Scope of Work For

Project 14-030
Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation

Prepared for

Air Quality Research Program (AQRP)
The University of Texas at Austin

by

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1. Statement of Work

1.1 Introduction

Biogenic volatile hydrocarbons (BVOCs) are important precursors in atmospheric chemistry that lead to formation of ozone and secondary particulate matter in Southeast Texas [1-4]. Among the BVOCs emitted, isoprene is the most important for ozone formation in Southeast Texas due to its large emission quantities [1] and fast reaction rates with oxidants. Ozone air quality predictions thus depend on accurate isoprene and other BVOC emission estimates from regional vegetation. For either regional or global scale air quality modeling, the latter emissions, particularly isoprene, are estimated via various biogenic emission modeling systems, such as the Global Biosphere Emissions and Interactions System (GloBEIS) [5], Biogenic Emissions Inventory System version 3 (BEIS3) [6] or Model of Emissions of Gases and Aerosols from Nature (MEGAN) model [7, 8]. Modeling isoprene emissions requires various input parameters, particularly biomass distribution, leaf temperatures, and photosynthetically active radiation (PAR) levels, including their recent history. While these have been relatively well characterized, the influence of drought on isoprene emissions due to (i) effects of reduced soil water availability, and (ii) prolonged high temperatures on the photosynthetic production of the biochemical isoprene precursor inside the leaves has been less well represented in these emission models. As Texas regularly experiences drought episodes, including a severe drought in 2011, it is necessary to better understand the capability of current emission models in estimating BVOCs under drought conditions, and improve the drought effect parameterization.

A number of studies have shown that drought will affect emissions of BVOCs due to its impact on plant physiological processes [e.g., 9, 10-25], triggering responses such as reduction in stomatal conductance and photosynthesis rates. Higher ambient temperature and reduced stomatal conductance can also lead to higher leaf surface temperature, which further affects the BVOC emissions. In GloBEIS 3, the influence of drought on isoprene emission is accounted for using a simple linear parameterization that scales the emission rates based on the widely used Palmer Drought Severity Index (PDSI). In MEGAN 2.1, isoprene emission rate is scaled by the difference between soil moisture (volumetric water content) and the wilting point. Both approaches were derived based on limited observations and the appropriateness of these simple, linear parameterizations has not been extensively field tested yet. The most recent version of the BEIS3 model (version 3.14) does not consider drought impacts on biogenic emissions.

Field and laboratory measurements have shown that different tree species respond differently to drought conditions. While most plants are generally drought sensitive, some Texas grown oak species appear to be drought adapted. Field measurements carried out by Dr. Schade's research group during the extreme drought in Texas in 2011 (Figure 1) showed that the response of leaf-level photosynthesis and isoprene emissions was already significantly different between oak species when drought conditions began in spring (April/May 2011). For post oak (*Quercus stellata*) leaves, photosynthesis rate remained high and isoprene emission rate remained at previously established standard emission rates until the drought deepened during August 2011 when both started to decrease. For water oak (*Quercus nigra*) and southern red oak (*Quercus falcata*) leaves, photosynthesis rates and isoprene emission rates were already lower than standard in the beginning of the growing season. This species-dependent behavior under drought conditions is not accounted for in current BVOC emission models, and possibly a more sophisticated drought response model may be required to accurately predict isoprene emissions. The Schade group's field measurements

(Figure 2) also showed that there are obvious seasonal variations in the optimum isoprene emission temperature, and sustained high isoprene emission rates at high leaf temperatures (above 40 ^{o}C), particularly in the drought-adapted species post oak. While both GloBEIS and MEGAN include optimal temperature adjustments based on past temperature [8], these parameterized adjustments may need to be further evaluated because they were insufficient in these field-grown oak cases.

Our project's objectives are:

i. to evaluate the BVOC emission model, MEGAN 2.1, with a focus on isoprene predictions, using either their default or an updated drought parameterization scheme based on recently collected data during drought seasons and select, newly to be collected laboratory data;
ii. to evaluate the capability of the WRF model in predicting meteorological conditions for air quality simulations under drought conditions; and
iii. to evaluate the sensitivity of CMAQ ozone predictions in Southeast Texas when using different drought parameterizations for isoprene emissions.

1.2 Task Description

1.2.1 Task 1: Perform regional meteorology simulations using the Weather Research and Forecast (WRF) model.

Dr. Ying's group will perform the WRF simulations for two seven-month episodes (April to October, during which isoprene emissions from trees are most significant) in the extreme drought year 2011 and a relatively wet precipitation year, 2007. Dr. John Nielsen-Gammon will perform initial test simulations and provide a set of recommended WRF configurations to better predict meteorology under drought conditions in Southeast Texas. Model simulated wind speed, wind direction, surface temperature, relative humidity, and soil moisture content will be evaluated against all available observations using statistical measures to examine model performance. Model performance statistics to evaluate WRF model results will be based on Emery et al.[18], including mean fractional bias (MB), gross error (GE) and root mean square error (RMSE) (see Table 1 in Section 1.2.5). Soil moisture predictions will also be compared with the 25-km gridded surface soil moisture data from the Advanced Microwave Scanning Radiometer (AMSR-E) onboard NASA's Earth Observing System (EOS) Aqua satellite. Necessary adjustments to the WRF code and configurations will be made by Dr. Nielsen-Gammon based on the model performance, and an additional set of simulations will be made and evaluated by Dr. Ying.

The nested WRF modeling will use the Regional Planning Organization (RPO) domains as defined in http://www.tceq.texas.gov/airquality/airmod/rider8/modeling/domain. Three nested domains will be used (na_36km, sus_12km, tx_4km). Lambert Conformal Conic projection parameters, and other details such as vertical domain structures, can also be found from the above link. Initial and boundary conditions for WRF modeling will mostly be taken from the North American Regional Reanalysis (NARR) data (available from National Oceanic and Atmospheric Administration (NOAA), http://www.esrl.noaa.gov/psd/data/gridded/data.narr.html) with 32-km horizontal resolution and 3-h time resolution. National Land Cover Database 2011 (NLCD 2011) will be used as an alternative to the default WRF land use/land cover (LULC) data. We will also consider using the LULC data from the ENVIRON/Pacific Northwest National Laboratory (PNNL) for final WRF simulations if they become available early enough for the project and are proven to have significant advantages over the NLCD2011 dataset.

Our initial intent for soil moisture is to perform simulations using the Noah land surface model (LSM), with a one-month land surface model spin-up using initial land surface conditions interpolated from the North American Land Data Assimilation System (NLDAS) archive. In addition, satellite-derived soil moisture data from TCEQ will be used as initial conditions in final WRF run if they become early enough in the project and prove to be more accurate in describing the spatial and temporal distribution of soil moisture than the NLDAS dataset. The Noah LSM is widely used in both research and operational forecasting. We will also test the Community Land Model, Version 4, with prescribed vegetation phenology (CLM4SP) [26], to determine whether its more sophisticated handling of biospheric effects on land surface processes provides more realistic land surface fluxes and soil moisture profiles. CLM4SP was developed for use in global climate models and has been adapted for use in WRF.

1.2.2 Task 2: Perform field and laboratory measurements on common Texas tree species

1.2.2.1 Introduction

The research group of Dr. Schade in the department of Atmospheric Sciences at Texas A&M has repeatedly been assessing field-grown, mature isoprene-emitting trees (mostly oak species) in the Houston metropolitan area, including Sam Houston National Forest. As part of regular weekly field trips, in-situ leaf-level photosynthesis rates are measured and leaf-emitted VOCs are simultaneously sampled onto ¼" OD glass cartridges filled with adsorbents. The group is using a Perkin-Elmer ATD400 thermal desorber connected to a HP5890 GC with FID and an Rtx624 column, operated using ChemStation software, to analyze the trapped BVOCs (see QAPP).

For field sampling, a leaf-level photosynthesis analyzer (CIRAS-2, PP-Systems, Amesbury, MA) is used, modified to accommodate the adsorbent cartridges by splitting the leaf sample cuvette outflow. Leaf level emissions are sampled onto the adsorption cartridge using a 2-way isolation valve and flow controller (1 slpm FC) after leaf physiology has adapted to preset cuvette conditions (i.e. CO_2 concentration, light level, temperature and humidity levels; most commonly, "standard conditions" mean 400 ppm CO_2, 30 °C, 1000 µmol photons m^{-2} s^{-1}, and non-saturating humidity, typically 50-70% relative). Pump, valve, and FC are powered using 12 VDC dry lead acid batteries. An individual measurement is generally completed within 15-20 min and 3-4 different leaves on the same branch per tree are measured to acquire adequate statistics (see QAPP).

1.2.2.2 Field Measurements

As part of this project, field measurements will be used to

- augment the data base of leaf-level isoprene emissions from field-grown, isoprene emitting tree species common in Texas, and
- acquire new leaf-level isoprene emissions from field-grown plateau Live Oak (*Quercus fusiformis*) at the *Freeman Ranch* field site, as a function of
    - soil moisture at field sites (measured)
    - drought conditions at field sites (determined from online data bases, such as the *droughtmonitor* and Texas A&M's Office of the State Climatologist's high resolution, experimental drought maps at http://atmo.tamu.edu/osc/drought/, and
    - time of year.

Two to three field trips each month, one to each field site the Schade group maintains outside Houston city limits, during the summer of 2014, i.e. June through October, will be dedicated to this project. Tree species measured will include

- post oak (*Q. stellata*)
- water oak (*Q. nigra*), and
- sweetgum (*liquidambar styraciflua*)

In addition, two field trips will be scheduled in collaboration with the director of the *Freeman Ranch* near San Marcus, TX, to obtain photosynthesis measurements and isoprene sampling from plateau (also called "escarpment" or "Texas") live oak (*Q. fusiformis*). One of these trips is intended to obtain data before the oak trees undergo seasonal drought stress and will thus likely be executed in June 2014. The second trip will be scheduled for a period well into seasonal drought stress for the same trees as determined via the same drought monitoring tools listed above.

Both the field and greenhouse measurements will be in-situ leaf-level measurements of plant physiological parameters (leaf temperature, CO_2 (assimilation) and H_2O (transpiration) exchange rates, stomatal conductance, and leaf internal [CO_2], and simultaneously emitted isoprene. The instrument employed is a 2010 model CIRAS II leaf photosynthesis analyzer with a 2.85 cm^2 leaf area cuvette attachment (http://www.ppsystems.com/ciras2_portable_photosynthesis_system.htm). The typical data acquisition and sample protocol is as follows:

1. equilibrate instrument in the field; obtain neutral "no-leaf" reading (zero fluxes)
2. insert leaf in cuvette and wait for CO_2 setpoint to be reached (5 min)
3. wait for leaf to equilibrate to cuvette conditions (3-10 min)
4. record equilibrium readings and sample volatiles (3 min)
5. confirm leaf equilibrium after sampling (1 min)
6. zero and balance the 2-channel NDIR analyzer regularly as required during field data acquisition (approximately hourly)
7. repeat 2.-5. for the next leaf

In the field, all measurements are taken from attached, intact leaves on the sun-exposed side of the tree that can either be reached from the ground or via a ladder. Sampling commences when targeted leaves have experienced full sun conditions for at least an hour prior to any measurements, and shaded leaves are avoided unless for comparative purposes. Thus, work does not usually begin before 10:00 h local standard time (LST) and typically ends before 18:00 h LST.

All physiological data is stored inside the CIRAS II system every ten seconds, and averaged over one minute of equilibrium conditions for further processing. All adsorbent cartridges with or without VOC samples loaded are kept inside a cooled glass container until they are processed upon return to the laboratory (see QAPP).

All fluxes are calculated using flow-through approach, in which

$$\text{Flux} = V/\rho \times (C_{in} - C_{out}) \qquad [\text{g/s}] \qquad (1)$$

V is the flow-through rate, ρ is air density, and C is the mixing ratio of the trace gas of interest. While the CIRAS II calculates the water and carbon fluxes internally, we use the instrument's recorded flow rate, V, in conjunction the measured mixing ratio difference between an empty cuvette measurement and a leaf measurement to calculate isoprene fluxes.

1.2.2.3 Greenhouse Measurements

Tree seedlings were acquired from nurseries in Oklahoma and Louisiana. In spring 2014, we potted 100 seedlings each of Post Oak (*Quercus stellata*) and Water Oak (*Quercus nigra*) into a topsoil-sand mixture (2:1) augmented with a slow release fertilizer. The seedlings are stored and developing/growing in a Texas A&M University greenhouse on campus (Biology Department *Horticulture Greenhouse* (HTGH) on Lamar Street, east campus) where they will remain during the complete duration of this project.

Phase I: Plant development (ongoing)
As the seedlings get established, we need to water them evenly until the leaves have fully developed. We expect some mortality due to the late start of the project but are confident that at least 50% of all plants will develop normally, more than needed for this study. Once a subset of healthy trees has been established, all trees and pots will be tagged. The soil mix will be investigated in detail to determine soil density and texture, water holding capacity, organic carbon content, and performance with soil moisture sensors used to monitor development during the greenhouse experiment.

Phase II: Establishing baselines for the different species (beginning in June)
After the leaves have fully expanded, we will use the first 4-8 weeks to measure leaf-level physiology and isoprene emissions on 2-4 seedlings throughout the day. All seedlings will remain well-watered during this period. Specific attention will be paid to

- potential effects on emissions from using the cuvette itself, such as through injuring trichomes when placing it on a leaf (if such effects can be excluded the number of leaves and seedlings measured per day can be increased);
- capturing the diurnal cycle of the individual leaf since both photosynthesis and isoprene emission are affected by circadian rhythms, and isoprene may additionally be affected by precursor pool size variations; and
- the variability of these baseline emissions, which determines the minimum amount of leaves and seedlings required to be followed in the subsequent phases of the project in order to establish statistically significant differences between treatments.

Phase III: Drought experiment (August onward)
In this phase the independent variable will be the amount of water supplied to the plant. We expect to operate 3 different water regimes:

1. Control. Watering commences 4-6 times per week. The amount of water will be calculated based on the soil water holding capacity, keeping > 60% water filled pore space (WFPS) in the pot at all times.
2. Intermediate conditions. Decrease watering schedule to one to two times a week simulating typical east Texas mesic conditions of rainfall every 5-10 days, keeping WFPS at half or less of that in the control group.
3. Drought. Withhold water for 3-5 weeks depending on plant development. Rewater subset of drought-stressed plants at the end of that period to simulate heavy rain, and to avoid killing all plants. Monitor the recovery.

Temperature and light in the greenhouse are natural (glass roof), so will follow ambient conditions but will be monitored inside the greenhouse using a CSI data logger and sensors. The same logger will be used to monitor 12 soil moisture probes distributed in the plant pots and selected leaf temperatures. Both soil moisture probes and leaf temperature sensors will be moved once to twice during the greenhouse study to avoid a continuous effect on seedlings. The logger will record data at 10-second intervals and store 1-minute averages and some standard deviations.

All greenhouse measurements will be in-situ and will use the same CIRAS II leaf photosynthesis analyzer employed during field measurements. All conclusions will be based on the leaf level measurements.

1.2.3 Task 3: Evaluate drought parameterizations for isoprene emissions

Leaf-level isoprene emission rates measured in the field and laboratory will be compared with predictions using the current MEGAN parameterizations [8] by Dr. Schade. Dr. Schade with collaboration from Dr. Guenther of PNNL will also evaluate the data against a new drought parameterization from Dr. Guenther and drought parameterization based on data collected in Task 2. Soil moisture responses will be analyzed using the measured volumetric soil moisture and calculated WFPS. Since the expected response is a drop in isoprene emission rates but may vary between species, between individuals, and between field-grown mature, and greenhouse grown trees, no single response function is expected to model observed responses, an optimal formation most suitable for regional biogenic emissions modeling will be proposed. We will explore both linear and non-linear response functions, as well as potential thresholds.

Observed meteorological parameters will be used for the emission calculations whenever possible. The absorbed fraction of PAR (fPAR) at 8-day, 250 m resolution will be used for leaf-level emissions calculations and will be statistically downscaled from the Moderate Resolution Imaging Spectroradiometer (MODIS) 1-km resolution products [28] by Dr. Gao's group. Since the Normalized Difference Vegetation Index (NDVI) is highly correlated to both LAI and fPAR [29, 30], the downscaling will be carried out by applying the empirical relationships developed between LAI (and also fPAR) and the low resolution NDVI (1 km) to the high resolution NDVI (250m). The LAI and fPAR fields will also be used for regional BVOC modeling (Task 5).

1.2.4 Task 4: Perform regional BVOC modeling using MEGAN 2.1

The MEGAN 2.1 model will be applied to generate biogenic emissions for the two seven-month episodes in 2007 and 2011 by Dr. Ying's group. Meteorological inputs needed to run the models will be taken from outputs generated from Task 1. The gridded plant functional type distributions and emission factors will be based on the default North American dataset in MEGAN 2.1 provided by Dr. Guenther. 8-day LAI for 2007 and 2011 will be acquired from the Moderate Resolution Imaging Spectroradiometer (MODIS) 1-km resolution products [19] and prepared by Dr. Gao during Task 3. The LAI in urban areas will be replaced with values recommended by TCEQ staff. Urban mask file will be acquired from TCEQ. We will also consult Dr. Sorin Popescu in the Ecosystem Science and Management Department at TAMU for recommendations about appropriate LAI for Texas urban areas. Per discussion with TCEQ, several other land use/land cover database might also be available for the project. Including the 30-m resolution data developed by ENVIRON/Pacific Northwest National Laboratory (PNNL) and the Texas Parks and Wildlife Department (TPWD) 10-m resolution data for Texas ecosystems (might be useful to update base MEGAN emission rates). Depending on TCEQ's initial evaluation of the datasets and their model-readiness, they can be adopted for this project.

Five different biogenic emission fields will be generated:

1) Emission for 2007, wet year, no drought correction needed
2) Emission for 2011, dry year, without drought correction
3) Emission for 2011, dry year, with original MEGAN 2.1 parameterization
4) Emission for 2011, dry year, with Dr. Guenther's new drought parameterization
5) Emission for 2011, dry year, with the optimal parameterization generated in Task 3

Simulated biogenic emissions will be visualized hour by hour. Monthly averaged emissions will be calculated and compared with historical data to ensure the results are in reasonable ranges. The differences in isoprene emissions and other BVOC emissions will be studied, focusing on the seasonal variations and inter-annual differences between drought and wet years, and the differences among different parameterization schemes. The emissions of other BVOCs will be speciated for the Carbon Bond 2005 (CB05) chemical mechanism to be used for Task 5. Simulated biogenic emissions will be visualized hour by hour. Monthly averaged emissions will be calculated and compared with historical data to ensure the results are in reasonable ranges.

In addition to the above simulations using WRF derived PAR, an additional set of two sensitivity simulations will be conducted with satellite-derived PAR data from TCEQ: S1) Emissions for 2007, satellite derived PAR; and S2) Emissions for 2011, satellite derived PAR with optimal parameterization generated in Task 3. If significant differences in isoprene emissions are found between simulations (S1) and (1) and/or simulations (S2) and (5), these two sets of emissions will be applied in 1.2.5.

1.2.5 Task 5: Perform air quality simulations to evaluate the different BVOC drought parameterizations on ozone and isoprene concentrations

The most recent version of the CMAQ model (CMAQ 5.0) with the CB05 chemical mechanism will be used to study the impact of different drought parameterizations for isoprene emissions on regional ozone air quality in Southeast Texas. Meteorological fields generated in Task 1 and biogenic emissions fields generated in Task 4 will be used for the CMAQ simulations. A three-level nested domain will be used (rpo_36km, tx_12km, tx_4km), following the RPO Comprehensive Air Model with Extensions (CAMx) domains used by the TCEQ for ozone air quality modeling. Map projection parameters, and other details such as vertical domain structures, are described in detail in: http://www.tceq.texas.gov/airquality/airmod/rider8/modeling/domain. Emissions will be generated using the 2008 and 2011 National Emissions Inventory (NEI) and adjusted to represent 2007 and 2012 emissions using the NEI Air Pollutant Emissions Trends Data (http://www.epa.gov/ttn/chief/trends/). Biogenic emissions will be generated for the 2007 and 2011 episodes directly, driven by WRF simulated meteorology (or satellite-derived PAR if it becomes available) for these two years. The VOC emissions will be speciated for CB05. The speciation profiles provided with the NEI will be used directly. In addition to the NEIs, emission inventories provided by TCEQ will be used if they become available during the project in proper format. Initial condition/boundary condition (IC/BC) based on CMAQ's default IC/BC files, representing clean conditions will be used for 36-km simulations. For 12 and 4-km simulations, IC and BC will be based on simulation results of the parent domain. The impact of initial condition decreases as simulation goes on. First five days of simulation results will not be used in subsequent analysis to avoid initial condition impact. Likewise, 36-km boundary condition only impacts areas near the boundaries of the 36 km domain and they are not expected to affect evaluation of isoprene emissions in this study. More detailed boundary conditions derived from global models are not necessary.

Five sets of simulations will be conducted using the five sets of BVOC emissions generated in Task 4. Two additional sets of simulations will be conducted if isoprene emissions derived from satellite PAR are significantly different from the WRF-based estimations. Predicted isoprene concentrations from different BVOC mechanisms will be compared with each other and with observations, including hourly VOC concentrations measured by the automatic gas chromatography (AutoGC) systems. Ozone, nitrogen oxides (NOx) and carbon monoxide (CO) from all available TCEQ's continuous air monitoring stations (CAMS) and from the Air Quality System (AQS) developed by the United States Environmental Protection Agency (US EPA) (available from http://www.epa.gov/ttn/airs/airsaqs/detaildata/downloadaqsdata.htm) will also be used to compare model predictions with observations. Detailed inter-model comparisons will also be made to formaldehyde, MACR and MVK, which have significant contributions from isoprene oxidation and can indirectly affect ozone formation. The impact on isoprene and ozone will be analyzed through time series and statistical analyses. Statistical methods will include computation of metrics of bias and error between predictions and observations for ozone and precursors using the guidance of U.S. EPA (2007). Statistical measures are shown in Table 1.

Table 1: Definition of Model Performance Statistical Measures

Statistical Measures	**Definition**
Mean bias	$\mathrm{MB} = \frac{1}{N}\sum_{i=1}^{N}(C_{m,i} - C_{o,i})$
Gross error	$\mathrm{GE} = \frac{1}{N}\sum_{i=1}^{N}\lvert C_{m,i} - C_{o,i} \rvert$
Root mean square error	$\mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_{m,i} - C_{o,i})^2}$
Normalized mean bias	$\mathrm{NMB} = \frac{\sum_{i=1}^{N} C_{m,i} - C_{o,i}}{\sum_{i=1}^{N} C_{o,i}}$
Normalized mean error	$\mathrm{NME} = \frac{\sum_{i=1}^{N} \lvert C_{m,i} - C_{o,i} \rvert}{\sum_{i=1}^{N} C_{o,i}}$
Mean normalized bias	$\mathrm{MNB} = \frac{1}{N}\sum_{i=1}^{N}\frac{C_{m,i} - C_{o,i}}{C_{o,i}}$

Normalized gross error	$\mathrm{NGE} = \frac{1}{N}\sum_{i=1}^{N}\frac{\left|C_{m,i} - C_{o,i}\right|}{C_{o,i}}$
Mean fractional bias	$\mathrm{MFB} = \frac{2}{N}\sum_{i=1}^{N}\frac{C_{m,i} - C_{o,i}}{C_{m,i} + C_{o,i}}$
Mean fractional error	$\mathrm{MFE} = \frac{2}{N}\sum_{i=1}^{N}\frac{\left| C_{m,i} - C_{o,i} \right|}{C_{m,i} + C_{o,i}}$
Accuracy of paired peak	$\mathrm{APP} = \frac{C_{p,opeak} - C_{o,opeak}}{C_{o,opeak}}$
Accuracy of unpaired peak	$\mathrm{AUP} = \frac{C_{p,ppeak} - C_{o,opeak}}{C_{o,opeak}}$

Note: C_m is the model-predicted concentration i, C_o is the observed i, and N equals the number of prediction-observation pairs drawn from all monitoring stations. The subscripts ppeak and opeak are the hours when predicted and observed peak concentrations occur.

A modified CMAQ with source-tracking capability will be used in the simulation to determine contributions of biogenic and anthropogenic isoprene emission sources to isoprene and isoprene oxidation products concentrations at urban, suburban and rural receptor sites under drought and wet conditions [4].

1.2.6 Task 6: Project Report and Presentation

A project report will be developed during the course of the work that fully documents the field and laboratory measurements of BVOC emissions, evaluation of the drought parameterizations and regional emission and air quality modeling results during Task 1 to 5. Conclusions will include recommendations on drought parameterizations for BVOC modeling and WRF model configurations for drought conditions, as well as recommendations for longer-term research. A draft will be submitted to AQRP and TCEQ for review. A final report to address comments received from the draft review will be submitted to AQRP at the end of the project.

1.3 Timeline

The overall timeline of the project is shown in the following table (Table 2). Detailed timeline for Task 2 and 3 are shown in Table 3.

Table 2: Project Timetable

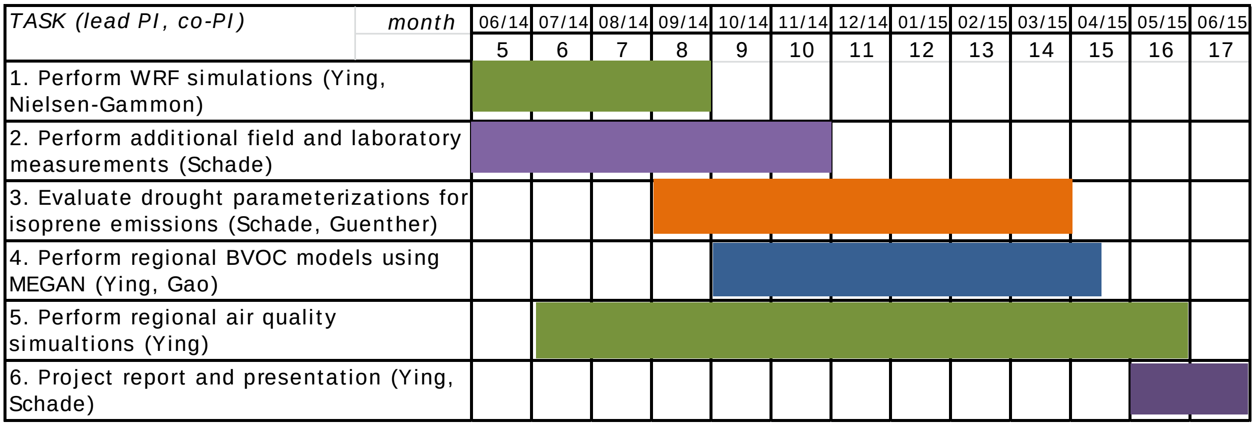
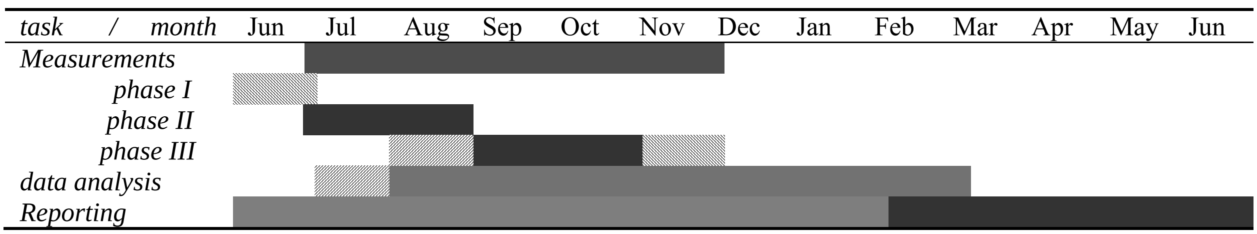


Table 3: Detailed Timetable for Task 2 (shading represents spin-up and -down times (line pattern), or presence and intensity of activity (light and dark grey color))



For Task 2 and 3, the following individual achievements (tasks list) are suggested as milestones, as tasks to be achieved in this order and within the time frame given to assure that the objectives of this project can be addressed.

a) June 2014
    a. assess seedling mortality rates
    b. maintain water status of all living seedlings
    c. begin leaf-level physiology and isoprene emission baseline measurements
    d. send out purchase orders for consumables
    e. execute 1st field trip to Freeman ranch for *Q. fusiformis* measurements, and two regular field trips
b) July 2014
    a. commence baseline measurements (phase II)
    b. maintain water status of all seedlings
    c. set up data logger for greenhouse gas environmental monitoring and soil moisture monitoring
    d. execute two regular field trips
c) August/September 2014
    a. evaluate baseline measurements
    b. select and mark trees for intermediate and drought treatments
    c. begin treatment schedule
    d. execute 2nd field trip to Freeman ranch for *Q. fusiformis* measurements, and two regular field trips
    e. suggest preliminary drought response parameterization based on field data in Sep. 2014

d) October/November/December 2014
    a. compare baseline to treatment measurements
    b. analyze observed drought responses of seedlings and field-grown mature trees
    c. execute two regular field trips in October
    d. submit data files to UT
e) spring 2015
    a. analyze drought response relationships; compare isoprene field data to seedling data
    b. provide (final) drought response parameterization
    c. submit data files to UT
    d. submit final report to UT

1.4 Deliverables

Monthly progress reports; draft and final project report. Other electronic data for WRF, MEGAN and CMAQ modeling, including all input and output files. Detailed deliverables and their due dates are listed below:

1. Executive summary. Due date: May 30, 2014.

2. Quarterly Reports. Quarterly Reports will provide a summary of the project for each reporting period. Due dates are listed in Table 4:

Table 4: Due dates for Quarterly Reports

Report	Period Covered	Due Date
Quarterly Report #1	June, July, August 2014	Friday, August 30, 2014
Quarterly Report #2	September, October, November 2014	Monday, December 1, 2014
Quarterly Report #3	December 2015, January & February 2015	Friday, February 27, 2015
Quarterly Report #4	March, April, May 2015	Friday, May 29, 2015
Quarterly Report #5	June, July, August 2015	Monday, August 31, 2015
Quarterly Report #6	September, October, November 2015	Monday, November 30, 2015

3. Technical Reports. Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word document. Due dates are listed in Table 5:

Table 5: Due dates for technical reports

Report	Period Covered	Due Date
Technical Report #1	Project Start – July 31, 2014	Friday, August 8, 2014
Technical Report #2	August 1 - 31, 2014	Monday, September 8, 2014
Technical Report #3	September 1 - 30, 2014	Wednesday, October 8, 2014
Technical Report #4	October 1 - 31, 2014	Monday, November 10, 2014
Technical Report #5	November 1 - 30 2014	Monday, December 8, 2014
Technical Report #6	December 1 - 31, 2014	Thursday, January 8, 2015
Technical Report #7	January 1 - 31, 2015	Monday, February 9, 2015

Technical Report #8	February 1 - 28, 2015	Monday, March 9, 2015
Technical Report #9	March 1 - 31, 2015	Wednesday, April 8, 2015
Technical Report #10	April 1 - 28, 2015	Friday, May 8, 2015
Technical Report #11	May 1 - 31, 2015	Monday, June 8, 2015

4. Financial Status Reports. Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the AQRP FY14-15 FSR Template found on the AQRP website. Due dates are listed in Table 6.

Table 6: Due dates for financial status reports

Report	Period Covered	Due Date
FSR #1	Project Start - July 31, 2014	Friday, August 15, 2014
FSR #2	August 1 - 31, 2014	Monday, September 15, 2014
FSR #3	September 1 - 30, 2014	Wednesday, October 15, 2014
FSR #4	October 1 - 31, 2014	Monday, November 17, 2014
FSR #5	November 1 - 30 2014	Monday, December 15, 2014
FSR #6	December 1 - 31, 2014	Thursday, January 15, 2015
FSR #7	January 1 - 31, 2015	Monday, February 16, 2015
FSR #8	February 1 - 28, 2015	Monday, March 16, 2015
FSR #9	March 1 - 31, 2015	Wednesday, April 15, 2015
FSR #10	April 1 - 28, 2015	Friday, May 15, 2015
FSR #11	May 1 - 31, 2015	Monday, June 15, 2015
FSR #12	June 1 - 30, 2015	Wednesday, July 15, 2015
FSR #13	Final FSR	Wednesday, August 15, 2015

5. Draft Final Report. A Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will include an Executive Summary. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Due Date: Monday, May 18, 2015

6. Final Report. A Final Report incorporating comments from the AQRP and TCEQ review of the Draft Final Report will be submitted to the Project Manager and the TCEQ Liaison. It will be written in third person and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources. Due Date: Tuesday, June 30, 2015.

7. Project Data. All project data including but not limited to QA/QC measurement data, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion.

8. AQRP workshop. A representative from the project will present at the AQRP Workshop in June 2015.

Expected Final Products

An approvable final report for this project will be prepared and submitted by the end of this project. Multiple conference papers and/or peer-reviewed journal papers (e.g., papers in journal Atmospheric Environment) on isoprene emission characterization and WRF/CMAQ modeling of isoprene under drought and wet conditions are expected to be produced after completion of this project. Data acquired from field experiment will be included in monthly technical report and final report. The following list shows the products from each task:

Task 1: 1) Optimal WRF configures of to predict meteorology and soil moisture under drought conditions. 2) An updated WRF model if any changes are made to the source code. 3) Simulated meteorology and soil moisture fields for 2007 and 2011, and the model performance evaluate of these predicted fields with all available data. All WRF modeling files, including raw input data to generate initial and boundary conditions, land use/land cover data, and WRF output files will be submitted to TCEQ for archive.

Task 2: Quality assured isoprene flux data, including both from field-grown, mature trees and greenhouse –grown seedlings. Within- and among-species variability of isoprene standard ("basal") emissions, temperature-response and drought-response of isoprene emissions will be documented.

Task 3: 1) Parameterizations of soil moisture response for isoprene emissions calculation based on fluxes measured in Task1. 2) Evaluation of predictive strength of the new drought parameterizations as well as the current parameterization in MEGAN 2.1 and an updated parameterization from Dr. Guenther.

Task 4: 1) Modeled isoprene emission fields for 2007 and 2011. For 2011, at least three different fields will be provided, using the original MEGAN 2.1 parameterization, the updated parameterization from Dr. Guenther and the optimal parameterization developed in Task 3. 2) LAI and PAR data for both modeling years. 3) emission fields for other biogenic emissions for the two years. All MEGAN modeling files, including MODIS LAI datasets, satellite PAR, processed meteorological fields, PFT fields, emission factor fields, and MEAGN intermediate and final output files will be submitted to TCEQ for archive.

Task 5: Simulated isoprene (and its oxidation products, MVK and MACR) and ozone concentrations for 2007 and 2011. At least five sets of results will be provided 1) 2007 (no drought effect); 2) 2011 without drought effect; 3) 2011 with the original MEGAN 2.1 drought parameterization; 4) 2011 with Guenther's new parameterization; 5) 2011 with the optimal parameterization derived in this study (Task 3). Performance evaluation of the predicted isoprene and its oxidation products and ozone will be documented. All CMAQ modeling files, including initial and boundary conditions for nested domains, photolysis rates, emissions, raw CMAQ output files, processed time series at monitors and corresponding observations, will be submitted to TCEQ for archive.

1.5 References

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