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A STUDY OF PHOTOCHEMICAL PROCESSES OF THE HOUSTON-GALVESTON METROPOLITAN AIRSHED WITH EPA CMAQ

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1. INTRODUCTION

Compared with typical ozone evolution patterns in a clear summer day in other US cities, air quality observations in the Houston-Galveston area show rapid transient high ozone events that significantly violate the National Ambient Air Quality Standards. We investigate meteorological processes and photochemical production of ozone for the Houston-Galveston area using the EPA's Models-3 CMAQ modeling system. Utilizing available meteorological and emissions data, we characterize the CMAQ's performance for the Texas Air Quality Study (TexAQS) 2000 field experiment period.

2.0 CMAQ SYSTEM IMPLEMENTATION AND PROCESSING

In the following, we describe implementation of the CMAQ system (Byun and Ching, 1999) and processing steps used in the present study.

2.1 Meteorological Simulations

We have used Nielson-Gammon (2002) TexAQS "driver" MM5 simulation restults in which a set of soil moisture availability values was specified to decrease during the model integration, to simulate evaporation of rain that fell just prior to the TexAQS period, August 22-September 2, 2000. The one-way nested simulations for the 36-km, 12-km, and 4-km resolution domains centered for the Houston-Galveston area have been made with lower-tropospheric nudging of water vapor, MRF planetary boundary layer mixing scheme, and the slab soil model with the 43 vertical levels.

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The soil moisture availability is specified to decrease during the model integration, to simulate evaporation of rain that fell just prior to the ozone episode. A new subroutine was added to the MM5 to permit model restarts with updated soil moisture. The driver model runs are expected to produce generally accurate daytime lower tropospheric temperatures and winds. Most days of the episode, the meteorological fields appear to be adequate for driving the particular combination of mixing and chemical processes that lead to high ozone on each of those days (Nielsen-Gammon, 2002). The MM5 data was further processed with the meteorological-chemistry interface processor (MCIP2) to generate meteorological input for the CMAQ system.

2.2 Emissions Processing

EPA has released the SMOKE Tool as a part of the Models-3 Computational Framework, replacing the original Models-3 Emissions Projection and Processing System (MEPPS). The SMOKE Tool is coded in the SAS© and Arc/Info languages, and has been configured to operate from the Models3 Study Planner and to provide input files in the required formats to SMOKE (Coats and Houyoux, 1996). However, the implementation and operation of the Models-3 framework require expensive third party software and experienced operator. In addition, the cost of installing the SAS and Arc/Info for a UNIX workstation is very expensive. Therefore, we have installed the SMOKE Tool on a Windows PC without using the Models-3 framework. SMOKE Tool was used to generate the necessary inputs for SMOKE for the grid allocation processing, such as to define grid, to generate coverages, and to generate surrogates.

For all the three 36-km, 12-km, and 4-km domains, we have generated emissions data for CB-4 and SAPRC chemical mechanisms. We

processed mobile, area, point, and biogenic emissions with the MM5/MCIP processed meteorology data and the NET96 inventory. For area emissions, SMOKE converts inventory pollutants to hourly and gridded emissions of the chemical species data. For mobile emissions, we imported emissions data from the NET96 mobile source inventory. For biogenic emissions processing, we have used county-based vegetation data because the EPA's BELD gridded data are based on a different map projection. For the point source processing, the inventory pollutants were converted to the hourly and gridded emissions of the chemical mechanism species. We used the "layer fraction method" to calculate plume rise.

Comparison between the CB-4 and SAPRC emissions shows comparable results for the explicit VOC species, such as ethylene, while CB-4's OLE species emissions need to be compared with OLE1 and OLE2 in the SAPRC mechanism.

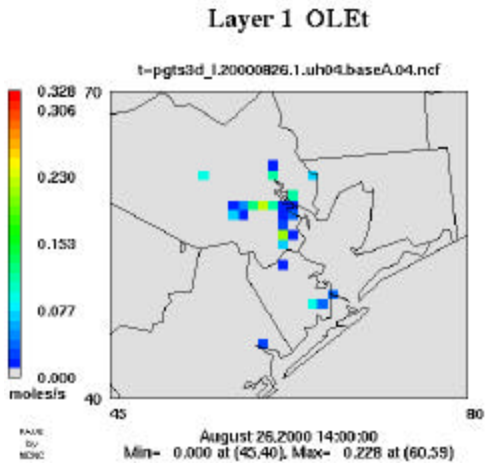

Figure 1a. Olefin emissions in CB-4.

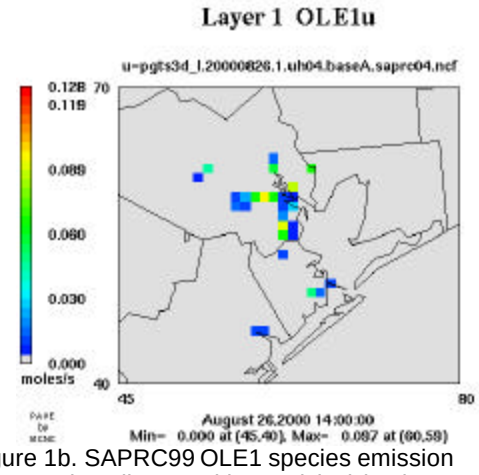

Figure 1b. SAPRC99 OLE1 species emission representing alkenes with reactivity k(OH)<7x10^4 ppm/min.

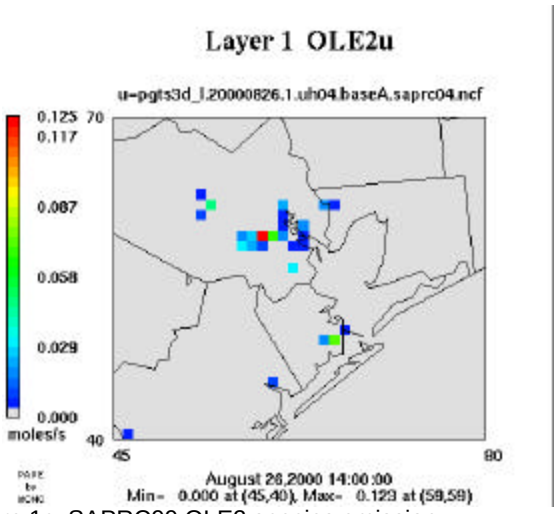

Figure 1c. SAPRC99 OLE2 species emission representing alkenes with reactivity k(OH)>7x10^4 ppm/min.

As an alternative, we have processed CAMx-ready emissions data used for the CAMx simulations by the Texas Commission for Environmental Quality (TCEQ) for CMAQ. This was necessary because the EPA 96 NEI is too old to represent the realty. Projection of the data for the year 2000 is possible, but it would be less reliable and TCEQ has invested significant resources to generate the most up-to-date emissions data for the TexAQS 2000 period. This allows use of more realistic emissions data in the simulations and provides an opportunity comparing the CMAQ results for a large emissions sensitivity cases, from 96NEI to current TCEQ emissions data. However, the CAMx-ready emissions data is only available for the CB-4 mechanisms and at 12-km and 4-km resolutions. To convert CAMx-ready emission data into CMAQ input data, we set up the processing steps such as unit conversion, species renaming and coordinate conversion. For both area and point sources, we have to read the CAMx-ready emission in binary data format, rename the species, and convert the units accordingly to CAMQ needs. For point sources, we have rearranged the set of point sources such as Major emission and Major stack parameters, MEPSE emission and MEPSE stack parameters. These inputs are processed with the ECIP to generate CMAQ-ready emissions data.

There were large differences between the two emissions data set. For example, NEI 96 shows overestimates of NOx emissions at some point sources, which has been cleaned up since.

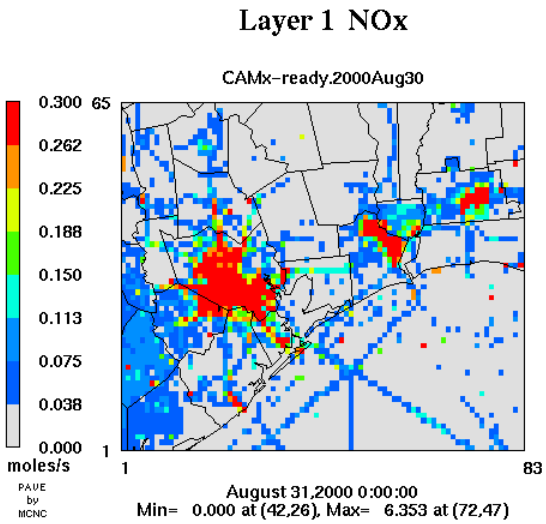

Figure 2. NOx emissions from TCEQ's CAMx-ready data for August 31, 00 UTC

2.3 CMAQ Processing

CMAQ simulations were performed for the episode August 23 – September 1, 2000 for the three domains described in Table 1. Profile boundary conditions were provided for Domain1 runs, while boundary conditions for the nested runs (Domain 2 and Domain 3) were provided from modeled results for the coarser domains. In order to provide more realistic initial conditions for the CMAQ runs, the model was allowed a spin-up time of two days, then restarted with initial conditions from hour 24 of August 24th, 2000. This procedure increased the reliability of the modeled results for August 23rd and August 24th, 2000.

Table 1: Domain characteristics for CMAQ runs

Domain	Cell	x-orig(m)	y-orig (m)
36-km	50x50	-216000	-1620000
12-km	92x92	-24000	-1500000
4-km	83x65	356000	-1228000

3.0 CMAQ SIMULATION RESULTS FOR TEXAQS 2000

3.1. Effect of minimum mixing height

By default, if the mixing height values from MM5 are missing or zero (for stable boundary layer), the Meteorology-Chemistry Interface Processor Version 2 (MCIP2) automatically assigns a value of the order of 16m (height of middle of the first layer). This may affect the pollutant distribution in CMAQ and can create unusually high surface concentrations of pollutants at night. CMAQ simulations were performed to study the effect of mixing height on air quality modeled results: the first set of runs used mixing height values passed through directly from MM5 with adjustment for minimum mixing heights to 16m; the second used meteorology with internally computed stable boundary layer in MCIP that includes adjustment to the minimum mixing heights of 50m, instead of 16m. Simulation results show that the increase of the minimum mixing height leads to reduction on ozone over a large area. The differences occurred at different times in the episode.

3.2. Comparison between the CB-4 and SAPRC simulations with 96 NEI

Houston ozone chemistry is greatly influenced by the very high olefin emissions from the Ship Channel petrochemical industries. Several monitoring sites in the Houston-Galveston area show rapid transient high ozone events (THOEs) that significantly violate the National Ambient Air Quality Standards. Recent science research projects led by the TCEQ have revealed that THOEs might be related with the large amount of co-located unsaturated volatile hydrocarbons (olefins) and NO_x emissions from industrial sources concentrated in the Houston Ship Channel area.

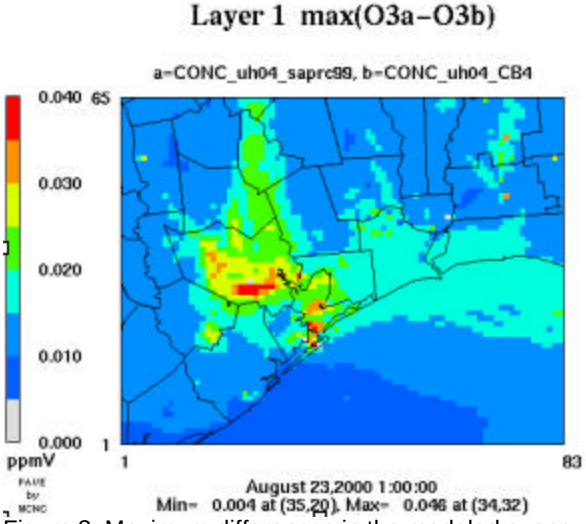

Figure 3. Maximum differences in the modeled ozone concentrations between SAPRC99 and CB4 mechanisms.

Because of the high reactivity of the olefin species, we need to compare mechanism differences between Carbon-Bond 4 and SAPRC-99 chemical mechanism. The simulations with the SMOKE-processed NEI 96 emissions data show significant differences between the CB-4 and

SAPRC mechanisms in the Ship Channel areas, where significant amount of olefin emissions exists (Figure 3). Also, except for the several point sources with large NOx emissions and a few sites with THOE trend, CMAQ compares with the observation quite favorably (Figure 4).

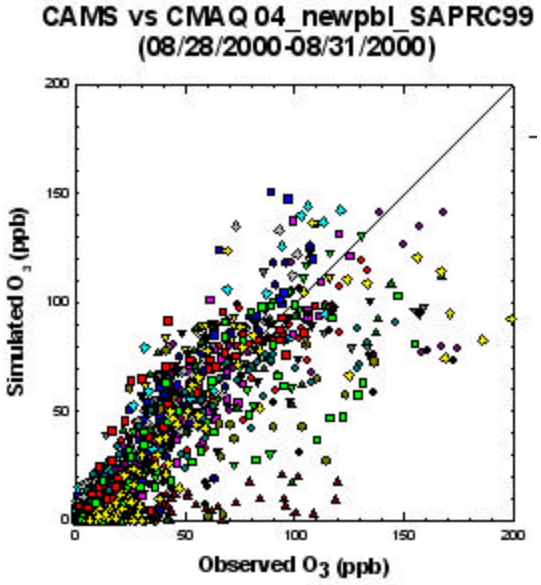

Figure 4. Evaluation of CMAQ with SAPRC mechanism against CAMS observations.

3.3. Simulation with CAMx-ready CB-4 emissions data

As stated before, the VOC emissions uncertainty in the Houston-Galveston area is large. In particular, unsaturated hydrocarbon emissions may be grossly underestimated. It is suggested that alkene emissions in inventories are significantly (factor of 3-10) lower than those expected from the aircraft measurements of formaldehyde concentration during the TexAQS 2000. With such emissions, models will not accurately simulate observations. Recognizing the shortcomings, TCEQ has modified the olefins emissions from several large point sources in the Ship Channel to have similar magnitude as the NOx emissions. We adapted this data for the CMAQ simulations.

Although the CMAQ simulation results with the TCEQ CB-4 emissions data show a very good correlation with the observation without the obvious problem in the NOx emissions, it fails to simulate high ozone conditions (Figure 5).

4.0 CONCLUSIVE REMARKS

TCEQ has been improving the CAMx simulation by further modifying the meteorology and emissions inputs as well as adaptation of 1-km flexi nesting and using the 70% of the MM5's PBL height predictions. It is yet to be studied if the current bias we observe in the CMAQ simulations can be corrected with the adaptation of the new MM5 "driver-run" simulations, or adaptation of the finer grid size in the CMAQ simulations, or the adaptation of the SAPRC mechanism.

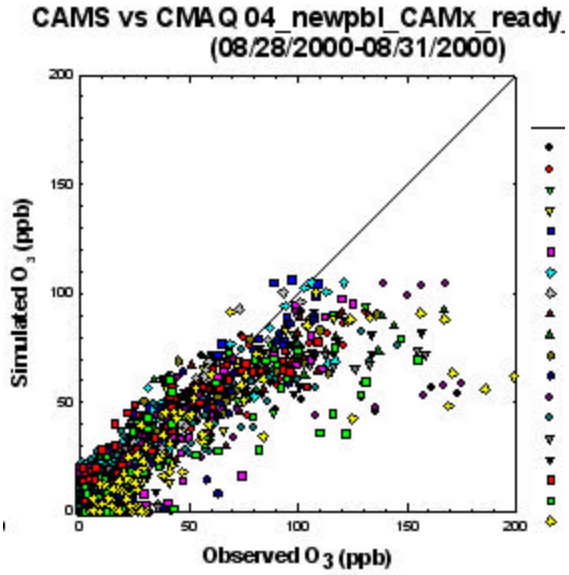

Figure 5. Evaluation of CMAQ with CAMx-ready CB-4 emissions data against CAMS observations.

5.0 ACKNOWLEDGEMENT

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