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**	1/8/2015
REPORTING PERIOD	**From:** December 1, 2014 **To:** December 31, 2014	**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. We understand that the FSR and Invoices are due to the AQRP by the 15th of the month following the reporting period shown above.

Detailed Accomplishments by Task

Team members continued to coordinate, review, and discuss by telecoms the specific tasks assigned to each group. This report presents the progress achieved by the parallel efforts from the University of Colorado (CU) and the University of Maryland (UMD)/NASA Goddard teams.

The CU team continued their efforts in identifying P3 and DC8 aircraft sampling periods arising from clearly identifiable sources. These periods will then be used for further study by WRF and CMAQ. As discussed in the report last month, the CU team identified Sept. 25 for the initial analysis. This team started this analysis by quantifying CH2O/CO slopes from the final DISCOVER-AQ data for 4 specific CH_2O source regions where: 1) petrochemical refinery emissions were dominant over the Baytown Exxon Mobil petrochemical complex; 2) biogenic isoprene emissions were dominant over West Houston and Conroe; 3) where an unknown source, possibly from CH_2O photochemical production downwind of the Baytown complex was dominant over Smith Point; and 4) where automotive and urban sources mixed with residual CH_2O from the previous night together with transported CH_2O were dominant over the center of Houston over Moody Tower. Similar to the report last month, this analysis started by displaying the time series of CH_2O, CO, propene, and pressure altitude during the second circuit (shown in Fig. 1).

Figure 2 depicts the airborne CH_2O data acquired during the 1st and 2nd circuits superimposed on a map of the Houston Metropolitan Area. The CH_2O measurements are color-coded and sized by the measured CH_2O mixing ratios. The enhanced CH_2O in the boundary layer over the bay and at Smith Point during the 2nd circuit (starting time around 12 noon local) is clearly evident relative to corresponding measurements during the 1st circuit (starting time around 9 am local). The 1st circuit, however, reflects significantly higher CH_2O and propene (not shown here) levels right over the Exxon-Mobil Baytown petrochemical complex, which is not evident during the 2nd circuit. This behavior, which represents an ideal case for further analysis using WRF-CMAQ modeling, most likely reflects direct emission sources of CH_2O and its precursors (ethene and propene) right over the Exxon-Mobil Baytown petrochemical complex during the 1st circuit followed by the prevalence of secondary CH_2O production downwind over the Bay and at Smith Point during the 2nd circuit. Although this will require some additional analysis to confirm this hypothesis, this ideal case when coupled with forthcoming analysis from the 3rd circuit, will

enable us to check and update the latest petrochemical emission inventory for the Exxon-Mobil Baytown petrochemical complex as well as a check on our knowledge of the meteorology and chemistry. Similar to last month's report focusing on the 1st circuit, Figure 3 in this report presents CH_2O-CO regression plots for the 2nd circuit during the Sept. 25 flight for various sampling domains.

In parallel, the UMD/NASA Goddard team continued to update and improve their WRF and CMAQ model simulations. WRF is being re-run to improve the model representation of sea and bay breezes. A new modeling technique has been implemented and includes: higher resolution meteorological initial and boundary conditions (North American Mesoscale 12 km model instead of the North American Regional Reanalysis, which has a horizontal resolution of 40 km), and the inclusion of a 1 km horizontal resolution domain. We are performing observational nudging on all model domains. The new modeling technique involves running WRF iteratively, where we first run WRF performing analysis nudging based on the NAM 12 km, and then re-run WRF performing analysis nudging based on the previous WRF simulation. This modeling technique prevents the relatively coarse NAM 12 km model from degrading the high-resolution WRF modeling domains (4 km and 1 km modeling domains). The initial WRF run has been completed and the iterative 4 km and 1 km runs are anticipated to be completed within a week.

Preliminary Analysis

The initial 1 km horizontal resolution WRF simulation (not the iterative 1 km WRF run, which is currently running) did a better job capturing the sea and bay breeze circulations than our initial 4 km simulation (Figures 4 and 5).

Data Collected

Final data from the DISCOVER-AQ and NASA SEAC^{4}RS Houston field deployments are in the NASA data archive. Data from the former is publicly available online.

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Computer maintenance throughout the month of December prevented us from finishing the WRF iterative simulations. Computers maintenance has been completed and we anticipate the WRF iterative simulations to be completed within a week.

Goals and Anticipated Issues for the Succeeding Reporting Period

We will finish the WRF iterative simulation, evaluate the model results with observations including performing a statistical comparison between the new WRF iterative run and the original WRF run, and prepare input files for new CMAQ simulations. The CU team will continue their efforts in providing to the UMD/Goddard team interesting time periods for further analysis. Initial efforts will focus on P3 sampling on September 25, 2013.

Detailed Analysis of the Progress of the Task Order to Date

We don't anticipate delays in the completion of this project.

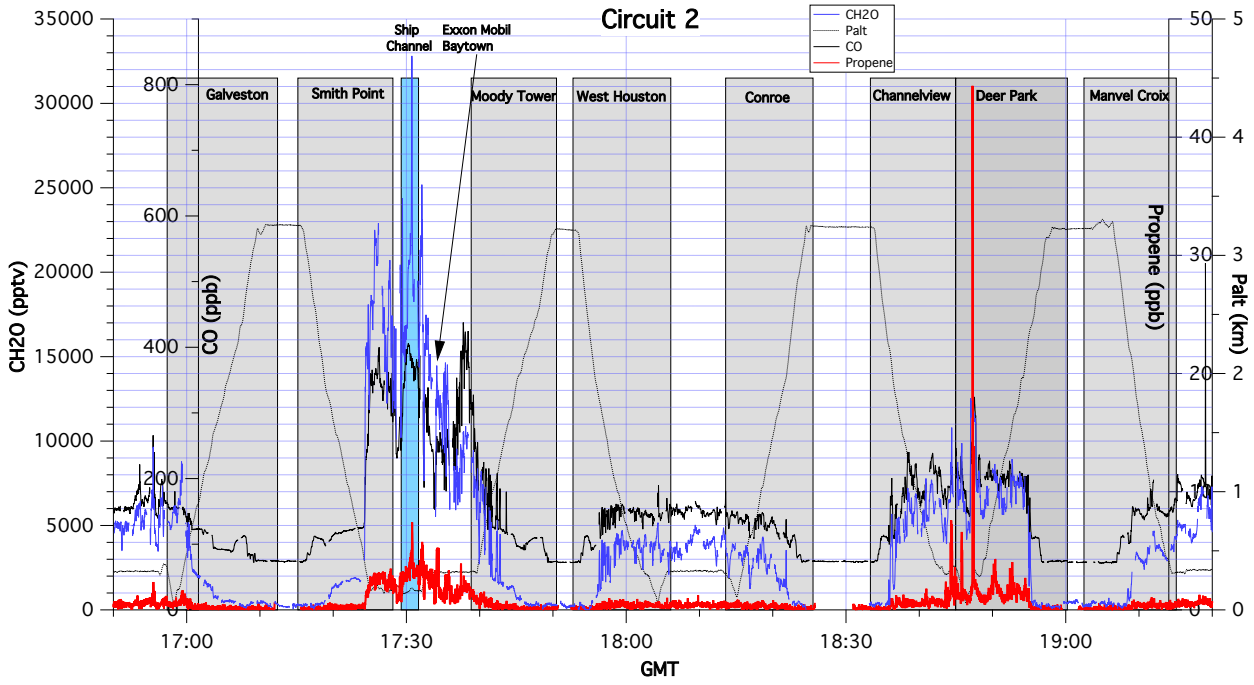

Figure 1: Time series of final archived data for the 1-second concentrations of CH_2O (blue), CO (black), and propene (red), along with pressure altitude (Palt) for the second circuit measured on the NASA P3 on September 25, 2013 at various sites in the Houston, Texas metropolitan area. The Fried group at the University of Colorado acquired the CH_2O measurements while the CO and propene were measured respectively, by the Diskin DACOM group at NASA Langley and the PTRMS instrument from the Armin Wisthaler group formerly at University of Innsbruck. The significantly elevated concentrations of all 3 gases are evident near the Exxon Mobil Baytown petrochemical facility and near the petrochemical facilities around Channelview and Deer Park. This plot is illustrative of the many trace gases, whose time series are being studied.

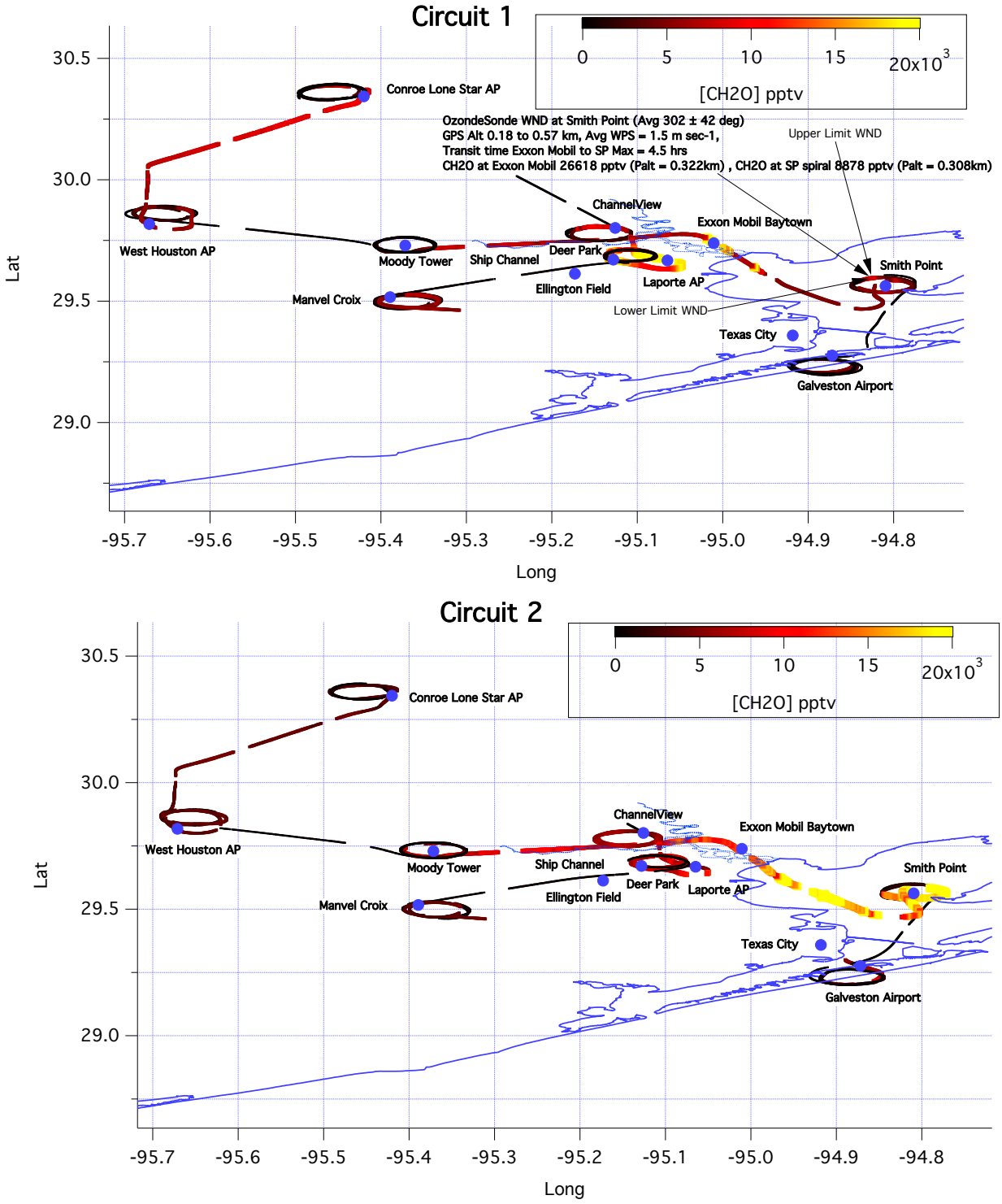

Figure 2: Map of the Houston Metropolitan Area with the P3 aircraft flight tracks, color-coded and sized by the measured CH_2O mixing ratios, superimposed for the 1st and 2nd circuits of the September 25, 2013 flight. The various spiral-sampling sites are shown. To enhance the visibility of the measurements at various locations, the color scale is capped at 20 ppb. However, as can be seen in Fig. 1 in this report and Fig. 1a in last month's report, the CH_2O mixing ratios exceed this value in certain locations. The upper panel also depicts the wind direction and its spread measured at Smith Point. Although the altitudes in these plots are not immediately obvious, Fig. 1 shows that the aircraft spiraled down over Smith Point to pressure altitudes < 0.4km and maintained this altitude over the Exxon-Mobil complex, over the Ship Channel, until the base of the Moody Tower spiral up.

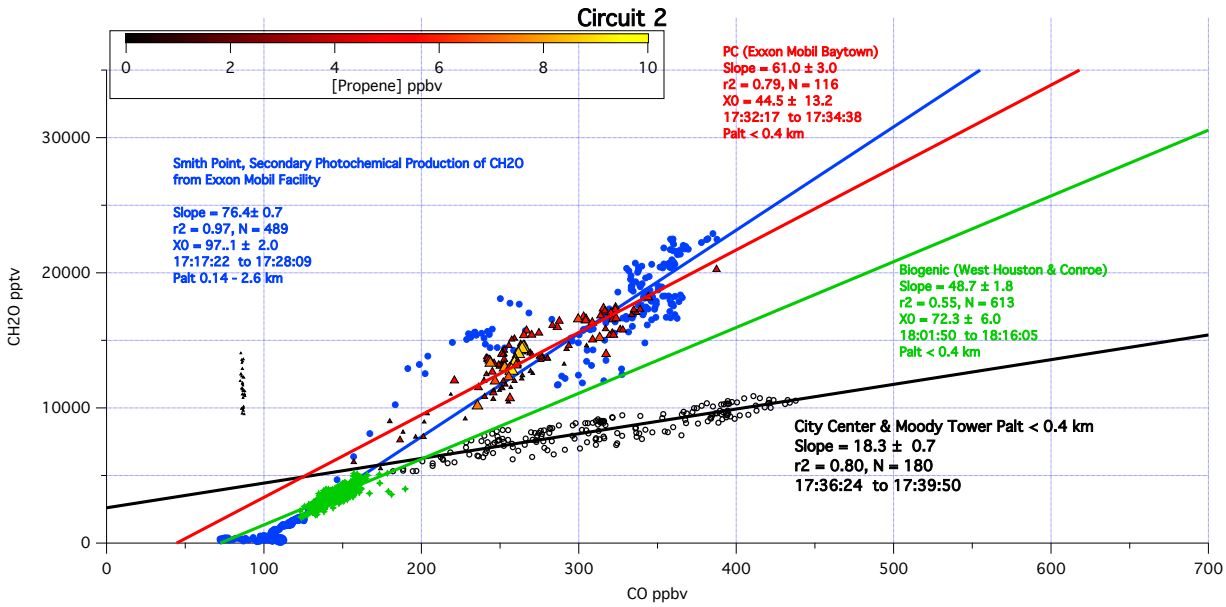

Figure 3: Linear regression slopes of CH_2O versus CO (units of ppt/ppb) for the 4 specific CH_2O sources observed during the 2nd circuit. These events are: 1) petrochemical refinery emissions near the Baytown Exxon Mobil petrochemical complex (red PC regression); 2) biogenic isoprene emissions (green Biogenic regression) near West Houston and Conroe; 3) potentially secondary photochemical production of CH_2O downwind of the Baytown complex (blue regression) over Smith Point; and 4) automotive and urban emission sources over the center of Houston over Moody Tower mixed with residual CH_2O from the previous night as well as transported sources from other regions. These regions were respectively identified by elevated: propene (PC trace); isoprene (biogenic trace); photochemical production of CH_2O at Smith Point (blue trace); and by the lack of elevated isoprene and propene but elevated black carbon, benzene and SO_2 over the city center (City Center Moody Tower black trace). The X_0 values denote the X-intercept, indicating the background CO concentrations that correlated with CH_2O. Very similar to the regression plot in last month's report, the City Center trace shows a distinctly different intercept indicative of the presence of residual background CH_2O, most likely from the previous night and transported from other regions.

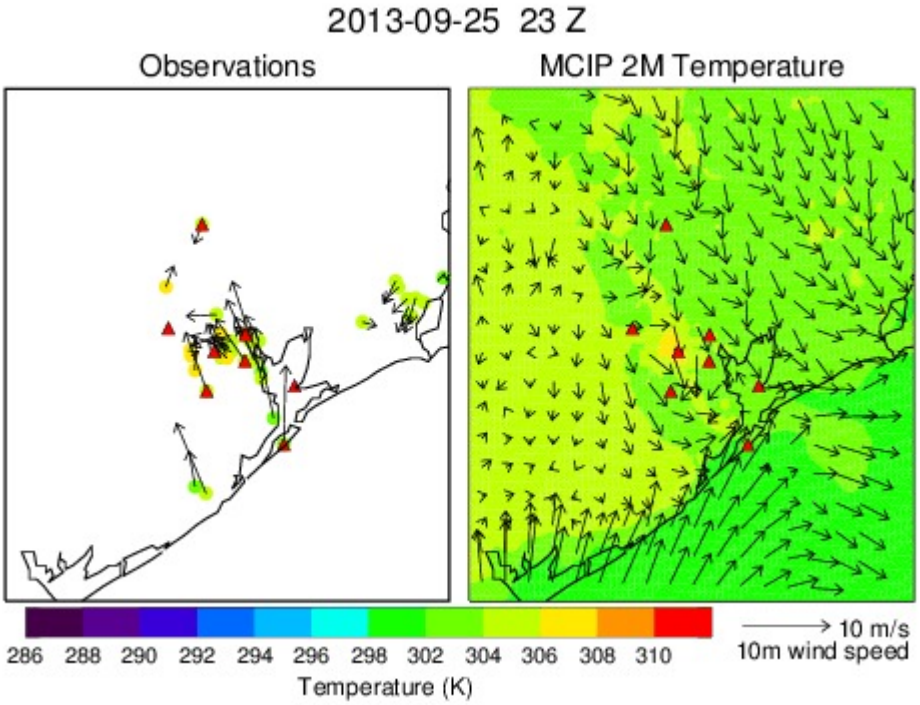

Figure 4: Observed (left) and WRF diagnosed (right) 2K temperature and 10 m wind velocity at 22 UTC 25 September 2013 from the original 4 km WRF simulation. WRF simulated weaker sea and bay breezes than observed

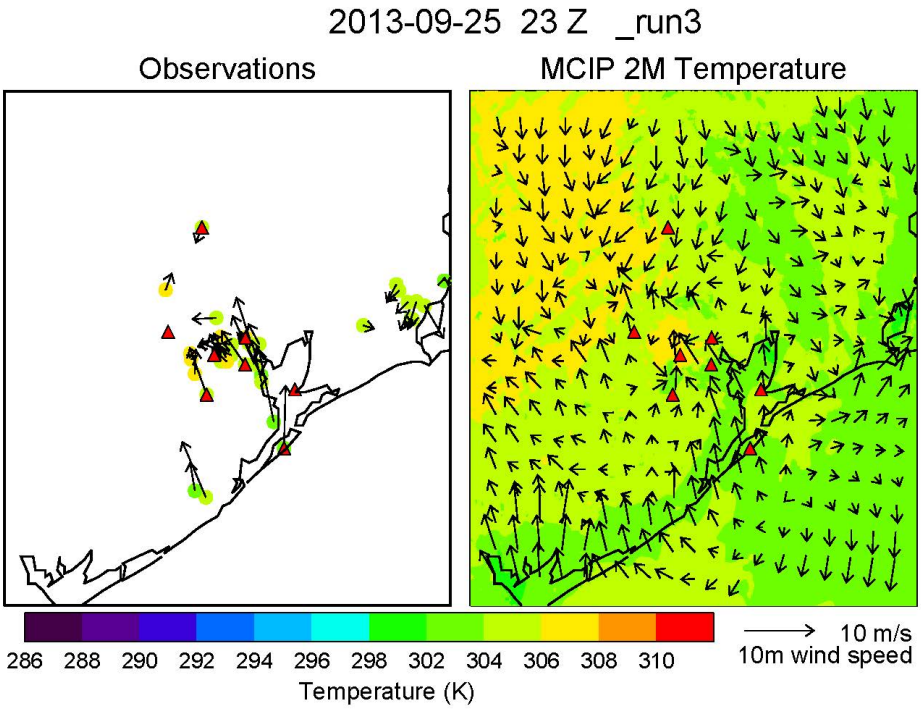

Figure 5: Observed (left) and WRF diagnosed (right) 2 m temperature and 10 m wind velocity at 23 UTC 25 September 2013 from the new 1 km WRF simulation. Strength of WRF simulated bay and sea breezes in agreement with observations.

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