Monthly Technical Report

PROJECT TITLE	Constraining NO_x Emissions Using Satellite NO_2 Measurements Over The Southeast Texas	**PROJECT #**	14-014
PROJECT PARTICIPANTS	University of Houston	**DATE SUBMITTED**	4/8/2015
REPORTING PERIOD	**From:** Mar. 1, 2015 **To:** Mar. 31, 2015	**REPORT #**	1
University of Houston		**Invoice #** N/A	**Amount** $0.00

A Financial Status Report (FSR) and Invoice will be submitted separately from each of the Project Participants reflecting charges for this Reporting Period. I understand that the FSR and Invoice are due to the AQRP by the 15th of the month following the reporting period shown above.

Detailed Accomplishments by Task

1. Finished CMAQ simulations (with NEI2008) and calculated statistics.
2. Preparation of NEI2011 is finished. The QA/QC is expected to be done shortly.
3. OMI NO_2 daily data for 09/2013 were processed (filtered and regridded).

Preliminary Analysis

We have finished a set of CMAQ simulation with NEI 2008 while we are working to finish the preparation of NEI 2011. The purpose is to develop a set of scripts/codes for analyzing CMAQ results. The re-run of CMAQ with NEI 2011 for 09/2013 should be quick.

The statistics for ozone is shown in Table 1. The statistics are based on CAMS data. The results are quite consistent across the variables. The OA cases have better IOA than No-OA case, while the differences between the 1Hr-OA and 3Hr-OA are quite small.

Table 1 Statistics of hourly surface ozone

Case	N	Corr	IOA	RMSE	MAE	MB	O_M	M_M	O_SD	M_SD
No-OA	33308	0.72	0.78	14.9	12.3	9.3	24.4	33.7	16.5	14.1
3Hr-OA	33308	0.73	0.82	14.0	11.3	7.0	24.4	31.4	16.5	16.5
1Hr-OA	33308	0.72	0.81	14.4	11.6	7.2	24.4	31.6	16.5	16.7

- N – data points; Corr – Correlation; IOA – Index of Agreement; RMSE – Root Mean Square Error; MAE – Mean Absolute Error; MB – Mean Bias; O – Observation; M - Model; O_M – Observed Mean; M_M – Model Mean; SD – Standard Deviation
- Units for RMSE/MAE/MB/O_M/M_M/O_SD/M_SD: ppb

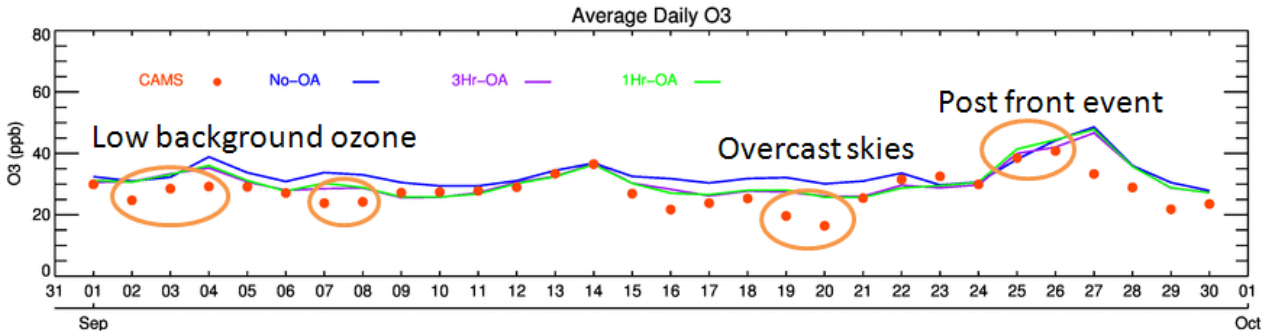

Figure 1. Daily average ozone time series

We also analyzed the ozone event on 09/25, Figure 2 and 3 show the combined wind-ozone plot at 10 CST and 13 CST.

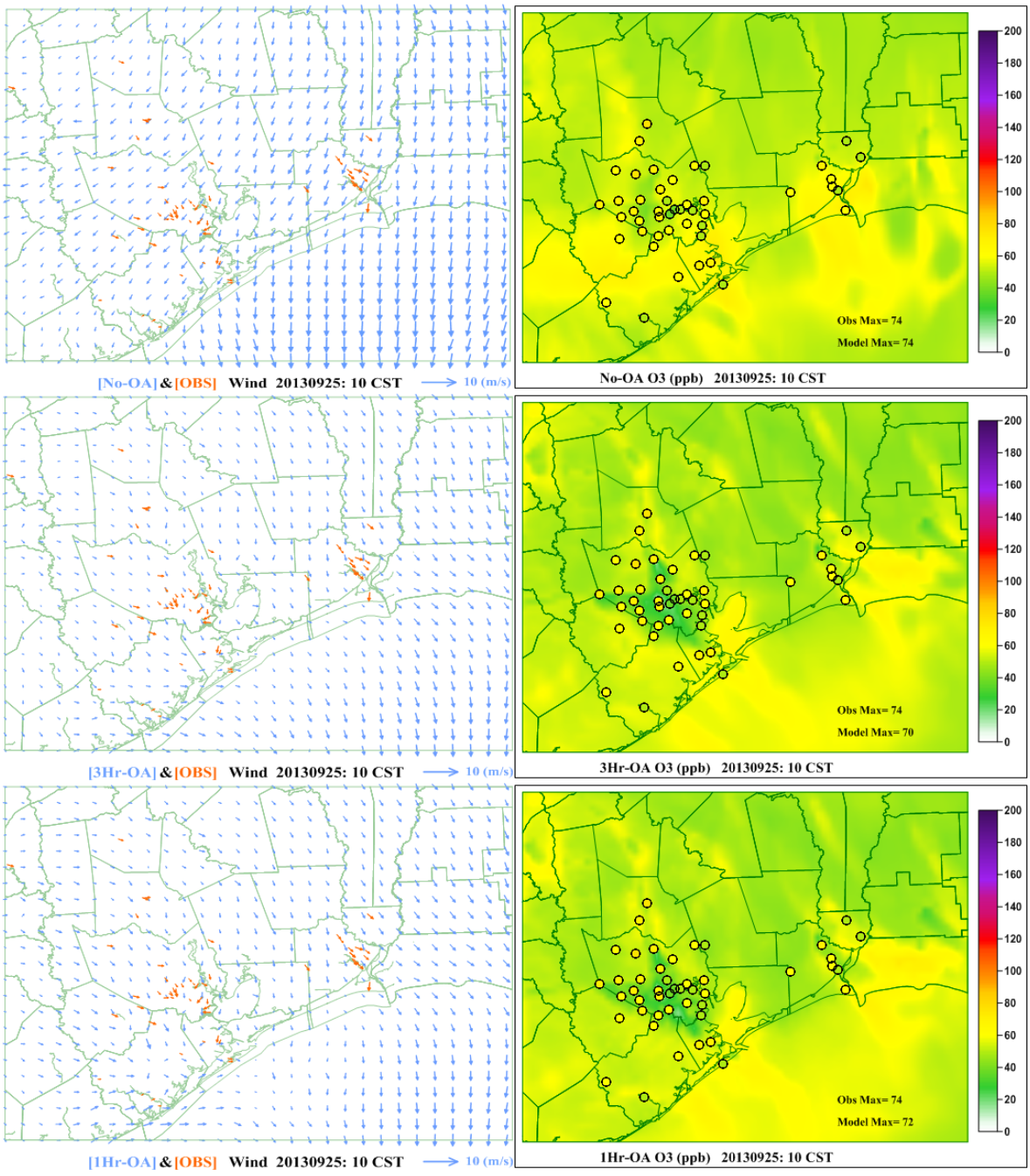

Figure 2. Ozone concentrations (left) and wind plots (right) at 09/25_10 CST for three simulation cases: “No-OA” (top), “3Hr-OA” (middle), and “1Hr-OA” (bottom). Ozone observation is in small circle; wind observation is indicated by an orange arrow.

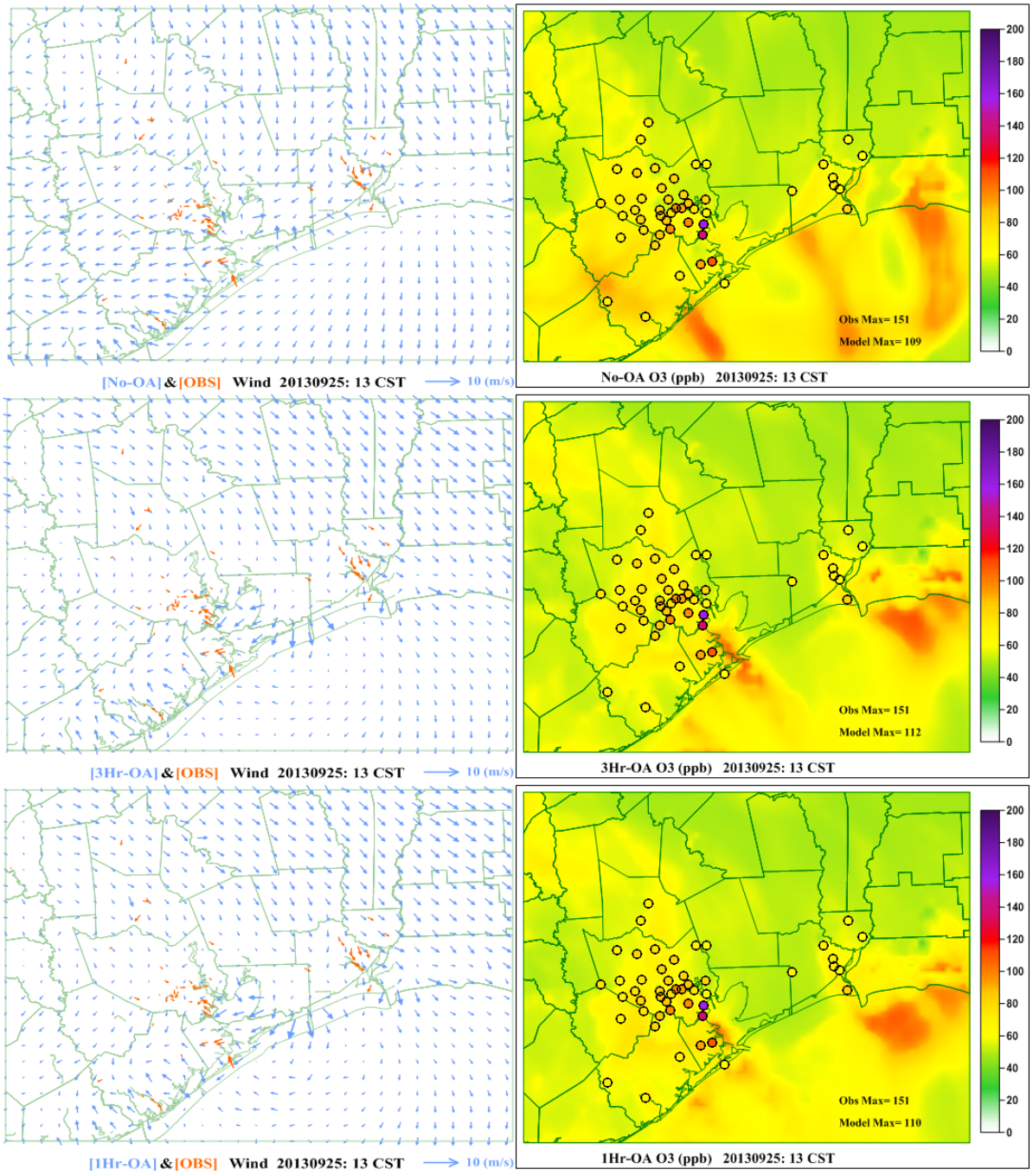

Figure 3. Ozone concentrations (left) and wind plots (right) at 09/25_13 CST for three simulation cases: “No-OA” (top), “3Hr-OA” (middle), and “1Hr-OA” (bottom). Ozone observation is in small circle; wind observation is indicated by an orange arrow.

Emission processing

Emission inventory migration from NEI2008 to NEI2011 have been finished. We expect to finish the QA/QC work in the near future.

The U.S. Environmental Protection Agency (EPA) has developed an air quality modeling platform for 2011 based on the 2011 National Emissions Inventory, version 1 (2011NEIv1). The platform consists of all the emissions inventories and ancillary data files used for SMOKE emissions modeling system needed to run the air quality model. The emission inventory from the platform is based on the 2011NEIv1, although there are some differences between the platform inventories and the 2011NEIv1 emissions.

The NEI 2011 platform verson 6.1 was developed in November 2014. It includes all the criteria air pollutants and precursors (CAPs) and the following hazardous air pollutants (HAPs): chlorine (Cl), hydrogen chloride (HCl), Benzene, Acetaldehyde, Formaldehyde and Methanol (BAFM). The NEI 2011 platform version 6.1 improved the NEI 2011 v6 with newer data and methods. Another revision v6.2 includes a few newer inventories and especially the latest mobile emissions using the Motor Vehicle Emissions Simulator (MOVES) 2014.

While some of the emissions data were developed specifically for this project and include improvements over the NEI 2011 platform v6.2 for this time period, the majority of the inventory data were from the NEI 2011 platform v6.1. A brief summary of the emissions data used in this emissions modeling platform follows:

- 2011 platform v6.1 represents all platform sectors (area, nonroad, and so on) other than Onroad mobile sources
- For Onroad mobile source emissions, the latest 2011 platform v6.2 based on the latest Motor Vehicle Emissions Simulator (MOVES) 2014 was used.

Table 1 lists the sectors that we used to represent the year 2011 air pollutant emissions for this emission modeling system, and any notes on data preparation.

As a QA/QC, we provided area sector comparison of the two inventories below. Figure 4 shows the area emissions from NEI2008 and NEI2011, as well as the differences in percentage. The reduction is evident everywhere. The intensity also decreased in Houston area.

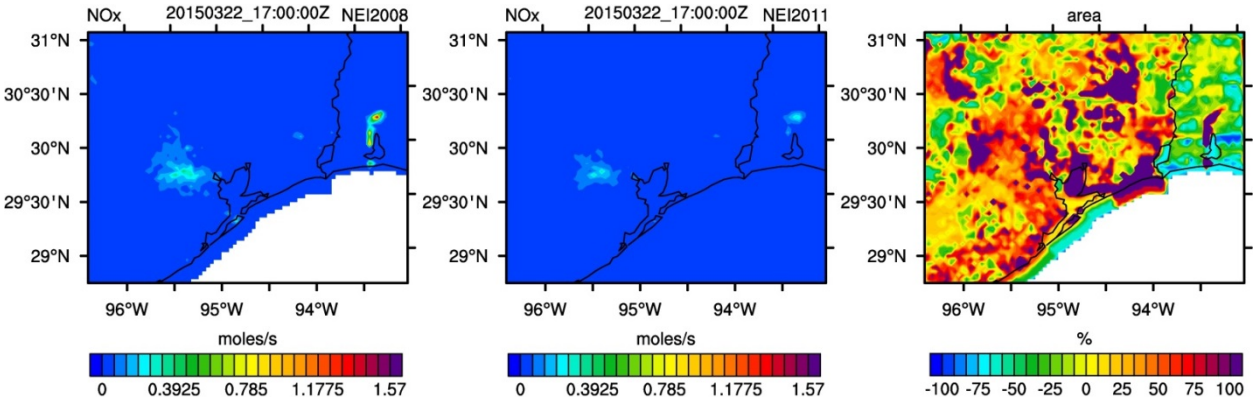

Figure 4. Area emission. On the left is NEI2008, middle is NEI2011, and right is the difference in percent.

Table 1. Platform sectors for the NEI 2011 platform

Platform Sector	Abbreviation	Description
EGU non-peaking units	ptegu	2011 NEI point source EGUs determined to operate as non-peaking units. Hourly 2011 CEMS are not used since the year of modeling is 2014.
EGU peaking units	ptegu_pk	Same as ptegu sector, but limited to EGUs that are determined to operate as peaking units. Hourly 2011 CEMS are not used since the year of modeling is 2014.
Point source oil and gas	pt_oilgas	2011NEIv1 point sources with oil and gas production emissions processes. Annual resolution.
Remaining non-EGU point	ptnonipm	All 2011NEIv1 point source records not matched to the ptegu, ptegu_pk, and pt_oilgas sectors, except for offshore point sources that are in the othpt sector. Includes all aircraft emissions and some rail yard emissions. Annual resolution.
Agricultural	ag	NH_3 emissions from 2011NEIv1 nonpoint livestock and fertilizer application, county and annual resolution.
Area fugitive dust	afdust	PM_{10} and $PM_{2.5}$ from fugitive dust sources from the 2011NEIv1 nonpoint inventory including building construction, road construction, and agricultural dust, and road dust. County and annual resolution.
Nonpoint oil and gas	np_oilgas	2011NEIv1 nonpoint sources from oil and gas-related processes. County and annual resolution.
Residential Wood Combustion	rwc	This is a new sector in 2011NEIv1. NEI nonpoint sources with Residential Wood Combustion (RWC) processes. County and annual resolution.
Class 1 & 2 CMV and locomotives	c1c2rail	Locomotives and primarily category 1 (C1) and category 2 (C2) commercial marine vessel (CMV) emissions sources from the 2011NEIv1 nonpoint inventory. Midwestern states' CMV emissions, including Class 3 sources, are from a separate year 2010 emissions inventory. County and annual resolution.
Commercial marine	c3marine	Category 3 (C3) CMV emissions projected to 2011 from year 2002 values. These emissions are not from the 2011NEIv1, but rather were developed for the rule called "Control of Emissions from New Marine Compression-Ignition Engines at or Above 30 Liters per Cylinder", usually described as the Emissions Control Area- International Maritime Organization (ECA-IMO) study: http://www.epa.gov/otaq/oceanvessels.htm. (EPA-420-F-10-041, August 2010). U.S. states-only emissions (zero in Midwest); see othpt sector for all non-U.S. emissions. Treated as point sources to reflect shipping lanes, annual resolution.
Remaining nonpoint	nonpt	2011NEIv1 nonpoint sources not otherwise removed from modeling or included in other platform sectors; county and annual resolution.

Nonroad	nonroad	2011NEIv1 nonroad equipment emissions developed with the National Mobile Inventory Model (NMIM) using NONROAD2008 version NR08a. NMIM was used for all states except California and Texas, which submitted their own emissions to the 2011NEIv1. County and monthly resolution.
Onroad RatePerDistance	rateperdistance	EPA ran MOVES2014 for 2011 in emissions factor mode. The MOVES lookup tables include on-network (RatePerHour) to represent exhaust and most evaporative emissions during running, tirewear, and brakewear modes. These data include the reference county and reference fuel month assignments that EPA used for the MOVES simulation.
Onroad RatePerHour	rateperhour	EPA ran MOVES2014 for 2011 in emissions factor mode. The MOVES lookup tables include off-network (RatePerDistance) that represents emissions from extended idling and APU operation. These data include the reference county and reference fuel month assignments that EPA used for the MOVES simulation.
Onroad RatePerVehicle	ratepervehicle	EPA ran MOVES2014 for 2011 in emissions factor mode. The MOVES lookup tables include off-network starts/stops (RatePerVehicle) that represents emissions from start exhaust and most evaporative emissions that occurs off-network. These data include the reference county and reference fuel month assignments that EPA used for the MOVES simulation.
Onroad RatePerProfile	rateperprofile	EPA ran MOVES2014 for 2011 in emissions factor mode. The MOVES lookup tables include off-network (RatePerProfile) that represents emissions from evaporative fuel vapor venting. These data include the reference county and reference fuel month assignments that EPA used for the MOVES simulation.
Non-US Point	othpt	Point sources from Canada's 2006 inventory and Mexico's Phase III 2012 inventory, annual resolution. Mexico's inventory is year 2012 and grown from year 1999 (ERG, 2009; Wolf, 2009). Also includes all non-U.S. C3 CMV and U.S. offshore oil production, which are unchanged from the 2008 NEI point source annual emissions.
Non-US nonpoint and nonroad	othar	Annual year 2006 Canada (province resolution) and year 2012 (grown from 1999) Mexico Phase III (municipio resolution) nonpoint and nonroad mobile inventories.
Non-US onroad	othon	Year 2006 Canada (province resolution) and year 2012 (grown from 1999) Mexico Phase III (municipio resolution) onroad mobile inventories, annual resolution.
Biogenic	biog	No updates made (Stay constant)

OMI NO_2 data processing

We obtained OMI tropospheric NO_2 daily observations (level2) and managed to filter out noisy values. In order to visualize and compare the OMI data with the model output (and perform inverse modeling), we should firstly remove the influence of a priori gas profile from OMI, and secondly project the level2 product on a longitude-latitude grid using a reliable gridding approach.

In order to perform the first task, following the approach described in Duncan et al. (2014), we first used the variable called "scattering weight" that is included in the OMI NO_2 granules. Scattering weights are available for various pressure levels stretching from the surface to the top of the atmosphere. We summed over all model layers the product of the scattering weight and model partial column (molecules/cm^2) in each model layer. This sum divided by tropospheric NO_2 column from model is called the air mass factor (AMF) of the model (AMFM). Subsequently, we divided the product of OMI tropospheric NO_2 and AMF of the satellite from the data file by AMFM to obtain a modified form of OMI tropospheric NO_2. It is worth mentioning that during the process another flag for AMF of the satellite was used to remove unreliable AMF values. This task is indeed required and neglecting it would result in an underestimation of NO_2 vertical columns in urban regions and an overestimation in rural regions resulting from using a coarse priori guess (here $2.5^o \times 2.5^o$ degree from GEOS-Chem).

In order to do the second task, we used a new algorithm (Kulmann et al. 2014) to grid the granules over the domain. While a level3 product has been provided by NASA, its spatial resolution is too coarse ($0.25^o \times 0.25^o$ degree) for inverse modeling in a regional scale. Consequently, using the recent algorithm that estimates NO_2 by a continuous differentiable, parabolic spline surface, we were able to map NO_2 in a very dense grid. The approach has been set up for our model domain for September of 2013. The following figure is the result of mapped OMI tropospheric NO_2 in 4km spatial resolution with and without applying AMF (Figure 5).

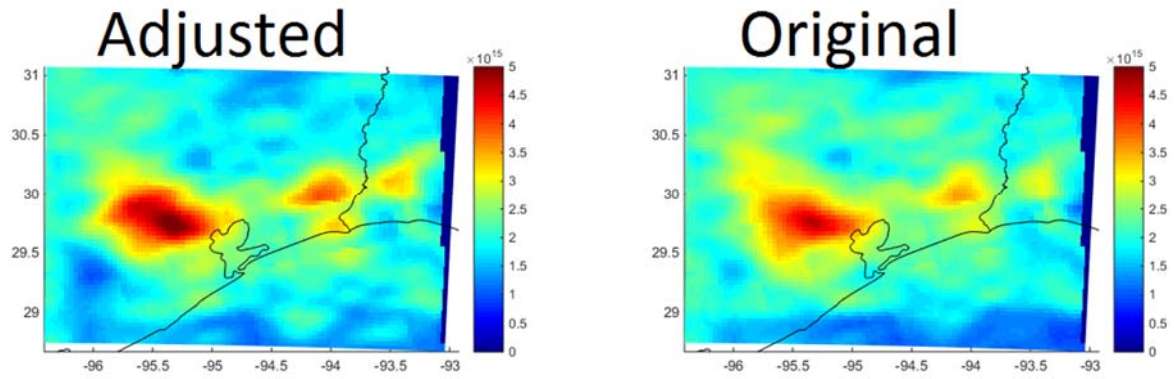

Figure 5. Left: mapped and adjusted OMI tropospheric NO_2 using the grid method and removing priori guess in 4km spatial resolution; right: mapped OMI tropospheric NO_2 using the grid method without performing the first step in the same resolution.

As far as we know, this is the first time that 1) one has used the grid algorithm for inverse modeling; additionally the figure demonstrates the most detailed OMI map for Houston and 2) no one has shown the difference between with and without considering AMF (even though they addressed this issue in the previous publications). We believe this figure can share a crucial message to air quality community, which is the fact that removing the influence of priori profile can undeniably have considerable impacts (both in magnitude and distribution) on OMI NO_2.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

We finished our emission preparation based on NEI2011 and we are working to QA/QC the final emission files to see if they are ready for CMAQ run.

Goals and Anticipated Issues for the Succeeding Reporting Period

We expect to finish the emission QA/QC work as well as the CMAQ re-run. We will repeat the analyses for the new CMAQ run and see the difference between NEI2008 and NEI2011.

Detailed Analysis of the Progress of the Task Order to Date

The completion of each of the project tasks and the draft and final reports are expected to be on the schedule from the Work Plan schedule.

Submitted to AQRP by: Yunsoo Choi

Principal Investigator: Yunsoo Choi