Scope of Work For

Project 14-008
Soil Moisture Characterization for Biogenic Emissions Modeling in Texas

Prepared for

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

by

Elena McDonald-Buller
Center for Energy & Environmental Resources
The University of Texas at Austin
Austin, Texas 78758
ecmb@mail.utexas.edu
512-471-2891

Christine Wiedinmyer
National Center for Atmospheric Research

Chris Emery
ENVIRON International Corporation

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Project Title: Soil Moisture Characterization for Biogenic Emissions Modeling in Texas

Principal Investigators: Elena McDonald-Buller (PI); Rong Fu (Co-PI)

Overview

The role of isoprene and other biogenic volatile organic compounds (BVOCs) in the formation of tropospheric ozone has been recognized as critical for air quality planning in Texas. In the southwestern United States, drought has become a recurring phenomenon and, in addition to other extreme weather events, can impose profound and complex effects on human populations and the environment. Understanding these effects on vegetation and biogenic emissions is important as Texas concurrently faces requirements to achieve and maintain attainment with the National Ambient Air Quality Standard (NAAQS) for ozone in several large metropolitan areas. Previous research has indicated that biogenic emissions estimates are influenced by potentially competing effects in model input parameters during drought and that uncertainties surrounding several key input parameters remain high. The primary objective of the project is to evaluate and inform improvements in the representation of one of these key input parameters, soil moisture, through the use of simulated and observational datasets. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) will be used to explore the sensitivity of biogenic emission estimates to alternative soil moisture representations.

Technical Context and Motivation

Isoprene and monoterpenes are quantitatively among the most important BVOCs emitted globally from vegetation (Fehsenfeld et al., 1992; Guenther et al., 1995; Guenther et al., 2006). In 2008, biogenic emissions accounted for 29% and 40% of the total VOC emissions inventories in the Dallas-Fort Worth and Houston-Galveston-Brazoria ozone nonattainment areas, respectively. Recognition of the role of BVOCs in tropospheric ozone and organic aerosol formation has been critical for air quality planning efforts in the state.

The National Oceanic and Atmospheric Administration, National Climatic Data Center (NOAA - NCDC) divides Texas into 10 climate regions. Most large metropolitan areas in the state are located within one of four climate regions, shown in Figure 1: North Central Texas (Dallas-Fort Worth; sub-tropical steppe or semi-arid savanna), South Central Texas (Austin and San Antonio; sub-tropical sub-humid mixed prairie, savanna and woodlands), East Texas (sub-tropical humid mixed evergreen-deciduous forestland) and Upper Coast (Houston; sub-tropical humid marine prairies and marshes) (Texas Water Development Board, 2012). Both temperature and precipitation gradually decrease inland from the Gulf of Mexico and across the state (Texas Water Development Board, 2012). Figure 2 shows the 12-month Standardized Precipitation Index (SPI) and selected annual precipitation distributions as the departure from normal during 2006 through 2011. Interannual variability in precipitation and the onset and persistence of drought in eastern Texas are evident.

Recent air quality modeling for attainment demonstrations in Texas has relied on estimates of biogenic emissions from the Global Biosphere Emissions and Interactions System (GloBEIS; Yarwood et al., 2010); MEGAN (Guenther et al., 2012) has been utilized widely for estimating biogenic emissions throughout the U.S. as well as globally. Differences exist between the pathways and representations of input parameters that could be expected to influence biogenic emissions estimates. As an example, GloBEIS uses the Palmer Drought Severity Index (PDSI) as the basis for a drought activity factor. MEGAN instead employs an activity factor based on soil moisture and wilting point. Guenther and Sakulyanontvittaya (2011) suggest that the use of soil moisture in MEGAN offers advantages over the use of the PDSI in GloBEIS, including the ability to obtain observations from field measurement and laboratory studies or predictions from models such as the Community Land Model (CLM4).

Figure 1. Thirty-six land cover/land use types in eastern Texas (Source: Popescu et al., 2011) with boundaries of Texas climate divisions (Source: National Oceanic and Atmospheric Administration) and developed metropolitan areas shown in red.

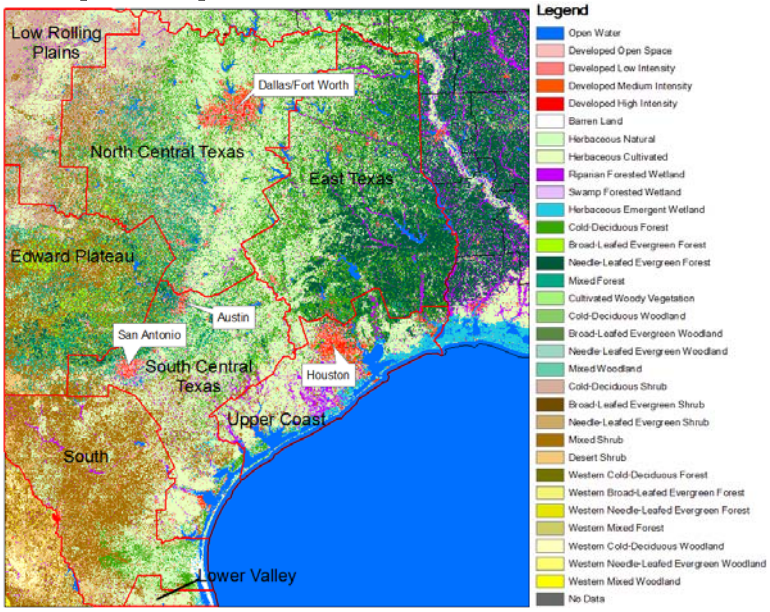
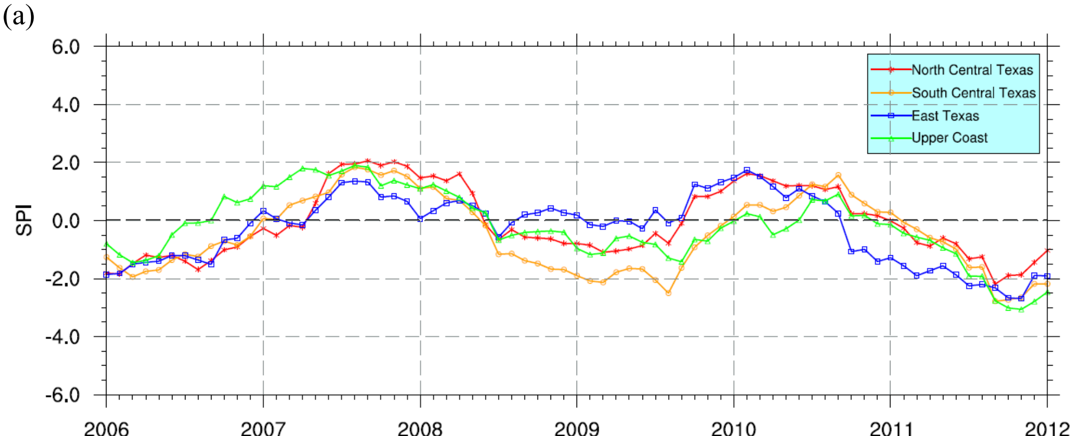
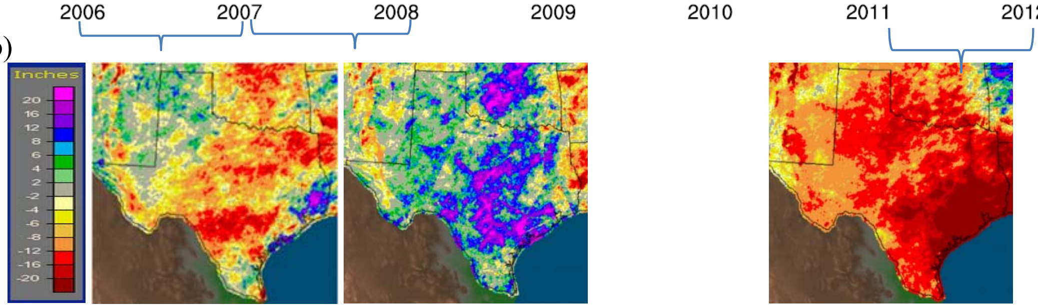


Figure 2. (a) 12-month SPI for four Texas climate regions. Positive SPI values suggest wet conditions while negative suggest drought. Source: National Climatic Data Center. (b) Annual precipitation distribution (as departure from normal in inches) for Texas during 2006, 2007, and 2011. Source: National Weather Service – Advanced Hydrologic Prediction Service.

(a)



(b)



Objective

The primary objective of the project is to evaluate and inform improvements in the representation of soil moisture through the use of simulated and observational datasets. The Model of Emissions of Gases and Aerosols from Nature (MEGAN) will be used to explore the sensitivity of biogenic emission estimates to alternative soil moisture representations. This work will be a collaboration between two research teams at the University of Texas at Austin: Dr. McDonald-Buller's at the Center for Energy and Environmental Resources and Dr. Rong Fu's of the Jackson School of Geosciences. Project tasks are described in detail below.

Task 1. Investigation and Evaluation of Soil Moisture Datasets

This work will consider in situ and remote sensing observational datasets as well as model simulations of soil moisture for the multi-state 12-km domain shown in Figure 3, with an emphasis on datasets available for the four eastern Texas climate divisions shown in Figure 1. An initial literature search will be conducted to identify observational datasets available for 2006-2012, which includes 2007 and 2011, the wettest and driest years on record in Texas during 2001-2012 (http://climatexas.tamu.edu/images/files/fnep_climdiv.txt).

Figure 3. The analysis of soil moisture will be conducted for the 12-km (blue) grid domain (Source: http://www.tceq.texas.gov/airquality/airmod/rider8/modeling/domain).

Observation-based datasets are anticipated to include, but may not be limited, to the following: (1) the North American Land Data Assimilation System (NLDAS) and (2) root zone and surface soil moisture drought indicators from the Gravity Recovery and Climate Experiment (GRACE) Data Assimilation System (Houborg et al. 2012). Additional soil moisture data may be available from the Soil Climate Analysis Network (SCAN) and others that form the International Soil Moisture Network (ISMN).

Simulations of soil moisture are important supplements to observational data, providing, for example, estimates in areas without available measurement sites. A review of soil moisture modeling approaches in the literature will be conducted. It is anticipated that off-line simulations with the newly developed Noah land surface model with multiparameterization options (Noah-MP) developed by Cai et al. (2014) and/or the Community Land Model (CLM) will be considered for this project.

Task 2. Comparison of Simulated and Observed Soil Moisture

Simulations of soil moisture from the selected model(s) will be compared with observations across the 12-km domain. To the extent possible, the team will develop suitable approaches for the reconciliation of spatial (vertical and horizontal) and temporal differences between model predictions and observational data to facilitate comparisons. Probability distributions produced by the simulations will be evaluated against NLDAS and GRACE surface and root zone soil moisture products. To the extent possible, the same surface forcings will be applied in the simulations as the NLDAS to investigate the performance of the models given realistic meteorological inputs. Detailed soil moisture budget differences between the simulations and NLDAS will be analyzed to identify sources of model biases. Comparisons will include an analysis of spatial gradients and rate of change of predicted soil moisture contents during representative, mostly rain-free periods to investigate the ability of the model applications to capture drying of soils during drought. Additional model comparisons will be considered if other soil moisture datasets with sufficient spatial and temporal resolution in eastern Texas are identified in Task 1.

Task 3. Preparation of MEGAN Simulations

MEGAN2.1, the most recent release, estimates emissions rate (F_i) of chemical species i from terrestrial landscapes in unit of flux (μg m^{-2} ground area h^{-1}) as:

$$F_i = \gamma_i \sum \varepsilon_{i,j} \chi_j \qquad (1)$$

where $\varepsilon_{i,j}$ (μg m^{-2} ground area h^{-1}) is the standard emission factor representing the net primary emission rate for vegetation type j with fractional coverage χ_j, γ_i is the emission activity factor that accounts for emission changes due to deviations from standard environmental and phonological conditions (Guenther et al., 2012; Guenther et al., 2006). Emission factors are specified for 19 compound classes (147 compounds lumped by emission responses to changes in environmental conditions) based on 15 CLM4 Plant Functional Types (PFTs) for more than 2000 ecoregions (Lawrence et al. 2010; Guenther et al., 2012). The overall activity factor (γ_i) accounts for variations in parameters including light (γ_p), temperature (γ_T), leaf area index (γ_{LAI}), leaf age (γ_A), soil moisture (γ_{SM}), and CO_2 inhibition (γ_C). Activity factors for light, temperature and LAI are separated into a light-dependent fraction (LDF) and a light-independent fraction (LIF) that are summed in the calculation of the overall activity factor:

$$\gamma = \gamma_A \gamma_{SM} \gamma_C (LDF \cdot \gamma_{LAI\_LDF} \cdot \gamma_{P\_LDF} \cdot \gamma_{T\_LDF} + (1 - LDF) \cdot \gamma_{LAI\_LIF} \cdot \gamma_{T\_LIF}) \qquad (2)$$

MEGAN requires geo-gridded files for driving variables, including emission factors, PFT distribution maps, LAI, solar radiation/photosynthetically active radiation, air temperature, soil moisture, wind speed, humidity and CO_2 concentrations (Guenther et al., 2012; Guenther and Sakulyanontvittaya, 2011).

It is anticipated that meteorological parameters, except Photosynthetically Active Radiation (PAR), will be obtained from the National Centers for Environmental Prediction (NCEP) North American Regional Reanalysis (NARR) products, as described by Huang et al. (2013). Hourly surface insolation from the Geostationary Operational Environmental Satellite (GOES), generated by University of Alabama in Huntsville) with a spatial resolution of 4-km will be re-gridded into a 1-km grid and converted to PAR based on a conversion factor of 0.45 (McNider, 2013; ENVIRON, 2011). The default version of MEGAN2.1 is configured to accept the 8-day composite LAI product (MCD15A2) from the Moderate Resolution Imaging Spectroradiometer (MODIS). For the study described by Huang et al. (2013), Dr. McDonald-Buller's team modified MEGAN to accept the more recent MODIS 4-day composite LAI product (MCD15A3). In addition, land use/land cover data with 30-m resolution across the eastern half of the state from a recent TCEQ-sponsored effort (Popescu et al., 2011) have been mapped to MEGAN's 16 PFTs.

Task 4. Sensitivity of Biogenic Emission Estimates to Soil Moisture
Sensitivity studies will be conducted using alternative representations of soil moisture within MEGAN for selected periods with varying climatic conditions during 2006-2012. Analysis of biogenic emissions will focus primarily on isoprene and monoterpenes for the growing seasons (April-October) in the four climate regions in eastern Texas (Figure 1) and comparisons within and between other states within the 12-km domain (Figure 3). The objectives will be to investigate temporal and spatial variations of biogenic emissions using maps and graphics, such as time series or box and whisker plots, that show monthly mean and percentile emissions estimates and to conduct targeted case studies of the variability between each of the four eastern Texas climate regions and within the 12-km domain.

Schedule
The project is composed of five tasks. The proposed schedule is presented in Table 1.

Table 1. Schedule of project activities

ID	Task	Apr.-May. 2014	June-July 2014	Aug-Sept. 2014	Oct.-Nov. 2014	Dec. 2014-Jan. 2015	Feb.-Mar. 2015	Apr.-May 2015	June 2015
1	***Investigation and Evaluation of Soil Moisture Datasets***	X	X	X	X				
2	***Comparison of Simulated and Observed Soil Moisture***				X	X	X		
3	***Preparation of MEGAN Simulations***			X	X	X			
4	***Sensitivity of Biogenic Emission Estimates to Soil Moisture***				X	X	X		
5	***Reporting***	X	X	X	X	X	X	X	X

Deliverables
AQRP requires certain reports to be submitted on a timely basis and at regular intervals. A description of the specific reports to be submitted and their due dates are outlined below. One report per project will be submitted (collaborators will not submit separate reports), with the exception of the Financial Status Reports (FSRs). The lead PI will submit the reports, unless that responsibility is otherwise delegated with the approval of the Project Manager. Report templates found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed; all reports will be written in the third person. The Technical, Draft Final, and Final Reports will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources.

Executive Summary
At the beginning of the project, an Executive Summary will be submitted to the Project Manager for use on the AQRP website. The Executive Summary will provide a brief description of the planned project activities, and will be written for a non-technical audience.
Due Date: Friday, May 30, 2014

Quarterly Reports
The Quarterly Report will provide a summary of the project status for each reporting period. It will be submitted to the Project Manager as a Word doc file. It will not exceed 2 pages and will be text only. No cover page is required. This document will be inserted into an AQRP compiled report to the TCEQ.

Due Dates:

Report	Period Covered	Due Date
Quarterly Report #1	March, April, May 2014	Friday, May 30, 2014
Quarterly Report #2	June, July, August 2014	Friday, August 30, 2014
Quarterly Report #3	September, October, November 2014	Monday, December 1, 2014
Quarterly Report #4	December 2015, January & February 2015	Friday, February 27, 2015
Quarterly Report #5	March, April, May 2015	Friday, May 29, 2015
Quarterly Report #6	June, July, August 2015	Monday, August 31, 2015
Quarterly Report #7	September, October, November 2015	Monday, November 30, 2015

Technical Reports

Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison as a Word doc using the AQRP FY14-15 MTR Template found on the AQRP website.

Due Dates:

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

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:

Report	Period Covered	Due Date
FSR #1	Project Start - May 31	Monday, June 16, 2014
FSR #2	June 1 - 30, 2014	Tuesday, July 15, 2014
FSR #3	July 1 - 31, 2014	Friday, August 15, 2014
FSR #4	August 1 - 31, 2014	Monday, September 15, 2014
FSR #5	September 1 - 30, 2014	Wednesday, October 15, 2014
FSR #6	October 1 - 31, 2014	Monday, November 17, 2014
FSR #7	November 1 - 30 2014	Monday, December 15, 2014
FSR #8	December 1 - 31, 2014	Thursday, January 15, 2015
FSR #9	January 1 - 31, 2015	Monday, February 16, 2015
FSR #10	February 1 - 28, 2015	Monday, March 16, 2015
FSR #11	March 1 - 31, 2015	Wednesday, April 15, 2015
FSR #12	April 1 - 28, 2015	Friday, May 15, 2015
FSR #13	May 1 - 31, 2015	Monday, June 15, 2015
FSR #14	June 1 - 30, 2015	Wednesday, July 15, 2015
FSR #15	Final FSR	Wednesday, August 15, 2015

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

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

Project Data
All project data will be submitted to the AQRP Project Manager within 30 days of project completion. This archive for the project will include all observational soil moisture data, input/job scripts/output for the soil moisture modeling, input/job scripts/output for the biogenic emissions modeling with MEGAN, and software files associated with the analysis and presentation of results in the final report. The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information. All data will be submitted for inclusion in the AQRP archive at the Texas Advanced Computing Center (TACC) and retained for seven years.

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

References:

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