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**	8/11/2015
REPORTING PERIOD	**From:** August 1, 2015 **To:** August 31, 2015	**REPORT #**	5

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 July 1-31, 2015, the team at University of Maryland College Park has accomplished the following tasks:

(1) Updated the box model mechanism from CB05 to CB05-TUCL with updated toluene and chlorine chemistry (CB05-TUCL is the mechanism used in the CMAQ model) so that the mechanisms in the box model and CMAQ are now the same.

(2) Compared the updated and previous version box model results and found some difference in $P(O_3)$ and radical concentrations.

(3) Completed the CMAQ process analysis run with model output results along the P-3B track, which include primary radical production rate (Q), loss rate of radicals due to their reactions with NOx (L_N), ozone production rate ($P(O_3)$), ozone loss rate ($L(O_3)$), net ozone production rate (net(O_3)= $P(O_3)$-$L(O_3)$), P(Ox), L(Ox), and net(Ox).

(4) Started to compare the box model to CMAQ with regard to ozone production and its sensitivity to NOx and VOCs and the results will be include in the next monthly report.

Preliminary Analysis

We compared the ozone production rate ($P(O_3)$), ozone loss rate ($L(O_3)$), and net ozone production (net $P(O_3)$) in the old and updated versions of chemical mechanisms and found a difference of ~25% in both $P(O_3)$ and net $P(O_3)$ (Figure 1). While we continue to look into the reasons causing the differences, we believe the differences are mainly caused by the different OH and RO_2 concentrations calculated the two mechanisms as indicated in Figure 2.

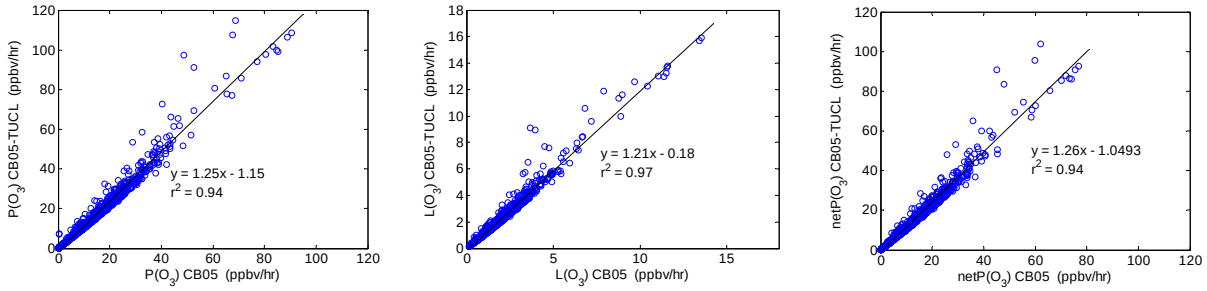

Figure 1. Comparison ozone production rate ($P(O_3)$) (left), ozone loss rate ($L(O_3)$) (middle), and net ozone production (net $P(O_3)$) (right) in the old (CB05) and updated (CB05-TUCL) versions of the chemical mechanisms.

We compared the major radical species, OH, HO_2 and RO_2, in the output of the two different chemical mechanisms and found that HO_2 concentration in the two mechanisms is about the same, but OH concentration increases by about 10% and RO_2 concentration increase by about 5.5% in the CB05-TUCL mechanism (Figure 2). While we are still looking into the causes for the increase in OH and RO_2, but we think the increases in OH and RO_2 concentrations are the main reasons causing the increase of $P(O_3)$ and net $P(O_3)$ as shown in Figure 1.

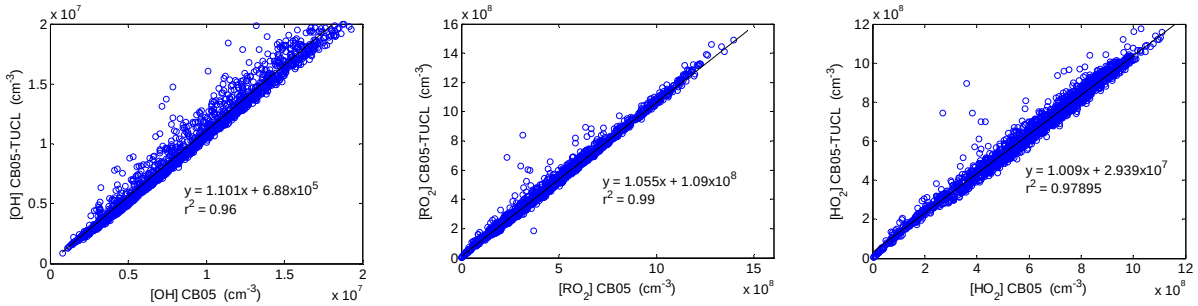

Figure 2. Comparison OH concentration (left), RO_2 concentration (middle), and HO_2 concentration (right) in the old (CB05) and updated (CB05-TUCL) versions of the mechanisms.

Data Collected

None.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

We found some increases in $P(O_3)$ and net $P(O_3)$ in the box model output after we update the CB05 mechanism to the CB05-TUCL mechanism that is used in the CMAQ model. Initial check points the increase of OH and RO_2 radical concentrations are the causes for the increase in $P(O_3)$. We will compare other calculated species to see if there are other differences.

Goals and Anticipated Issues for the Succeeding Reporting Period

(1) Continue the data analysis for the CMAQ process analysis run to calculate ozone production and its sensitivity to NOx and VOC and compare them with the box model results.

(2) Continue looking into possible other reasons causing the increase in $P(O_3)$ after the update of the chemical mechanism in the box model.

(3) Complete the sensitivity analysis of the box model to investigate the uncertainty associated with the use of CMAQ-calculated alkanes and alkenes to constrain the box model.

(4) Prepare for the draft of final report.

Detailed Analysis of the Progress of the Task Order to Date

We have completed the CMAQ process analysis run and update the box model mechanism to CB05-TUCL to be consistent with the CMAQ model. Everything regarding the Task Order schedule and progress is going generally well. As scheduled, we will prepare the draft final report by the end of this month.

Submitted to AQRP by: Xinrong Ren

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