Quality Assurance Project Plan

Project #18-005
Next steps for improving Texas biogenic VOC and NO emission estimates

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

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The University of California, Irvine and Ramboll have prepared this QAPP following EPA guidelines for a Quality Assurance (QA) Category III Project: Measurement and Research Model Development and Application. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

QAPP Requirements: The QAPP describes the project description and objectives, project organization and responsibilities, model selection, model design, model coding, model calibration, model validation, model evaluation, model documentation, scientific approach, sampling procedures, measurement procedures, quality checks, data analysis, interpretation and management, and reporting procedures, as prescribed in the applicable NMRL QAPP Requirements template (https://www.tceq.texas.gov/airquality/airmod/project/quality-assurance).

QA Requirements:
- Technical Systems Audits - Not Required for the Project
- Audits of Data Quality – 10% Required
- Report of Findings – Required in Final Report

Approvals Sheet

This document is a Category III Quality Assurance Project Plan for the following project: *Next steps for improving Texas biogenic VOC and NO emission estimates*. The Principal Investigator for the project is Alex Guenther and Co-Principal Investigator are Greg Yarwood.

Electronic Approvals:

This QAPP was approved electronically on October 15, 2018 by Elena McDonald-Buller, The University of Texas at Austin.

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Project Manager, Texas Air Quality Research Program

This QAPP was approved electronically on October 19, 2018 by Vincent M. Torres, The University of Texas at Austin.

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This QAPP was approved electronically on October 15, 2018 by Alex Guenther, University of California, Irvine.

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1.0 Project Description and Objectives

1.1 Purpose and Objectives

The overall goal of this project is to improve numerical model predictions of regional ozone and aerosol distributions in Texas by reducing uncertainties associated with quantitative estimates of biogenic VOC (BVOC) and NO emissions from Texas and the surrounding region. Although there have been significant advancements in the procedures used to simulate these biogenic emissions, there are still major uncertainties that limit predictability of Texas air quality simulations. This includes significant gaps in our understanding of biogenic emissions and their implementation in numerical models including isoprene, monoterpene and sesquiterpene emission factors and soil NO emissions. Therefore, we propose to improve the capability of the Model of Emissions of Gases and Aerosols from Nature (MEGAN, Guenther et al., 2012) framework to estimate emissions of these compounds. To accomplish this, we will conduct high quality measurements of isoprene, monoterpene and sesquiterpene emission factors at eastern Texas field sites near San Antonio, Dallas, and Houston and integrate these results, and those from other studies, into MEGAN. The version of the code resulting from this project will be MEGAN3.1

The primary output of the proposed research will be a more accurate approach for estimating biogenic VOC and NO emissions. Outcomes will include improved biogenic emission estimates and a better understanding of the current inconsistencies in various biogenic emission observational datasets and model simulations. The overall benefit of this project will be more accurate VOC and NO emission estimates for the Texas air quality simulations that are critical for scientific understanding and the development of regulatory control strategies that will enhance efforts to improve and maintain clean air.

The project has the following objectives:

- Conduct field measurements of isoprene, monoterpene and sesquiterpene emissions of important eastern Texas plant species resulting in improved emission factorsand investigate the variability within and among species and vegetation types.
- Update the MEGAN model to version MEGAN3.1 by incorporating an improved soil NO emission estimation approach and integrating the emission factor data from objective 1 into MEGAN emission factor processor.
- Investigate sensitivity of updated biogenic emissions estimated for Texas and surrounding regions.

1.2 Measurements to be evaluated

BVOC emission factors are the BVOC (e.g., isoprene, a-pinene, others) emission rates (moles per m2 leaf area per second) expected at a given set of standard environmental conditions (e.g., temperature of 30 C, solar photon flux density of 1000 micromoles per m2 leaf area per second). These emission factors are a key input for BVOC emission models. Values are uncertain for Texas (and other) vegetation.

1.3 Model development and application

The MEGAN3 model has an outdated (based on 1990s scientific understanding and capabilities) soil NO emission model that will be updated by incorporating an improved soil NO emission approach (based on recent studies) and integrating new emission factor data that will be obtained as part of this project. The sensitivity of the model to these changes will be assessed for 2013 because of the availability of aircraft observations for comparison.

2.0 Organization and Responsibilities

2.1 Project Personnel

The project will be directed by Dr. Alex Guenther (Principal Investigator) of the University of California, Irvine and Dr. Greg Yarwood of Ramboll (Co-Principal Investigator) for the Texas Air Quality Research Program (AQRP). Other staff members instrumental to the technical work include Mr. Tejas Shah and Dr. Ling Huang of Ramboll. Project participants and their responsibilities are listed in Table 1.

2.2 Project Schedule

An overall schedule of project activities by task is shown in Table 2. The schedule assumes a start date of August 1, 2018 and end date of August 31, 2019.

Table 1. Project participants and their key responsibilities.

Participant	Key Responsibilities
Alex Guenther	Principal Investigator (PI) from the University of California, Irvine will provide overall supervision and integration of the technical work and will be responsible for the preparation and submission of the monthly progress, quarterly progress, and final reports. He will have overall responsibility for project quality assurance and specific responsibility for quality assuring the field study work to measure emission factors.
Greg Yarwood	Co-PI from Ramboll will provide coordination with PI Dr. Guenther and staff members at Ramboll. Dr. Yarwood will consult with staff members at Ramboll on the MEGAN model development and assessment and advise on results reporting in collaboration with Dr. Guenther. He will review reporting deliverables and contribute to overall project quality assurance.
Tejas Shah	Lead Ramboll's contribution to the Task 4 MEGAN3 model sensitivity testing and evaluation task with assistance from staff members at Ramboll. He will be responsible for quality assuring updates to the MEGAN model code.
Ling Huang	Work with Dr. Guenther on the MEGAN3 model improvements in Task 3, with Dr. Huang carrying out modification to the MEGAN3 code.

Table 2. Schedule of project activities (tasks are bolded).

ID	Task	Aug 2018	Sept 2018	Oct 2018	Nov 2018	Dec 2018	Jan 2019	Feb 2019	Mar 2019	Apr 2019	May 2019	Jun 2019	July 2019	Aug 2019
1	***Measure BVOC EF***					X	X	X	X	X	X	X		
2	***MEGAN improvements***													
2a	*Soil NO model*			X	X	X	X							
2b	*BVOC EF*									X	X	X		
3	***Assessment of MEGAN Performance***										X	X	X	
R	*Monthly Technical & Financial Progress*	X	X	X	X	X	X	X	X	X	X	X	X	X
R	*Quarterly*		X			X			X			X		
R	*Draft Final*											X	X	
R	*Final*													X
R	*AQRP Workshop*													X

3.0 Scientific approach

Geron et al. (2001) assessed the measurements used to develop isoprene emission factors and concluded that most of the isoprene data suffered from a lack of recorded light/temperature growth conditions, self-shading of leaves in branch enclosures, perturbed enclosure measurement environments including low CO2 and high stress, no measurements of vegetation stress or physiological status, and variable time of day and season. Of particular concern was the lack of information on leaf growth environment, especially light and temperature, and the expected bias towards sampling shaded foliage. When examining species previously classified as low emitters, Geron et al. found that sun-lit leaves of these species had similar emissions as other high isoprene emitters. They concluded that any interspecies differences that may exist were obscured by the variability due to these other factors, especially differences in the light environment of the measured leaves.

Although some recent studies have classified their samples as representing "sun leaves", Niinemets et al. (2010) has shown that leaves classified as "sun leaves" can have very different light environments that can lead to isoprene EFs that vary by more than a factor of 2 and that this variability is highly correlated (r^2=~0.9) with the light environment as measured by the daily average integrated quantum flux density. The MEGAN3 approach enables estimation of EF for individual plant species and accounts for within canopy variation in isoprene EF driven by daily average integrated quantum flux density.

We will measure isoprene, monoterpene and sesquiterpene emission factor by following the measurement protocols described by Niinements et al. 2011. This includes making all EF measurements under controlled short-term light (1000 umol m-2 s-1) and temperature (30°C) environment, characterizing the long-term light and temperature environment (using the approach of Niinements et al. 2010), physiology (by measuring photosynthesis and transpiration with a LICOR 6400 gas exchange system), stress (by measuring chlorophyll and maximum quantum efficiency of photosystem II with a Photosynq multispeQ flourometer), specific leaf area and mass (using a scale for mass and a digital image analysis for leaf area), and by following the measurement protocols of Niinemets et al. (2011). Measurements will be made during late May to late June in eastern Texas at urban and rural sites around San Antonio, Dallas, and Houston. Lahr et al. (2015) has shown that oak and sweetgum leaves in the Houston area are mature with a representative isoprene emission rate. We will deploy a four-person field team to operate three BVOC emission factor measurement systems. A fifth person will be based in our UC Irvine laboratory to receive and immediately analyze samples shipped from the field. The three BVOC emission measurement systems will include two isoprene emission survey systems for rapid and accurate measurements of isoprene emissions and one glass cuvette system for accurate comprehensive BVOC measurements of monoterpenes and other BVOC (see section 11).

The isoprene survey systems will use an in-situ measurement so there will be no samples to store and ship. These systems will be used to characterize the dominant known isoprene emitters in eastern Texas including Quercus stellata (post oak), Q. virginiana (southern live oak), Q. fusiformis Liquidambar styraciflua (sweetgum), and at least 3 others such as Q. nigra (water oak), Nyssa sylvatica (blackgum), and Platanus occidentalis (American sycamore). Additional field measurements will be made in Irvine, CA for comparison. At least 3 replicate measurements will be made on 8 leaves of 6 trees of each of the 7 species for a total of more than 1000 measurements.

The comprehensive BVOC emission measurement systems will collect BVOC on solid absorbent tubes (Markes Stainless Steel tubes with 180 mg total absorbent with Tenax TA 35/60, Carbograph 5TD, 5 mm quartz wool) and shipped to Irvine CA for analysis within 48 hours during which samples will be at room temperature or below. This approach has successfully been used to measure isoprene, monoterpene and sesquiterpene emission factors (e.g., Harley et al. 2014). Target plant species will include at least 24 dominant eastern Texas tree species which, in addition to the 7 isoprene-emitting species listed in the previous paragraph, includes species such as Pinus taeda (loblolly pine), Q. marilandica (blackjack oak), Fraxinus pennsylvanica (green ash), Prosopis glandulosa (honey mesquite), Taxodium distichum (bald cypress), Carya illinoinensis (Pecan), Ulmus crassifolia (Cedar elm), and Juniperus ashei (ashe juniper). In addition, we will quantify emissions of at least 4 dominant Texas urban trees such as Fraxinus velutina (Arizona ash), Magnolia grandiflora, Lagerstroemia indica (crape myrtle), Triadica sebifera (Chinese Tallow tree), Catalpa bignonioides, Celtis occidentalis (hackberry), and Cinnamonum camphora (Camphor). At least two replicate measurements will be made on 3 leaves of 2 trees of these 22 tree species (at least 360 measurements). Finally, we will measure emission from at least 8 dominant Texas crops such as cotton, corn, sorghum, wheat, alfalfa, coastal bermuda grass, peanuts, and soybeans. At least 3 replicate measurements will be made on 3 leaves of 3 plants of these 8 species (at least 140 measurements).

After collecting each set of 10 samples, a measurement “blank” will be collected to quantify any background BVOC. The “blank” tubes will be handled in exactly the same way as the samples except that the sample pump will not be turned on. As the study plan calls for >500 measurements, we will collect > 50 blanks.

4.0 Sampling procedures

Two measurement systems, consisting of LICOR 6400 environmental control and gas exchange systems integrated with in-situ portable gas chromatographs as described by Geron et al. 2016, will be used for rapid measurement of a large number of isoprene EFs. We will use all of the QA/QC procedures described by Geron et al. 2016.

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In order to extend EF measurements to monoterpenes and sesquiterpenes, we will use an additional measurement system, shown in Figure 1, consisting of a custom-made glass-cuvette gas exchange system similar to the system described by Harley et al. (2014). BVOC will be collected on solid absorbent tubes and shipped to Irvine CA for analysis within 48 hours by GC-TOFMS/FID using an approach based on EPA method TO-17. This approach has successfully been used to measure isoprene, monoterpene and sesquiterpene emission factors (e.g., Harley et al. 2014). We will use QA/QC procedures established for EPA method TO-17 along with those described by Harley et al. 2014.

5.0 Measurement procedures

The objectives of BVOC emission factor enclosure measurements are to quantify representative emission factors for the dominant vegetation types for input to emission models. Our vegetation enclosures employ environmental monitoring and control during the measurements so that emission are measured at a specified temperature and light level. The measurements can be either laboratory- or field-based. Whole plants, branches, or individual leaves can be enclosed.

To measure CO_2 and H_2O concentrations (for photosynthesis and transpiration rates) an infrared gas analyzer (e.g., LiCor 6400, LiCor 840) is used. Individual biogenic VOCs will be measured by either focusing on solid adsorbents (with subsequent analysis in our Irvine laboratory using gas chromatography (GC) and flame ionization (FID) and mass spectrometer (MS) detection) or in-situ using a GC with a portable photoionization detector.

Sample collection of solid absorbent cartridges with analysis by GC-FID and GC-MS: BVOC will be collected on solid absorbent cartridges consisting of glass tubes packed with Tenax TA and carbograph 5TD and transported to our Irvine laboratory for analysis**.** The smaple will be collected using GilAir mass flow controlled pumps which automatically correct for measured temperature and pressure. The cartridge tubes collected in the field will be loaded into a thermally desorbing autosampler (TD-100, Markes International, Inc). The VOCs will be cryofocused at -10 °C on a cold trap and then transferred to the column (30 m, DB-5) of a gas

chromatograph (GC, model 7890B, Agilent Technologies, Inc) equipped with time-of-flight mass spectrometer (Markes BenchTOF-SeV) and flame ionization detector (TD-GC-FID/TOFMS). During the thermal desorption, the tube will be heated to 285 °C for 6 min with helium carrier gas. Helium will be used as the carrier gas with at a flow rate of 1.2 mL min^{-1}, and a multi-step temperature ramp was used from -30 °C to 260 °C. The response to isoprene and β-pinene will be calibrated by loading known amounts into cartridge tubes followed by analysis with the same protocols of the field samples.
The analytical system has a detection limit of ~1 pg for most BVOC. The overall detection limit for the atmospheric samples, however is somewhat higher than the limit of the analytical system because the background levels for cartridges exposed to air (i.e., blanks) in the absence of drawn flow for the corresponding time period (i.e., samples) which have typical concentrations of ~10 pg. These results corresponded to an approximate uncertainty in the analytical method of 2 ppt for a 3-L sample. The precision for most BVOC is ~10%. Additional uncertainty of 5% is introduced by the uncertainty in the measured flow rate of the VOC sampler. Overall measurement uncertainty is <20%. The primary hydrocarbon calibration gases are based on NIST prepared and certified standard cylinders of n-butane and benzene (10 ppbv in N_2). We will use the concept of effective carbon number (ECN) to correct the FID response for different BVOC. A characterized multi-component standard will be used to determine retention times and retention indices for individual compounds. The GC-MS-FID system will be calibrated daily with calibrations standards, replicate measurements, and blanks (to determine any background offsets). For adsorbent cartridges analyzed using a GC-MS-FID system, both MS and FID signals can be utilized for quantification and identification. Standard calibrations (between 2 and 4 replicates) will be loaded with each series of adsorbent cartridges. These contain verified concentrations of isoprene and camphene with resulting peak areas that are comparable to field samples. From these calibration chromatograms, selected ion monitoring (SIM) chromatograms are established to determine the MS response for those compounds. Based on ratios of other chemical species' ion fragments relative to camphene and isoprene, SIM response factors are generated, so that concentrations can be determined from analyzing specific ions (e.g., m/z=93 for a monoterpene) rather than the total ion or FID signal. This is necessary for cases in which co-elution occurs.

6.0 Quality Metrics

Data quality requirements: Leaf enclosure emissions measurements typically have demonstrated variations between 15% and 300% in repeated measurements within the same enclosure. The low end of this range represents measurements made at constant environmental conditions. The upper end represents measurements made under different light and temperature regimes, and measuring individual specimens within the same species under varying phonological stages. The measurement accuracy must be at least as good as the lower range of natural variability, and so we need to have accuracy within ~15%. The BVOC emission rate from a dynamic (air-purged) vegetation enclosure is calculated by the following equation:

$$ER = Q\left[\frac{C_{out} - C_{in}}{m_{dry}}\right]$$

Where *ER* is the emission rate (ugC m_{dry}^{-1} hr^{-1}), C_{out} and C_{in} are the outlet and inlet concentrations respectively of the compound of interest (in ugC l^{-1}), *Q* is the volumetric flow rate of the air purging the enclosure (in l min^{-1}) and m_{dry} is the dry leaf mass (grams). If the inlet air is sufficiently clean (VOCs removed so $C_{in} \approx 0$) the procedure is greatly simplified.

Each of the terms used in calculating an emission rate need to be checked for accuracy. The enclosures flow rates (Q) are checked daily using a Dry-Cal Definer volumetric flow meter (BIOS, Butler NJ), corrected to standard conditions of temperature and pressure. The enclosure temperature, humidity and light sensors are checked weekly using handheld temperature, RH and quantum sensors. Certified VOC standards are used to develop response factors for both the GC methods. These are inter-compared with laboratory GC methods, which are in turn compared to NIST certified standards. The dry mass of leaves is determined using a standard laboratory balance, which is verified using known weights.

Enclosure blanks (samples collected through the empty enclosure) will be collected and analyzed weekly. On a monthly basis, gas-phase standards containing VOC of interest are analyzed before and after passing through empty enclosure systems to quantify wall losses within the enclosure.

7.0 Data management

7.1 Types of data from measurements: The proposed measurement activities will generate field observations of BVOC emission factors along with and ancillary data. A variety of post-processing will be conducted including temporal averaging, calibration, and filtering. These additional processes will generate reduced datasets.

7.2 Standards for data and metadata format and content: The raw data from each instrument will be output in the format provided by the instrument manufacturer. Calibration factors will be used to convert raw data into concentration data. Emissions will be calculated by combining concentration, flow and biomass/area data. The reduced data will be saved in the MEGAN3 EFP data format (comma separated ASCII data).

7.3 Policies for access and sharing: All reduced data will be archived and available for download from the MEGAN data archive (bai.ess.uci.edu/megan). The results will be published in peer reviewed scientific journals including details on the technical aspects. We will clearly notify this data access and sharing policy in the publications.

7.4 Policies for re-use, re-distribution, and the production of derivatives: The policy for re-use, re-distribution, and the production of derivatives is that citation of the source of the data is required such as the original publication, provided it exists, or “personal communication” with PI.

7.5 Plans for archiving data, samples, and other research products, and for preservation of access of them: Multiple copies of raw and processed data will be stored in different media such as hard drives, DVD, and cloud storage along with metadata (laboratory notebooks, log sheets, etc.) and archived at the PI’s institution (University of California, Irvine) for a minimum period of five years.

8.0 Model Selection

The project is specifically focused on the continuing development of the MEGAN model and its application to Texas air quality planning and management. MEGAN is highly relevant to air quality modeling, offering high spatial and temporal resolution, consistency across geopolitical boundaries, and flexible options for the chemical speciation of emissions. The Texas AQRP has been instrumental in the evolution of MEGAN. Two previous AQRP Projects 14-016 (Yarwood et al., 2015) and 16-011 (Yarwood et al., 2017) have served as the foundation for the development of the next generation of the model. A major goal of this project is to complete development of the next generation global-scale model for future TCEQ applications, including in the development of biogenic emissions estimates and boundary conditions for its air quality modeling domain.

9.0 Model Design

The Model of Emissions of Gases and Aerosols from Nature (MEGAN) is designed to provide inputs of all important biogenic VOC on the temporal and spatial scales required for regional air quality and global earth system models. The model considers all BVOC emissions regardless if they occur in natural ecosystems or managed landscapes including urban areas. The current version, MEGAN3 is updated from MEGAN2.0 (Guenther et al., 2006) and MEGAN2.02 (Sakulyanontvittaya et al., 2008) to include additional compounds, emission types, and controlling processes. Additional advancements in characterizing previously unaccounted compounds (e.g., Jud et al. 2016), heterogeneity in the vertical distribution of isoprene emitting trees (Bryan et al. 2015), quantifying BVOC response to stress (e.g., Karl et al. 2008, Kaser et al. 2013, Ghirardo et al. 2016, and reconciling isoprene and monoterpene emission factors (e.g., Emmerson et al. 2016) during the past 5 years were incorporated into MEGAN3.

Isoprene and monoterpene emissions in Texas have previously been estimated using GloBEIS, which was developed as a more flexible alternative to the USEPA BEIS model that was the only widely used tool for biogenic emission modeling. GloBEIS is no longer being developed or supported. The flexible framework and key features have been incorporated into the MEGAN model, which has been used for biogenic emission modeling in Texas. These features include the ability to 1) use landcover data developed for the state of Texas, 2) account for environmental conditions prevalent in Texas (e.g., drought), and 3) update emission factors and other model components.

9.1 Conceptual Model

MEGAN estimates emissions by combining an estimate of the emission capacity of a landscape based on landcover variables with an estimate of emission activity that may be related to variations in landcover, weather and other factors (e.g., Guenther et al., 2012). The emission capacity represents the expected emission at a standard set of conditions, i.e., a leaf temperature of 30 °C and photosynthetically active radiation (PAR) of 1000 µmol m-2 s-1. MEGAN uses simple mechanistic algorithms to account for the major known processes controlling biogenic emissions. Emissions observed under experimental conditions are adjusted using emission activity algorithms to account for deviations from standard conditions during the periods of interest.

9.2 Algorithms and Equations

PAR and temperature are widely recognized as the most important factors controlling the emissions of isoprene and monoterpenes and the short-term response of isoprene and monoterpene emissions to changes in these controlling variables is reasonably well known. Algorithms have also been introduced to account for the response of isoprene to past PAR and temperature, although this is considerably less understood in comparison to short-term responses. An additional complexity is that PAR and temperature vary considerably with canopy depth and for sun and shade leaves at the same canopy depth and so a canopy environment model is required to estimate conditions for sun and shade leaves at 5 canopy depths. Other algorithms account for variations in leaf age and amount, carbon dioxide and drought.

MEGAN3.1 development will include additional algorithms to simulate biogenic NO emission. Soil type, temperature, soil moisture, and nitrogen inputs are recognized as the major factors controlling biogenic NO emission. Temperature and soil moisture for driving biogenic NO emissions will be the same as those used for biogenic VOC. Gridded inventories of nitrogen fertilizer and nitrogen deposition similar to those available for use with the community GEOS-chem model will be used.

9.3 Model Data

The current MEGAN inputs, including emission factors, landcover (plant functional type [PFT], LAI), weather (PAR, temperature, wind speed, humidity, soil moisture) and atmospheric composition (CO2) will continue to be used although the emission factors will be modified to account for new categories and compounds. Additional landcover (canopy vertical heterogeneity) and atmospheric composition (ozone) inputs will be added but will be optional so that the model can be run with existing input data.
MEGAN allows users to either output emissions of individual compounds or provide output in the categories used by some of the common atmospheric chemistry reaction schemes (e.g., SAPRCII, SAPRC99, RADM2, RACM, or CBMZ).

10.0 Model Coding

The program to be updated is the MEGAN biogenic emissions model. The new version will be referred to as the MEGAN3.1 code. The MEGAN3.1 code and requirements are similar to that used for MEGAN2.1 and MEGAN3 and will be able to run within the same computing environments that have historically been used for MEGAN2.1 and MEGAN3.

Requirements for Model Code Development

Code development will be directed by a single Ramboll staff member, with input from the UCI Principal Investigator and assistance from one or two other Ramboll staff members as needed to develop and test specific process modules. The lead developer will oversee construction of all facets of the new code, ensure seamless integration among new subroutines and within the MEGAN program flow, and lead all testing and quality assurance steps. The lead developer will maintain close communication with Ramboll’s co-Principal Investigator to report progress, technical issues, and possible solutions.

Basic process testing and debugging will be performed by first running new subroutines inside a standalone test-bed driver program. Functionality, interfacing, performance and design constraints for the new module will be evaluated. Good Fortran coding practices such as clear and complete comments and a structured programming approach as well as Fortran compile-time checks will help to confirm that the subroutines are coded properly.

Upon successful testing, the new subroutines will be implemented into the MEGAN model and tested by running short (~1 day) test cases. This testing will focus on identifying implementation bugs and performance issues. Potential alternatives will be considered and tested to improve speed.

Final MEGAN3.1 system evaluation will be conducted by applying the updated model for two existing modeling datasets as described in Section 5.

Computer Hardware and Software Requirements
MEGAN3.1 is expected to be run on workstations and cluster environments running common distributions of the Linux operating system with Csh/sh scripting language and Fortran 90 compiler. For example, the code will be able to run on a GNU/LINUX x86_64 computer with PGI compiler. The MEGAN3.1 model code will not support parallelization. MEGAN preprocessors are expected to be run on either workstations with Linux or on computers using the Windows operating system.

Requirements for Code Validation
Tejas Shah (Ramboll) will be responsible for conducting audits of data quality at a level of at least 10% of the data generated by the updated software. Temporary diagnostic output code will be written in the test-bed system to allow for a visual inspection of model inputs and outputs components and intermediate variables going into the modified algorithms and solvers.

10% of model inputs will be reviewed by comparison of each variable's values in the original input data set with its values after they have been read into the model. We will perform quality assurance checks to ensure that as the model calculations proceed, the calculations are performed correctly. Following the calculation of key intermediate variables within the model, at least 10% of the intermediate variable data will be reviewed visually and assessed for reasonableness. If any values are found to lie outside their expected range, we will use print statements in the code and/or debugging tools to determine the origin of the unexpected value and correct the model code if an error is found. The visual inspection of model inputs and intermediate variables will be performed by a member of the team who did not participate in the development of the model code. Finally, model outputs will be evaluated as outlined in the next paragraph below.

The emission rate estimates from the MEGAN3.1 model will be compared to emission flux measurements obtained from the SAS field study campaigns. Also, data generated by MEGAN3.1 will be compared to the output from the MEGAN3 and MEGAN2.1 version to ensure that design changes result in expected outcomes. MEGAN sensitivity results will be evaluated visually using graphical systems to identify and report the impact of the program changes. Emission rates will be graphically and statistically compared to available measurement data to gauge impacts to model performance. The objective of the model evaluation will be to determine if the model predictions agree with reported isoprene and monoterpene emissions within the uncertainties of the observations. This will be used to evaluate success in achieving the project objective of reducing uncertainties associated with quantitative estimates of BVOC emissions from Texas and the surrounding region.

The Ramboll co-Principal Investigator will work closely with the chief code developer and lead researcher to review all new code developments. Results of all tests and QA/QC procedures will be documented in the Final Report that is one of the project deliverables.

11.0 Model Calibration

The MEGAN model emission factors will be based on emissions data including the enclosure data obtained as part of this study. The uncertainties of the emission estimation technique have been constrained with comparisons with other emission estimates and with the comparison of chemical transport models with satellite observations for two previous AQRP Projects 14-016 (Yarwood et al., 2015) and 16-011 (Yarwood et al., 2017). Although limitations were identified, earlier versions of the model have shown to perform within reason for the U.S. and to be within the uncertainties of other models, such as BEIS model (Warneke et al. 2010).

Sensitivity studies will systematically examine how individual and collective modifications to the MEGAN model influence estimates of biogenic VOC and NO relative to the baseline configuration. Spatial mapping and descriptive summaries will be created for this project to facilitate the detection of anomalies and evaluation of reasonableness. The team members have extensive experience with the development of the MEGAN model, its application, and evaluation of uncertainties surrounding the model inputs. They will apply expert judgment in the calibration of the model investigating in particular how updates to model input parameters or use of alternative input datasets affect emissions estimates relative to the baseline configuration. In cases where an expected directional change in model predictions is inconsistent with changes in input data resources or anomalously small or large emissions estimates are evident, further investigation of discrepancies will be conducted and reconciliation approaches will be pursued. No further calibration of the MEGAN model will be performed as part of this project.

12.0 Model Validation

Approach

The objective of Task 3 is to investigate MEGAN3.1 model sensitivity and evaluate model emission estimates using aircraft BVOC observations. We will carry out emissions sensitivity modelling in support of the Task 3. We will then select a small number of best estimate and/or sensitivity test MEGAN3.1 emission inventories for comparison against aircraft flux data from SAS and evaluate them. The purpose of the evaluation is to constrain the MEGAN3.1 emissions using the SAS aircraft flux data. The evaluation using aircraft flux measurements will assess MEGAN3.1 configurations including alternative emission factor data and model simulations with and without algorithms accounting for individual drivers of BVOC emission variability.

Aircraft Data

During the SAS 2013 summer field campaign, the National Center for Atmospheric Research (NCAR) C-130 aircraft and the National Oceanic and Atmospheric Administration (NOAA) P-3 aircraft measured terpenoid (isoprene and total monoterpenes) concentrations over Texas and surrounding states using proton transfer reaction spectrometer (PTR-MS) systems and speciated monoterpenes using gas chromatograph mass spectrometry (GC-MS) (in-situ fast-response GC-MS on the NCAR C-130 and canister sampling with laboratory GC-MS analysis for the NOAA P-3).

Fast response VOC measurements were made on the NCAR C-130 during the 2013 Nitrogen, Oxidants, Mercury, and Aerosol Distributions, Sources, and Sinks (NOMADSS) study using a custom-designed airborne PTR-MS developed at NCAR and described by Karl et al. (2013). During flights focused on BVOC fluxes, a limited suite of VOC measurements were targeted in order to increase sensitivity. Measurements typically included isoprene, total terpene, methanol, and methacrolein plus methyl vinyl ketone). A fast GC-MS measured isoprene, methyl butenol, a-pinene and other speciated monoterpenes, methanol, and many other VOC with a time resolution of about 5 minutes. In AQRP Project 14-016, spatially resolved eddy covariance fluxes were obtained from wavelet analysis along flight tracks flown in the mixed layer (Yarwood et al., 2015; Yu et al. 2017). These fluxes will be used to evaluate the MEGAN3.1 BVOC emission inventories.

The aircraft data used in this project are described in detail in Kaser et al. (2015), Warneke et al. (2016), and Yu et al. (2017). Kaser et al. (2015) and Warneke et al. (2016) provide descriptions of the instruments and data collection methods for all data that will be used in this project. References given in these two papers describe the calibration and QA/QC for each instrument on the C-130 and P-3 aircraft. 100% of the aircraft data that will be used in this study have undergone extensive QA/QC by the research groups who collected the data during the SAS Study.

The SAS aircraft data are archived in data repositories at NCAR and NOAA. A master list of data from SAS is posted at http://data.eol.ucar.edu/master_list/?project=SAS and contains the C-130 terpenoid data used in this project. The data manager for the NCAR C-130 data is Steve Williams (sfw@ucar.edu). Data from the NOAA P-3 are posted at http://esrl.noaa.gov/csd/groups/csd7/measurements/2013senex/P3/DataDownload/ and are managed by Ken Aikin (kenneth.c.aikin@noaa.gov).

MEGAN3.1 Performance Evaluation

We will use C-130 aircraft flux data to evaluate emissions developed with the MEGAN3.1 model. MEGAN3.1 emissions will be extracted along the C-130 flight segments for each of the sensitivity test inventories. The MEGAN3.1 emissions of isoprene, monoterpenes and other species of interest will be paired in space and time with the aircraft flux data and modelled and measured fluxes will be compared. MEGAN.1 model performance will be reviewed using both graphical and statistical methods. Graphical methods will include spatial maps and time-series comparing model predictions to observations. Graphics may be developed using a mix of several plotting applications, including GIS, PAVE, Surfer, and NCAR/NCL. Statistical methods will include computation of metrics for bias and error between predictions and observations for isoprene and total monoterpene emission rates. Standard statistical metrics as described in EPA air quality modelling guidance (EPA, 2014) will be calculated (Table 12-1).

Consistent with EPA Modelling Guidance (EPA, 2014), we will use multiple statistical metrics in the model performance evaluation. At a minimum, we will evaluate the root mean square error (RMSE), normalized mean bias (NMB), normalized mean error (NMB), and the correlation coefficient (r) or coefficient of determination (r^2). Linear regression analysis (e.g., coefficient of determination, r^2) will be used to examine the model's ability to capture observed variability. The results of the comparisons will be used to inform the development of the emission factor database and the MEGAN3.1 model. From the MEGAN3.1 performance evaluation, we will select the best-performing and/or sensitivity test inventories for evaluation with an air quality model.

We will use meteorological data from AQRP Project 14-016 (Yarwood et al., 2015) which was adapted from a 2013 Texas ozone forecast modeling application developed by Ramboll for the

TCEQ (Johnson et al., 2013). The modeling domain consists of a 36 km continental-scale grid and a nested 12 km grid. The regional 12 km grid used in the forecasting project to cover Texas and surrounding states encompasses nearly all of the overland flight tracks of the C-130 and P-3 made during June-July 2013 (Figure 12-1).

The 2013 WRF model output was evaluated against surface and aircraft observations during Project 14-016 (Yarwood et al., 2015) and found to be acceptable for the purpose of the project.

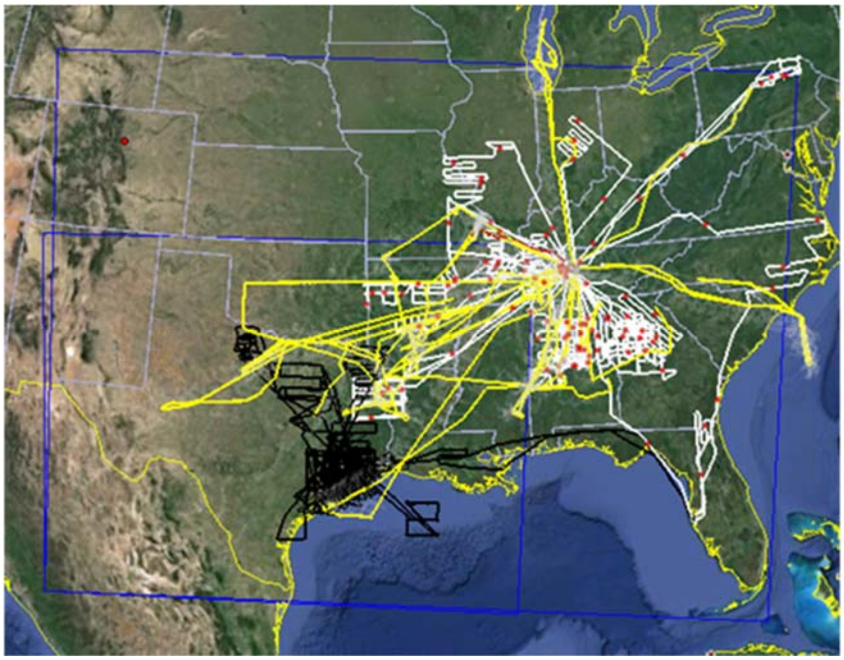

Figure 12-1. WRF and MEGAN3.1 12 km modeling grid and aircraft flight paths. Aircraft flight paths: SAS C-130 (yellow), SAS P-3 (white), and TEXAQS 2006 (black). TCEQ 12 km grid extent (smaller blue domain), and expanded 12 km grid (larger blue domain).

MEGAN3.1 will be run from June 1-July 15, 2013 to simulate the period when C-130 and P-3 aircraft data are available. The Weather Research and Forecasting (WRF) (Skamarock et al., 2008) was run in hindcast mode to output the meteorological fields (Yarwood et al., 2015) that will be used to drive the June-July 2013 MEGAN3.1 emissions.

The WRF 2013 meteorological database was evaluated against observed weather data as part of AQRP Project 14-016. WRF performance was found to be comparable to that of similar regional meteorological model applications. Of note for MEGAN emission inventory development is that comparison of WRF modeled surface downward shortwave radiation (DSW) with visible satellite images for the C-130 flights and solar radiation measured at TCEQ monitoring sites indicated that, despite the presence of cloud-radiation feedback, WRF underestimated the observed cloud field and overestimated DSW. Underestimating clouds and overestimating the available shortwave radiation very likely introduced a high bias in the MEGAN isoprene emissions through a high bias in PAR and affected the partitioning of surface heat and moisture fluxes. This model performance issue is typical of WRF simulations at moderate spatial resolution and must be taken into account in the interpretation of MEGAN3 and CAMx modelling results.

For the selected MEGAN3.1 emission inventories, we will compare modeled and measured fluxes at the surface and along the C-130 and P-3 aircraft flight tracks. The aircraft flight paths were mapped to grid cells within the 12 km modelling domain during AQRP Project 14-016. For the grid cells containing aircraft transects, we will document the model's performance in simulating measured isoprene and other BVOC fluxes.

Table 12-1. Definition of performance metrics for MEGAN3.1 modeling.

Metric	Definition[1]
Mean Bias (MB)	$\frac{1}{N}\sum_{i=1}^{N}(P_i - O_i)$
Mean Error (ME)	$\frac{1}{N}\sum_{i=1}^{N}\lvert P_i - O_i\rvert$
Root Mean Squared Error (RMSE)	$\sqrt{\frac{\sum_{i=1}^{N}(P_i - O_i)^2}{N}}$
Normalized Mean Bias (NMB) (-100% to +∞)	$\frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N} O_i}$
Normalized Mean Error (NME) (0% to +∞)	$\frac{\sum_{i=1}^{N}\lvert P_i - O_i\rvert}{\sum_{i=1}^{N} O_i}$
Coefficient of Determination (r^2) (0 to 1)	$\left(\frac{\sum_{i=1}^{N}(P_i - \overline{P})(O_i - \overline{O})}{\sqrt{\sum_{i=1}^{N}(P_i - \overline{P})^2 \sum_{i=1}^{N}(O_i - \overline{O})^2}}\right)^2$

[1]P_i and O_i are the predicted and observed values (O_i,P_i) at the i^{th} site paired in space and time and N is the number of observed/modeled data pairs.

The MEGAN3.1 model performance evaluation will inform the development of MEGAN3.1. The AQRP Project 14-016 MEGAN2.1 emissions developed with EFvA2015 inputs will serve as a baseline for MEGAN3.1 model performance. Metrics from Table 12-1 will serve as the basis for comparison of model performance in simulating measurements along the aircraft flight tracks. Configurations of MEGAN3.1 that cause significant degradation in model performance metrics will be reviewed. For example, a configuration of MEGAN3.1 that caused the average isoprene NMB along the C-130 flight tracks to decrease from -16% in the baseline run to -40% would be reviewed with the purpose of understanding the cause of the change in isoprene performance and determining whether some component of MEGAN3.1 or its inputs should be revised. All conclusions regarding model performance will be clearly documented in the final report.

13.0 Model Perfomance Evaluation

Per requirements for Category III projects, audits of 10% of data for data quality will be performed, and the results of the QA evaluation will be reported in the Final Report.

Assessment Process for Emission Factor Database

A member of the research team who did not develop the MEGAN3 emission factor database or conduct model simulations will review at least 10% of the emissions data for quality assurance purposes. The Ramboll project manager will review the emission factor results using graphical displays of raw emission factor output. This will result in audits of well in excess of 10% of model inputs and outputs. Results of all tests and QA/QC procedures will be documented in the Interim and Final Reports that comprise the project deliverables.

Assessment Process for MEGAN3.1 Code Development
A member of the research team who did not develop the MEGAN3.1 model will review at least 10% of the model code for quality assurance purposes. The Ramboll project manager will review the model code. This will result in audits of well in excess of 10% of model inputs and outputs. Results of all tests and QA/QC procedures will be documented in the Interim and Final Reports that comprise the project deliverables.

Assessment Process for MEGAN3.1 Modeling
A member of the research team who did not develop the MEGAN3.1 model input datasets or conduct model simulations will review at least 10% of the input data and model output for quality assurance purposes. The Ramboll project manager will review all results from the MEGAN3.1 model applications using graphical displays of raw model output as well as the model performance evaluation products. This will result in audits of well in excess of 10% of model inputs and outputs. Results of all tests and QA/QC procedures will be documented in the Interim and Final Reports that comprise the project deliverables.

14.0 Model Documentation
The existing MEGAN documentation and User's Guide will be revised to reflect the updates to the MEGAN code and emission factor preprocessor made during this project. This will include the following:

- Model description including the underlying assumptions and equations/algorithms used in the model. A flow chart will be provided to give an overview of the model including inputs and outputs. Individual routines and parameter values and sources will be described. Limiting conditions, including spatial domain, will also be described.

- Model specifications including hardware and software requirements, programming language and memory requirements

- The emission measurement database and emission factor preprocessor will be described in detail including procedures for updating the emission measurement database.

- A copy of the source code, including embedded comment statements, as well as input and output files will be provided as a digital appendix to the User's Guide. The existing MEGAN3 description of the availability of input data and procedures for processing these data will be updated to reflect new datasets.

15.0 Reporting
As required, monthly technical, monthly financial status, and quarterly reports as well as an abstract at project initiation and, near the end of the project, the draft final and final reports will be submitted according to the schedule below. Dr. Guenther or his designee will electronically

submit each report to both the AQRP and TCEQ liaisons and will follow the State of Texas accessibility requirements as set forth by the Texas State Department of Information Resources (http://aqrp.ceer.utexas.edu/). Principal investigators Guenther and Yarwood anticipate attending and presenting at the AQRP data workshop. Draft copies of any planned presentations (such as at technical conferences) or manuscripts to be submitted for publication resulting from this project will be provided to both the AQRP and TCEQ liaisons per the Publication/Publicity Guidelines included in Attachment G of the subaward. Final project data and associated metadata will be prepared and submitted to the AQRP archive. Each deliverable and required deadline for submission are presented below.

Abstract: At the beginning of the project, an Abstract will be submitted to the Project Manager for use on the AQRP website. The Abstract will provide a brief description of the planned project activities, and will be written for a non-technical audience.

Abstract Due Date: nnn, 2018

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

Quarterly Report Due Dates:

Report	Period Covered	Due Date
September 2018 Quarterly Report	July, August, September 2018	September 28, 2018
December 2018 Quarterly Report	October, November, December 2018	December 31, 2018
March 2019 Quarterly Report	January, February, March 2019	March 29, 2019
June 2019 Quarterly Report	April, May, June 2019	June 28, 2019

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the FY18-19 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Aug2018 MTR	Project Start - August 31, 2018	September 8, 2018
Sep2018 MTR	September 1 - 30, 2018	October 8, 2018
Oct2018 MTR	October 1 - 31, 2018	November 8, 2018
Nov2018 MTR	November 1 - 30 2018	December 8, 2018
Dec2018 MTR	December 1 - 31, 2018	January 8, 2019

Jan2019 MTR	January 1 - 31, 2019	February 8, 2019
Feb2019 MTR	February 1 - 28, 2019	March 8, 2019
Mar2019 MTR	March 1 - 31, 2019	April 8, 2019
Apr2019 MTR	April 1 - 28, 2019	May 8, 2019
May2019 MTR	May 1 - 31, 2019	June 8, 2019
Jun2019 MTR	June 1 - 30, 2019	July 8, 2019
Jul2019 MTR	July 1 - 31, 2019	August 8, 2019
Aug2019 MTR	August 1- Project end	Project end date

Financial Status Reports (FSRs): Financial Status Reports will be submitted monthly to the AQRP Grant Manager (Maria Stanzione) by each institution on the project using the FY18-19 FSR Template found on the AQRP website.

FSR Due Dates:

Report	**Period Covered**	**Due Date**
Aug2016 FSR	Project Start - August 31, 2018	September 15, 2018
Sep2016 FSR	September 1 - 30, 2018	October 15, 2018
Oct2016 FSR	October 1 - 31, 2018	November 15, 2018
Nov2016 FSR	November 1 - 30 2018	December 15, 2018
Dec2016 FSR	December 1 - 31, 2018	January 15, 2019
Jan2017 FSR	January 1 - 31, 2019	February 15, 2019
Feb2017 FSR	February 1 - 28, 2019	March 15, 2019
Mar2017 FSR	March 1 - 31, 2019	April 15, 2019
Apr2017 FSR	April 1 - 28, 2019	May 15, 2019
May2017 FSR	May 1 - 31, 2019	June 15, 2019
Jun2017 FSR	June 1 - 30, 2019	July 15, 2019
Jul2017 FSR	July 1 - 31, 2019	August 15, 2019
Aug2017 FSR	August 1 - 31, 2019	September 15, 2019
FINAL FSR	Final FSR	October 15, 2019

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. It will also include a report of the QA findings.

Draft Final Report Due Date:

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.

Final Report Due Date: August 1, 2019

Project Data: All project data including but not limited to QA/QC measurement data, metadata, databases, modeling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (). The data will be submitted in a format that will allow AQRP or TCEQ or other outside parties to utilize the information. It will also include a report of the QA findings.

AQRP Workshop: A representative from the project will present at the AQRP Workshop August 2019.

Presentations and Publications/Posters: All data and other information developed under this project which is included in published papers, symposia, presentations, press releases, websites and/or other publications shall be submitted to the AQRP Project Manager and the TCEQ Liaison per the Publication/Publicity Guidelines included in Attachment G of the Sub-award.

16.0 References

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