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	2/9/2015
REPORTING PERIOD	**From:** January 1, 2015 **To:** January 31, 2015	REPORT #	4

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

Team members continued to coordinate, review, and discuss by telecoms the specific tasks assigned to each group. 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, and data from the first two P3 circuits were presented. In this report we present data for the 3rd circuit (Fig 1), and for completeness we show the results from all 3 circuits superimposed on a map of the Houston Metropolitan area in Figs. 2a, 2b, 2c. In all 3 cases back trajectories (not shown) show similar Northwest to Southeast flow. Figures 2 show the progression in CH_2O concentrations as a function of time of day. We note that the CH_2O scales in 2A and 2B are limited to a maximum value of 20 ppbv to show the enhancements more clearly, even though concentrations attained levels as high as 35 ppbv. The scale on the 3rd circuit, which was not limited, is approximately a factor of 2 higher than the 1st two circuits. These plots show the direct emissions of CH_2O and its fast reacting precursors during circuit 1 (local starting time ~ 9am) from petrochemical sources in and near the Ship Channel, the photochemical production of CH_2O downwind of these sources during the 2nd circuit (12 noon local time), and the decay during the 3rd circuit (local time ~2:30 pm) as well as enhanced dispersal as the boundary layer continues to grow throughout the day. As will be shown in a future report, plots of O_3 vs CO show the expected anti-correlation between ozone and CO (negative slope) over the bay to the Moody tower spiral during the 1st circuit, which is indicative of O_3 titration from fresh emissions. However, during the second circuit, such plots yield positive slopes, indicative of ozone production. As mentioned in previous reports, this temporal behavior represents an ideal 1st case to study using WRF-CMAQ in an effort to: 1) understand the sources of CH_2O; 2) determine the relative contributions of direct versus 2nd photochemical sources; 3) provide new estimates of emission rates for CH_2O and its hydrocarbon precursors; and 4) assess our current knowledge of the photochemistry. Because this analysis relies quite heavily on WRF-CMAQ results, we now present progress in this area by the UMD/NASA Goddard team.

We completed re-running WRF to improve the model representation of sea and bay breezes using a new modeling technique, higher resolution meteorological initial and boundary conditions (North American Mesoscale 12 km model), and the inclusion of a 1 km horizontal resolution domain. We performed observational nudging on all model domains and ran WRF iteratively. For the iterative simulation, 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 (4 km and 1 km) WRF modeling domains. MCIP was run to create meteorological input files for CMAQ for all four domains (36, 12, 4 and 1 km). We analyzed WRF model output alongside temperature and wind velocity observations.

Preliminary Analysis

The final iterative 1 km horizontal resolution WRF simulation did a better job capturing the sea and bay breeze circulations than our initial 4 km simulation (Figures 3 and 4). The following statistics were calculated to evaluate the model diagnosed 2-m temperature and 10-m wind speed and direction for the September 24-26, 2013 period and are shown in Table 1: mean bias, normalized mean bias, normalized mean error, and root mean square error. The 2 m temperature and 10 m wind speed and direction statistical analysis between the observations and the original 4km simulation and the initial and final iterative 1 km and 4 km simulations are shown in Tables 2-4. The final iterative 1 km WRF run produced the lowest mean bias and normalized mean bias for temperature and wind speed than the other simulations. The first iterative 1 km simulation produced the lowest mean bias and normalized mean bias for wind direction.

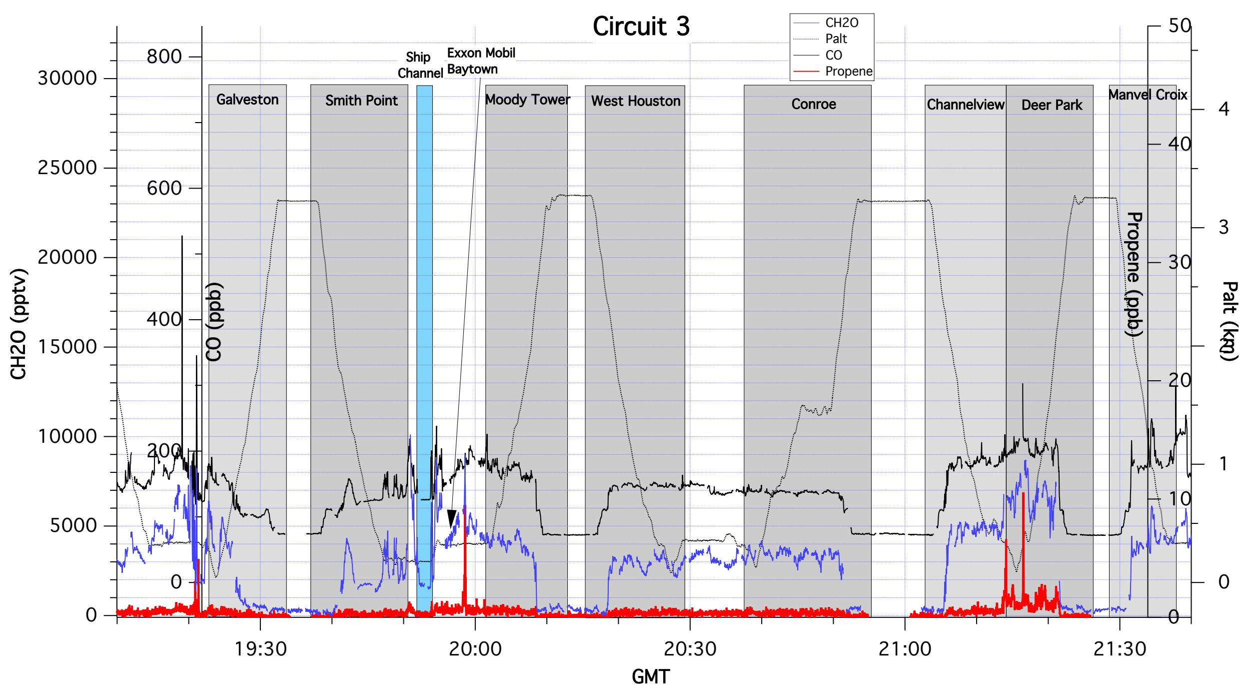

Figure 1: Time series plot of 1-second P3 CH_2O measurements from the DFGAS instrument (blue lines), the CO measurements from the NASA DACOM instrument (black lines) and the PTRMS propene measurements from Armin Wisthaler's group (red lines).

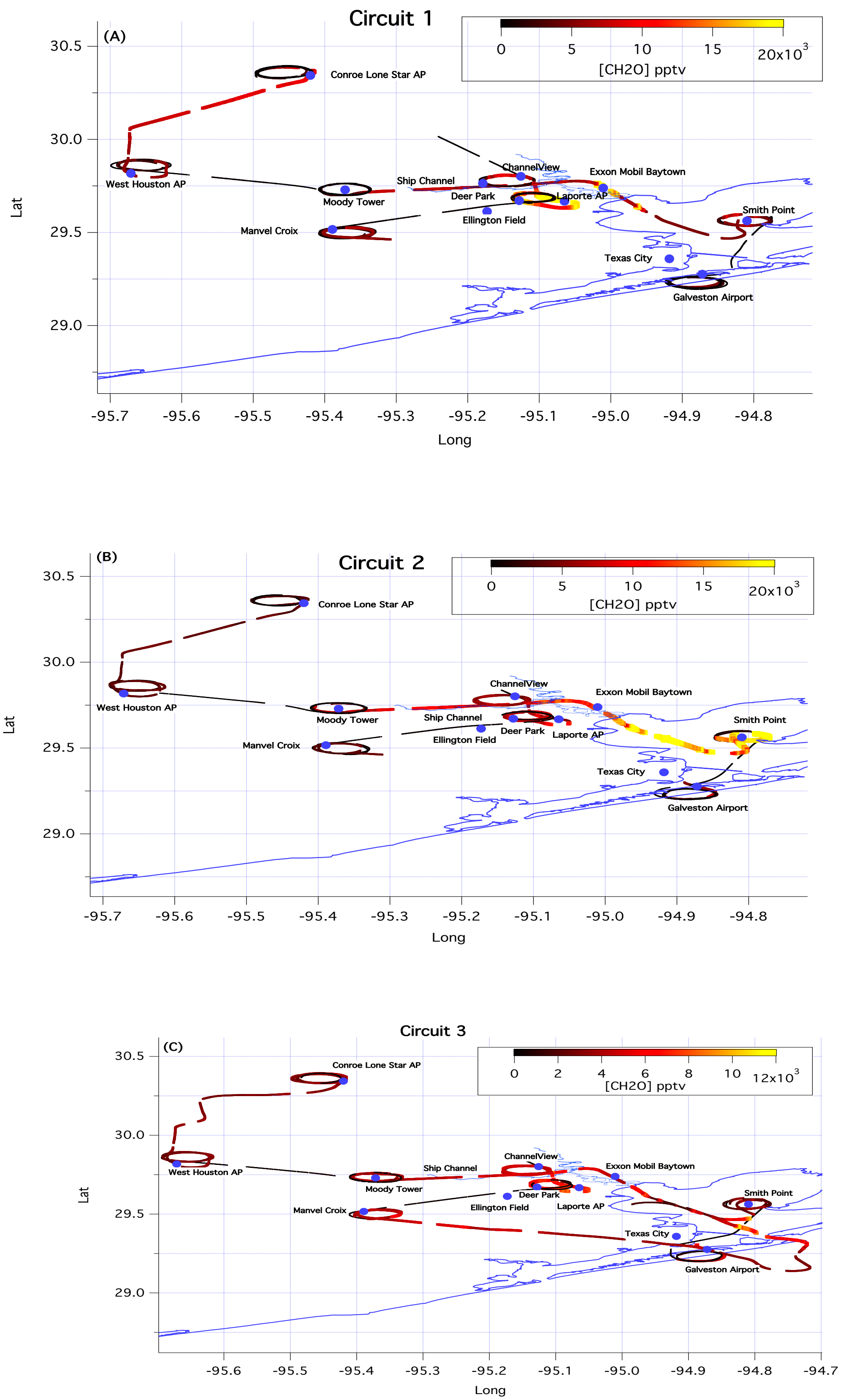

Figure 2A, B, C: CH_2O distributions over the Houston Metropolitan Area showing the source emissions during the 1st circuit, enhanced photochemical production of CH_2O during the 2nd circuit, and the decay during the 3rd circuit. The respective local starting times are (9 am, 12 noon, 2:30 pm).

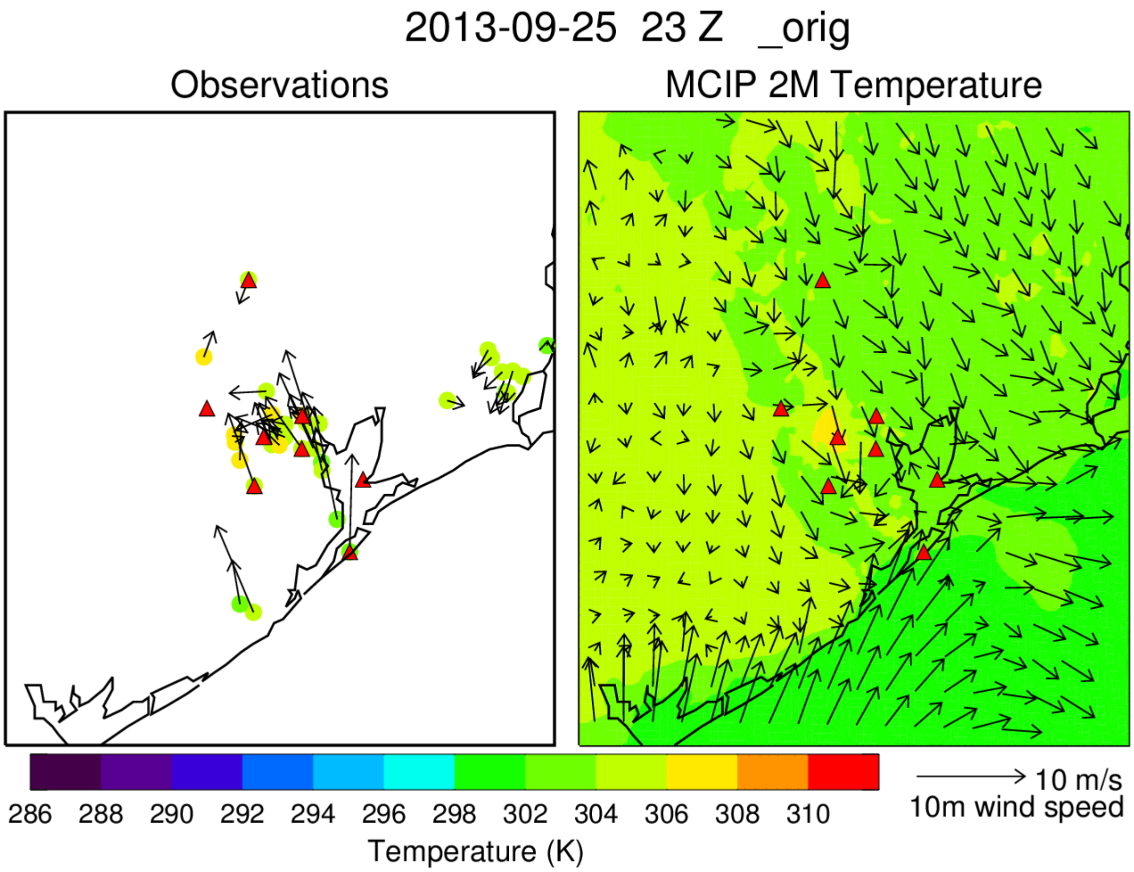

Figure 3: Observed (left) and WRF diagnosed (right) 2-m temperature and 10-m wind velocity at 23 UTC 25 September 2013 from the original 4 km WRF simulation. WRF simulated weaker sea and bay breezes than observed.

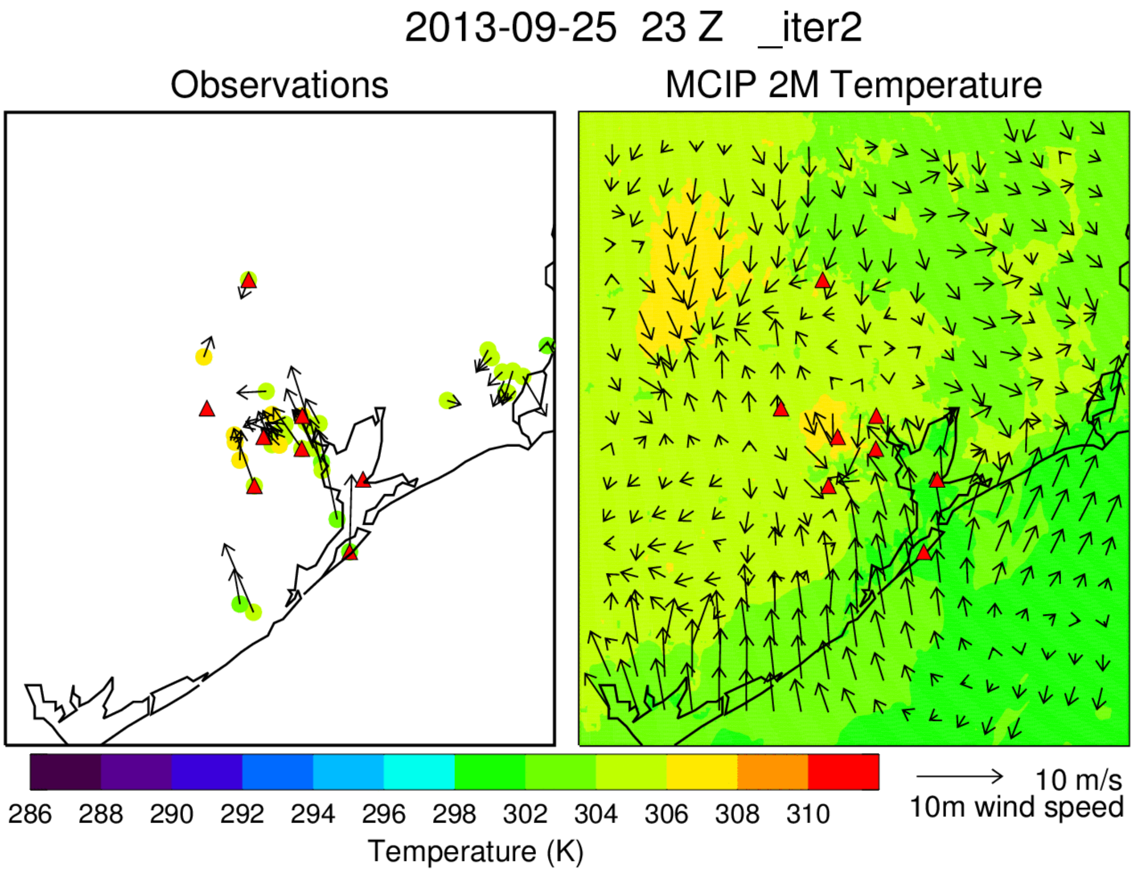

Figure 4: Observed (left) and WRF diagnosed (right) 2-m temperature and 10-m wind velocity at 23 UTC 25 September 2013 from the new 1 km WRF simulation. Strength of WRF simulated bay and sea breezes are in better agreement than in the original simulation (Figure 3).

Statistic	**Equation**
Mean Bias	$MB = \frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)$
Normalized Mean Bias	$NMB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i} \times 100\%$
Normalized Mean Error	$NME = \frac{\sum_{i=1}^{N}\lvert M_i - O_i \rvert}{\sum_{i=1}^{N} O_i} \times 100\%$
Root Mean-Square Error	$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2}$

Table 1. Definition of the statistics calculated in Tables 2-4. In these equations M represents the model results, O represents the observations, and N is the number of data points.

Temperature					
Stat	Iter 2 1 km	Iter 2 4 km	Iter 1 1 km	Iter 1 4 km	Original 4km
MB (K)	-0.134	-0.574	-0.193	-0.528	0.805
NMB	-0.045	-.191	-0.064	-0.176	0.268
NME	-0.366	0.382	0.361	0.377	0.410
RMSE	1.40	1.472	1.39	1.45	1.56

Table 2. Temperature mean bias (MB), normalized mean bias (NMB), normalized mean error (NME), and root mean square error (RMSE) for the original 4 km simulation, the 4 and 1 km simulations for the initial iterative WRF simulation (Iter 1) and the final iterative WRF simulation (Iter 2) based on observations from ~40 sites in the Houston metropolitan area on September 24, 25, and 26.

Wind Speed					
Stat	Iter 2 1 km	Iter 2 4 km	Iter 1 1 km	Iter 1 4 km	Original 4km
MB(m/s)	-0.467	-0.518	-0.511	-0.514	-0.677
NMB	-13.9	-15.5	-15.2	-15.3	-20.2
NME	44.1	43.6	44.4	43.3	50.2
RMSE	1.93	1.90	1.96	1.90	2.22

Table 3. Same as Table 1, but for wind speed.

Wind Direction					
Stat	Iter 2 1 km	Iter 2 4 km	Iter 1 1 km	Iter 1 4 km	Original 4km
MB (deg)	-3.27	2.5	-2.39	3.32	-39.6
NMB	-51.5	40.7	-37.5	52.3	-623
NME	850	825	874	813	1109
RMSE	90.0	87.7	92.7	87.0	100

Table 4. Same as Table 1, but for wind direction.

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
Begin CMAQ simulations.

Detailed Analysis of the Progress of the Task Order to Date
We don't anticipate delays in the completion of this project. The next reporting period will identify additional sampling days for further analysis. The proposing team will address if the exceedingly high CH_2O levels observed during September 25 is anomalous relative to the rest of the P3 sampling month, and if so, why.

Submitted to AQRP by: Alan Fried

Principal Investigators: Alan Fried and Chris Loughner