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	6/8/2015
REPORTING PERIOD	From: May 1, 2015 To: May 31, 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 May 1-31, 2015, the team at University of Maryland College Park has accomplished the following tasks:

- (1) Data analysis of the box modeling for ozone production and its sensitivity to NOx and VOCs.
- (2) Preparation of the progress report to be report at the AQRP workshop.

Preliminary Analysis

Figure 1 shows net ozone production rate ($P(O_3)$) calculated using the box model results along the P-3B flight track. There are several $P(O_3)$ hot spots over the Houston Ship Channel and its downwind over Galveston Bay. This is as what we would expect because of large emissions of ozone precursors (NOx and VOC) from the Houston Ship Channel. The highest $P(O_3)$ up to ~70 ppbv hr⁻¹ were observed over Galveston Bay on September 25, 2013, consistent with high ozone levels observed cross the Houston area on that day.

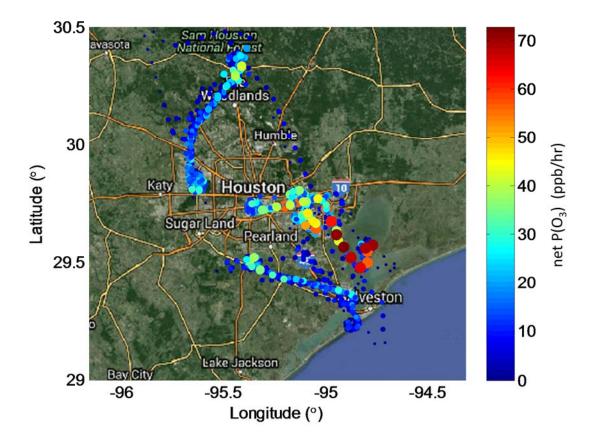


Figure 1. Net ozone production rate ($P(O_3)$) calculated using the box model results along the P-3B flight track. The size of dots is proportional to $P(O_3)$.

We used a method developed by Larry Kleinman [Kleinman, L. I., The dependence of tropospheric ozone production rate on ozone precursors, *Atmos. Environ.*, 39(3), 575–586, 2005] to examine the sensitivity of ozone production to NOx and VOCs. In this method, ozone production is a function of NOx and VOC and the sensitivity of ozone production can be determined by an indicator L_N/Q , where L_N is radical loss due to NOx, and Q is total primary radical production. Because the radical production rate is about the same as the radical loss rate, this ratio represents the fraction of radical loss due to NOx. It was found that if the ratio > 0.5, P(O₃) is VOC-sensitive. If the ratio < 0.5, P(O₃) is NOx-sensitive.

Figure 2 shows the indicator L_N/Q of ozone production sensitivity along the P-3B flight track. As we can see P(O₃) was mainly VOC-sensitive over the Houston Ship Channel and its surrounding urban areas due to large NOx emissions. Over the areas away from the center of the city with relatively low NOx emissions, P(O₃) was usually NOx-sensitive.

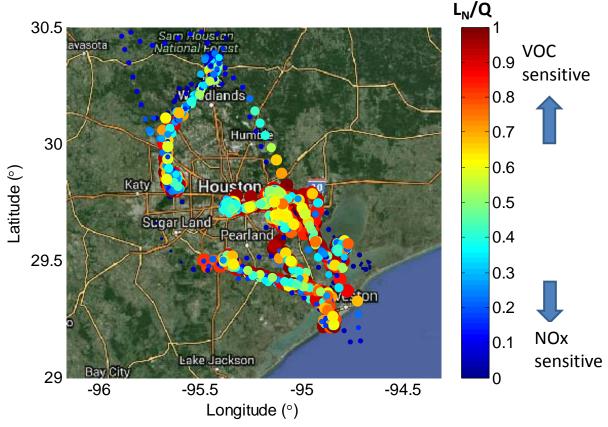


Figure 2. Ozone production sensitivity indicator, L_N/Q , along the P-3B flight track. P(O₃) is VOC-sensitive when $L_N/Q > 0.5$, and NOx-sensitive when $L_N/Q < 0.5$.

We looked at the diurnal variations of $P(O_3)$. A broad $P(O_3)$ peak in the morning with significant $P(O_3)$ in the afternoon was obtained (Figure 3). We noticed that high $P(O_3)$ mainly occurred with $L_N/Q > 0.5$ (i.e., in the VOC sensitive regime).

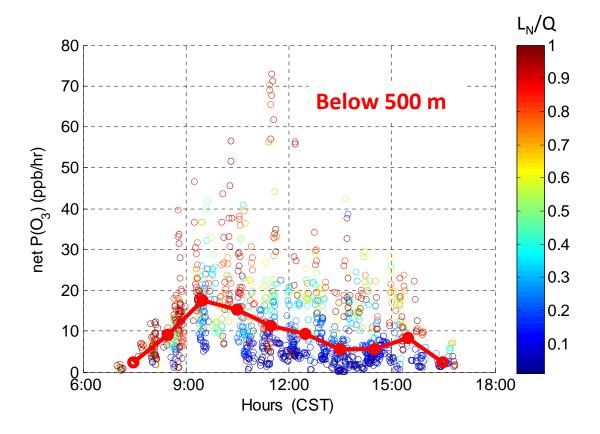


Figure 3. Diurnal variation of ozone production rate colored with the indicator L_N/Q . The solid red circles represent the median values in hourly bins of P(O₃). Data are limited with the pressure altitude less than 500 m to represent the lowest layer of the atmosphere.

The diurnal variation of L_N/Q indicates that $P(O_3)$ was mainly VOC sensitive in the early morning and then transited towards the NOx sensitive regime later the day (Figure 4). High $P(O_3)$ in the morning was mainly associated with VOC sensitive due to high NOx levels in the morning. Even though $P(O_3)$ was mainly NOx sensitive in the afternoon, there were periods when $P(O_3)$ was VOC sensitive.

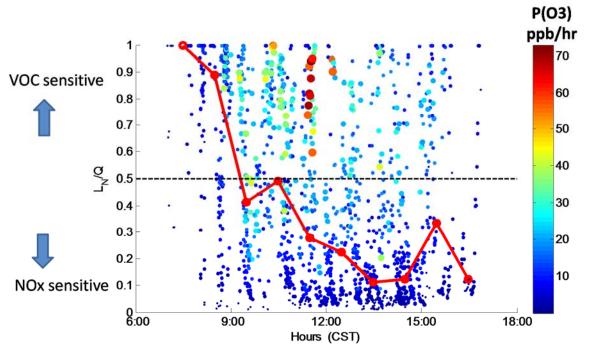


Figure 4. Diurnal variation of the indicator L_N/Q of ozone production rate sensitivity colored with ozone production rate. The solid red circles are the median values in hourly bins of L_N/Q .

Data Collected

None.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments Due to incomplete measurements of VOC on the P-3B, we used the CMAQ-calculated alkanes and alkenes to constrain the box model. We acknowledge there will be some uncertainty associated to this and we propose a sensitivity analysis to investigate the uncertainty.

Goals and Anticipated Issues for the Succeeding Reporting Period

- (1) To attend the AQRP workshop and present the results from this project.
- (2) To investigate ozone production and its sensitivity to NOx and VOCs at each vertical profile locations.
- (3) CMAQ process analysis to map the ozone production efficiency (OPE) and nitrogen oxides (NOx) and VOC limited areas throughout the Houston metropolitan area.

(4) 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.

Detailed Analysis of the Progress of the Task Order to Date

We have finished the data analysis program and are preparing the project progress report to be presented at the upcoming AQRP workshop. 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 RenPrincipal Investigator:Xinrong Ren