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**	3/9/2015
REPORTING PERIOD	**From:** February 1, 2015 **To:** February 28, 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. We 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

As discussed in last month's report, the initial task of the CU (University of Colorado) team in February was to investigate the relationship of the exceedingly high measured CH_2O levels on September 25 to the rest of the aircraft sampling month (Sept. 4 to Sept. 26). Because of the magnitude of the CH_2O levels (up to 33 ppbv during the 2nd circuit and 26 ppbv during the 1st circuit) observed at select locations in the boundary layer near and downwind of the Exxon-Mobil Baytown facility on this day relative to more typical values < 10 ppbv observed throughout the rest of the month, the project team deemed it important to simultaneously investigate this aspect while finishing the development of the WRF-CMAQ model that will be employed in tackling the other major project goals: 1) understanding the sources of CH_2O and its temporal trends; 2) determining the relative contributions of direct versus 2nd photochemical sources of CH_2O from highly reactive volatile organic compounds (HRVOC's) downwind; 3) providing new estimates for the emission rates of CH_2O and its hydrocarbon precursors; and 4) assessing our current knowledge of the photochemistry. Our 2nd Quarterly report submitted in late February provided plots of the measured CH_2O distributions from the NASA P3 aircraft during the DISCOVER-AQ study on Sept. 25 over the entire Houston Metropolitan area versus the rest of the month. For space reasons these plots will not be repeated here, but they clearly show that Sept. 25 stands out. This is in agreement with the 24-hour canister sampling measurements of ethene (one of the HRVOC CH_2O precursors) by the State of Texas at the HRM3 sampling site (west end of the Channelview spiral along the Ship Channel) and the Lynchburg Ferry site. Throughout the month of September prior to Sept. 25, the 24-hour ethene average at the HRM3 site ranged between 2 and 4 ppbv, but on Sept. 25 this jumped to 10 ppbv. In addition, the 1-hour auto-GC measurements of ethene on this day and into the early morning hours of Sept. 26 at HRM3 ranged between 0.2 and 109 ppbv. Mark Estes at the TCEQ, who provided us with these plots, believes such high levels resulted from a narrow ethene plume emitted near the eastern end of the Ship Channel. Clearly, Sept. 25 reveals anomalously high emissions of both CH_2O and its precursors relative to the rest of September, and this will be further studied and discussed in subsequent reports.

Preliminary Analysis

Our 2nd Quarterly report submitted in late February also included results of the WRF-CMAQ simulations with different horizontal resolutions. For completeness, we repeat these results here. Initial WRF-CMAQ simulations at horizontal resolutions of 36, 12, and 4 km produced a weaker bay breeze than observed on September 25 that resulted in lower ozone concentrations along the western coastline of Galveston Bay and points inland to the north and west. We re-ran WRF with a revised technique and a fourth modeling domain with a horizontal resolution of 1 km to improve the model representation of the sea and bay breezes. The new run used 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 nudged all domains, whereas previously we only nudged the 36 km domain. In addition we used a WRF iterative technique, where we first ran WRF performing analysis nudging based on the NAM 12 km, and then re-ran WRF performing analysis nudging based on the previous WRF simulation. This modeling technique prevented the relatively coarse NAM 12 km model from degrading the high-resolution WRF modeling domains (4 km and 1 km modeling domains). The new WRF run simulated a stronger bay breeze along the western coastline of Galveston Bay that is in better agreement with observations than our initial simulation (Figure 1).

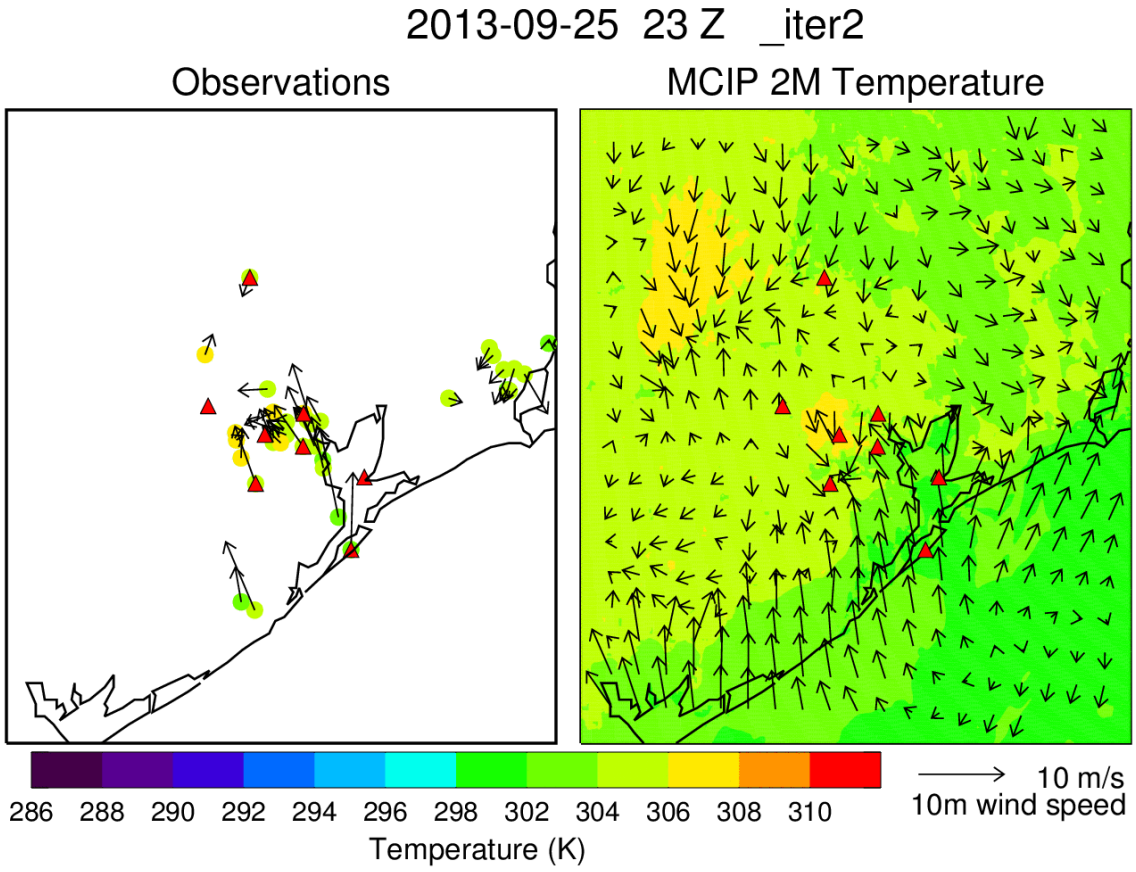

Figure 1: Observed (left) and WRF diagnosed (right) 2 m temperature and 10 m wind velocity at 23 UTC 25 September 2013 from the new 1 km WRF simulation.

New CMAQ simulations based on the new and improved WRF simulation have been completed for the 36, 12, and 4 km domains, and the CMAQ simulation for the 1 km domain is currently underway. Overall, the new 4 km CMAQ simulation is in better agreement with the observations than the original simulation (Figure 2). For maximum 8-hour average ozone on September 25, a

high model bias is present at Galveston and a low model bias is present at La Porte Sylvan Beach in both the original and new 4 km CMAQ simulations. The new 4 km CMAQ simulation did not capture the observed high ozone over Channelview and Deer Park during the 2nd and 3rd circuits and Moody Tower on the 3rd circuit (Figure 3). Figure 4 presents our initial comparisons of CMAQ model simulations (20-minute averages) and comparisons with 1-minute averaged measurements for CH_2O for this day.

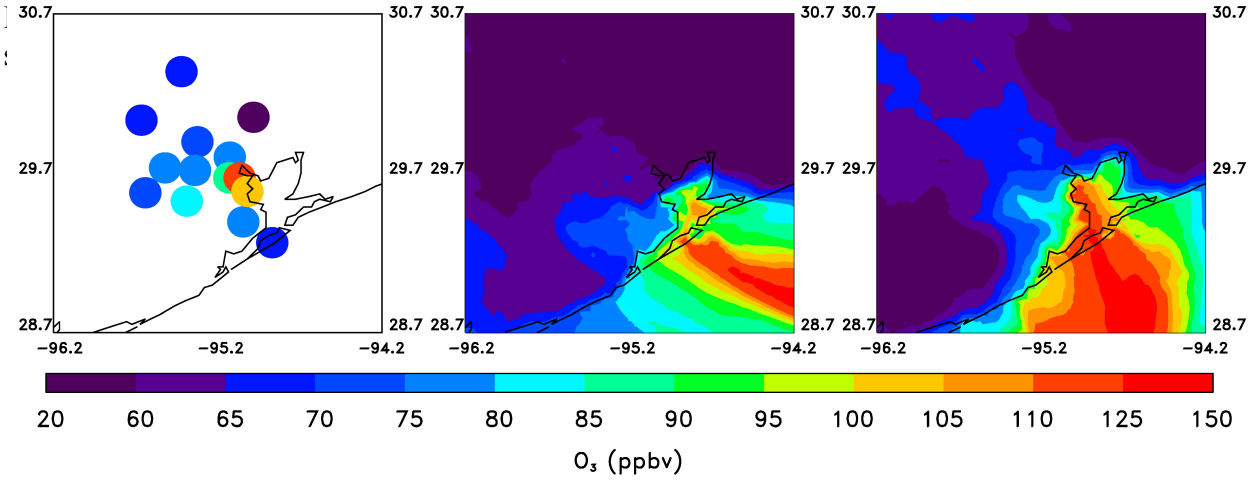

Figure 2: Eight-hour average ozone maximum from observations (left), original 4 km CMAQ simulation (middle), and new 4 km CMAQ simulation on 25 September 2013.

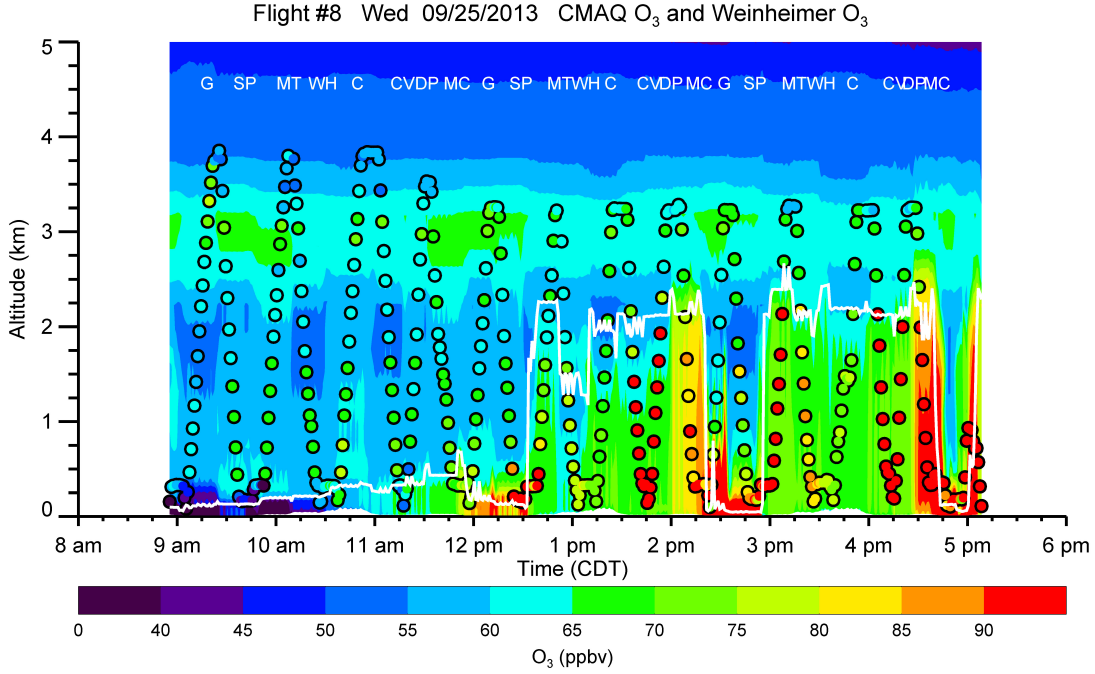

Figure 3: CMAQ simulated (background) and observed (overlay) ozone concentrations along a flight track on 25 September 2013. The white line shows the location of the top of the boundary layer as calculated by the WRF model. The white letters at the top of the figure, "G", "SP", "MT", "WH", "C", "CV", "DP", and "MC" stand for the spiral locations Galveston, Smith Point, Moody Tower, West Houston, Conroe, Channelview, Deer Park, and Manvel Croix, respectively. CMAQ results are from the new 4 km horizontal resolution domain

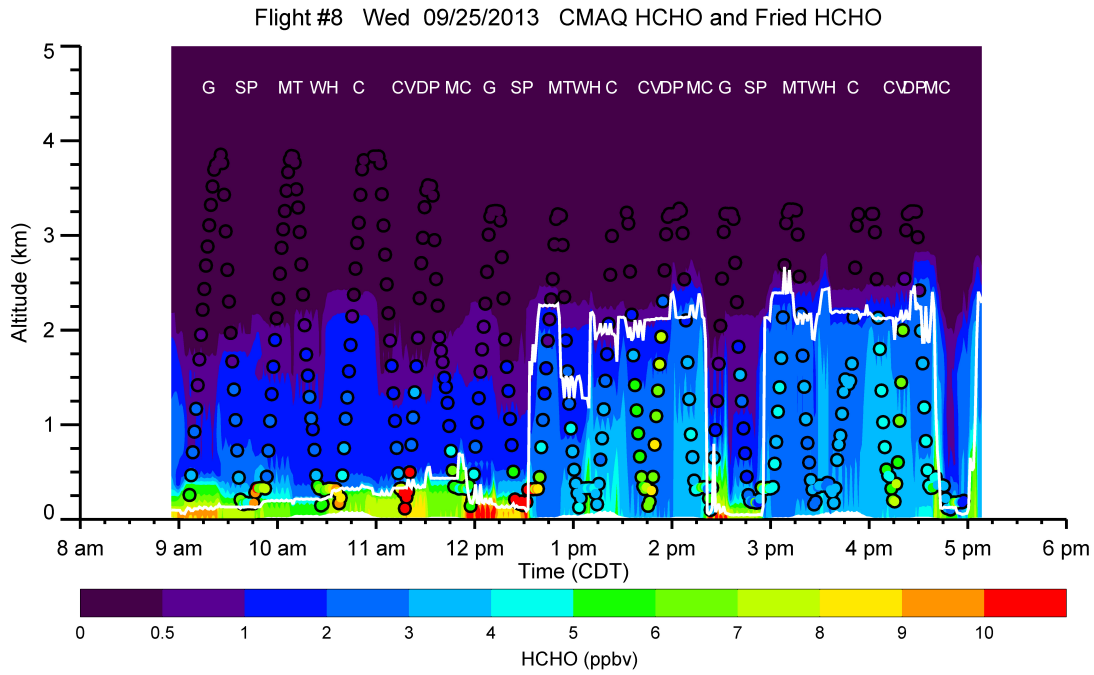

Figure 4: Same format as Fig. 3, only for formaldehyde.

As can be seen, the model on Sept. 25 shows a low CH_2O bias relative to the measurements throughout the boundary layer over Channelview (CV) during the 1st and 2nd circuits and over Deer Park (DP) during all three circuits. This will be further evaluated and discussed in subsequent reports.

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
We don't anticipate any issues for the next reporting period. Some of the goals that we will try to accomplish include: 1) continued CMAQ simulations and comparisons with aircraft observations of CH_2O for Sept. 25 and other days; 2) comparisons of aircraft CH_2O observations over Deer Park for Sept. 25 with the rest of the September sampling period; and 3) comparisons of our Deer Park CH_2O missed approach observations with 24-hour DNPH sampling results, where available.

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

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