# Monthly Technical Report

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| **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** | 6/8/2015 |
| **REPORTING PERIOD** | **From:** May. 1, 2015<br>**To:** May. 30, 2015 | **REPORT #** | 1 |
| | University of Houston | **Invoice #**<br>N/A | **Amount**<br>$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 $15^{th}$ of the month following the reporting period shown above.

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**Detailed Accomplishments by Task**

1. Finished inverse modeling to update NOx in NEI2011. The new inventory is named as NEI2011n
2. Finished CMAQ simulations with NEI2011n and calculated ozone statistics.
3. Evaluated model tropospheric $NO_2$ column using satellite $NO_2$ column.

**Inverse Modeling**

The Bayesian inversion was used to update the emission parameters of NOx using OMI $NO_2$ data, with CMAQ simulation as the forward model. In the inverse model, NOx emissions are separated into four sectors: area, biogenic, mobile and point sources. The relationship between the observation vector y (here OMI) and state vector x (here emissions) can be described as:

$$y = Kx + \varepsilon$$

where the K matrix (Jacobian matrix) represents NOx sensitivities to the state vector defined by CMAQ model, and ε is the error term. In order to calculate the Jacobian matrix for each sector, we made use of the Brute force method. According to this approach, sensitivity is measured based on the corresponding gas concentration ($NO_2$) changes in respect to emission changes (NOx). Mathematically expressing, the sensitivity can be given by:

$$S = \frac{NO_2^{+d} - NO_2^{-d}}{2d}$$

where $d$ is the fraction of change, and $NO_2$ is the simulated tropospheric $NO_2$ column. We set $d$ to 100% which means two simulations with double $NO_x$ emissions and without the $NO_x$ emissions have been conducted for each sector.

The uncertainties for each sector were set to 50% for area, mobile and point sources and to 300% for biogenic emission. The uncertainty for OMI was $1.4 \times 10^{15}$ molec.cm$^{-2}$ based on Bucsela et al., (2013). Then a posteriori state ($\hat{x}$) vector can be computed by:

$$\hat{x} = x_a + (K^T S_\varepsilon^{-1} K + S_a^{-1})^{-1} K^T S_\varepsilon^{-1} (y - K x_a)$$

where $x_a$ is the a priori state vector, $S_a$ is the estimated error covariance matrix for $x_a$, and $S_\varepsilon$ is the error covariance matrix for observation errors.

## Old and Updated NOx Emissions by Sector

The old and updated NOx emission by sector is shown in figure 1. The top row plots are for old (priori) NOx emission while bottom row shows the updated (posteriori) NOx emission. The four plots in each row represent the four sectors: area, biogenic, mobile and point (from left to right). In updated emission, NOx decreased in three anthropogenic sectors and increased in biogenic sector. Both reduction and enhancement have not occurred evenly over the domain.

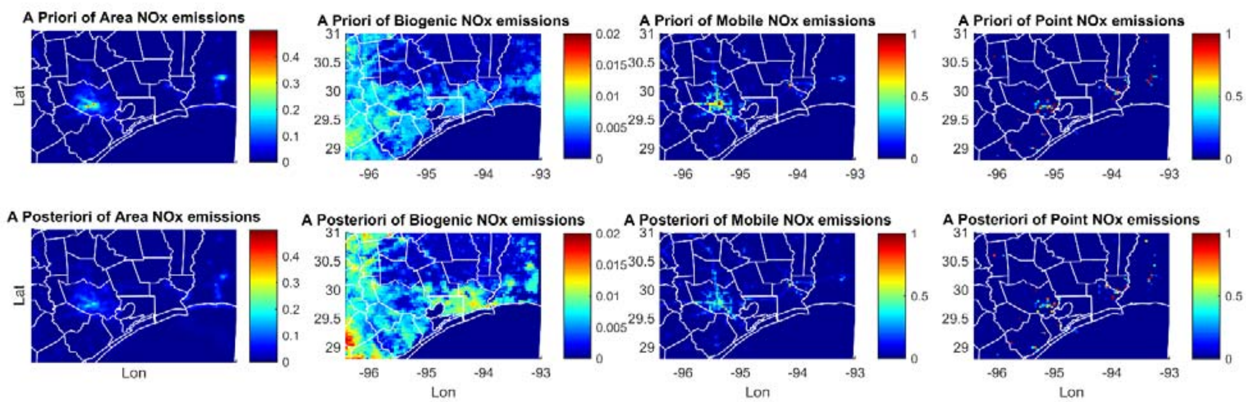


Figure 1. Old (top row) and updated (bottom row) NOx emissions.

The old and updated total NOx emission is shown in figure 2.

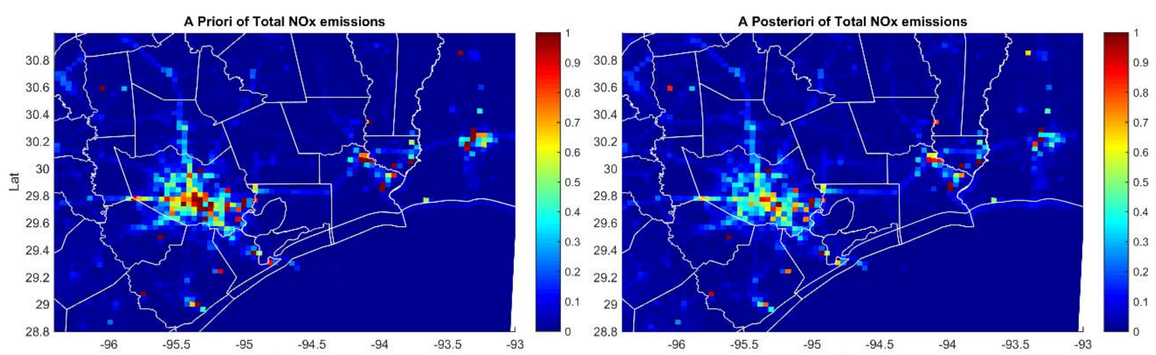


Figure 2. Old (left) and updated (right) total NOx emissions.

## Surface Ozone Statistics Using NEI 2011 and NEI 2011n

We have finished a pair of CMAQ simulations with NEI 2011 and NEI2011n over Southeast Texas. The meteorology is “1Hr-Objective Analysis (OA)” case. In this meteorology, OA is run at 1-hr interval input.

The statistics for ozone is shown in Table 1. The statistics are based on CAMS data.

**Table 1 Statistics of hourly surface ozone**

| Case | N | Corr | IOA | RMSE | MAE | MB | O_M | M_M | O_SD | M_SD |
|---|---|---|---|---|---|---|---|---|---|---|
| NEI2011 | 33308 | 0.74 | 0.79 | 14.6 | 12.0 | 9.3 | 24.4 | 33.7 | 16.5 | 14.2 |
| NEI2011n | 33308 | 0.76 | 0.80 | 14.4 | 11.7 | 9.2 | 24.4 | 33.7 | 16.5 | 15.2 |

- 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

It can be seen that the updated emission slightly improved surface ozone statistics, with correlation increased by 0.02 and IOA by 0.01. The mean bias shows a small decrease.

## Ozone Vertical Profile from Aircraft Measurement

Ozone aloft were compared to measurements from NOAA aircraft P3B. The comparison of aircraft data with model results is more complicated since the aircraft is moving in a 3-Dimensional space. To compare model to observations, we need to find the model data matching the location and time of aircraft point measurement. We have developed in-house codes to match model results with aircraft and ozone-sonde measurements. Since aircraft data have much higher frequency than model output, we aggregated all the aircraft data points in one grid cell during 1-hour period to match model output.

Figure 3 shows the modeled vertical profiles and the measurements (red dots) on 09/25/2013. Nine hourly profiles are displayed to give the ozone evolution from ground up to 4-km height. The updated NEI20011n case underperformed the original NEI2011 one only in the first plot (08 CST). Its performance in the 2$^{nd}$ plot (09 CST) is generally better, underperforming only in a small section: 400-1000m height. The updated case outperformed the original one in all following hours (10-16 CST), sometimes reducing the bias by over 10 ppb.

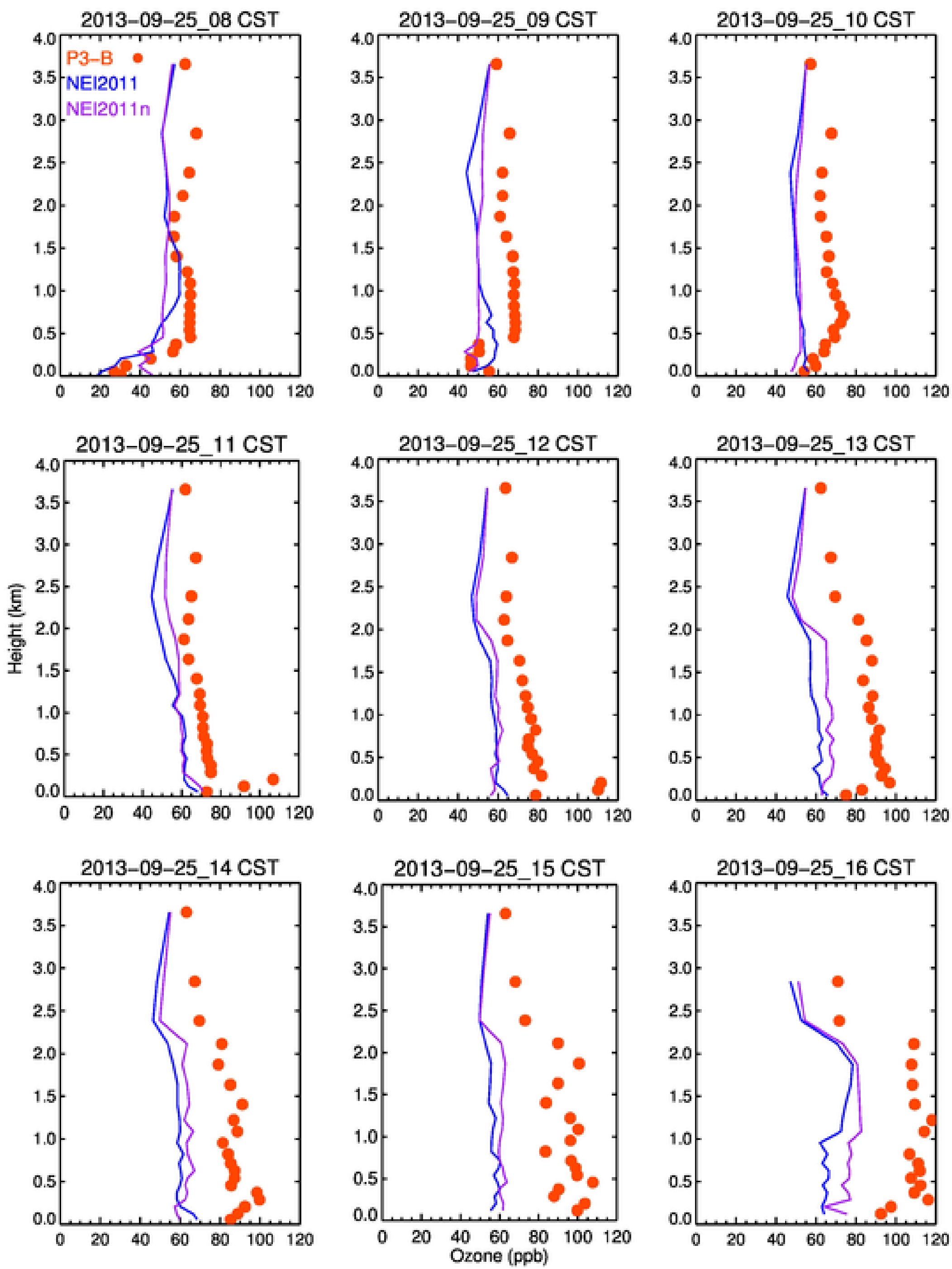


**Figure 3**: Ozone vertical profile – modeled vs. measurements; measurements are aggregated over model grid cells and averaged hourly

### CMAQ and OMI $NO_2$ Comparison

By using the profile of simulated $NO_2$ and the height of tropopause from OMI data, the simulated tropospheric $NO_2$, which is the sum of partial $NO_2$ concentrations from the surface to top of the troposphere, is calculated. The simulated tropospheric $NO_2$ using the original NEI2011 and the updated one are compared to OMI tropospheric $NO_2$. Figure 4 shows the spatial $NO_2$ from original NEI2011 (top left) and NEI2011n (top right). The second row of the figure depicts OMI tropospheric $NO_2$ which has been adjusted for conducting an apples-to-apples comparison based on the simulated tropospheric $NO_2$. The third row demonstrates the ratio of simulated tropospheric $NO_2$ to OMI tropospheric $NO_2$. High values in ratio means overprediction of the model and vice versa.

Indeed, the updated $NO_2$ matched better with OMI data. This is also expected as OMI data are used to modify the original NEI2001.

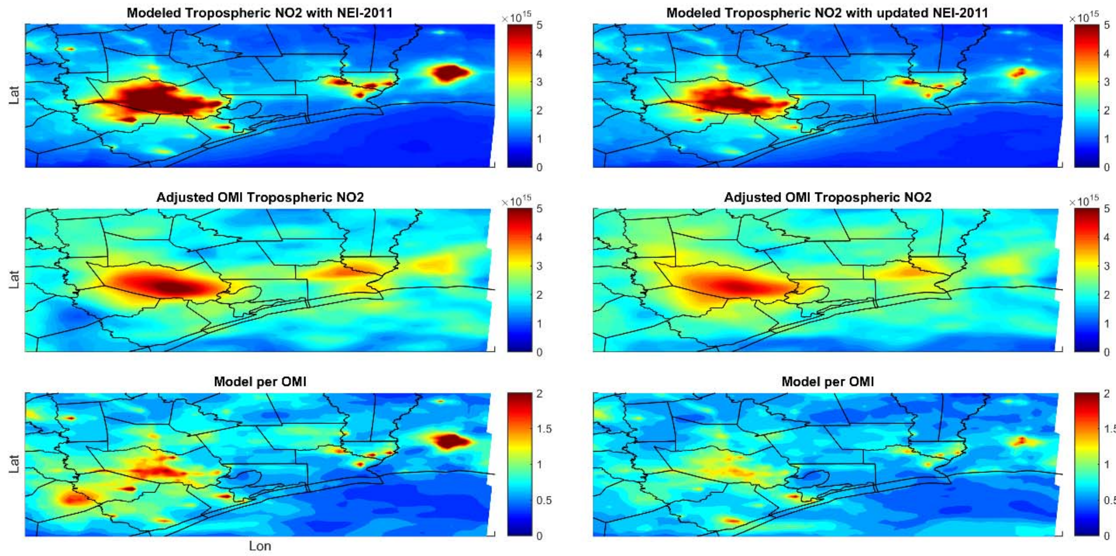


**Figure 4**: Comparison between $NO_2$ columns (average over September of 2013). Left – NEI2011; Right – NEI2011n

## Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

We have not encountered any problems in May.

## Goals and Anticipated Issues for the Succeeding Reporting Period

We expect to finalize all the analyses and prepare for the final report.

## 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.

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Submitted to AQRP by: Yunsoo Choi

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