# AQRP Monthly Technical Report

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| **PROJECT TITLE** | Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation | **PROJECT #** | 14-030 |
| **PROJECT PARTICIPANTS** | Qi Ying, Gunnar W. Schade, John Nielsen-Gammon, Huilin Gao | **DATE SUBMITTED** | 9/9/2014 |
| **REPORTING PERIOD** | **From:** August 1, 2014<br>**To:** August 31, 2014 | **REPORT #** | 2 |

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.

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**Detailed Accomplishments by Task**

**Task 1: Meteorology simulation with WRF.**
Base case WRF simulations for April - October for 2007 and 2011 have been completed. The simulations are initialized using the North American Regional Reanalysis (NARR) data alone. Land surface processes were simulated using the Noah land surface model.

**Task 2: Perform field and laboratory measurements on common Texas tree species**
*<u>Note</u>: Due to an additional project start delay from June to July and the unanticipated need to move all our seedlings to a different greenhouse in July, all monthly milestones described in the QAPP had to be moved by one month ahead*

The original July (now August, 2nd reporting month) milestones were addressed as follows:

a. commence baseline measurements – completed/ongoing
b. maintain water status of all living seedlings – though the water regime was improved, the main obstacle we encountered was/is to keep the oak seedlings alive; the plants have suffered different stresses that have so far made it very difficult to determine a steady basal isoprene emission; it was and is necessary to bring the plants to a healthy state first, before applying the drought treatment. The first step taken to decrease the mortality rate was to determine the amount of water that the plants needed; this was done by watering the plants and repeatedly measuring photosynthesis rate while weighing the plants in/with their pots; this allowed us to determine approximate daily water use by the plants, then use this information to provide the proper amount of water to improve the viability of the plants. Figure 1 shows an example of how we evaluated the optimum photosynthesis point (after which photosynthesis decreases). As can be seen, biological variability is likely to add a complication to our measurement results.

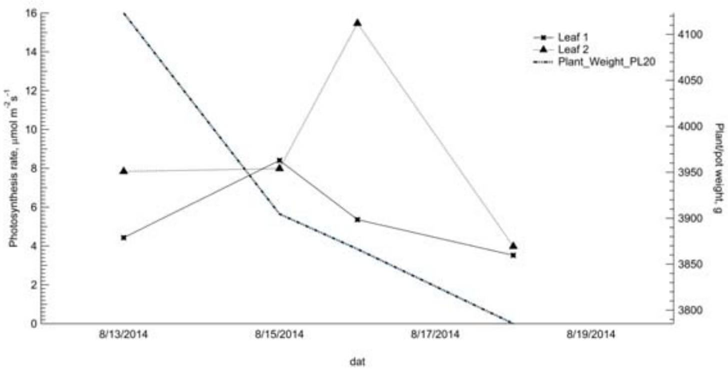


**Figure 1**: Photosynthesis rates and plant+pot weight of a post oak seedling. The bar graph represents weightings, the two lines the photosynthesis development over the same period.

c. set up data logger for greenhouse gas environmental monitoring and soil moisture monitoring – completed

As a first step, we carried out a calibration of the soil sensors in the laboratory for the particularly soil mix used in this experiment; the (unfertilized) soil mix was analyzed by TAMU's Soil, Water, and Forage Testing Laboratory in the Department of Soil and Crop Sciences (report attached); it is a sandy loam with low organic matter (<1%), low salt content, and neutral pH; the soil sensor calibrations are listed in Table 1 and an example is shown in Figure 2.

**Table 1**: Soil sensor calibration equations

| Sensor | Equation |
|---|---|
| 1 | $y=23.351x^2 + 9.4919x$ |
| 2 | $y = 15.774x^2 + 9.8896x$ |
| 3 | $y = 0.4623x^2 + 9.5968x$ |
| 4 | $y = -53.741x^2 + 11.517x$ |
| 5 | $y = 137.81x^2 + 4.524x$ |
| 6 | $y = -30.989x^2 + 11.194x$ |
| 7 | $y = 212.39x^2 + 4.9658x$ |
| 8 | $y = 47.355x^2 + 9.1722x$ |
| 9 | $y = 57.628x^2 + 8.4329x$ |
| 10 | $y = 6.3512x^2 + 10.445x$ |

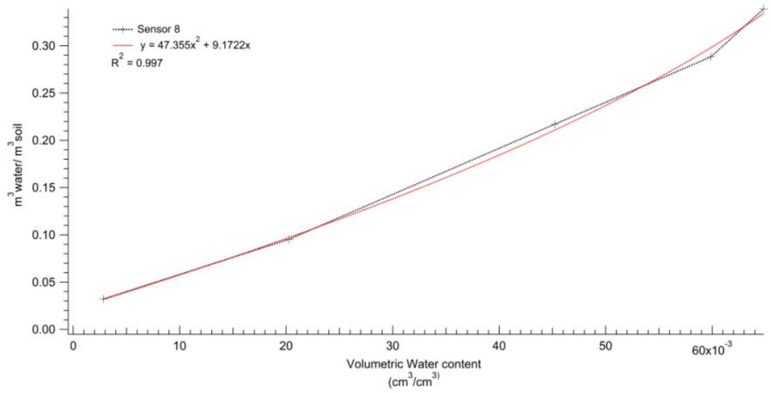


**Figure 2**: Example calibration curve, sensor 8. A wet vs. dry weighing procedure using a calibrated volume was used to determine volumetric water content.

The data logger was deployed to the greenhouse early September after a major Asbestos removal process. It is recording data at 1-min intervals.

d. execute two regular field trips – we executed our first field trip to the Freeman Ranch near San Marcos in mid-August; due to scheduling conflicts, no extra field trips were executed in August, but some extra measurements were performed in early September.

**Task 3: Evaluate drought parameterization for isoprene emissions –** Not started yet.

**Task 4: Perform regional BVOC modeling using MEGAN –** Not started yet.

**Task 5: Perform regional air quality simulations**

Emissions for 2011 have been processed using 2011 NEIv1 and the same procedures the EPA process the emissions. Particularly, mobile emissions were successfully processed using SMOKE-MOVES with tabulated emission factors based on MOVES simulations done by the EPA. The emissions were calculated using the base case WRF results. New mobile and point source emissions have to be generated with updated WRF results for future CMAQ simulations. There is a problem processing the nonpoint emissions with the EPA supplied scripts. The problem appeared when trying to integrate the toxics emission inventory with criteria emission. We are contacting EPA to resolve this issue.

**Preliminary Analysis**

**Task 1:** The model performance for temperature, relative humidity and wind speed is generally within the WRF model performance in previous studies. However, we noticed poor model performance of surface temperature during severe cold weather event that affected majority part of the central and eastern US during the first two-weeks of April 2007. We performed a new simulation with sea surface temperature (SST) updated daily using satellite observations and noticed improved model performance (see Table 2 and Figure 3) on temperature and wind speed, although relative humidity is slightly worse. We will use satellite SST in all future simulations.

**Table 2** Model performance of 2 m temperature, relative humidity and 10 m wind speed based on results at ~100 weather stations in the 4-km WRF domain for April 1-29, 2007.

| | Temp. (K) | | Precip. (cm) | | Wind (m/s) | | RH (%) | |
|---|---|---|---|---|---|---|---|---|
| | base case | SST | base case | SST | base case | SST | base case | SST |
| avg_obs | 290.3 | 290.3 | 1.3 | 1.3 | 4.27 | 4.27 | 71.8 | 71.8 |
| avg_pre | 292.5 | 292.5 | 1.1 | 1.0 | 4.80 | 4.69 | 65.3 | 64.2 |
| MB* | 2.2 | 2.0 | -0.2 | -0.3 | 0.53 | 0.43 | -7.1 | -7.6 |
| RMSE | 3.7 | 3.5 | 3.1 | 3.0 | 2.16 | 2.13 | 19.1 | 19.4 |
| GE | 2.9 | 2.7 | 1.5 | 1.4 | 1.69 | 1.66 | 14.5 | 14.7 |

*Mean bias, MB=$\frac{1}{N}\sum_{i=1}^{N}(C_{m,i} - C_{o,i})$; Root mean square error, RMSE=$\sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_{m,i} - C_{o,i})^2}$; Gross error, GE=$\frac{1}{N}\sum_{i=1}^{N}|C_{m,i} - C_{o,i}|$. $C_m$ is the model-predicted concentration *i*, $C_o$ is the observed *i*, and N equals the number of prediction-observation pairs draw from all monitoring stations.

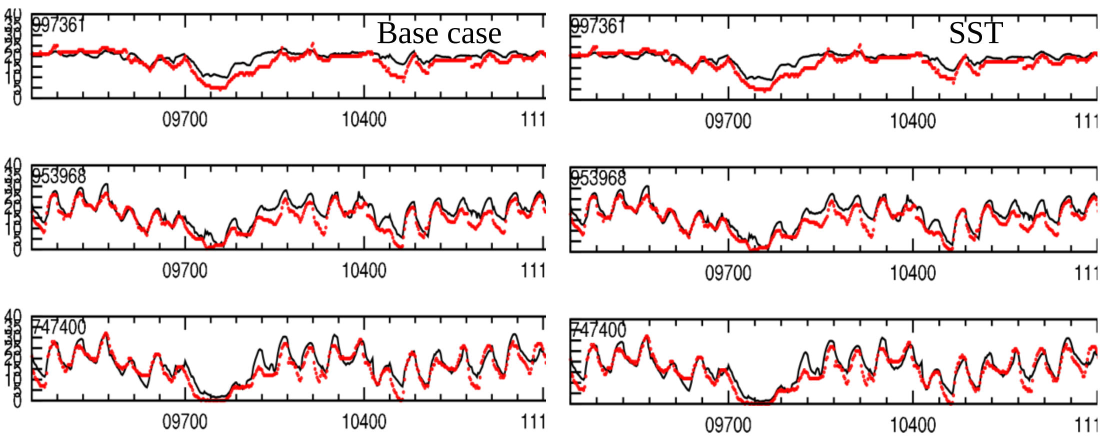


**Figure 3:** Temperature time series at three stations in the 4-km domain in the first three weeks of April, 2007. Red dots are observations and black lines are predictions. Units are $^{o}$C. The panels on the left are base case simulation results and the panels on the right at simulations using satellite SST.

**Task 2:** Mortality rates have further increased, likely due to the additional stress factors from the move of all seedlings to a different greenhouse, in and out of said greenhouse during Asbestos abatement, partial over-watering, and pest exposure as a result of the move. Current seedling availability is listed in Table 3.

Measured standard basal emissions (PAR=1000 µmol $m^{-2}$ $s^{-1}$, leaf T = 30 °C) of isoprene obtained so far include plateau life oak – 64±5 nmol $m^{-2}$ $s^{-1}$ (1 sd, field data on eight leaves, three trees) water oak – 36±7 nmol $m^{-2}$ $s^{-1}$ (1 sd, greenhouse data on 6 leaves, two seedlings), and post oak 30±10 nmol $m^{-2}$ $s^{-1}$ (1 sd, greenhouse data on 12 leaves, four seedlings). Emissions of water oak and post oak are relatively low, which we attribute to the stress the seedlings have undergone, also reflected in their relatively low photosynthesis rate. While the soil has a slow release fertilizer in it, we will begin adding fertilizer to the watering schedule in September.

**Table 3**: Tree seedlings available for our study; "viable" are seedlings with, currently, large enough and healthy leaves to be clamped into our leaf-cuvette (2.5 $cm^2$ leaf area)

| Species | alive | "viable" |
|---|---|---|
| **Post oak** | 19 | 6 |
| **Water oak** | 43 | 6 |

## Data Collected

1. Leaf-level photosynthesis and isoprene emissions data for *Quercus fusiformis*, obtained at the Freeman Ranch near San Marcos in August 2014
2. Leaf-level photosynthesis data for water oak and post oak seedlings in the greenhouse during week 3 of August and week 1 of September 2014, the latter including isoprene emissions using our carbon adsorbent cartridges (see above)
3. Meteorology observation data from NCDC for 2007 and 2011. Soil moisture data from the TAMU soil moisture data base.

## Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

1. In lieu of purchasing a new logger as outlined in the proposal, we have decided to use our existing CR1000 logger since it will not be occupied in another project as expected
2. Comparing the proposed Tenax® cartridges to our carbon adsorbent cartridges when sampling isoprene during leaf-level measurements in the field and the greenhouse, we decided to use a lower sampling volume than with carbon adsorbent cartridges. The reason for this change lies in the fact that we know from experience that isoprene mixing ratios under measurement conditions can exceed the determined breakthrough concentrations of the Tenax® cartridges as shown in Figure 4a, if we used the standard 500 mL volume. Figure 4b shows the latest calibration curve (July 2014) for the carbon adsorbent cartridges for comparison. For the above reported measurements, we have used the carbon adsorbent cartridges. Typical isoprene mixing ratios exiting the CIRAS 2 leaf cuvette are between 20 and 200 ppb and better signal to noise-ratios are obtained at 500 mL sample size.

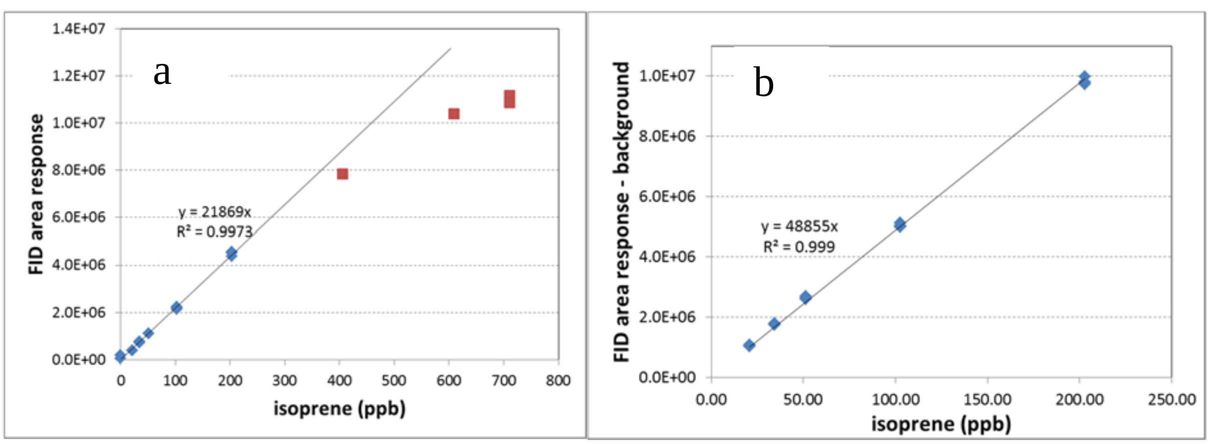


**Figure 3**: (a) Tenax® cartridge calibration curve for a sample size of approx. 200 mL. Note breakthrough above ca. 250 ppb. (b) Carbon adsorbent combination (Carbopack B + Carbotrap X) cartridge calibration (sample size: 500 mL) curve shows consistency at least up to 200 ppb.

**Goals and Anticipated Issues for the Succeeding Reporting Period**

Goals

Task 1: Perform WRF modeling for 2011 using soil moisture from North American Land Data Assimilation System (NLDAS) archive and the CLM4 land use model; determine the most suitable model results for CMAQ and emission simulations based on time series and statistical analysis.

Task 2: 1) Execute field work; 2) continue leaf-level measurements in the greenhouse, and begin drought treatments if satisfactory baseline measurements are obtained in September; 3) execute $2^{nd}$ field trip to Freeman Ranch, preferably when drought is detected mid to end September

Task 4: Start a test MEGAN biogenic emission simulation for 2011 (test run with base case WRF results).

Task 5: Finish generating all anthropogenic emissions;

**Detailed Analysis of the Progress of the Task Order to Date**

Task 1: Due to delayed start of the project, we are behind schedule slightly. We expect Task 1 to be completed by end of October instead of September, as stated in the work plan. However, we will start Task 4 in October 2014 as planned, generating biogenic emissions with completed WRF runs at that time. We don't expect a delay in Task 4 at this point.

Task 2: Due to delayed start of the project, we are one month behind schedule.

Task 5: On schedule.

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Submitted to AQRP by: Qi Ying

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