3 uses the solar radiation fields processed through GOES satellite data analysis, observed temperatures, and land use land cover data specifically developed for the HGA (TCEQ, 2002).

Figure 1 shows how the Texas EI was processed in the SMOKE and EPS2 systems. The emissions modeling domain for the comparison was set up for the HGA 2-km grid domain (166 x 130 cells) which covers southeastern Texas, the eastern part of Louisiana and the Gulf of Mexico as shown in Figure 2. The Texas EI was processed for the period of the TexAQS 2000 Experiment (Aug. 23rd - Sept. 1st, 2000). The CB-IV mechanism was used to speciate VOC emissions.

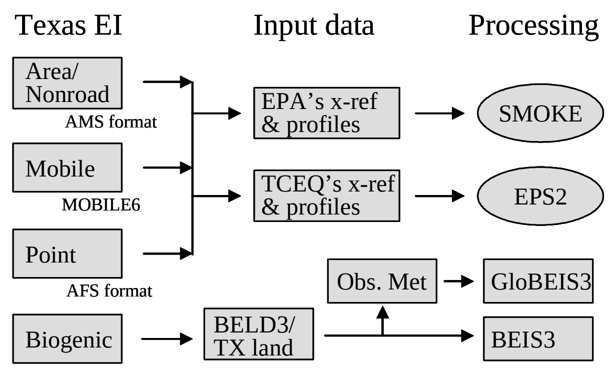

Fig. 1 Emissions modeling of the Texas emissions inventory used to compare SMOKE and EPS2 results based on U.S. EPA- and TCEQ cross-reference and profile data for each step of spatial allocation, chemical speciation and temporal allocation, respectively.

3.0 RESULTS AND DISCUSSIONS

Each step of spatial allocation, chemical speciation, temporal allocation and biogenic emissions processing were compared between the SMOKE and EPS2 systems.

3.1 Spatial Allocation

Surrogate data is used to determine spatial distributions of area and nonroad mobile emissions. Since on-road mobile emissions in the Texas EI are prepared with the link-based MOBILE6 outputs, they do not need to use surrogate data for the gridding.

The GIS emissions shape files from the U.S. EPA (ftp://ftp.epa.gov/EmisInventory/emiss_shp/) were processed with the SMOKE Tool to prepare 15 surrogates used for the spatial allocation in SMOKE. Similarly, EPS2 uses 24 surrogates developed by TCEQ (Funk et al., 2002). Since HGA is adjacent to the Gulf of Mexico and includes the Ship Channel area, the Texas EI involves all onshore and offshore emissions. However, the SMOKE system is not able to grid the onshore and offshore emissions correctly because surrogates for these can not be generated from the current U.S. EPA's emission shape files. If the emissions data are processed in SMOKE without any revision in the surrogate data, the offshore emissions become inland emissions. In order to prevent the emissions from being misplaced, TCEQ's surrogate data for EPS2 were used for the onshore and offshore emissions.

Figure 2 compares spatial distributions of the Texas area and nonroad mobile emissions for EPS2 and SMOKE. Differences in area emissions and around major roads are noticeable.

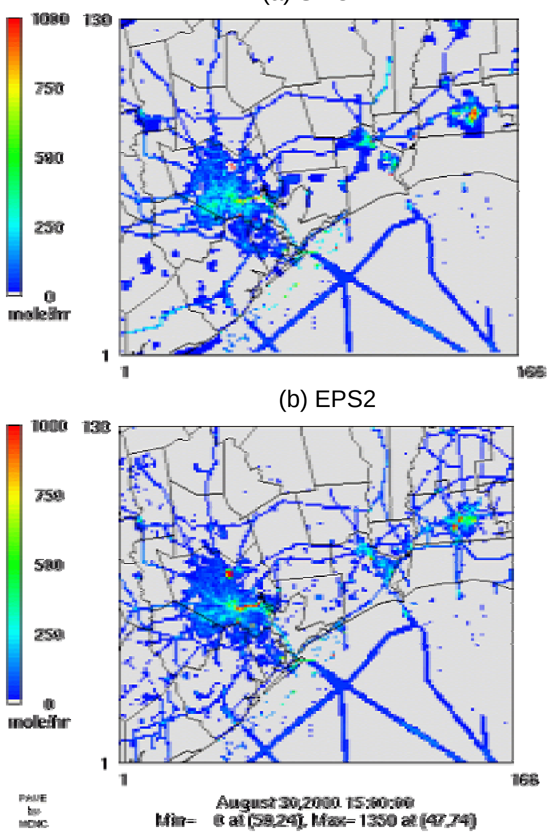

Fig. 2 Spatial distributions of area and nonroad mobile NO emissions processed by (a) SMOKE and (b) EPS2. TCEQ's surrogates were used to process onshore and offshore emissions in SMOKE.

3.2 Chemical Speciation

The chemical split factors are applied to speciate the lumped VOC emissions into individual species. SMOKE assigns a speciation profile prepared by U.S. EPA based on the SCC (Source Classification Code) of the source. Similarly EPS2 uses the TCEQ-developed profiles for chemical speciation. However, EPS2 uses the cross-reference data for each set of FIPS (Federal Information Processing System) and SCC codes to assign a chemical profile to the VOC emissions. Therefore, the exact same source and amount of VOC emissions in two counties may result in different emission rates of individual species. Also EPS2 uses special profiles for additional emissions to adjust the targeted VOC species (TCEQ, 2002).

Figure 3 compares total SMOKE and EPS2 emission rates of each species for the domain. Nonroad mobile emissions (Fig 3(a)) show an almost uniform ratio of EPS2 to SMOKE emissions rates (about 0.9) after chemical speciation. Fig. 3(a) indicates that SMOKE generates around 10% more emissions than EPS2 for the same species. In Fig 3(b), EPS2 shows relatively higher emissions for some CB-IV species such as ALD2, OLE, and XYL than SMOKE for NEGU point emissions. The ratios of EPS2 and SMOKE for species vary from source to source according to the split factors applied to the source.

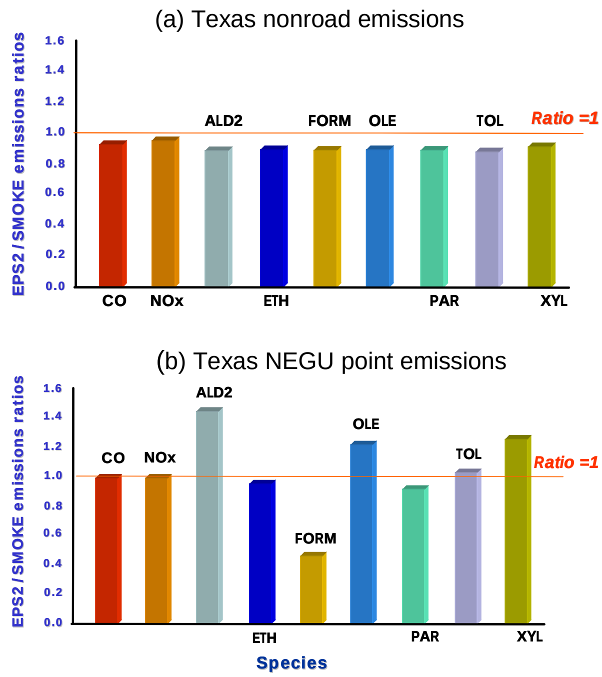

Fig. 3 Examples of the chemical speciation results for (a) Texas nonroad mobile and (b) Texas NEGU point emissions.

3.3 Temporal Allocation

To obtain hourly emissions, the peak ozone day and annual average emissions for area/ nonroad mobile and point sources are allocated with the monthly, weekly, and weekday/weekend temporal profiles.

SMOKE presents more diurnal fluctuations for the nonroad mobile emissions compared to EPS2 as shown in Fig 4(a). Specifically, SMOKE shows over 30% higher NO emission rates in daytime for nonroad mobile emissions. Fig 4(b) compares olefin emissions for the EGU point sources. SMOKE shows around 20% higher emission rates, but the variation patterns are quite similar. Usually, EPS2 does not present diurnal variations for the

NEGU point emissions. On the contrary, SMOKE displays the diurnal variations to the emissions as shown in Fig 3(c).

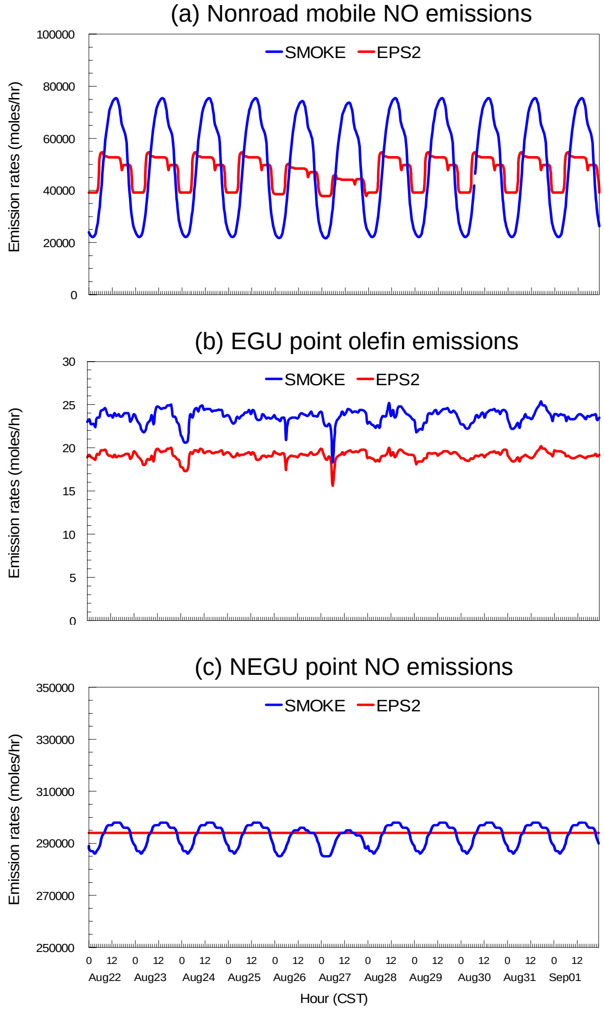

Fig. 4 Examples of temporal variations for (a) nonroad mobile NO, (b) EGU point olefin, and (c) NEGU point NO emissions after SMOKE and EPS2.

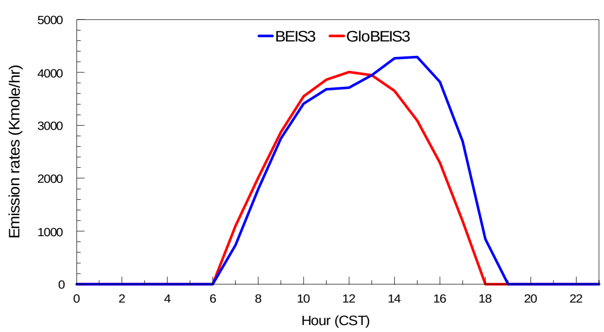

Fig. 5 Averaged diurnal variations of the isoprene emissions from BEIS3 and GloBEIS3 during the period of Aug 22 ~ Sept 1, 2000.

3.4 Biogenic Emissions

Figure 5 compares temporal variations of isoprene emissions from GloBEIS3 and BEIS3. While GloBEIS3 shows symmetric sinuous diurnal isoprene emission patterns, BEIS3 presents slightly skewed emissions rates in late afternoon. Both BEIS3 and GloBEIS3 results show relatively similar spatial distributions for isoprene while somewhat different spatial patterns for other species such as paraffins and olefins.

4. CONCLUSIONS

SMOKE and EPS2 present different emission rates of each VOC species for Texas EI after spatial allocation, chemical speciation, and temporal allocation due to different inputs of cross-reference and profile data. Also different LULC and meteorological data used in BEIS3 and GloBEIS3 show different biogenic emission patterns. To test the system algorithm differences in SMOKE and EPS2, in a future study the spatial surrogates, chemical split factors and temporal profiles will be harmonized.

5. REFERENCES

Funk, T.H., Stiefer, P.S., and Chinkin, L.R., 2001: Development of Gridded Spatial Allocation Factors for The State of Texas, Final Report 3, STI-900570-2114-FR3, Prepared for Texas Natural Resource Conservation Commission, August 31, 2001. (ftp://www.tnrcc.state.tx.us/pub/OEPAA/TAD/Modeling/HGAQSE/Contract_Reports/EI/)

Kim, S., and Byun, D.W., 2003: Prototyping the Texas emissions inventory preparation system for the SMOKE system, 12th International Emission Inventory Conference, San Diego, April 29 - May 1, 2003. (http://www.epa.gov/ttn/chief/conference/ei12/poster/kim.pdf)

Texas Commission on Environmental Quality, 2002: Attachment 3 – Emissions Inventory Development and Modeling for the August 25-September 1, 2000 Episode November 15, 2002. (ftp://ftp.tnrcc.state.tx.us/pub/OEPAA/TAD/Modeling/HGAQSE/Modeling/Doc/TSD_PHASE1/attachment3-emissions_inventory.pdf)

Texas Natural Resource Conservation Commission, 2002: Development of Source Speciation Profiles from the TNRCC 2000 Point Source Database, August 30, 2002. (ftp://www.tnrcc.state.tx.us/pub/OEPAA/TAD/Modeling/HGAQSE/Contract_Reports/EI/)