AQRP Monthly Technical Report

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

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
Task 1: Meteorology simulation with WRF. Completed.

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 spring 2015 milestones were addressed as follows:

a. <u>Analyze drought response relationships:</u> could not be addressed yet since measurements so far have been unsuccessful (see previous monthly reports).
   <u>Compare isoprene field data to seedling data:</u> With data input from UT, courtesy of Gary McGaughey and Elena McDonald-Buller, we have begun to look closer at the soil moisture data at our field sites as compared to soil moisture estimates from two models the UT group is using as inputs for running isoprene emission model scenarios. In Figures 1-6, we show comparisons with our local measurements. In all cases, the comparison is a problematic one because local measurements may not be representative of all soils in the pixel, for which model data was retrieved, neither may local rainfall correspond to total rainfall in said pixel. Additionally, local measurements are performed at a single depth, while the model considers a range of depths. In the case of Houston, the comparison is surprisingly good considering that the local soil has a higher clay content than either of the other sites. Both for The Woodlands and Sam Houston National Forest, it appears that local soil moisture values are significantly lower than what the models calculate. In both cases, the local soils are sandy loams / loamy sands that dry rapidly after rains, and it appears that the models may assume an average higher clay content, explaining higher water holding capacity and lower slopes (of 0-10 cm water content) during periods between rain events.

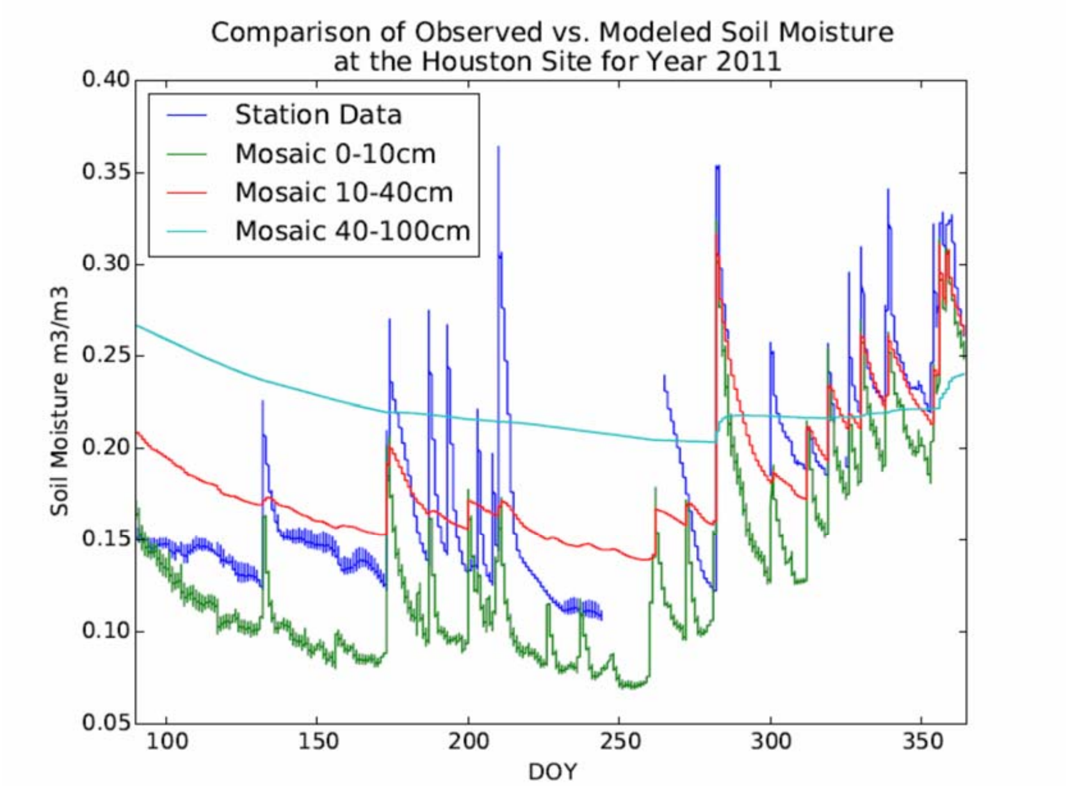

Figure 1: A&M measured 10-cm soil moisture data near Jefferson Davis S, north of downtown Houston as compared to MOSAIC model data

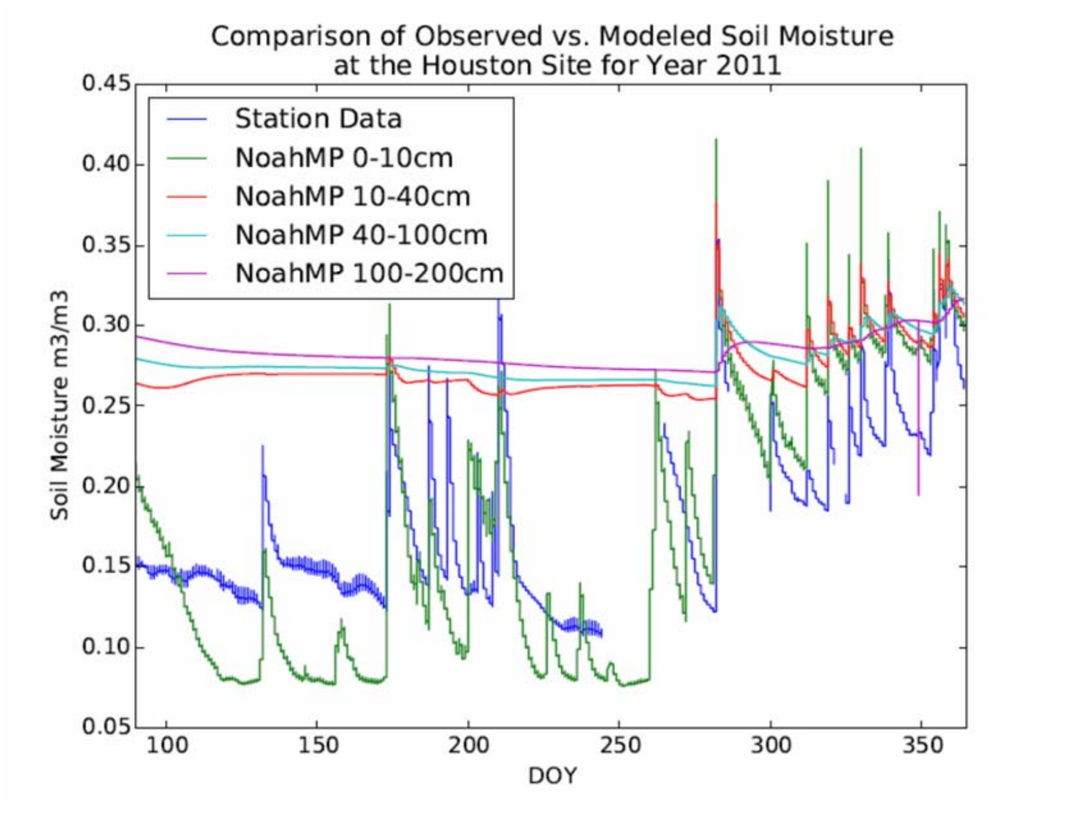

Figure 2: Same as Fig. 1, but compared to NoahMP model data

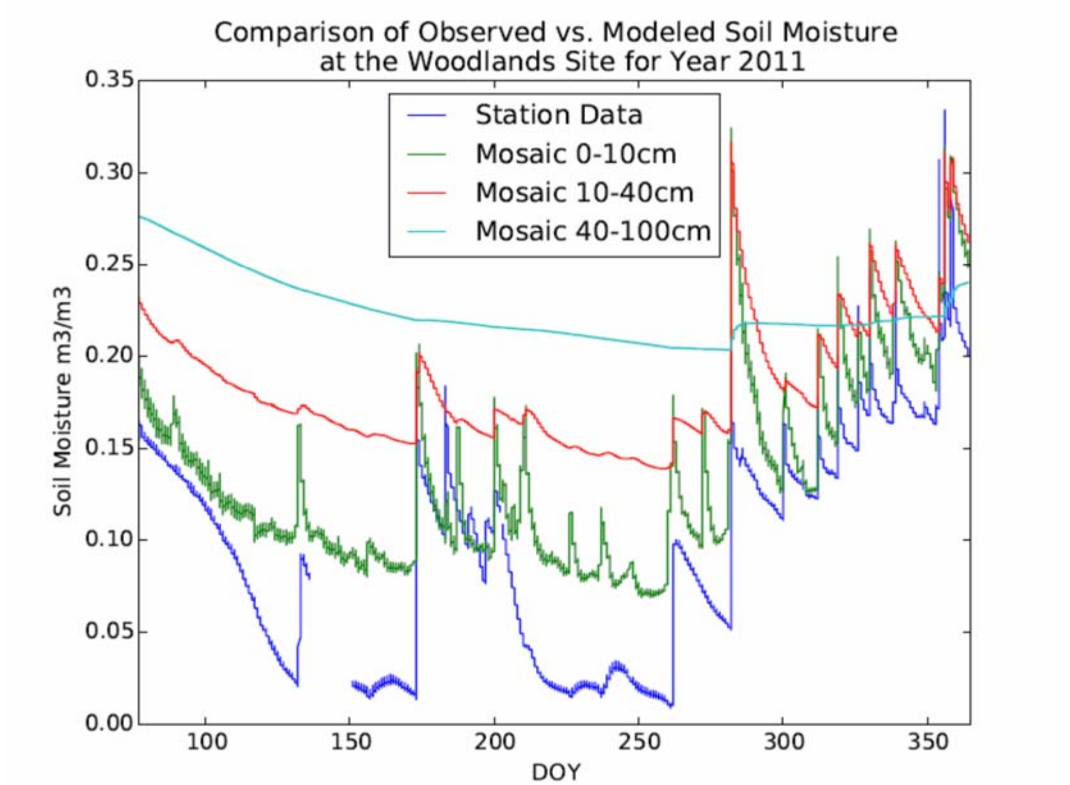

Figure 3: Same as Fig. 1, but using data for A&M's site in The Woodlands behind McCullough Junior HS, approximately three miles west of HWY 45.

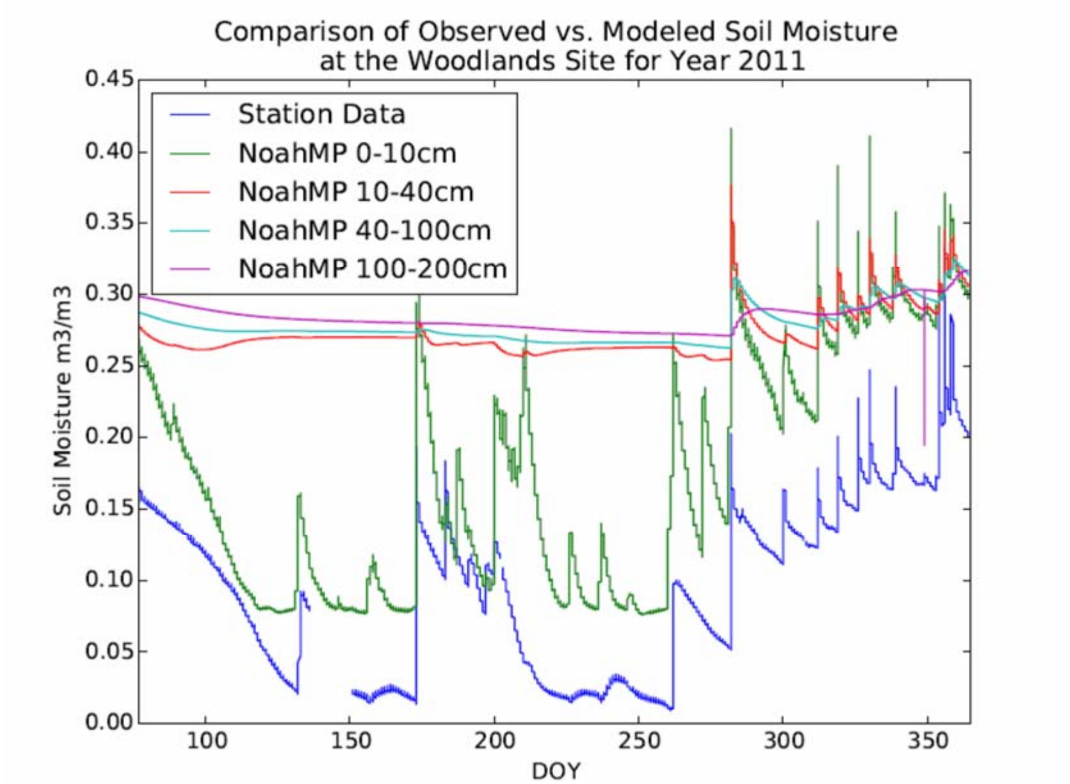

Figure 4: Same as Fig. 2, but using data for A&M's site in The Woodlands behind McCullough Junior HS, approximately three miles west of HWY 45.

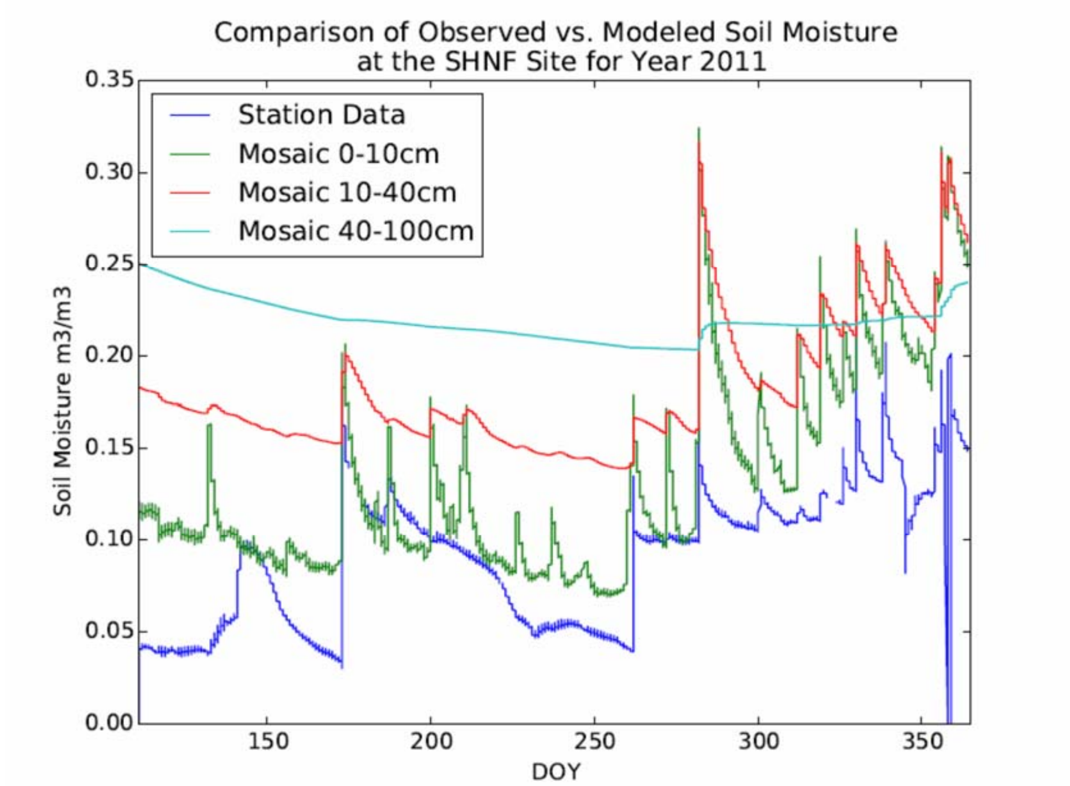

Figure 5: Same as Fig. 1, but using data for A&M's site in Sam Houston National Forest, also approximately three miles west of HWY 45.

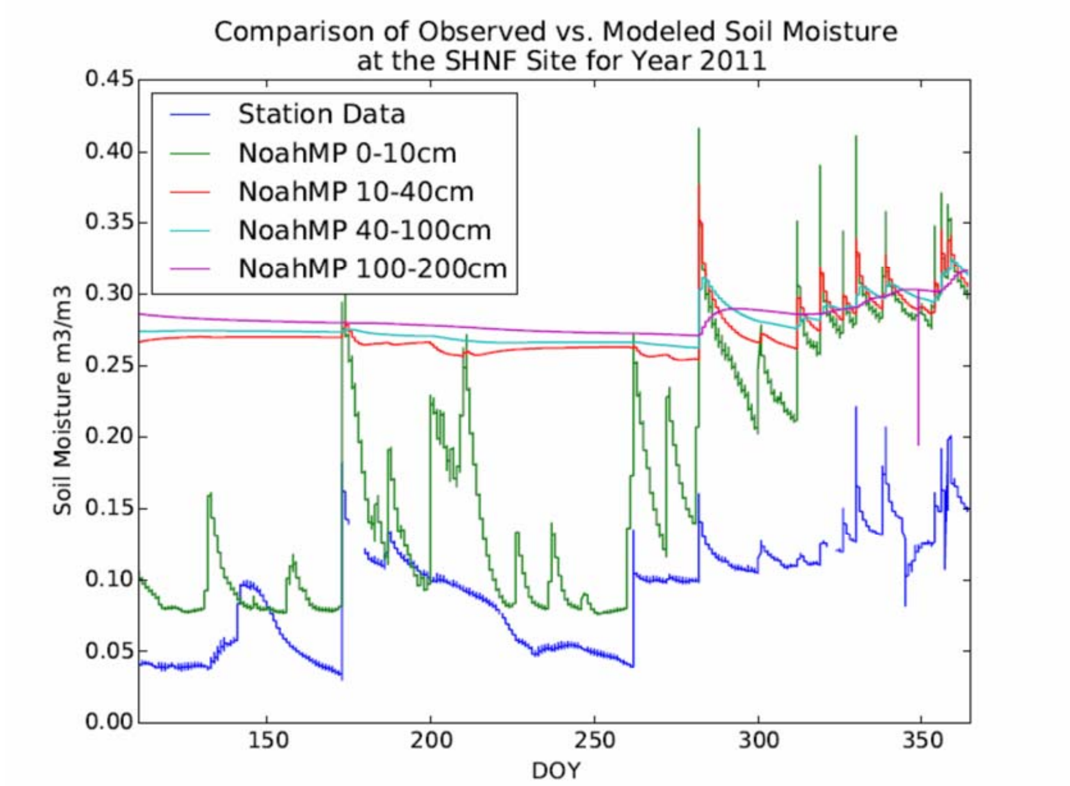

Figure 6: Same as Fig. 2, but using data for A&M's site in Sam Houston National Forest, also approximately three miles west of HWY 45.

b. provide final drought response parameterization: could not be addressed yet due to inconclusive data collected on seedlings last summer/fall; however, a first set of new measurements was conducted on freshly erupted leaves in mid March 2015, it showed low photosynthesis rates and no isoprene emissions, meaning leaves were still developing and isoprene synthase development was incomplete or its activity negligible
c. submit data files to UT: we refer to the new data format submitted for approval with our January monthly report

Task 3: Evaluate drought parameterization for isoprene emissions – Currently MEGAN significantly over-predicts isoprene emissions under both wet and dry conditions. Once we have a new drought parameterization from Task 2, we can compare that with the default parameterization to see the differences in isoprene emissions (from a relative perspective). However, we will not be able to compare the predicted isoprene concentrations with observations to determine which drought parameterization is better.

Task 4: Perform regional BVOC modeling using MEGAN – Completed. Both base case and the drought parametrization case have been completed for all three domains.

Task 5: Perform regional air quality simulations

a. We performed base case CMAQ simulation for July 2007. Summer ozone concentrations in 2007 is lower than those in 2011 and the model does not suffer the over prediction problem.
b. We performed additional simulations to try to understand why ozone concentrations are over-predicted in summer 2011.
   1) We compared vertical ozone profiles taken at urban Houston and compared with model predictions. Ozone profiles were available for June and August. However, most of the soundings are made on days without ozone prediction problem. June 24 is the day with over-predictions, and the predictions are higher than observation at all elevations up till 16 km. Mixing height seems reasonable, both at about 3-4 km.

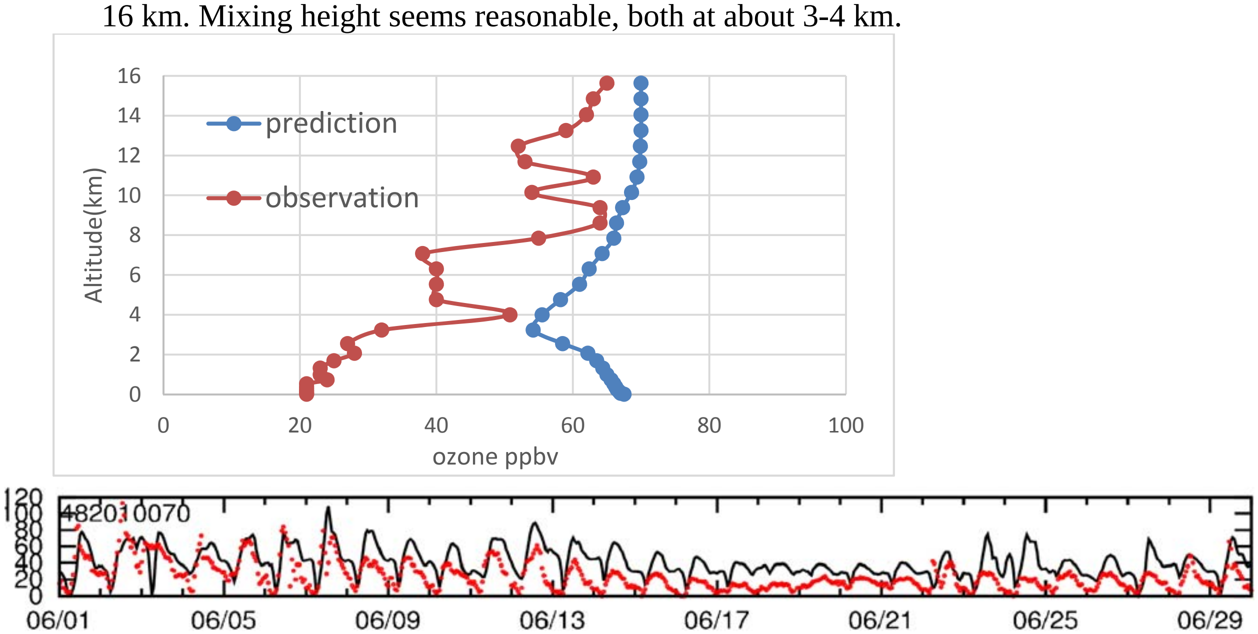

Figure 7: Predicted time series of ozone at the HROC site (closest to UH), and the vertical ozone profile on June 24, 2011, at 1900 UTC.

2) We did two sensitivity simulations, modifying the vertical diffusion coefficient but those two simulations have little impact on predicted peak surface concentrations.
3) We used the process analysis feature in CMAQ to study ozone formation in DFW region. This area shows significant over-predictions in July, 2011. Process analysis shows this region has the higher ozone production rate than other urban regions.

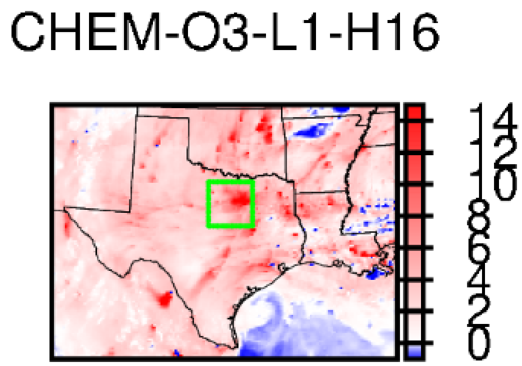

Figure 8: Ozone formation due to chemistry at 1600 CST, July 20, 2011 (units are ppb/hr).

Process analysis information at all the grid cells within the green box are averaged, so that horizontal advection contributions are minimized. The following figure shows the comparison of the averaged process rates on July 19 (good prediction) and July 20 (significant over prediction) at the surface layer (~0-35 m) and at layer 3 (~85-170 m). The largest difference appears to be the horizontal and vertical advection. On July 20, the advection contributions are much lower.

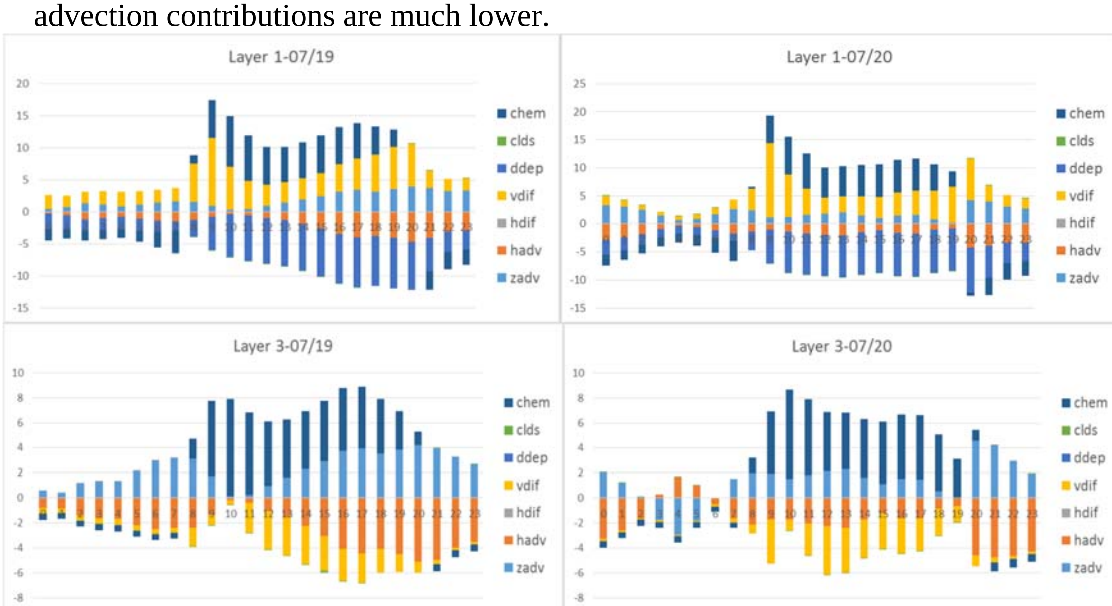

Figure 9: Process analysis for ozone on July 19 and July 20.

Preliminary Analysis

Task 2: Figures 1-6 show an overall encouraging correspondence of soil moisture levels between local measurements and models that integrate over a much larger area incorporating the local measurement point. However, critical for an evaluation of the isoprene algorithm is not just getting soil moisture right, but the confirmation that local wilting points are captured correctly, since the algorithm uses both these inputs. Whether the wilting point is getting closer in a particular location also depends on a tree species' (average) rooting depth, which may be higher for some isoprene emitters than others. If the model captures soil moisture correctly at one depth, but not at other depths due to a non-representative soil texture at a measurement site (or in the model), the onset of the effect on local or regional isoprene emissions maybe misjudged even though the response function used is correct/representative. Unfortunately, this is an issue that cannot be resolved via our greenhouse measurements, which are geared towards the actual response function evaluation.

Task 5: Preliminary process analysis shows there is no significant difference in ozone formation rate (from chemistry) for a large ozone over-prediction day and a previous day with good ozone predictions in the DFW. Instead, large difference in horizontal and advection rates suggest that is caused by the difference in predicted meteorological conditions. However, more analysis should be carried out for other days and other regions (e.g. the HGB region).

Data Collected

1. 1st set of measurements on new leaves erupting in spring on greenhouse-based seedlings

Identify Problems or Issues Encountered and Proposed Solutions or Adjustments

Goals and Anticipated Issues for the Succeeding Reporting Period

<u>Goals</u>

Task 2: 1) after a lit. search completed in March, derive a better estimate of total, or a depth profile of soil moisture data during the 2011 field season in order to better relate isoprene emissions to soil moisture; 2) continue caretaking of the greenhouse-based seedlings, monitoring the new leaf growth as ambient insolation increases; monitor newly acquired and potted post oak and other seedling for leaf growth, including routine physiology and isoprene emissions sampling begun in March 2015.

Task 5: 1) perform additional isoprene observation vs. prediction analyses for daily isoprene at PAMS sites to check the extent of the isoprene over-prediction problem; 2) perform additional sensitivity runs to solve the ozone over-prediction problem; 3) finish base case simulation for 2007 and 2011, with the current input data sets and model configurations.

Detailed Analysis of the Progress of the Task Order to Date

Task 2: Major delay on task 2 due to inconclusive data last summer/fall. Commencing new measurements this spring, awaiting leaf maturation.

Task 5: We will have to move on to finish CMAQ modeling for 2011 and 2007 using two different MEGAN emission datasets generated previously. Ozone prediction issue in 2011 will still be analyzed and we will update the CMAQ simulations if improvements are found. We expect to complete all four sets of simulations in early May. We will choose days will satisfactory ozone model performance for additional analysis of soil moisture on isoprene emission and ozone.

Submitted to AQRP by: Qi Ying

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