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**	12/4/2014
REPORTING PERIOD	**From:** November 1, 2014 **To:** November 30, 2014	**REPORT #**	2

Detailed Accomplishments by Task

Team members coordinated and reviewed by telecoms the specific tasks assigned to each group. The CU team initiated their efforts to identify P3 and DC8 aircraft sampling periods arising from clearly identifiable sources. These periods will then be used for further study by WRF and CMAQ. Because of the large and dynamic pollution levels trapped in a shallow boundary layer, 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 near 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. Figures 1a, 1b, which are illustrative of the types of plots being generated and studied, will be used as starting points to arrive at updated emissions as well as checks on our knowledge of the meteorology and chemistry.

The UMD / NASA Goddard team updated the modeling technique and began WRF simulations down to a horizontal resolution of 1 km based on preliminary WRF and CMAQ simulations run down to a horizontal resolution of 4 km.

Preliminary Analysis

A comparison between observations and WRF and CMAQ simulations run down to a horizontal resolution of 4 km reveals that the model simulated weaker sea and bay breezes than observed. For September 25, the model simulated the sea breeze front just onshore over Galveston, while observations reveal the bay breeze front pushing farther inland.

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

We are currently re-running WRF with different model inputs and options to try to improve the model representation of the sea and bay breeze circulations. We are now using the North American Mesoscale (NAM) 12 km model for initial and boundary conditions instead of the

North American Regional Reanalysis (NARR), which has a horizontal resolution of 40 km. We are also nudging all domains, whereas previously we only nudged the 36 km domain. In addition we are now using a WRF iterative technique, 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).

Goals and Anticipated Issues for the Succeeding Reporting Period

The new WRF model simulation will be completed and analyzed with observations. Based on the conclusions of this analysis, we will either proceed to run CMAQ and calculate back trajectories with RIP or refine the WRF modeling technique and inputs and re-run WRF. The CU team will provide 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

The AQRP task order was executed over 4 months after the anticipated start date established in the Work Plan. Although we don't anticipate issues that will retard progress, the late start will necessitate pushing back the accomplishments of each Milestone.

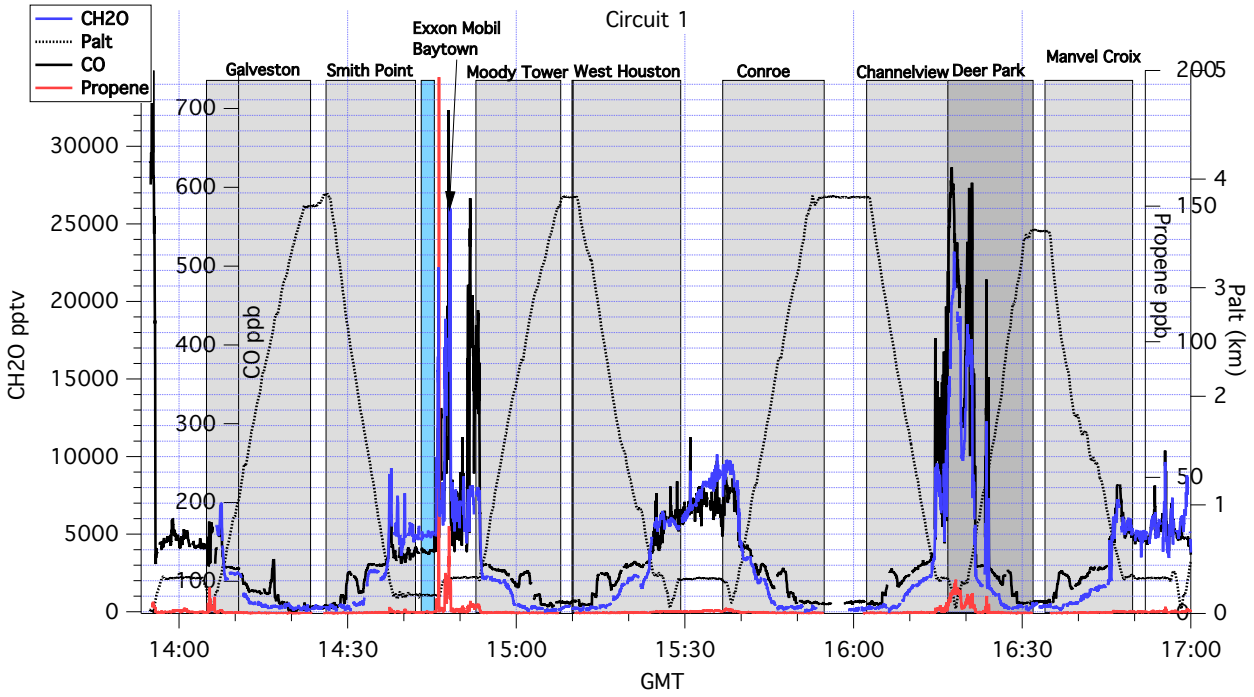

Figure 1a: Time series of final archived data for the 1-second concentrations of CH_2O, CO, and Propene, along with pressure altitude (Palt) for the first circuit measured on the NASA P3 on September 25, 2013 at various sites in the Houston, Texas metropolitan area. The Fried group at the University 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. This plot is illustrative of the many trace gases, whose time series are being studied.

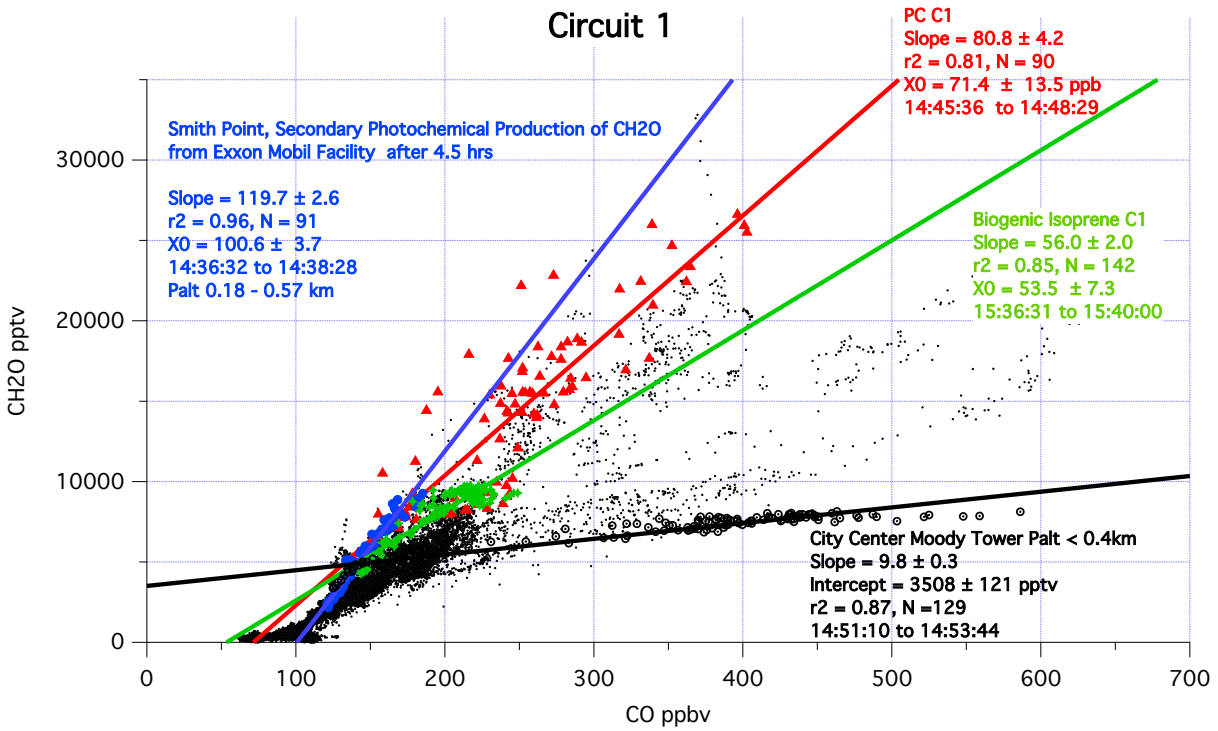

Figure 1b: Linear regression slopes of CH_2O versus CO (units of ppt/ppb) for the 4 specific CH_2O sources observed during the first circuit of Fig 1a. These events are: 1) petrochemical refinery emissions near the Baytown Exxon Mobil petrochemical complex (red PC C1 regression); 2) biogenic isoprene emissions (green Biogenic regression C1) near 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); low propene (reacted away) but favorable wind direction from the Baytown complex to Smith Point and the shallow boundary layer (<0.5 km from ozonesonde and CH_2O measurements) that confines the emissions and their products (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 trace). The X_0 values denote the X-intercept, indicating the background CO concentrations that correlated with CH_2O. In the case of the City Center trace, the distinctly different intercept indicates the presence of residual background CH_2O, most likely from the previous night and transported from other regions.

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