

AQRP Monthly Technical Report

PROJECT TITLE	Analysis of Ozone Production and Its Sensitivity in Houston Using the Data Collected during DISCOVER-AQ	PROJECT #	Choose an item. 14-020
PROJECT PARTICIPANTS	University of Maryland College Park	DATE SUBMITTED	5/8/2015
REPORTING PERIOD	From: April 1, 2015 To: April 30, 2015	REPORT #	3

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

During the period from April 1-30, 2015, the team at University of Maryland College Park has accomplished the following tasks:

- (1) CMAQ model output was extracted along the P-3B flight tracks for the month of September and was used as input to constrain the CB05 box model for long-lived species that were not measured on the P-3B.
- (2) Initial box model run has been conducted based on Carbon Bond Version 5 (CB05) mechanism.
- (3) We continued working on the programming of Matlab program that will be used to analyze the box model results for ozone production and its sensitivity to NO_x and VOCs.
- (4) The WRF and CMAQ statistical evaluation for Project #14-004 has been completed. The CMAQ simulation we will perform for this project will be based on the modeling technique and input files used in this project.

Preliminary Analysis

Figure 1 shows some comparison results between CB05 and CMAQ for the intermediate species: OH, HO₂, methylperoxy radical (MEO₂), and other higher alkylperoxy radicals (XO₂ that converts NO to NO₂). These intermediate are very important for the calculation of ozone production. Any differences in these species will contribute to the difference in ozone production in the CB05 box model and CMAQ model.

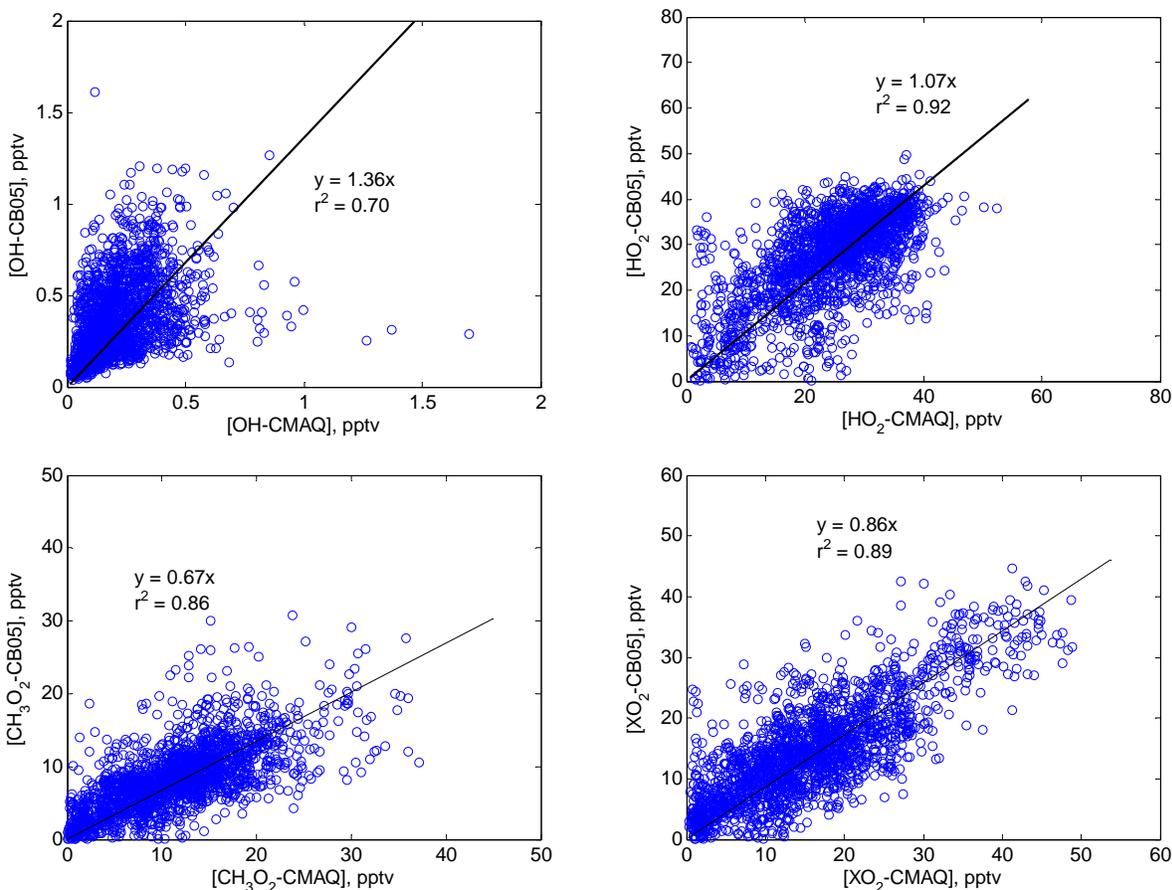


Figure 1. Comparison between CB05 and CMAQ for some intermediate species: OH, HO₂, methylperoxy radical (MEO₂), and other higher alkylperoxy radicals (XO₂ that converts NO to NO₂).

As we can see in Figure 1, there are some differences in these intermediates and this will result in differences in ozone production rates calculated using the CB05 box model and the CMAQ model results. We found the reasons for these differences are the differences in some precursors in the box model (measured on the P-3B) and the CMAQ model (calculated from emissions) as shown in Figure 2. We noticed the correlation between the P-3B measured NO_x (NO and NO₂) and the CMAQ modeled NO_x is particularly poor. As we know the intermediates shown in Figure 1 are very sensitive to NO and NO₂. We will compare these species again after the new CMAQ simulations with updated emissions files.

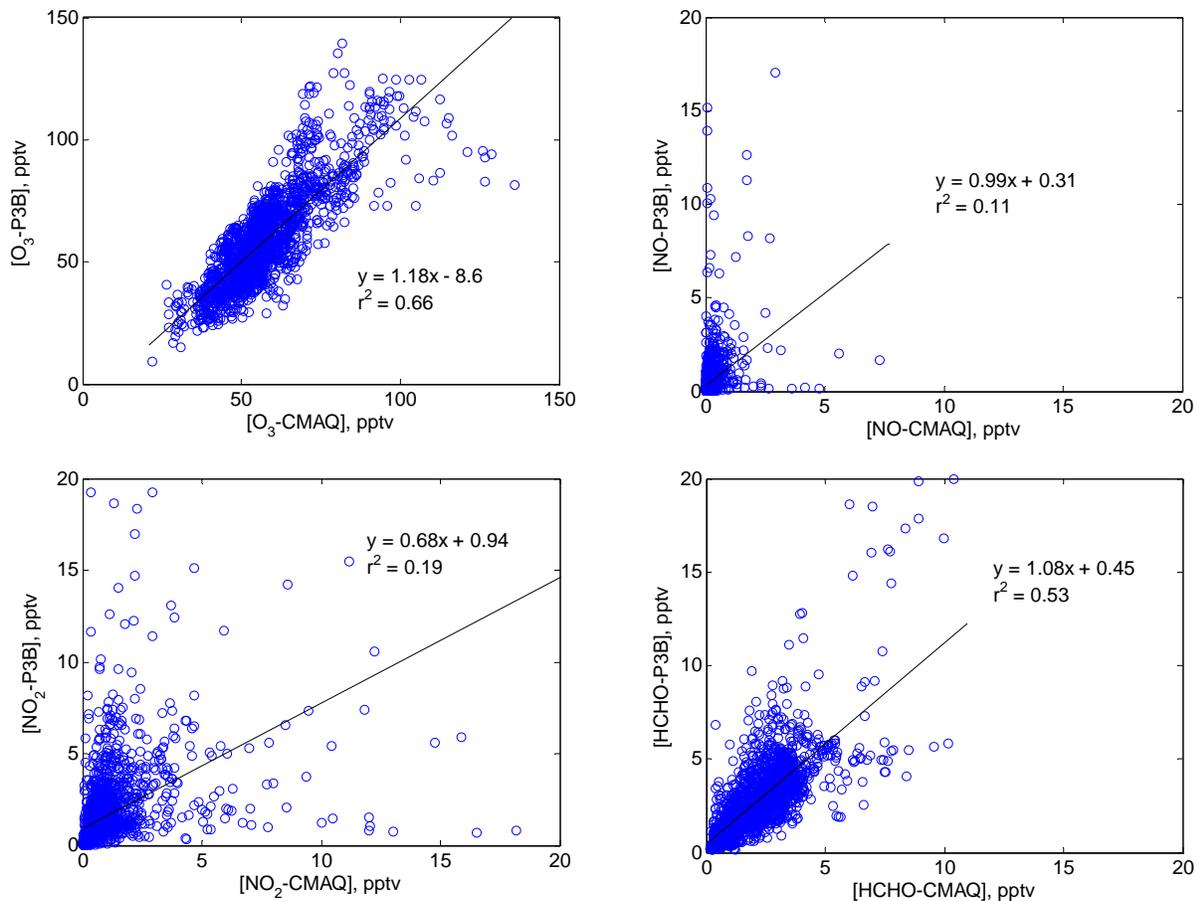


Figure 2. Comparison between P-3B observations and CMAQ model for some precursors: O_3 , NO, NO_2 , and formaldehyde (FORM).

Data Collected

None.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

In the CMAQ model, we identified a low bias in model emissions estimates and developed a plan for updating the emissions. These updated emissions input files will be used in CMAQ simulations for this project.

Goals and Anticipated Issues for the Succeeding Reporting Period

- (1) We will finish the Matlab code analyze the box modeling results to calculate ozone production and its sensitivity to NO_x and VOCs.
- (2) The CMAQ simulations will be re-run after the emissions input files are updated. The CB05 box model will also be re-run using the new CMAQ output files.
- (3) After updated input files for the CMAQ model run with process analysis are being prepared, we will run CMAQ with process analysis to map the ozone production

efficiency (OPE) and nitrogen oxides (NOx) and VOC limited areas throughout the Houston metropolitan area.

Detailed Analysis of the Progress of the Task Order to Date

We have run the box model with the CB05 mechanism using the initial CMAQ output. We will finish the data analysis program. The work with WRF-CMAQ modeling has generated some reasonable results and the model will be re-run with the updated emissions files. Everything regarding the Task Order schedule and progress is going well. There were no delays in completing tasks and project goals during this reporting period.

Submitted to AQRP by: Xinrong Ren

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