Prototyping the Texas Emissions Inventory Preparation System for the SMOKE System

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ABSTRACT

The Texas emissions inventory used for the Houston-Galveston Area (HGA) state implementation plan modeling studies by Texas Commission for Environmental Quality was processed with SMOKE and EPS2 systems and the results were compared.

SMOKE estimated higher total emissions than EPS2 for area source EI on the HGA modeling domain. Emissions from SMOKE were about 10% larger than EPS2, especially CO. After performing chemical speciation for CB-IV mechanism, SMOKE estimated higher emissions for PAR while EPS2 estimated higher emissions for TOL. Chemical speciation for point sources presented different emissions patterns for VOC species due to the use of different speciation factors.

The Texas Transportation Institute (TTI) MOBILE6 emissions based on link data were processed externally using EPS2 to facilitate further use of MOBILE6 output by combining with other source emissions in AQMs input-ready format. Compared with county-based NET96 data, TTI MOBILE6 emissions from HGA 8 counties showed around 20% lower emissions. Biogenic estimations using BEIS3 in SMOKE were also compared with GLOBEIS3 emissions used by TCEQ.

INTRODUCTION

The Texas Commission for Environmental Quality (TCEQ), Environ, University of Texas, and others have implemented emissions processing methods for building Texas emissions inventory (EI) used for the Houston-Galveston Area (HGA) state implementation plan (SIP) modeling studies. In particular, the inventory data, which include Houston-Galveston Ship Channel point-source speciated VOC emissions, are processed through the EPS2 system, GLOBEIS3, and EPA's MOBILE6 modified by TTI.

The emissions data are used with the CAMx air quality model to assess the efficacy of the emissions control strategies in HGA. As an alternative modeling tool, EPA's Community Multiscale Air Quality (CMAQ) modeling system, which includes the Sparse Matrix Operator Kernel Emissions (SMOKE) emissions processing system, is expected to gain more acceptances for air quality studies and eventually for the SIP process. To evaluate effects of different physical and chemical processes on air quality, the up-to-date Texas emissions data must be used. However, the current Texas EI data format and processing steps are tightly linked with the EPS2 system.

While the system has proven to be capable of providing necessary emissions input for CAMx operated by TCEQ, external organizations or university researchers have been unable to test emissions scenarios because they could not generate necessary model-ready emissions data for other air quality models. One of the key scientific benefits of using the SMOKE system is that it allows easy extension of the chemical mechanisms permitting investigation of the effects of the specific chemical components on ozone production.

In this paper, we described the implementation of area and point EI prepared in EPS2-ready format into SMOKE and compared some results from EPS2 and SMOKE using the EI. An external method to process link-based MOBILE6 emissions using EPS2 and to convert into SMOKE format before the merging with other emissions was applied. The results were compared with the county-based estimation using NET96. Also biogenic emissions from BEIS3 in SMOKE were compared with GLOBEIS3 output provided by TCEQ.

TEXAS EMISSIONS INVENTORY

Compared with National Emissions Inventory (NEI), TCEQ are currently using more updated and specified Texas EI for air quality modeling work in HGA ozone non-attainment area during the TexAQS 2000 period (Aug. 23rd ~ Sep. 1st, 2000). For this comparison study between SMOKE and EPS2, TCEQ's base case emissions inventories were used. TCEQ's area and point source EI were prepared in several categories by dividing geographically total emissions of each source type into five and six sub-emission types, respectively, as described in Table 1.

In the case of point sources, Texas and Louisiana EI were separately prepared for Electric Generating Utilities (EGU) and Non-EGUs using the Aerometric Information Retrieval System

(AIRS) Facility Subsystem work file format[1]. Link-based MOBILE6 output inventory from TTI was used as mobile emissions inventory.

GLOBEIS3 was used by TCEQ for the estimation of biogenic emissions. The results were compared with BEIS3 in SMOKE. Current TCEQ's EI contains emissions rates for only three raw species; a) NOx, b) VOC, and c) CO.

Table 1. Texas Emissions Inventory provided by TCEQ for the study of TexAQS 2000.

Source	EI category	Remarks
Area & nonroad	Texas area	Peak ozone day data, AIRS AMS/AFS file format (Texas: 2000; LA & offshore: 1999; ship: 1997)
	Texas nonroad	
	Louisiana all emissions	
	Off-shore	
	Elevated ship emissions	
Point	Texas EGU & NEGU (2)	Peak ozone day and hourly emissions data, AFS format (1999)
	Louisiana EGU & NEGU (2)	
	Off-shore	
	Texas upset	
Mobile	MOBILE6 output for HGA 8 counties	Link-based (2000), TTI
Biogenic	GLOBEIS3	BELD3

DATA PREPARATION FOR SMOKE

Area sources

As shown in Table 1, Texas area source EI was divided into five categories; a) Texas area, b) Texas nonroad, c) Louisiana all area, d) offshore, and e) elevated ship emissions. All of them were prepared in AMS (AIRS Area and Mobile Subsystem) work file format except elevated ship emissions in AFS (AIRS Facility Subsystem) work file format which were treated as point emissions. In order to use the area EI data file in EPS2-ready format, the header part describing file format and information is required in SMOKE to recognize the input file type. Since Texas EI file in EPS2-ready format does not include the header, it should be added before using in SMOKE.

There are several additional FIPS codes such as 98039, 98071, 98167, and 98245 in the area EI. TCEQ used the FIPS codes beginning with 9xxxx by adding 50000 to existing FIPS codes (e.g., 98039 = 48039+50000, for Brazoria County) to separate on-/off-shore emissions. Those FIPS codes should be revised or added into the state/county data file in SMOKE.

During the SMOKE run with the area EI, default temporal and gridding cross reference profile files were used. Temporal cross reference profiles were added for some SCCs of which cross reference profiles were not available from the x-ref file in SMOKE.

Point sources

Whereas other emissions such as area, biogenic and mobile sources are spatially distributed with surrogate data, point sources can be spatially allocated with their own location data. According to the EPS2 manual[2], the location of one point source can be presented as either UTM (km) or LAT-LON (decimal degrees). However, TCEQ EI data used LCP (Lambert Conformal Projection) coordinates to locate their point sources.

SMOKE is able to read the location of a point source in either coordinates[3], however there are some problems to directly use TCEQ's EI data in SMOKE without converting the location information, because TCEQ uses LCP coordinates while SMOKE uses UTM and LAT-LON coordinates when it reads EPS2-ready EI data. In AFS work file format used by EPS2 for point sources, UTM zone data is optional when LAT-LON coordinates are used. In other words, SMOKE considers point source EI to be prepared in LAT-LON coordinates if there is no UTM zone data available in the database like TCEQ's point EI. Therefore, TCEQ's LCP position values should be converted into LAT-LON coordinates prior to use in SMOKE. Like area sources, temporal cross reference profiles were added for some SCCs.

Mobile sources

TCEQ is currently using link-based MOBILE6 emissions from TTI for HGA 8-county area using VMT (Vehicle Mileage Traveled) data. While the current version of SMOKE (1.4 Beta) relies on county-based mobile emissions or MOBILE5, MOBILE6 emissions is based on link data and includes more vehicle and emission types for the estimation of air pollutant emitted from on-road vehicles.

Since the new version of SMOKE which is implemented with MOBILE6 is not available currently, we used an external method to process MOBILE6 emissions using the EPS2 system. Then it was merged with other source emissions previously processed by SMOKE. Instead of TCEQ's SAS code, FOTRAN code for data converting from MOBILE6 output to LBASE input format was used.

Biogenic emissions

In order to estimate biogenic emissions using BEIS3 in SMOKE, three BGUSE files in NetCDF format were prepared. The results were compared with GLOBEIS3 estimation provided by TCEQ.

RESULTS

TCEQ EI data using SMOKE and EPS2 systems were processed during the period of TexAQS 2000 to compare their results. The emissions modeling domains for this study were set up using TCEQ's model domain which covers southeastern Texas and some parts of Louisiana and the Gulf of Mexico (Figure 1). The meteorological data was prepared by MCIP (Meteorology-Chemistry Interface Processor) using TAMU/TNRCC MM5 (Mesoscale Model) driver base simulation.

Area sources

Figure 1 compares spatial distributions between EPS2 and SMOKE using TCEQ's area source EI except elevated ship and offshore emissions. Offshore emissions inventory was not included during SMOKE processing due to a quite different spatial surrogating system.

During SMOKE processing, spatial allocation factors prepared by SMOKETOOL using old emissions shape file were employed. As shown on Figure 1(right), the northern part of Houston presents an empty emission hole inside which one red spot shows a very high emissions rate. In practice, the area represents the Houston Intercontinental Airport in which emissions are not spatially allocated well due to missing surrogate data for airport emissions with the current shape file. EPA's new emissions surrogate file will be examined and TCEQ's surrogate data will be also tested in the near future.

Compared with EPS2 as shown in Table 2, SMOKE shows somewhat higher emissions rates for area sources. Especially, CO and PAR emissions were 10~20% higher than EPS2. In the case of TOL, EPS2 estimations show about 30% higher emissions rates. The discrepancies of total emissions amounts for CO and NOx are thought to be due to different gridding surrogate file.

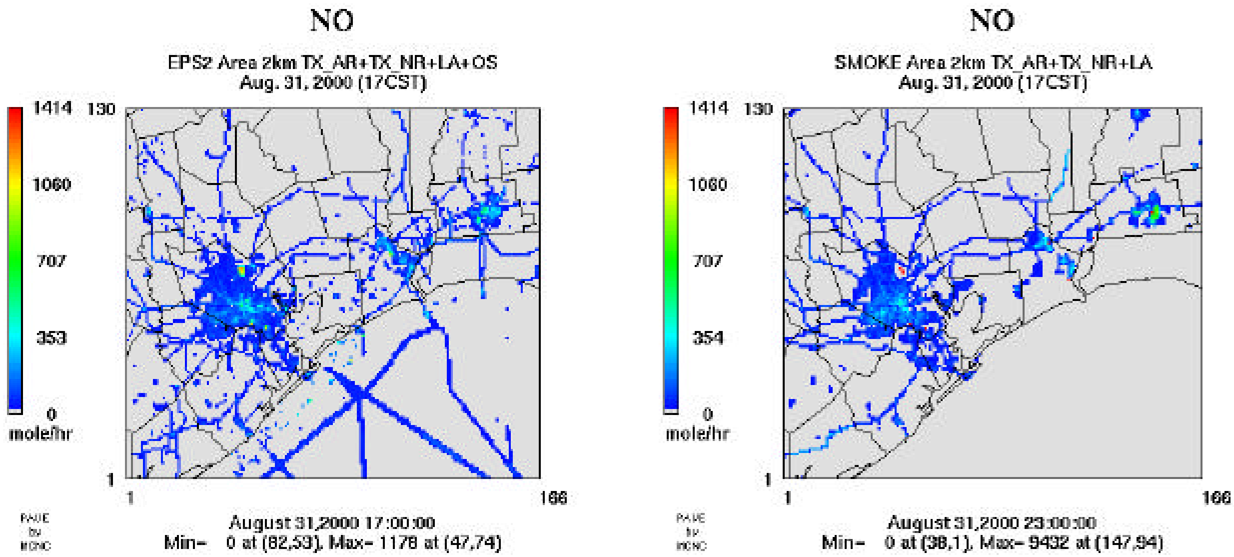

Figure 1. Spatial distributions of NO emissions from area sources processed by EPS2 (left) and SMOKE (right). Off-shore emissions were not included in SMOKE processing.

Table 2. Chemical speciation results of SMOKE and EPS2 for area source EI during TexAQS 2000.

(Unit: ton/day)

Species	Texas area		Texas nonroad		Louisiana		Total	
	SMOKE	EPS2	SMOKE	EPS2	SMOKE	EPS2	SMOKE	EPS2
CO	199.6	185.7	1373.9	1269.3	178.8	175.5	1752.3	1630.5
NO	43.5	52.3	173.8	164.3	56.9	53.4	274.2	269.9
NO2	4.8	5.8	19.3	18.2	6.3	5.9	30.5	29.9
ALD2	0.4	0.3	5.3	4.6	0.9	1.2	6.6	6.2
ETH	3.5	3.2	7.1	6.4	2.7	3.2	13.4	12.8
FORM	0.0	0.0	1.4	1.2	1.2	1.2	2.6	2.4
ISOP	0.0	0.0	0.1	0.1	0.0	0.0	0.1	0.1
OLE	2.1	1.9	5.0	4.5	1.5	1.7	8.7	8.2
PAR	143.1	113.2	76.4	67.6	42.7	41.7	262.3	222.6
TOL	26.1	41.2	11.6	10.2	4.1	4.3	41.9	55.7
XYL	22.3	23.3	16.3	14.7	4.2	5.0	42.8	43.0
Total	445.5	427.0	1690.2	1561.1	299.5	293.2	2435.2	2281.3

Point sources

Among several point inventories, spatial distributions of NO emissions from Texas non-electric generating utilities were compared as shown in Figure 2. Since point source emissions are spatially allocated on the domain with its own location data unlike other sources, EPS2 and SMOKE presents exact the same emissions pattern. However, different temporal allocation factors were used for EPS2 and SMOKE, the maximum emissions rates are different. As shown in Figure 3(left), temporal variation pattern is uniform in EPS2 while SMOKE shows slight hourly variation.

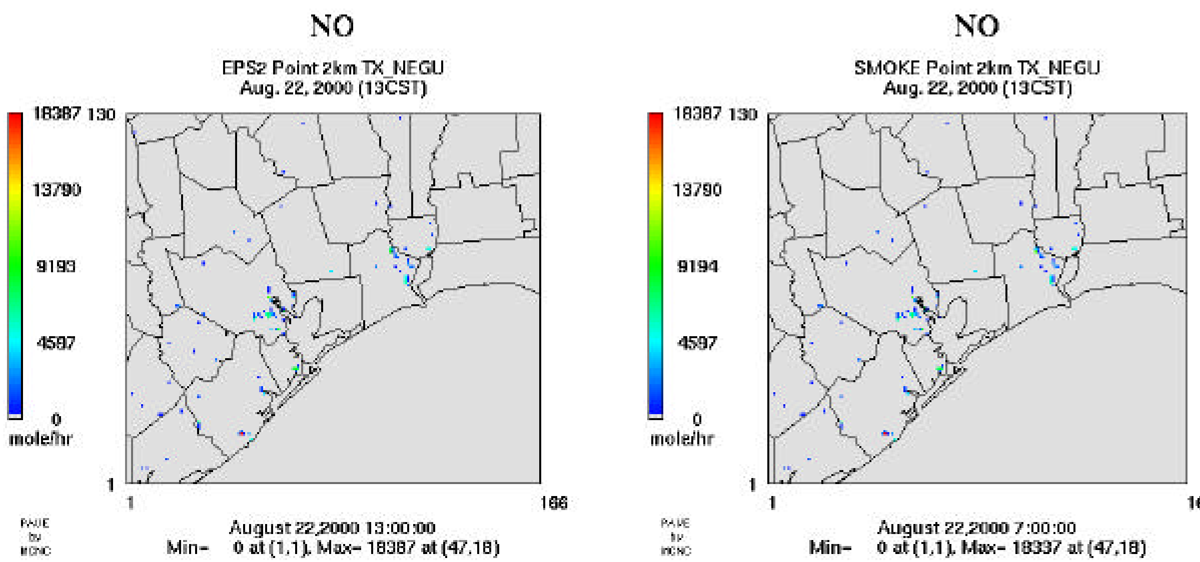

Figure 2. Spatial distributions of NO emissions from Texas non-electric generating utilities processed by EPS2 (left) and SMOKE (right)

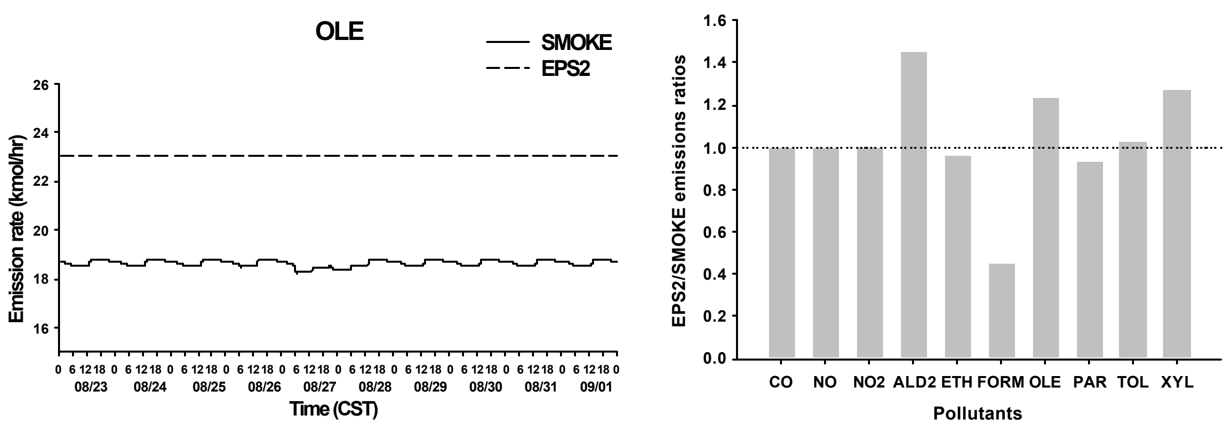

Figure 3. Temporal variations of OLE emissions (left) and EPS2/SMOKE emissions ratios (right) from Texas non-electric generating utilities.

Total emissions rates of each species from the domain during the period were compared by calculating ratios between EPS2 and SMOKE as shown in Figure 3(right). While CO and NOx emissions are same, VOC species presents different emissions rates after chemical speciation. EPS2 shows relatively higher emissions for ALD2, OLE, and XYL than SMOKE.

Mobile sources

Link-based MOBILE6 emissions inventory from TTI was pretreated using FORTRAN code and then inputted into LBASE, the first module of EPS2 to process link-based mobile EI.

Figure 4 presents MOBILE6 NO emissions rates in HGA 8 counties using VMT and link data. Compared with NET96 mobile emissions processed by SMOKE, NO emissions rates have been reduced by 20~30%, especially during afternoons and weekends, and show apparent peak emissions during morning rush hour.

Since MOBILE6 emissions were processed using EPS2, chemical speciation profiles and split factors prepared by EMSCVT, one of sub-modules in EPS2 providing chemical speciation data was applied. Once SMOKE becomes capable of processing link-based mobile emissions coupled with MOBILE6, the results may not be same due to different speciation factors uses. This influence will be also analyzed when it becomes available.

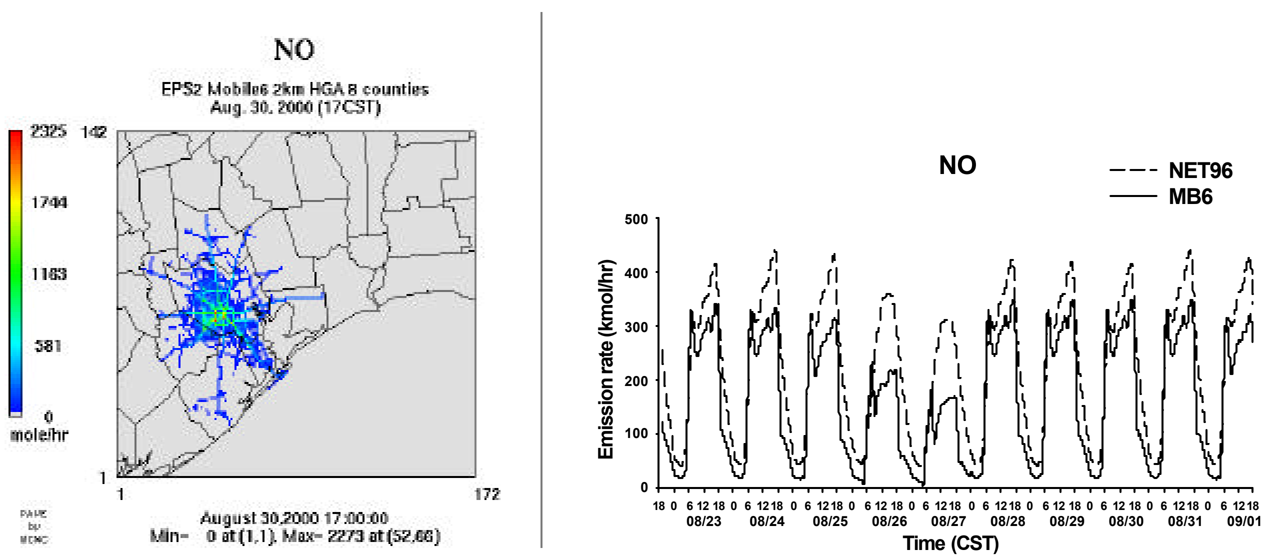

Figure 4. Spatial distributions of MOBILE6 NO emissions (left) and comparison of temporal emissions rates with NET96 (right).

Biogenic emissions

Figure 5 shows a comparison of ISOP and PAR emissions between GLOBEIS3 used by TCEQ and BEIS3 in SMOKE. Land use data for both GLOBEIS3 and BEIS3 was prepared using BELD3. In the case of meteorological data, SMOKE used MCIP output from MM5 and GLOBEIS3 used radiation estimated by satellite data analysis and observed temperature. While ISOP spatial distributions from both cases show similar emissions rates, maximum emissions rates of PAR from BEIS3 are largely different from GLOBEIS3. More details will be examined by comparing each estimation process and emissions factor of each species in GLOBEIS3 and BEIS3 afterwards and the influences will be also verified through air quality model simulations.

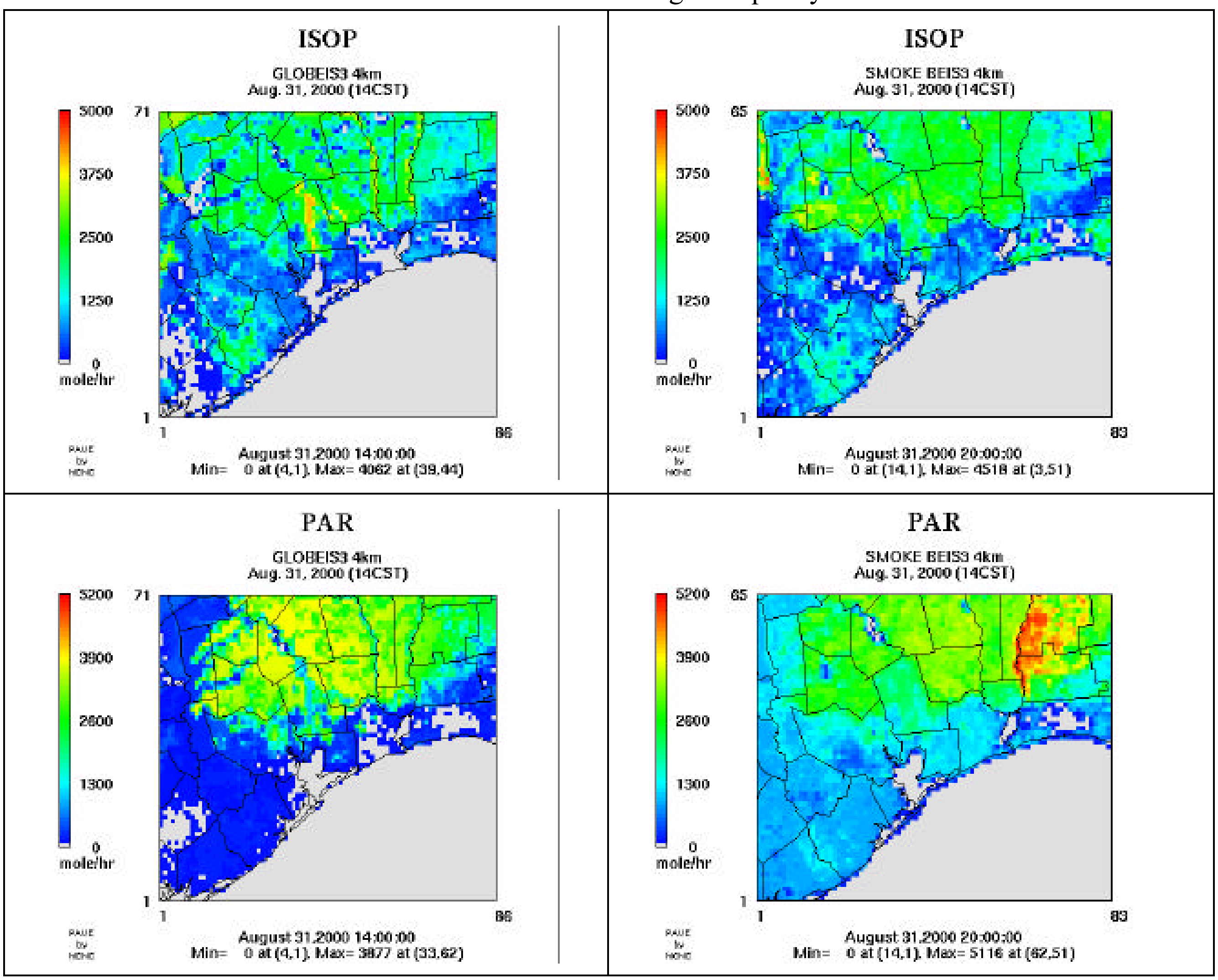

Figure 5. Comparison of ISOP (top) and PAR (bottom) emissions using GLOBEIS3 (left) and BEIS3 in SMOKE (right).

CONCLUSIONS

Texas emissions inventory used for the Houston-Galveston Area SIP modeling studies by TCEQ, two emissions preparation systems, SMOKE and EPS2, were compared for area and point source EI. Also mobile emissions between MOBILE6 and NET96 and estimations of biogenic emissions between BEIS3 in SMOKE and GLOBEIS3 were compared. The results were summarized as follows;

- SMOKE estimated a bit higher total emissions rates than EPS2 for area source. Especially, CO emissions from SMOKE were about 10% higher than EPS2. Chemical speciation showed SMOKE and EPS2 resulted in relatively higher speciated species; PAR for SMOKE, TOL for EPS2, respectively.
- EPS2 and SMOKE presented the same emissions amounts for CO and NOx for point sources, however ALD2, OLE, and XYL emissions in EPS2 were relatively higher than SMOKE.
- Compared with county-based NET96 mobile emissions, MOBILE6 showed around 20% lower emissions rates.
- GLOBEIS3 and BEIS3 showed different emissions patterns.

In the future these emissions data will be used to perform cross comparisons of SMOKE and EPS2 with CAMx and CMAQ.

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KEY WORDS
Texas Emissions Inventory
SMOKE
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MOBILE6

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