A numerical study to understand impact of meteorological fields on Houston's high O_3 problem using CMAQ/MM5

Fang-Yi Cheng, Soon-Tae Kim, Daewon Byun

Institute for Multi-dimensional Air Quality Studies, University of Houston, U.S.A.

1. Introduction

The Houston-Galveston-Brazoria area (HGB) has been known as the severe ozone (O_3) non-attainment regions in the states (Allen et al., 2002). The Houston's high O_3 concentration is mostly contributed from the petrochemical and industrial emission sources (e.g. Ship Channel) and also the emission source from urban activities such as mobile emissions. In addition, high O_3 concentrations can occur under certain meteorological conditions. Nielsen-Gammon (2002) pointed out that O_3 concentrations in the HGB area are sensitive to the wind speed and mixing layer height. For example, under shallow mixing layer and light wind conditions, the dispersion of air pollutants is limited in turn enhancing the O_3 concentrations.

In air quality modeling, correct representation of the local wind and planetary boundary layer (PBL) information are especially important to understand the transport and diffusion of pollutant behavior within the boundary layer. These processes are strongly dependent on the land surface characteristics. The default U.S. Geological Survey (USGS) 25-category land use (LU) data with MM5 (Grell et al. 1994) is outdated and inaccurate. For example, Houston is categorized as a complete impervious surface (Figure 1, panel a). With this dataset, MM5 predicted higher daytime maximum temperatures than the observations in the Houston downtown area (Cheng et al., 2004). In reality, Houston city has around 30% vegetation coverage realizing substantial evapotrasporation processes. Recently, the Texas Forest Service (TFS) hired Global Environmental Management (GEM) to generate an updated and more accurate land use and land cover (LULC) datasets for Houston and the surrounding eight county areas using the 30 meter resolution LANDSAT satellite imagery and ancillary datasets for the reference year 2000 (Figure 1, panel b) (GEM, 2003).

The objective of this study is to understand the effects of using different meteorological fields and emission inputs due to LULC differences on Houston's high O_3, and its precursor's condition.

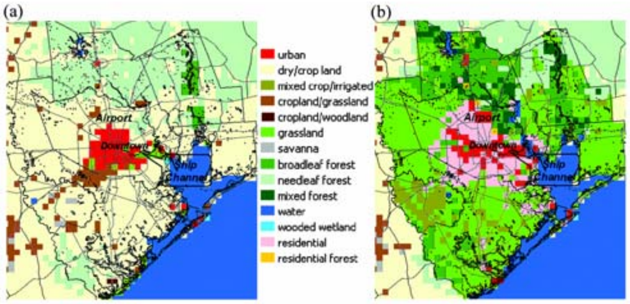

Figure 1. Dominant land use types at 4-km resolution from (a) original USGS 25-category and (b) TFS-LULC dataset.

2. Model configuration

2.1. Meteorology

MM5 Version 3 Release 6 (MM5v3.6.0) with Grell cumulus scheme for cloud condition; the medium-range forecast (MRF) boundary layer scheme for vertical diffusion and a comprehensive land surface model (Noah LSM) is utilized. Two MM5 simulations were performed with two different LU data (USGS and TFS LULC), which were named MM5-USGS (M1) and MM5-TFS (M2) respectively.

2.2. Emission

Anthropogenic emissions were prepared with the 2000 Texas Emissions Inventory (EI) provided by the Texas Commission on Environment Quality (TCEQ). TCEQ's Texas EI was specifically prepared for air quality modeling for the Houston-Galveston O_3 non-attainment area (Kim et al., 2003). The point source emissions were divided into low level sources and major elevated sources according to the stack parameters, such as stack height, exhausting gas temperature, and velocity. Biogenic emissions estimated using GloBEIS3 (Yarwood, 1999) were merged to the anthropogenic emissions for air quality simulations. Prior to input into CMAQ, the emissions inputs were converted into the CMAQ-ready format, applying the plume-rise with 3 sets of MM5: MM5-GOES (Nielsen-Gammon, 2003), MM5-USGS (M1) and MM5-TFS (M2). The emission input is named "E0", "E1" and "E2" respectively.

2.3. Air Quality Modeling

CMAQ (Byun and Ching, 1999; Byun and Schere, 2006) version 4.3 was used for air quality modeling. The CB4 chemical mechanism is applied. CMAQ used the same layer structure as MM5 (with 43 sigma layers) for the lowest 13 layers (around ~1100 m) but layers in the upper troposphere were collapsed to save computing time. We used 23 vertical levels in CMAQ.

To distinguish the influence of the meteorological changes on air quality simulations, and also to isolate the effects of the changes in the emission input due to the meteorological differences, several sensitivity studies were performed. The design of CMAQ sensitivity tests is to understand the meteorological and emission changes due to LULC differences on air quality simulation. There are three sets of the CMAQ sensitivity designs.

First, two CMAQ simulations were performed with two different meteorological fields (M1 and M2), and with "E0" emission input. The CMAQ simulation with the MM5-USGS (M1) dataset is named CMAQ-USGS (M1E0); the simulation with the MM5-TFS (M2) dataset is named CMAQ-TFS (M2E0). This sensitivity design is to confine the influence on air quality simulation the different meteorological fields due to the use of different LULC data.

Second, in order to study the effects of meteorological parameters (such as PBL heights, winds, and temperatures) on vertical allocation of point source emissions, the MM5-USGS (M1) and MM5-TFS (M2) simulations were used separately to determine emissions rates of ozone precursors for each vertical layer. The emission datasets were named EMI-USGS (E1) and EMI-TFS (E2) respectively. Two additional air quality simulations were performed using the meteorological conditions from MM5-TFS (M2), but with different emission datasets EMI-USGS (E1) and EMI-TFS (E2). The two air quality simulations are named CMAQ-TFS (M2E1) and CMAQ-TFS (M2E2).

Third, two CMAQ simulations were performed with consistent meteorological and emission datasets. The CMAQ simulation is performed with the M1 and E1 datasets (namely M1E1), to compare with the M2E2 simulation. With this setup, the meteorological and emission datasets are consistent for air quality simulations.

The Table 1 is the summary of the above 3 sensitivity comparisons. Sensitivity 1 focuses on the simulation M1E0 and M2E0. Sensitivity 2 focuses on the simulation M2E1 and M2E2. Sensitivity 3 focuses on the simulation M1E2 and M2E2.

Table 1. Lists of air quality sensitivity tests with different meteorological (MM5-USGS (M1), MM5-TFS (M2)) and emission inputs (E0, E1, E2).

Emission Meteorology	E0	E1	E2
MM5-USGS M1)	M1E0	X	M1E1
MM5-TFS (M2)	M2E0	M2E1	M2E2

3. Evaluation of model results

3.1 M1E0 V.S. M2E0

Figure 2a and 2b compare spatial distributions of ethylene from CMAQ-USGS (M1E0) and CMAQ-TFS (M2E0) simulations, respectively, at 0600 CST 30 August 2000. The corresponding plots for the PBL height are in Figure 2c and 2d. In the early morning along the Houston Ship Channel high emission area, the MM5-TFS (M2) simulation predicts deeper PBL heights (Figure 2d) than the MM5-USGS (M1) simulation (Figure 2c) because the area is represented as an urban (impervious) LULC type. The deeper mixing in turn produced lower ethylene concentrations at the surface (Figure 2b). It should also be noted that westerly winds prevailed at 0600 CST, which carried the emissions from the western side of the Houston Ship Channel area to the downwind side (East of the Ship Channel area). At a later time 1400 CST, under the well-mixed boundary layer condition, higher ethylene was simulated with the MM5-TFS data, particularly in the cell where shallow PBL height was predicted, because the high resolution TFS-LULC resolved the Ship Channel as a water body. With the northerly winds simulated for 1400 CST, the high ethylene concentrations were transported downwind or to the south.

At the La Porte site, the CMAQ-TFS (M2E0) simulation improves the prediction of maximum O_3 concentration especially on 30 of August 2000 (Figure 3). Both simulations over-predicted the NO_2 concentrations. The ethylene concentrations from the CMAQ-TFS (M2E0) simulation agreed better with the observed values than the CMAQ-USGS (M1E0) simulation. On 30 August 2000, the first peak in the morning and second peak in the early afternoon were also better captured in the CMAQ-TFS (M2E0) simulation. On the other hand, the CMAQ-USGS (M1E0) simulation showed high bias most of the time, corresponding to the shallower PBL heights predicted during the nighttime, as compared to the CMAQ-TFS (M2E0) simulation. The secondary species such as peroxyacetyl nitrate (PAN) and formaldehyde (HCHO) produced from the O_3 photochemistry, showed a significant improvement on 30 August 2000 in the MM5-TFS (M2) simulation. The peaks of HCHO and PAN improved for August 30 and 31 in the CMAQ-TFS (M2E0) simulation.

Most of the time during the episode, the precursor species were over-predicted in the CMAQ-USGS (M1E0) simulation, particularly on August 25, 28 and 31. NO_x and ethylene were over-estimated in the early morning when the mixing was confined in a shallow layer.

3.2 M2E1 V.S. M2E2 (sensitivity test with different emission datasets due to the usage of different meteorological inputs)

Considering the changes in the point source emissions with different plume-rise results due to the usage of different meteorological fields, two air quality simulations (M2E1 and M2E2) are compared. The sensitivity test shows that the CMAQ results are not significantly different between the plume-rise estimates due to the use of M1 and M2 meteorological data.

3.3 M1E1 V.S. M2E2

The previous sensitivity tests prove that the O_3 and its precursor's concentrations are not significantly affected by the emission plume-rise differences caused by the different meteorological data (M1 and M2) but by the difference in the meteorological fields mostly. The simulations show close result to the first sensitivity. The higher O_3 concentrations corresponded to the higher O_3 precursor's concentrations, which were distributed differently by the different wind transport and PBL mixing characteristics. The CMAQ-TFS (M2E2) with consistent inputs improved the high O_3 predictions slightly.

4. Conclusion

The USGS LULC dataset displays Houston as a large contiguous impervious surface while the TFS-LULC describes it as a congregation of narrow strips of impervious surface areas and isolated urban developments surrounded by the suburbs and residential vegetation LULC types. The meteorological simulation is improved with the use of a more accurate and updated land use map.

Overall, the peaks of O_3 precursors were higher and over-estimated in the Ship Channel emission source area in the CMAQ-USGS (M1E0) than the CMAQ-TFS (M2E0) simulation. The MM5-USGS (M1) simulation with the undeveloped land use type "grass" over the area predicted weaker mixing than the MM5-TFS (M2) simulation with the urban (impervious) surface type. The confined mixing over the Houston Ship Channel area resulted in over-prediction of the O_3

precursors such as NO_x and VOC species in the CMAQ-USGS (M1E0) simulation. With the correct representation of the LU type "urban" in the TFS-LU data, the mixing was enhanced and the precursor concentrations showed better agreement with the measurements. Mostly, the daily maximum O_3 concentration inside Harris County was better captured in the CMAQ-TFS (M2E0) simulation, especially on August 29, 30 and 31, due to the improvements of the actual surface conditions near the Ship Channel emission source area (major urban impervious type and surrounded by the residential and water body LULC types). With favorable wind conditions at night and in the early morning, the O_3 precursors were transported from the Ship Channel emission source towards the area with low mixing, trapping the pollutants in a confined shallow layer. There, a rapid development of O_3 occurred as the sunlight intensified in the morning and continued to increase throughout the afternoon as the sea breeze was counteracted by the weak northerly synoptic flow resulting in stagnant wind conditions.

Additional air quality simulations were performed with fixed meteorological data but with different emission inputs. Through this sensitivity study, we learned that the meteorological fields would affect the vertical allocation of the emissions, but its impact on the air quality simulation was not significant.

In this study, we demonstrated that the correct representation of the surface features was important for the simulation of realistic meteorological conditions, which were essential for air quality modeling to capture the local transport and mixing characteristics of air pollutants.

Reference:

Allen, D., Durrenberger, C. and Gary, M., 2002: Acceleration science evaluation of ozone formation in the Houston-Galveston area: meteorology.

Byun, D.W., and J. K. S. Ching, 1999: Science algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. EPA/600/R-99/030, U.S. EPA

Byun, D.W., and K. L. Schere, 2006: Review of the Governing Equations, Computational Algorithms, and Other Components of the Models-3 Community Multiscale Air Quality (CMAQ) Modeling System. Applied Mechanics Reviews, Volume 59, Number 2 (March 2006), pp. 51-77.

Cheng, F.-Y., D.W. Byun, and S.-T. Kim, 2004: Fine scale meteorological simulations of the Houston-Galveston Metropolitan area with LANDSAT-derived high-resolution land use and land cover datasets. Extended Abstract, Fifth Conf. on Urban Environment, Vancouver, BC, Amer. Meteor. Soc..

Grell, G., Dudhia, J. and Stauffer, D.R., 1994: A description of the fifth-generation Penn State/NCAR Mesoscale Model (MM5). NCAR Tech. Note NCAR/TN-398+STR, 117pp.

Kim, S.and Byun, D.W., 2003: Prototyping the Texas emissions inventory preparation system for the SMOKE system. Presented at the 12th International Emission Inventory Conference of U.S. EPA, San Diego, CA, April 29 - May 1, 2003.

Nielsen-Gammon, John W., 2002: Development of a conceptual model for meteorology and ozone formation in the Houston-Galveston Metropolitan area. Report to the Texas Natural Resource Conservation Commission, August 30, 2002.

Nielsen-Gammon, John W., 2003: Meteorological modeling for the August 2000 Houston-Galveston ozone episode: implementation and initial evaluation of GOES skin temperature assimilation, June 3, 2003.

Yarwood, G., G. Wilson, C. Emery, and A. Guenther, 1999: Development of GloBEIS – A State of the Science Biogenic Emissions Modeling System. Final Report, Prepared for Texas Natural Resource Conservation Commission.

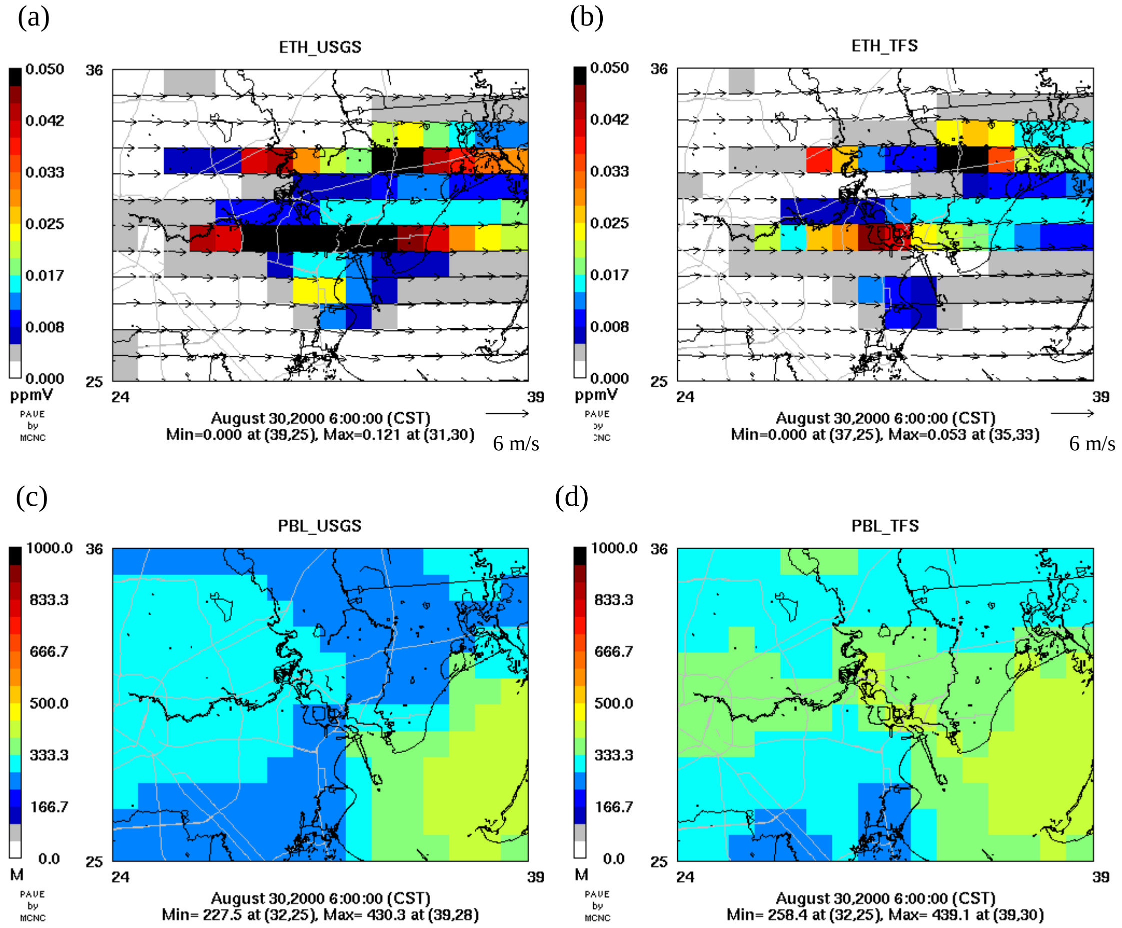

Figure 2. (a) and (b) are ethylene concentrations from CMAQ-USGS (M1E0) and CMAQ-TFS (M2E0) simulations, (c) and (d) and are the corresponding PBL height from MM5-USGS (M1) and MM5-TFS (M2) simulations at 0600 CST 30 August.

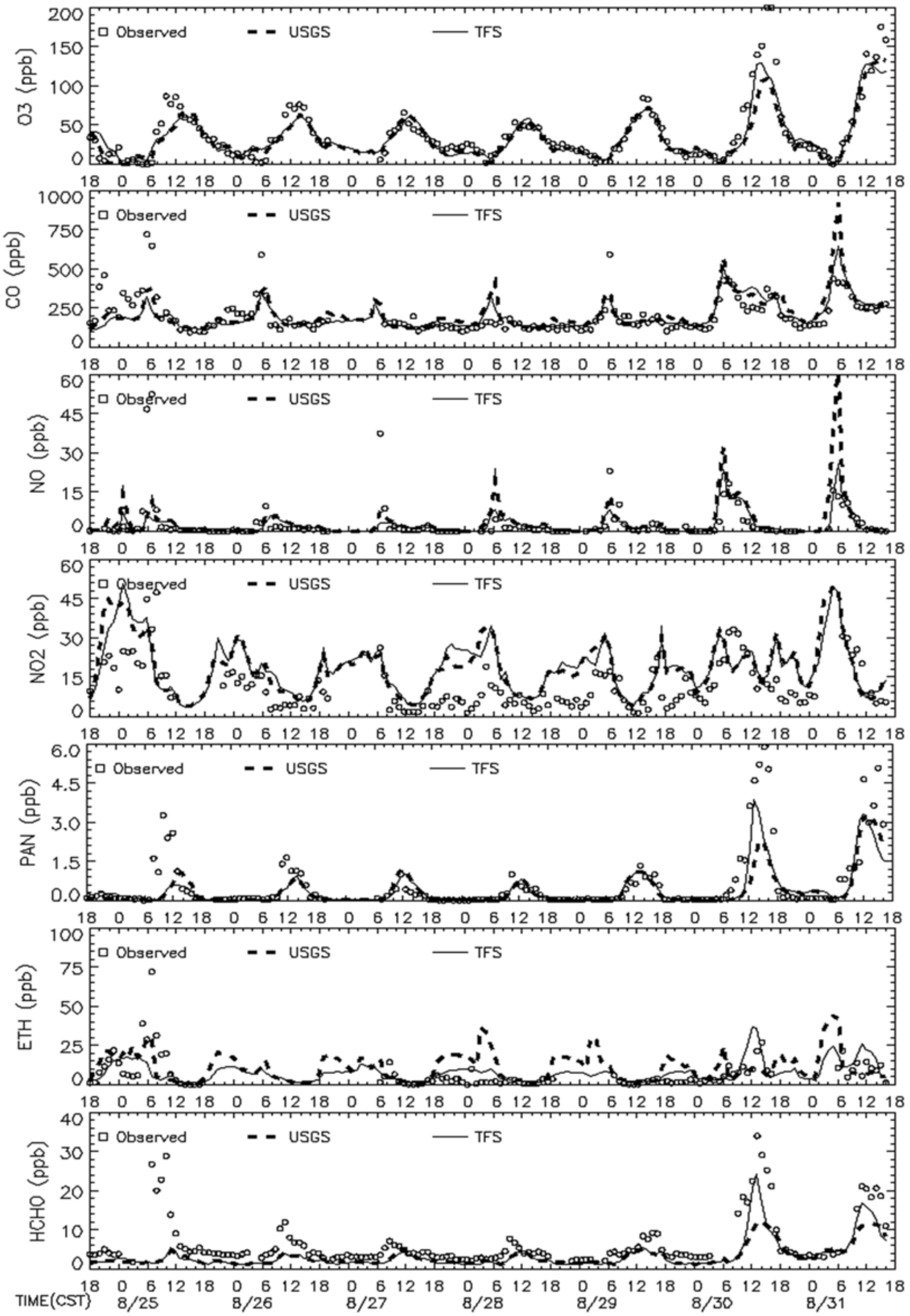

Figure 3. Time series comparison of observation and simulation for O_3, CO, NO, NO_2, PAN, ethylene (ETH) and formaldehyde (HCHO) concentrations at La Porte (608) site (dashed line is from M1E0 and solid line is from M2E0 simulations.)