AQRP Monthly Technical Report

PROJECT TITLE	Analysis of Airborne Formaldehyde Data Over Houston Texas Acquired During the 2013 DISCOVER-AQ and SEAC^{4}RS Campaigns	**PROJECT #**	14-002
PROJECT PARTICIPANTS	Alan Fried, Christopher P. Loughner, and Ken Pickering	**DATE SUBMITTED**	5/8/2015
REPORTING PERIOD	**From:** April 1, 2015 **To:** April 30, 2015	**REPORT #**	7

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

We completed comparing the 1 km CMAQ runs with P-3B observations, and included Smith Point surface ozone observations into our CMAQ – AQS comparisons.

Preliminary Analysis

A comparison of Smith Point surface ozone observations and AQS observations with a 1 km horizontal resolution CMAQ simulation of maximum 8 hour average ozone concentrations for September 24-26 are shown in Figures 1-3. Smith Point is of interest since it is the receptor of significant pollution plumes originating from the ExxonMobil Baytown and Shell Deer Park petrochemical facilities during part of this time period. Smith Point and surrounding regions over Galveston Bay during the above time period represent ideal first cases by which to test our forthcoming modeling analyses where we will: 1) assess the contributions of direct emissions versus secondary photochemical production of CH_2O; 2) estimate emissions of ethene, propene and CH_2O from these two facilities and compare with facility emission estimates; and 3) assess our photochemical mechanisms involving highly reactive alkenes.

The high bias in CMAQ on September 24 near Galveston may be due to the lack of iodine and bromine chemistry in the model, which destroys ozone. By contrast, the CMAQ model simulation shows a low bias near Galveston Bay on September 25, which we attribute to a low bias in emissions estimates near the ExxonMobil Complex and Deer Park. A comparison of CMAQ with CH_2O measurements made onboard of the P-3B reveals a low bias near the ExxonMobil Complex during the 1st and 2nd circuits, downwind of the ExxonMobil Complex over Smith Point, and in all three of the Deer Park spirals (Figure 4). In addition, CMAQ has a low bias of CO near the ExxonMobil Complex (Figure 5), downwind of the ExxonMobil Complex, and over Deer Park; a low bias of NO over the ExxonMobil Complex and Deer Park; and high biases in ozone over flaring combustion sources near the ExxonMobil complex from ozone titration with NO. The low model biases in CH_2O, CO, and NO near the ExxonMobil Complex and Deer Park suggests a low bias in model emissions estimates in these areas. Back-trajectories from the 1 km WRF output (to be included in the next report) reveal transport from

the northeastern edge of the Smith Point spiral from the ExxonMobil Complex and from the southern edge of the Smith Point spiral from Deer Park. Time-series comparisons of CH_2O, CO, NO, and O_3 between CMAQ and P-3B observations as the P-3B passes over the ExxonMobil Complex during the first spiral (Figure 5) and the northeastern edge of the Smith Point spiral on the 2nd spiral (Figure 6) displays model biases over and downwind of the ExxonMobil Complex corroborating with the analysis that emissions estimates are too low near the ExxonMobil Complex leading to less ozone production downwind of this emissions source region. Detailed CH_2O comparisons of Fig 5 with Fig. 6 will be the subject of another report.

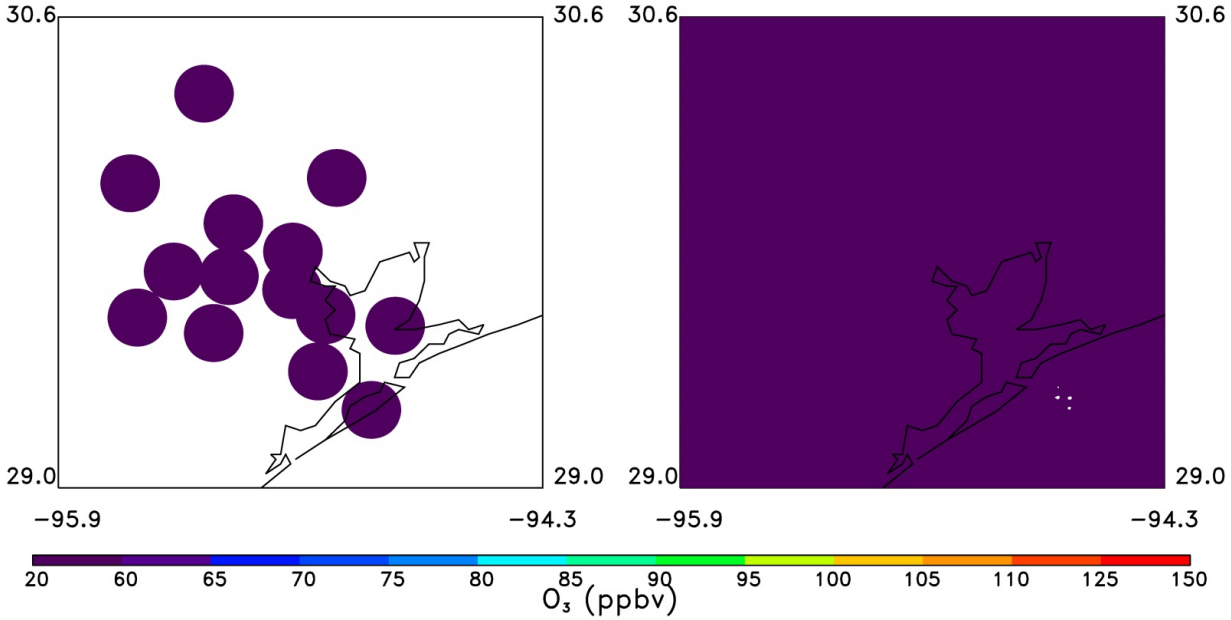

Figure 1: Eight-hour average ozone maximum from observations (left) and new 1 km CMAQ simulation on 24 September 2013.

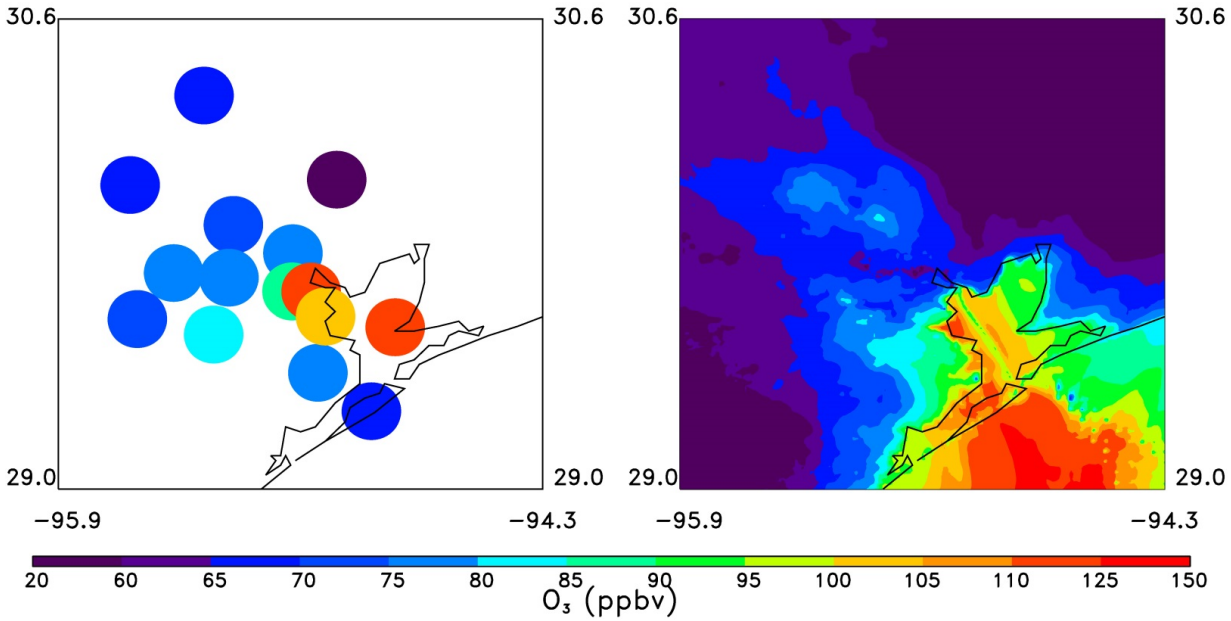

Figure 2: Eight-hour average ozone maximum from observations (left) and new 1 km CMAQ simulation on 25 September 2013.

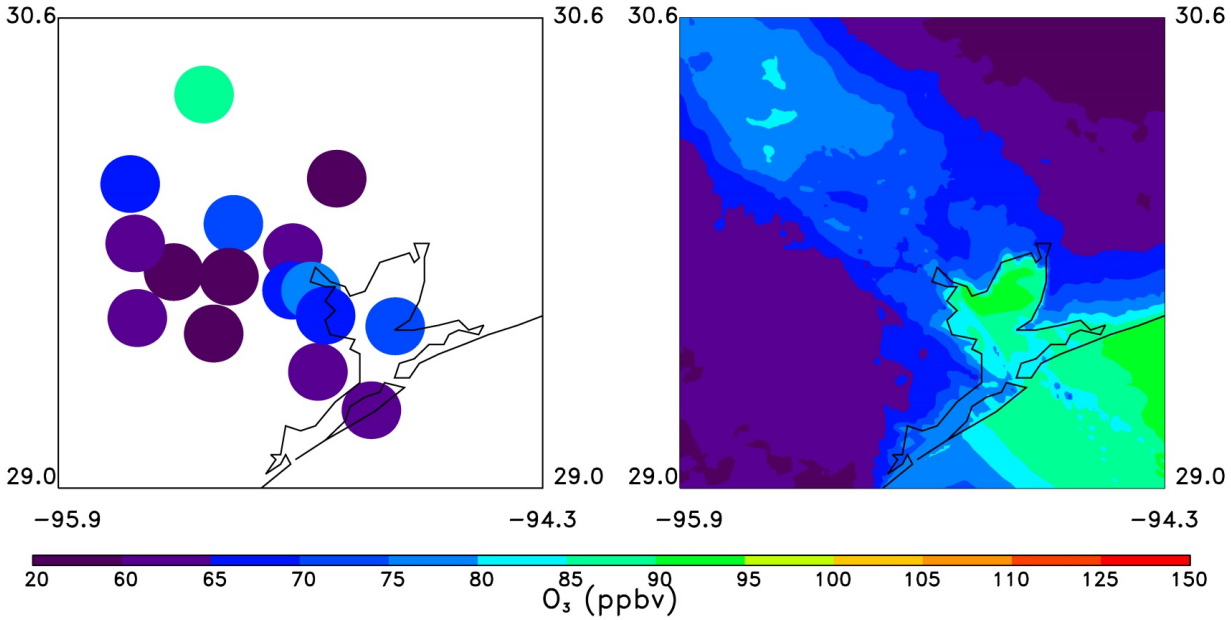

Figure 3: Eight-hour average ozone maximum from observations (left) and new 1 km CMAQ simulation on 26 September 2013.

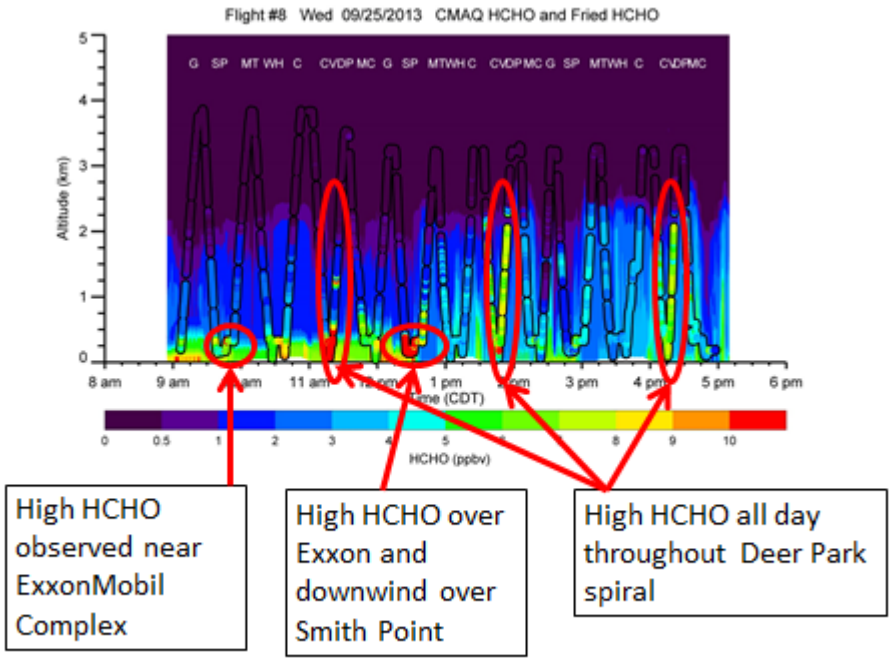

Figure 4: Annotated curtain of CMAQ CH_2O concentrations (background) along the NASA P-3B flight track (overlay) shows high CH_2O concentrations near the ExxonMobil Complex during the first circuit, downwind of the ExxonMobil Complex over Smith Point during the 2nd and 3rd circuits, and during all three of the Deer Park spirals.

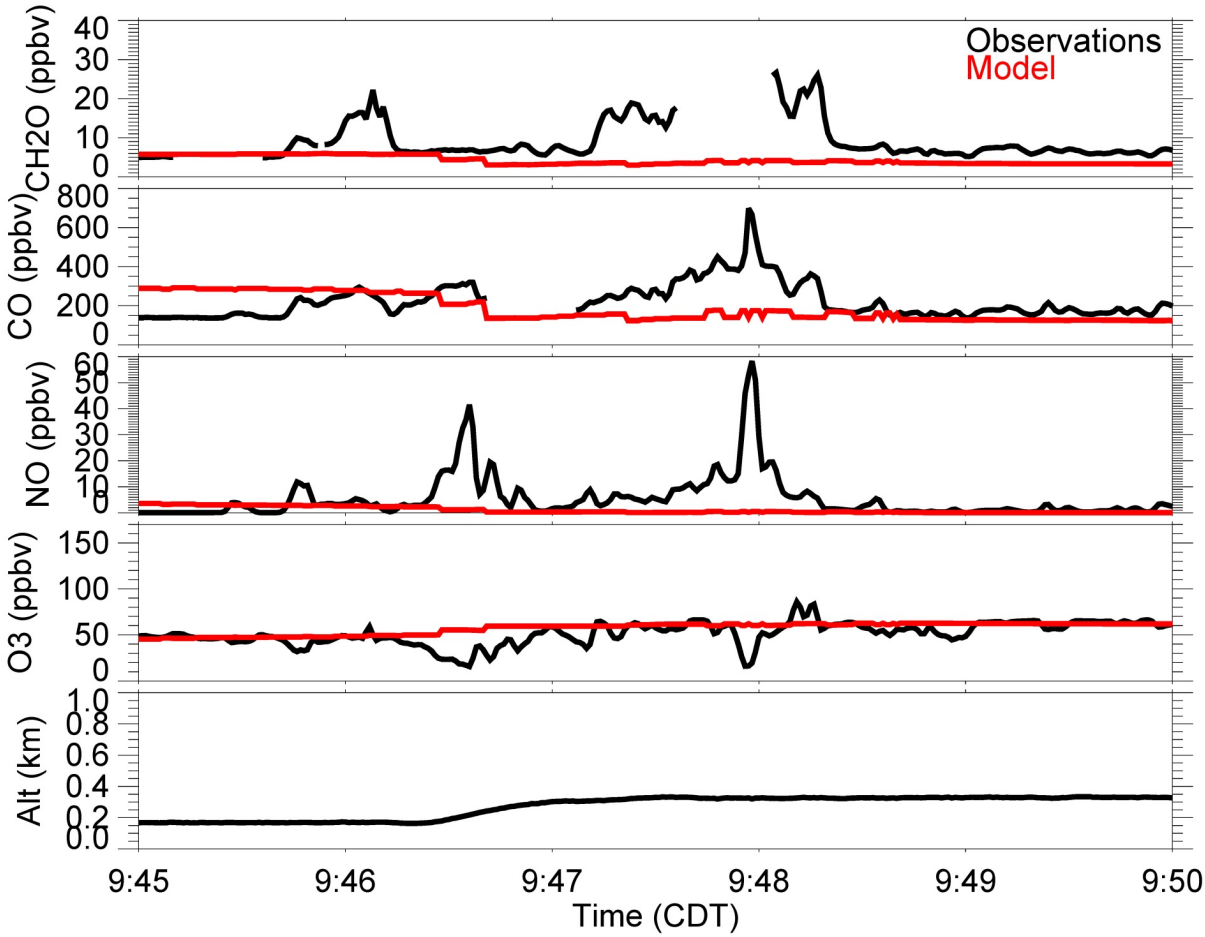

Figure 5: Time-series comparisons of P-3B and CMAQ CH_2O, CO, NO, and O3 near the ExxonMobil Complex during the 1st circuit on September 25.

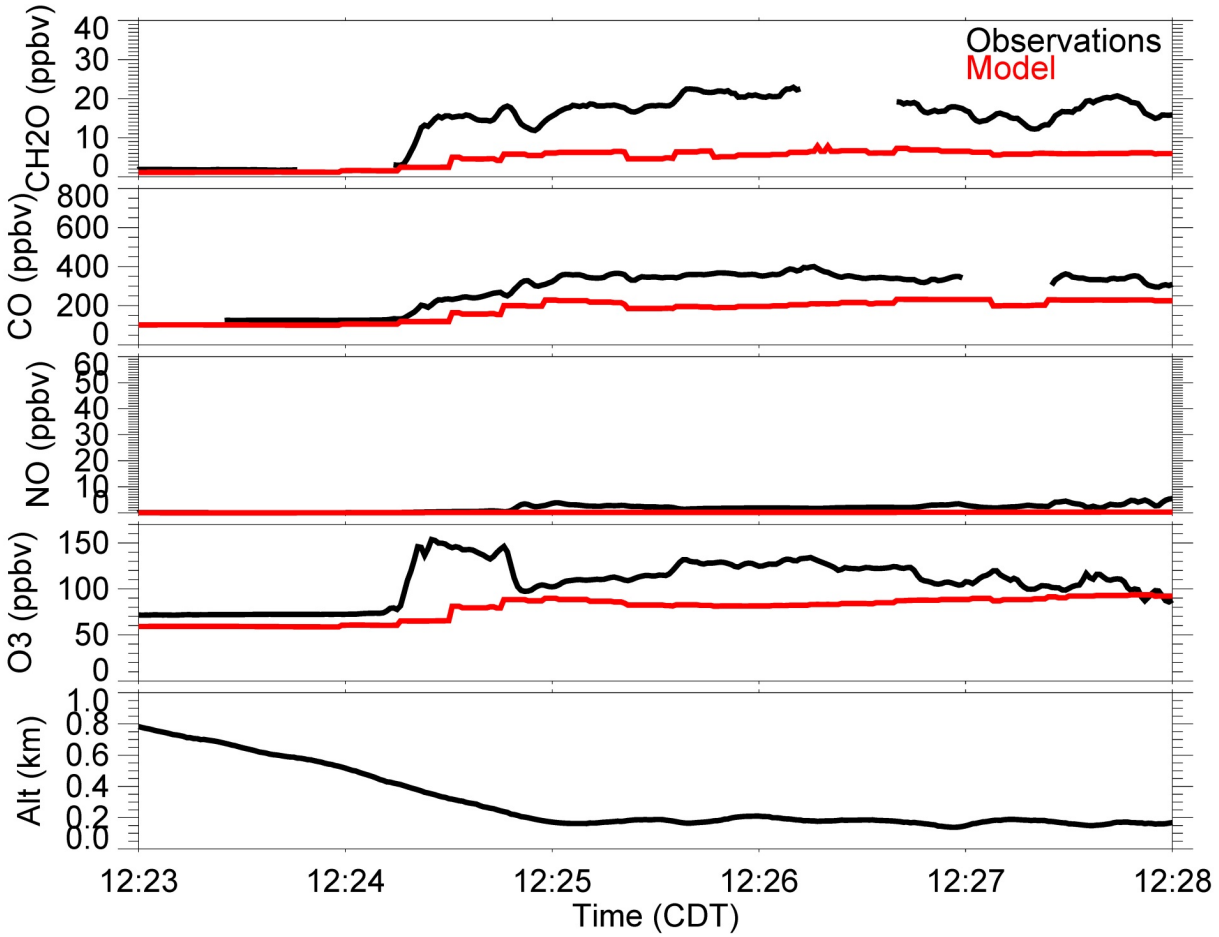

Figure 6: Same as Figure 5, but located on the northeastern edge of the Smith Point spiral, which was downwind of the ExxonMobil Complex, during the 2nd circuit.

Data Collected
None.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments
No problems encountered.

Goals and Anticipated Issues for the Succeeding Reporting Period
Improve emissions inventory (E) based on the following ratios for a new CMAQ simulation with process analysis:

- $\frac{E(CO)_{new}}{E(CO)_{old}} = \frac{\Delta[CO(source\ region - upwind)]_{observed}}{\Delta[CO(source\ region - upwind)]_{model}}$
- $\frac{E(CH_2O)_{new}}{E(CO)_{new}} = \frac{[CH_2O]_{observed}}{[CO]_{observed}}$
- $\frac{E(NO)_{new}}{E(CO)_{new}} = \frac{[NO]_{observed}}{[CO]_{observed}}$
- $\frac{E(propene)_{new}}{E(CO)_{new}} = \frac{[propene]_{observed}}{[CO]_{observed}}$

Detailed Analysis of the Progress of the Task Order to Date
We don't anticipate delays in the completion of this project.

Submitted to AQRP by: Alan Fried
Principal Investigators: Alan Fried and Chris Loughner