Quality Assurance Project Plan

Project 16 – 011
A Next Generation Modelling System for Estimating Texas Biogenic VOC Emissions

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

Prepared by

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Ramboll Environ and Alex Guenther, Independent Consultant, have prepared this QAPP following EPA guidelines for a Quality Assurance (QA) Category III Project: Measurement. It is submitted to the Texas Air Quality Research Program (AQRP) as required in the Work Plan requirements.

QAPP Requirements: Project Description and Objectives, Organization and Responsibilities, Model Design, Model Coding, Model Calibration, Model Verification, Model Evaluation, Model Documentation, Reporting, References

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 project: A Next Generation Modelling System for Estimating Texas Biogenic VOC Emissions. The Principal Investigators for the project are Dr. Greg Yarwood, Dr. Sue Kemball-Cook and Dr. Alex Guenther.

Electronic Approvals:

This QAPP was approved electronically on 9/6/2016 by Dr. Elena McDonald-Buller, The University of Texas at Austin.

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This QAPP was approved electronically on 9/6/2016 by Vincent M. Torres, The University of Texas at Austin.

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This QAPP was approved electronically on 09/17/2016 by Co-PI Dr. Greg Yarwood, Ramboll Environ.

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QAPP Distribution List

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Dr. Alex Guenther, Co-Principal Investigator

1.0 PROJECT DESCRIPTION AND OBJECTIVES

Ramboll Environ and Dr. Alex Guenther, Independent Consultant, have prepared this Quality Assurance Project Plan (QAPP) following EPA guidelines. The nature of the technical analysis and tasks to be conducted as part of this project are consistent with quality assurance (QA) Category III: Research Model Development or Application. The type of work that will be conducted in this study falls under the guideline of "Research Model Development and Application Projects."

1.1 Purpose of Study

Emissions of reactive gases from the earth's surface drive the production of ozone and aerosol and other atmospheric constituents relevant for regional air quality. Emissions of some compounds, including biogenic volatile organic compounds (BVOCs), are highly variable and can vary more than an order of magnitude over spatial scales of a few kilometers and time scales of less than a day. This makes estimation of these emissions especially challenging and yet accurate quantification and simulation of these fluxes is a necessary step towards developing air pollution control strategies and for attributing observed atmospheric composition changes to their causes.

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 BVOC emissions from Texas and the surrounding region. Although there have been significant advancements in the procedures used to simulate BVOC emissions, there are still major uncertainties that affect the reliability of Texas air quality simulations. This includes significant gaps in our understanding of BVOC emissions and their implementation in numerical models including 1) isoprene emission factors, 2) missing compounds, and 3) and unrepresented processes including canopy heterogeneity and stress induced emissions. For example, Texas AQRP project 14-016 (Yarwood et al., 2015) reported direct aircraft measurements of isoprene fluxes that were lower than the MEGAN predictions and Texas AQRP project 14-030 (Ying et al., 2015) summarized near surface isoprene concentrations that were higher than those predicted using MEGAN emissions with a chemistry and transport model. We propose to reconcile these and other observations by developing new emission factors and incorporating missing BVOC compounds and unrepresented BVOC emission processes into the Model of Emissions of Gases and Aerosols from Nature (MEGAN, Guenther et al., 2012) framework. To accomplish this, we will develop a transparent and comprehensive approach to assigning isoprene and monoterpene emission factors and will update MEGAN to include additional BVOC and processes including stress induced emissions and canopy heterogeneity. We expect the explicit representation of canopy heterogeneity and other processes will eliminate any significant difference between MEGAN isoprene emission estimates and aircraft flux measurements.

The primary output of the proposed research will be a flexible, transparent and more accurate approach for estimating BVOC emissions. The proposed work aims to reduce

BVOC emission uncertainties and develop an improved version of a model for estimating emissions of isoprene, monoterpenes and other significant BVOC from Texas. Outcomes will include improved BVOC emission estimates and a better understanding of the current inconsistencies in various BVOC observations and model simulations. The overall benefit of this project will be more accurate VOC 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.

1.2 Project Objectives

The project aims to reduce BVOC emission uncertainties associated with the absolute magnitude of the emissions and the response of the emissions to changes in plant stress (e.g., water and heat stress) and to improve the ability of biogenic emission estimation tools to better predict emissions of monoterpenes and responses to short- and long-term drought stress. This project will incorporate biogenic emission findings from previous Texas projects into a version of a biogenic model appropriate for Texas air quality applications. This will be accomplished by synthesizing results from previous Texas AQRP projects and other studies into a new version of MEGAN, a biogenic emissions model used for predicting BVOC emissions in Texas and other regions.

Our specific objectives include:

1. Develop a database system that provides a transparent approach for estimating BVOC emission factors.
2. Synthesize available isoprene and monoterpenes emission and concentration observations for Texas and surrounding regions, reconcile any discrepancies, and calculate Texas isoprene and monoterpene emission factor best estimates and ranges.
3. Develop a next generation BVOC emission model, MEGAN3, that includes missing compounds and unrepresented processes including stress induced (drought, extreme temperature and air pollution) emissions and canopy heterogeneity.
4. Investigate MEGAN3 model sensitivity and evaluate model emission and ambient concentration estimates using surface and aircraft observations and a photochemical model.

2.0 PROJECT ORGANIZATION AND RESPONSIBILITIES

2.1 Responsibilities of Project Participants

This project is being conducted by Ramboll Environ and Dr. Alex Guenther, Independent Consultant, under a grant from the Texas Air Quality Research Program (AQRP). The project Co-Principal Investigators (PIs) are Dr. Greg Yarwood and Dr. Sue Kemball-Cook of Ramboll Environ and Dr. Alex Guenther, Independent Consultant. The Co-PIs will assume overall responsibility for the research and associated quality assurance. Dr. Guenther will lead the development of the BVOC emission factor database system and will calculate terpenoid emission factors for Texas and surrounding regions. Dr. Guenther will also direct the development of MEGAN3. Dr. Kemball-Cook will oversee the Ramboll Environ effort in development of the BVOC database and MEGAN3 and the evaluation of the new inventories using a regional photochemical model. She will be responsible for project management and reporting. Dr. Yarwood will provide technical guidance and oversight. All Principal Investigators will contribute to the final report.

The project will be overseen by AQRP Project Manager Dr. Elena McDonald-Buller and TCEQ Project Liaison Mr. Doug Boyer. They will review the project deliverables and documentation. The personnel working on this project and their specific responsibilities are listed in Table 2-1 below.

Table 2-1. Project participants and responsibilities

Participant	Project Responsibility
Dr. Greg Yarwood (Ramboll Environ)	Co-Principal Investigator: Project oversight; responsible for providing technical guidance and review of reports and presentations
Dr. Susan Kemball-Cook (Ramboll Environ)	Co-Principal Investigator: Project oversight, management and reporting; responsible for Ramboll Environ effort in development of the BVOC database and MEGAN3 and the evaluation of MEGAN3 inventories using a regional photochemical model.
Dr. Alex Guenther (Independent Consultant)	Co-Principal Investigator: Lead researcher; responsible for development of the BVOC emission factor database system, calculation of terpenoid emission factors for Texas and surrounding regions, direction of the development of MEGAN3, and contributions to final report
Mr. Tejas Shah (Ramboll Environ)	Project Manager, Ramboll Environ: Responsible for development of emission factor database and update of MEGAN3 code.
Ms. Michele Jimenez (Ramboll Environ)	Develop emission factor database
Dr. Ling Huang (Ramboll Environ)	Develop MEGAN3 model code
Mr. Jeremiah Johnson (Ramboll Environ)	Conduct MEGAN3 and CAMx modeling and perform model evaluation

2.2 Project Schedule

The project schedule is shown in Table 2-2 below. Objectives 1-4 shown in Section 1.2 correspond to Tasks 1-4 in Table 2-1. Task 5 is dedicated to project management and reporting. Project documentation requirements are listed under Task 5.

Table 2-2. Schedule of project activities and deliverables.

Task	Task Name	Task Manager	Duration	2016					2017										
				8	9	10	11	12	1	2	3	4	5	6	7	8	9	10	11
				AUG	SEP	OCT	NOV	DEC	JAN	FEB	MAR	APR	MAY	JUN	JUL	AUG	SEP	OCT	NOV
Task 1	Develop Community BVOC EF Database System	AG/TS	4 mo		■	■	■	■											
Task 2	Terpenoid EFs for Texas and Surrounding Region																		
Task 2.1	Synthesize TX emissions data	AG	4 mo		■	■	■	■											
Task 2.2	Reconcile TX terpenoid emissions data	AG	4 mo			■	■	■	■										
Task 2.3	Calculate TX terpenoid EFs	AG	1 mo							■									
Task 3	Development of MEGAN3																		
Task 3.1	BVOC Emission Response to Stress	AG/TS	6 mo					■	■	■	■	■	■						
Task 3.2	Canopy Environment and Structural Heterogeneity	AG/TS	6 mo			■	■	■	■	■	■								
Task 3.3	Revise Emission Categories/Add New Compounds	AG/TS	3 mo								■	■	■						
Task 3.4	PFT Dependent Emission Traits	AG/TS	3 mo							■	■	■							
Task 3.5	Update Existing Parameters	AG/TS	2 mo						■	■									
Task 3.6	Clarify Existing Code	AG/TS	1 mo					■											
Task 3.7	Update MEGAN Documentation and User's Guide	AG/TS	2 mo											■	■				
Task 4	MEGAN3 Evaluation and Sensitivity Study	JJ/TS/SKC	3 mo									■	■	■					
Task 5	Project Management																		
Task 5.1	Contract, Work Plan, QAPP, Abstract	SKC	2 wk	■															
Task 5.2	Draft and Final Report	AG/SKC/TS/GY	2 mo											■	Draft	Final			
Task 5.3	AQRP Meeting Presentation	AG/SKC/TS/GY	3 wk												■	■			
Task 5.4	Compile and Submit Deliverables	SKC	1 wk														■		
Task 5.5	Monthly Technical Reports	SKC/TS	1 day		■	■	■	■	■	■	■	■	■	■	■	■	■		
Task 5.6	Financial Status Reports	SKC	1 day		■	■	■	■	■	■	■	■	■	■	■	■	■	■	
Task 5.7	Quarterly Reports	SKC/TS	1 day	■			■			■			■			■	■	■	■

3.0 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, MEGAN2.1 (Guenther et al. 2012), 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. 2014, Ghirardo et al. 2016, and reconciling isoprene and monoterpene emission factors (e.g., Emmerson et al. 2016) during the past 5 years will be 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[1]. 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.

3.1 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 Area Index (LAI) of 5 at an above canopy temperature of 30 °C and photosynthetically active radiation (PAR) of 1500 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.

3.2 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

[1] https://www.tceq.texas.gov/assets/public/implementation/air/sip/dfw/dfw_ad_sip_2015/AD/Adoption/DFW_SIP_Appendix_B_060315.pdf

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 development will include additional algorithms to simulate BVOC emission response to stress (high winds, temperature extremes, air pollution) and vertical heterogeneity in isoprene emitting fraction of vegetation. The latter accounts for the tendency of isoprene emitters to occur in either the overstory (under high PAR conditions) or understory (under low PAR conditions). The current emission categories will be revised to add more compounds (e.g., 3-pentanone, 1-penten-3-ol, methyl vinyl ketone, carbon tetrachloride, benzothiazole) and revise the grouping of compounds into categories that have similar atmospheric impacts (e.g., monoterpenes with similar reactivity). The current MEGAN approach of having a constant value of some parameters (e.g., light dependent fraction of monoterpenes) will be modified to account for the observed variability in these parameters for different plant functional types (e.g., tropical forests have a high fraction of light dependent a-pinene emission while most forests in Texas do not). Parameters in the existing MEGAN algorithms, including emission factors and coefficients in emission activity algorithms accounting for response to environmental conditions, will be updated based on recent studies (Kim et al. 2011, Seco et al. 2015, Emmerson et al. 2016 and other studies summarized by Guenther 2013). In addition, the existing code will be clarified with additional comments and code simplification to make it clear and minimize errors.

3.3 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.

Model outputs will remain the same with the exception of the potential to output some additional compounds. 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). If a user chooses to output emissions according to one of these chemical schemes, then there will be no change in the categories of compounds that are output by MEGAN2.1 or MEGAN3. If instead the user chooses to output individual compounds then MEGAN3 will have additional compounds in comparison to MEGAN2.1.

4.0 MODEL CODING

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

4.1 Requirements for Model Code Development

Code development will be directed by a single Ramboll Environ staff member, with input from the lead researcher and assistance from one or two other Ramboll Environ 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 Environ's co-Principal Investigators 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 system evaluation will be conducted by applying the updated model for two existing modeling datasets as described in Section 5.

4.2 Computer Hardware and Software Requirements

MEGAN3 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 MEGAN 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.

4.3 Requirements for Code Verification

We will conduct 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

Commented [CO1]: Is the temporary diagnostic output code intended to check 10% of the data generated? Is the visual inspection (of model inputs and outputs) the 10% check and will it be performed by an independent observer?

Looking to have a clear understanding of what the 10% check is comprised of and how it meets the definition of an audit of data quality defined in the TCEQ QMP as:
An examination of data to determine if the data objectives specified in the QAPP were met for the project. Audits of data quality entail tracing data through the steps of the collection, analysis, interpretation, and reporting processes to identify a clear, logical connection between the steps in the data management system for the project.

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 new MEGAN model will be run and thoroughly evaluated for the SAS field study campaigns (Section 5). ~~Data~~ More than 10% of the output data generated by MEGAN3 will be compared to the output from the MEGAN2.1 version to ensure that design changes result in expected outcomes. More than 10% of the MEGAN3 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 performance 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 assessment of MEGAN3 model performance will be reviewed by a project team member who did not participate in code development or carry out the model performance evaluation.

The Ramboll Environ 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.

5.0 MODEL CALIBRATION

Two models will be used in this study. The MEGAN3 model will be developed as part of the study and a photochemical model will be used as part of the testing and evaluation of MEGAN3.

5.1 MEGAN3

The Model of Emissions of Gases and Aerosols from Nature v3 (MEGAN) will be used to model fluxes of BVOCs. The MEGAN model emission factors will be based on emissions data including the enclosure data that form the basis for the current BEIS and MEGAN emission factors (e.g., Guenther et al. 1994), more recent enclosure and canopy flux tower data summarized by Guenther (2013), and the isoprene and monoterpene flux observations from the 2013 Southeast Atmosphere Study (SAS) study. No further calibration of the MEGAN model will be performed as part of this project.

5.2 CAMx Air Quality Model

The Comprehensive Air quality Model with Extensions v6.30 with IEEE compiler flag (CAMx; Ramboll Environ, 2016) will be used to model atmospheric concentrations of BVOCs. The CAMx model was calibrated for the 2013 modeling episode by Ramboll Environ during the development of the Near Real Time modeling platform (Johnson et al., 2014) and was extensively evaluated during AQRP Project 14-016 (Yarwood et al., 2015). No further calibration of the CAMx model will be performed as part of this project.

6.0 MODEL VERIFICATION

6.1 Approach

The objective of Task 4 is to investigate MEGAN3 model sensitivity and evaluate model emission and ambient concentration estimates using surface and aircraft observations together with a photochemical model. We will carry out emissions sensitivity modelling in support of the Task 2 isoprene and monoterpene emission factor database development and the Task 3 MEGAN3 development. Available isoprene and monoterpene emissions data will be compiled into the emission factor database and member of the research team who did not develop the MEGAN3 model will review at least 10% of the data for quality assurance purposes. Each emission factor will be assigned a quantitative score that represents a measure of the quality of the base data based on the uncertainty associated with the measurement technique, the number of replicates, and quality assurance procedures. The methodology for assigning this score will be developed as a task of this project. Database users will be able to select either the best emission factor estimate, based on the assigned score, or select the full range of emission factor values for a sensitivity study. Emission factors that make relatively large contributions to overall uncertainty in emission estimates can be identified and prioritized for future emission measurements that can be added to the database using the same procedures used for the initial database development. For the domain shown in Figure 6-1, a best estimate inventory will be developed, based on the quantitative scores discussed above, and evaluated with SAS aircraft flux data and concentrations calculated using a photochemical model. The purpose of the evaluation is to constrain the MEGAN3 emissions using the SAS aircraft flux and concentration data together with the photochemical model. The evaluation using aircraft flux measurements, described in section 6.3, will assess MEGAN configurations including alternative emission factor data and model simulations with and without algorithms accounting for individual drivers of BVOC emission variability (e.g., light, temperature, drought, stress, and canopy heterogeneity).

6.2 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). These fluxes will be used to evaluate the MEGAN3 emission inventories developed under Task 3.

On board the NOAA P-3, measurements of VOCs were made both by a custom-built PTR-MS instrument as well as from GC-MS analyses of whole air samples. While the PTR-MS measurements on board the C-130 were focused on determining terpenoid fluxes, the PTR-MS measurements on board the P-3 included a much broader suite of compounds to characterize anthropogenic, biogenic and biomass burning emissions as well as their oxidation products. These data were used to evaluate the photochemical model in AQRP Project 14-016 and will be used for the same purpose here.

The aircraft data used in this project are described in detail in Kaser et al. (2015) and Warneke et al. (2016). 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).

6.3 MEGAN3 Performance Evaluation

We will use C-130 aircraft flux data to evaluate emissions developed with the MEGAN3 model. MEGAN3 emissions will be extracted along the C-130 flight segments for each of the sensitivity test inventories. The MEGAN3 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 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 6-1).

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 model. From the MEGAN3 performance evaluation, we will select the best-performing and/or sensitivity test inventories for evaluation with an air quality model.

6.4 CAMx Model Performance Evaluation

The Comprehensive Air quality Model with Extensions v6.30 (CAMx; Ramboll Environ, 2016) will be used to model fluxes and atmospheric concentrations of BVOCs. The CAMx regional air quality model is an Eulerian photochemical grid model that can be applied over spatial scales ranging from sub-urban to continental. CAMx simulates the emission, dispersion, chemical reaction, and removal of pollutants in the troposphere by solving the pollutant continuity equation for each chemical species on a system of nested three-dimensional grids. The Eulerian continuity equation describes the time dependence of the average species concentration within each grid cell volume as a sum of all of the physical and chemical processes operating on that volume.

We will use the AQRP Project 14-016 2013 CAMx modeling platform (Yarwood et al., 2015), which was adapted from a 2013 Texas ozone forecast modeling application developed by Ramboll Environ 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 6-1).

The 2013 CAMx model was evaluated against surface and aircraft observations of ozone, and ozone precursors during Project 14-016 (Yarwood et al., 2015) and found to be acceptable for the purpose of the project. The model has a high bias for surface ozone that is most pronounced at coastal sites during periods of onshore flow. This suggests that the model is affected by bias in the model boundary conditions for ozone and/or precursors.

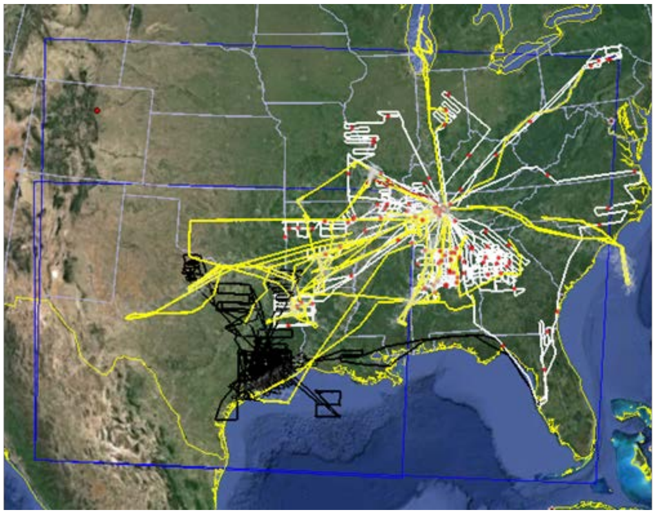

Figure 6-1. CAMx 12 km modeling grid and aircraft flight paths. Aircraft flight paths: SAS C-130 (yellow), SAS P-3 (white), and TEXAQS 2006 (black). TCEQ 12 km grid extent (smaller blue domain), and expanded 12 km grid (larger blue domain).

CAMx will be run from June 1-July 15, 2013 to simulate the period when C-130 and P-3 aircraft data are available. We will use Revision 2 of the Carbon Bond 6 CB6 chemical mechanism (CB6r2) (Yarwood et al., 2012). The Weather Research and Forecasting (WRF) (Skamarock et al., 2008) meteorological model was used in hindcast mode to develop the June-July 2013 meteorological fields required for input to CAMx (Yarwood et al., 2015).

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 emission inventories, we will compare modeled and measured concentrations at the surface and along the C-130 and P-3 aircraft flight tracks. We will evaluate CAMx modelled concentrations against aircraft measurements for the following species: OH, isoprene, 1st generation isoprene products, isoprene nitrates, terpenes, methanol, acetone, ozone and NOx. CAMx modelled NOx and ozone will be also evaluated against surface measurements. The purpose of this evaluation is two-fold:

1. Ensure that the model is functioning as expected and that the meteorological and other inputs are of acceptable quality and have been properly prepared
2. Evaluate the effect of the MEGAN3 emission inventories on model performance

The surface evaluation assesses CAMx model performance in simulating observed ground level ozone and NOx throughout the 12 km grid during the 2013 episode. Within Texas, monitoring data used for the model performance evaluation will come from the TCEQ's Continuous Air Monitoring Station (CAMS) sites. Outside Texas, we will use data from the Clean Air Status Trends Network (CASTNET) monitoring network sites, which are shown in Figure 6-2. We focus on evaluation at rural sites because the model's 12 km resolution may make it difficult to simulate ozone formation in urban areas with sufficient accuracy.

The aloft evaluation will compare CAMx modelled concentrations and fluxes with C-130 and P-3 aircraft data and modelled and observed values will be paired in time and space. The aircraft flight paths were mapped to grid cells within the CAMx 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 fluxes as well as measured concentrations of OH, isoprene, 1st generation isoprene products, isoprene nitrates, terpenes, methanol, acetone, ozone and NOx. Model performance will be stratified with respect to high and low isoprene and NOx regimes where the regime is defined by the observed values. A CAMx run that uses the base-case MEGAN emission inventory prepared with default inputs will be evaluated in this manner, as will CAMx runs that used the new MEGAN3 emission inventories. The performance of the CAMx runs will be compared and the effect of the MEGAN3 inventories on the CAMx model's ability to simulate the aircraft measurements will be determined.

In both surface and aloft evaluations, CAMx 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 the species listed above. Standard statistical metrics as described in EPA air quality modeling guidance (EPA, 2014) will be calculated (Table 6-1).

Consistent with EPA Modeling 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.

Table 6-1. Definition of performance metrics for MEGAN3 and CAMx 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.

For all CAMx runs, we will display the above metrics for CASTNET sites shown in Figure 6-2 and CAMS monitoring sites. The metrics will be applied to hourly model and observed data paired in time and space.

EPA's modelling guidance (EPA, 2014) recommends against the use of bright line tests to evaluate model performance. However, it is useful to place the present model runs within the context of previous modelling efforts. We will compare the value for each metric for the CAMx model runs to the regional air quality model performance metric ranges reported in Simon et al. (2012). We will perform this comparison with the intention of investigating performance rather than using the ranges as a pass/fail test for the CAMx simulations.

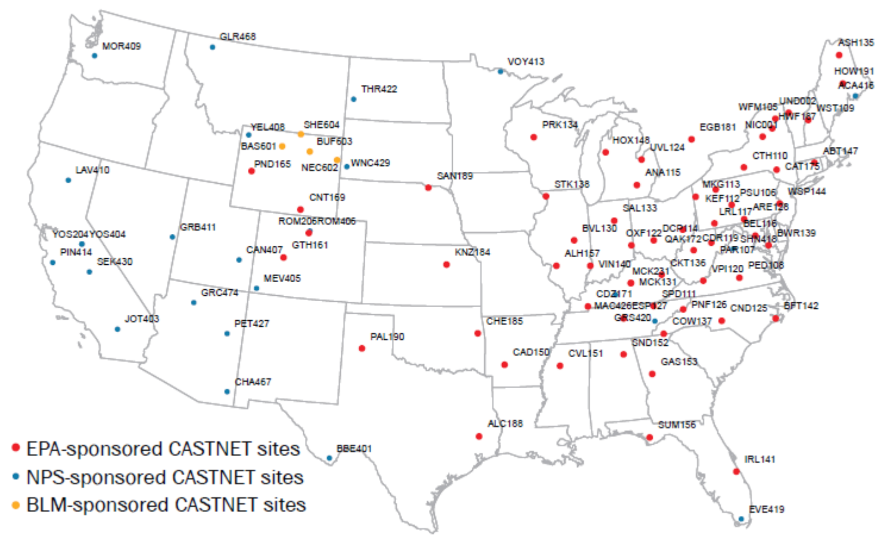

Figure 6-2. Location of CASTNet Sites. EPA figure[2].

The CAMx model performance evaluation will inform the development of MEGAN3. The AQRP Project 14-016 CAMx run using MEGAN2.1 emissions developed with EFvA2015 inputs will serve as a baseline for CAMx model performance in Project 16-011. CAMx performance in simulating measured species using the new MEGAN3 inventories will be compared with CAMx performance in the baseline run. Metrics from Table 6-1 will serve as the basis for comparison of model performance in simulating measurements along the aircraft flight tracks and at the surface.

Configurations of MEGAN3 that cause significant degradation in any of the CAMx performance metrics will be reviewed. For example, a configuration of MEGAN3 that caused the CAMx episode 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 or its inputs should be revised. We do not set targets or criteria for the performance metrics because we recognize that changes in MEGAN3 emissions may cause one aspect of CAMx performance to improve while another aspect worsens. We will consider the CAMx model performance as a whole as we use model performance to constrain the MEGAN3 configuration. All conclusions regarding model performance will be clearly documented in the final report.

[2] https://www3.epa.gov/castnet/docs/CASTNET_Factsheet_2013.pdf

7.0 MODEL 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.

7.1 Assessment Process for Emission Factor Database

A member of the research team who did not develop the MEGAN3 emission factor database and CAMx model input datasets or conduct model simulations will review at least 10% of the emissions data for quality assurance purposes. The Ramboll Environ 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.

7.2 Assessment Process for MEGAN3 Code Development

A member of the research team who did not develop the MEGAN3 model will review at least 10% of the model code for quality assurance purposes. The Ramboll Environ 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.

7.3 Assessment Process for MEGAN3 and CAMx Modeling

A member of the research team who did not develop the MEGAN3 and CAMx 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 Environ project manager will review all results from the MEGAN3 and CAMx model applications using graphical displays of raw model output as well as the model performance evaluation products described in Section 6.4. 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.

8.0 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 MEGAN2.1 description of the availability of input data and procedures for processing these data will be updated to reflect new datasets including those recently developed for TCEQ through AQRP project 14-016.

9.0 REPORTING

9.1 Project Documentation Requirements

The project documentation requirements are listed in Table 2-2. The required documentation is summarized below. The due date for each component of the documentation is shown in Table 2-2 and in Section 9.2.

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.

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 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.

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY16-17 MTR Template found on the AQRP website.

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 AQRP FY16-17 FSR Template found on the AQRP website.

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.

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. The Final Report will also include documentation of the specific quality assurance steps, associated findings, and any necessary corrective actions taken to rectify data quality issues related to the modelling described above.

AQRP Workshop Presentation: A representative from the project will present at the AQRP Workshop in the first half of August 2017.

All reports 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.

Report templates and accessibility guidelines found on the AQRP website at http://aqrp.ceer.utexas.edu/ will be followed.

9.2 Final Project Deliverables

The project deliverables will include all project data including but not limited to QA/QC measurement data, metadata, databases, modeling inputs and outputs, etc., All data will be submitted to the AQRP Project Manager within 30 days of project completion (September 29, 2017). 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.

The documentation deliverables are outlined in Section 9.1 and are listed below. The schedule for all deliverables is presented in Table 2-2.

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: Wednesday, August 31, 2016

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 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.

Quarterly Report Due Dates:

Report	**Period Covered**	**Due Date**
Aug2016 Quarterly Report	June, July, August 2016	Wednesday, August 31, 2016
Nov2016 Quarterly Report	September, October, November 2016	Wednesday, November 30, 2016
Feb2017 Quarterly Report	December 2016, January & February 2017	Tuesday, February 28, 2017
May2017 Quarterly Report	March, April, May 2017	Friday, May 31, 2017
Aug2017 Quarterly Report	June, July, August 2017	Thursday, August 31, 2017
Nov2017 Quarterly Report	September, October, November 2017	Thursday, November 30, 2017

Monthly Technical Reports (MTRs): Technical Reports will be submitted monthly to the Project Manager and TCEQ Liaison in Microsoft Word format using the AQRP FY16-17 MTR Template found on the AQRP website.

MTR Due Dates:

Report	Period Covered	Due Date
Sep2016 MTR	September 1 - 30, 2016	Monday, October 10, 2016
Oct2016 MTR	October 1 - 31, 2016	Tuesday, November 8, 2016
Nov2016 MTR	November 1 - 30 2016	Thursday, December 8, 2016
Dec2016 MTR	December 1 - 31, 2016	Monday, January 9, 2017
Jan2017 MTR	January 1 - 31, 2017	Wednesday, February 8, 2017
Feb2017 MTR	February 1 - 28, 2017	Wednesday, March 8, 2017
Mar2017 MTR	March 1 - 31, 2017	Monday, April 10, 2017
Apr2017 MTR	April 1 - 28, 2017	Monday, May 8, 2017
May2017 MTR	May 1 - 31, 2017	Thursday, June 8, 2017
Jun2017 MTR	June 1 - 30, 2017	Monday, July 10, 2017
Jul2017 MTR	July 1 - 31, 2017	Tuesday, August 8, 2017

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 AQRP FY16-17 FSR Template found on the AQRP website.

FSR Due Dates:

Report	Period Covered	Due Date
Sep2016 FSR	September 1 - 30, 2016	Monday, October 17, 2016
Oct2016 FSR	October 1 - 31, 2016	Tuesday, November 15, 2016
Nov2016 FSR	November 1 - 30 2016	Thursday, December 15, 2016
Dec2016 FSR	December 1 - 31, 2016	Tuesday, January 17, 2017
Jan2017 FSR	January 1 - 31, 2017	Wednesday, February 15, 2017
Feb2017 FSR	February 1 - 28, 2017	Wednesday, March 15, 2017
Mar2017 FSR	March 1 - 31, 2017	Monday, April 17, 2017
Apr2017 FSR	April 1 - 28, 2017	Monday, May 15, 2017
May2017 FSR	May 1 - 31, 2017	Thursday, June 15, 2017
Jun2017 FSR	June 1 - 30, 2017	Monday, July 17, 2017
Jul2017 FSR	July 1 - 31, 2017	Tuesday, August 15, 2017
Aug2017 FSR	August 1 - 31, 2017	Friday, September 15, 2017
FINAL FSR	Final FSR	Monday, October 16, 2017

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: Tuesday, August 1, 2017

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: Thursday, August 31, 2017

Project Data: All project data including but not limited to QA/QC measurement data, metadata, databases, modelling inputs and outputs, etc., will be submitted to the AQRP Project Manager within 30 days of project completion (September 29, 2017). 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. All project data including but not limited to QA/QC measurement data, metadata, databases, modelling inputs and outputs, etc., will be maintained by Ramboll Environ for a minimum of five years after the project ends.

AQRP Workshop: A representative from the project will present at the AQRP Workshop in the first half of August 2017.

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 Subaward.

10.0 REFERENCES

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