AQRP Project 16-011

A Next Generation Modeling System for Estimating Texas Biogenic VOC Emissions

Final Report

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EXECUTIVE SUMMARY

Emissions of reactive gases and particles from terrestrial ecosystems (biogenic emissions) drive atmospheric distributions of several constituents relevant for air quality and climate. Biogenic emissions tend to be 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 strategies for mitigating air pollution and climate change. Biogenic VOC emission estimation activities date back more than 50 years when Dr. Fritz Went made a first attempt to quantify biogenic VOC emissions into the atmosphere. A series of models was developed in the in the US, specifically BEIS, BEIS2, BEIS3, MEGAN and MEGAN2, using a similar framework and base data and yet the results often differed by more than a factor of two (Warneke et al. 2010). The BEIS models were intended to be used for regulatory air quality modeling with fixed landcover and parameters. MEGAN was designed to be more flexible and for use by both regulatory air quality modeling and scientific research. Comparison of these models has been complicated by emission factors, response functions and environmental conditions calculations that were difficult to extract from the models and to determine their origin. A transparent approach for determining emission factors and other variables and a modular approach for evaluating each model component would facilitate efforts to assess and improve biogenic emission models.

The goal of Texas Air Quality Research Program (AQRP) Project 16-011 was to improve numerical model predictions of regional ozone and aerosol distributions in Texas by reducing uncertainties associated with quantitative estimates of biogenic volatile organic compound (BVOC) emissions from Texas and the surrounding region. We aimed to reduce 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 incorporated biogenic emission findings from previous Texas projects into a version of a biogenic model appropriate for Texas air quality applications. Results from previous Texas AQRP projects and other studies were incorporated into a new version 3 of the Model of Emissions of Gases and Aerosols from Nature (MEGAN3).

Our specific objectives included:

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. Include in MEGAN3 missing compounds and unrepresented processes including stress induced (drought, extreme temperature and air pollution) emissions and canopy heterogeneity.

4. Investigate MEGAN3 sensitivity to data used for calculating emission factors and stress induced emission algorithms. Evaluate model emission and ambient concentration estimates using surface and aircraft observations and a photochemical model.

All four objectives were accomplished as summarized by the following:

MEGAN Emission Factor Processor
An Emission Factor Processor for MEGAN3 (MEGAN-EFP) was developed as an open source Python code to ingest driving variables and calculate landscape scale biogenic emission factors and other model drivers. The approach is flexible so that users can use any available landcover and emissions data and can investigate the performance of various datasets. A data quality rating system was implemented so that the user can choose to omit low quality data. The framework was implemented for BVOC emissions, specific leaf area and emission light dependence fraction and can be extended to include other plant and soil traits that can vary spatially. The emission factors calculated with the MEGAN-EFP are highly transparent in that the landcover and emission data that they are based on can be traced back to specific publications.

Texas Isoprene and Monoterpene Emissions Data
High quality enclosure measurements of isoprene emission were available for a large fraction of the tree species that comprise most of the total isoprene emission in Texas and were integrating into the MEGAN-EFP. Utilizing the MEGAN-EFP, it was determined that almost all of the Texas isoprene emitting trees are members of just three genera (oaks, sweetgum, tupelo/gum), all of which have had at least one species investigated with state-of-the-art techniques. The comparison also demonstrated that the differences between BEIS and MEGAN isoprene emission estimates are primarily due to the specific leaf area (the leaf area to leaf mass ratio) estimates and reconciled discrepancies between leaf enclosure and aircraft estimates of isoprene emission factors. The evaluation also indicated that one tree genera, the oaks, are highly diverse with many species in Texas and the surrounding region that have not been studied so the possibility exists that some of these oak species may emit isoprene at substantially different rates than those that have been studied. The assessment also revealed that there are no high quality isoprene emission data for tree species other than the high isoprene emitters in Texas and most other regions. This allows the possibility that some of the tree species thought to be non-emitters may actually have non-zero emission rates.
The available Texas monoterpene emissions data were incorporated into the MEGAN-EFP but there were no high quality enclosure measurements of monoterpene emissions for any Texas trees. Aircraft monoterpene flux measurements were incorporated into the database and currently are the best approach for constraining monoterpene emission factors.

MEGAN3 Model
The MEGAN model code was improved by making the code more modular and easy to follow, by removing unneeded code, by adding additional compounds that may have an important role in air quality and previously unrepresented processes, and by incorporating recent results into the existing algorithms and parameters. Also, an error in the soil NOx emissions code was fixed.

The resulting code, called MEGAN3, provides a modular framework that can be updated as additional knowledge and driving variables become available.

MEGAN3 Sensitivity and Evaluation

A comparison of MEGAN2.1 and MEGAN3, with the emission factors generated by the initial runs of the MEGAN-EFP, indicated that the MEGAN3 isoprene emissions were considerably lower than MEGAN2.1 and in better agreement with aircraft flux and concentration measurements. Within Texas and across the southeastern US, there was a reduction in monoterpene emissions calculated in MEGAN3 relative to MEGAN v2.1 that degraded agreement. Concentration comparisons using the Comprehensive Air quality Model with extensions (CAMx) indicate that estimates of monoterpenes aloft and surface ozone were often considerably lower using the MEGAN3 estimates. For surface ozone, the net effect on model agreement with observations was mixed and varied by site. CAMx underestimated the aircraft monoterpene concentration measurements using MEGAN v2.1 emissions and the underestimate became more pronounced using MEGAN3. The cause of the reduction of monoterpene emissions in MEGAN3 is not known, but is under investigation. Assessment of the new stress algorithms (high temperature, low temperature, high winds, high ozone) incorporated into MEGAN3 indicated that there was relatively little impact on isoprene and monoterpenes using the initial parameterizations. These stresses are expected to have a greater impact on other biogenic VOC.

Below, we list the conclusions of Project 16-011 and recommendations for further work.

Conclusions

- MEGAN3 can be used to provide biogenic emissions estimates that are more accurate than MEGAN2.1 as demonstrated by comparison to aircraft flux measurements. MEGAN3 also facilitates assessing and improving individual model components including emission factors, canopy and soil environment conditions, and response functions which should lead to improvements over alternative models that are based on outdated emission factors and model algorithms.
- The MEGAN3 framework can be used for assessing available landcover and emissions data and identifying gaps. The available landcover and emissions data that were incorporated for the initial database used for this project improved isoprene emissions for the regions investigated by the 2013 SAS aircraft study. Discrepancies between enclosure and aircraft measurements of isoprene emissions pointed out in previous studies were reconciled. Specific Leaf Area (ratio of leaf area to mass) was identified for the first time as a major reason for differences in BEIS and MEGAN isoprene emission estimates. Additional gaps were identified associated with isoprene, such as oak species emission diversity, and especially monoterpene emissions, for which there are few high quality data. Other compounds, including sesquiterpenes, oxygenated VOC, and semi-volatile compounds, may be important but are relatively unstudied.
- Distributions of tree species, the major source of isoprene and monoterpene emissions in Texas, can be adequately estimated with existing landcover data in forested regions.

Additional efforts are needed to improve tree species distributions in urban and savannah locations. This includes integrating all of the existing data into the MEGAN3 landcover database and developing new landcover data such as plant species composition data for non-forested landscapes. Isoprene and other VOC emission studies have focused on closed canopy forests. The performance of models in open canopies in savannas and shrublands, including those that dominate in Central Texas and other regions, has not been well characterized and the existing landcover data, canopy environment and isoprene response functions may not be suitable for these landscapes.

Recommendations for Future Work

- Forests are an important source of monoterpene emissions but the rates remain highly uncertain. High quality measurements of monoterpene emission factors should be conducted to characterize the dominant Texas vegetation. Emission factors for isoprene, including low or zero emissions, and other compounds, including sesquiterpenes and stress compounds, could be estimated by the same study.
- The oaks are a diverse genus and include some European species that do not emit isoprene. The isoprene EF of more of the dominant Texas oaks, including the savannah and shrub oaks that are relatively understudied, should be investigated with high quality measurements to quantify any within-genera variation.
- High quality measurements of isoprene emissions should be used to characterize at least one species in all dominant genera of Texas trees in order to identify non-emitters. If these measurements are not available then existing data, even low quality data that identifies plants as non-emitters should be used to assign a zero isoprene emission rate to these plants.
- The MEGAN3 stress-induced emission algorithms should be used to investigate the sensitivity of air quality model results for cases where stress events are suspected of impacting emissions. If these indicate air quality simulations are sensitive to stress-induced emissions, then additional studies should be conducted to improve the current parameterizations.
- Soil NO emissions are important in agricultural areas of Central Texas. Improved crop landcover and nitrogen fertilizer rate distributions should be incorporated into the MEGAN emission factor processor.
- Sub grid scale heterogeneity of highly reactive VOC may be important for quantifying ozone and PM and for effective comparisons of modelled VOC concentrations with TCEQ auto-GC data and should be investigated with field measurements of ambient concentrations and emission sources.
- BVOC concentrations in shrub and savannah regions, such as the Edwards plateau, should be measured to determine if these regions are a significant source of terpenoid emissions. If they are, then improved landcover and emissions data should be obtained for these landscapes along with an improved canopy environment model and canopy depth emission algorithm suitable for open canopies.

- Further development and testing of MEGAN3 is recommended, including integration of additional MEGAN-EFP landcover and emissions data especially non-tree landcover and compounds other than isoprene and monoterpenes.

1.0 INTRODUCTION

This document provides the final report for the Texas Air Quality Research Program (AQRP) Project 16-011, "A Next Generation Modeling System for Estimating Texas Biogenic VOC Emissions". The project Co-Principal Investigators (Co-PIs) are Dr. Greg Yarwood and Dr. Susan Kemball-Cook of Ramboll Environ and Dr. Alex Guenther. The AQRP project manager is Dr. Elena McDonald-Buller at the University of Texas, Austin. The project liaison for the Texas Commission on Environmental Quality (TCEQ) is Mr. Doug Boyer.

The overall goal of Project 16-011 was to improve numerical model predictions of regional ozone and aerosol distributions in Texas by reducing uncertainties associated with quantitative estimates of biogenic volatile organic compound (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. In this project, we developed new emission factors and incorporated missing BVOC compounds and unrepresented BVOC emission processes into the Model of Emissions of Gases and Aerosols from Nature (MEGAN) framework. To accomplish this, we developed a transparent and comprehensive approach to assigning isoprene and monoterpene emission factors and updated MEGAN to include additional BVOC and processes including stress induced emissions and canopy heterogeneity. We evaluated MEGAN BVOC emission inventories for Texas and surrounding regions using surface and aircraft observations and a photochemical model.

The overall benefit of this project is more comprehensive 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.

1.1 Background

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 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.

1.2 Overview of Approach

The project aimed 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 incorporated biogenic emission findings from previous Texas projects into a version of a biogenic model appropriate for Texas air quality applications. This was 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 included:

5. Develop a database system that provides a transparent approach for estimating BVOC emission factors.
6. 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.
7. 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.
8. Investigate MEGAN3 model sensitivity and evaluate model emission and ambient concentration estimates using surface and aircraft observations and a photochemical model.
9. Prepare recommendation as to whether MEGAN inputs developed in 3 and 4 above should be used in future TCEQ modeling.

1.3 Overview of Report

In Section 2, we describe the development and application of a transparent approach for estimating BVOC emission factor distributions. In Section 3, we report on our efforts to synthesize, reconcile and calculate isoprene and monoterpene (terpenoid) emission factors for Texas and the surrounding region. Section 4 describes the development of the MEGAN3 model. In Section 5, we provide an overview of the evaluation of MEGAN3 emissions against emission fluxes derived from SAS aircraft measurements. Section 5 also presents the photochemical modeling with default and updated MEGAN emission inventories and evaluation of modeled concentrations against surface and aircraft measurements. In Section 6, we present conclusions and recommendations for future work. Finally, Section 7 contains results of the data quality audits.

2.0 TASK 1: A TRANSPARENT APPROACH FOR ESTIMATING BVOC EMISSION FACTOR DISTRIBUTIONS

2.1 BVOC Emission Factor Estimation Approach

MEGAN calculates biogenic VOC emission rates as the product of an emission factor and an emission activity factor, similar to the approach used for anthropogenic VOC emission estimates (Guenther et al. 2012). BVOC emissions research has focused mostly on the identification and quantification of processes controlling variations in emission activity, which is not surprising since these studies are typically conducted with the intent to publish in the scientific literature and studies focused on emission factors are often considered relatively mundane and may be difficult to publish in leading journals. Yet it is clear that uncertainties in emission factors are an important contribution and may even dominate the total uncertainty in BVOC emission rate estimates (Arneth et al. 2011, Guenther 2013). The task of synthesizing relevant observations and compiling emission factors is challenging, due to the diverse measurement approaches and the immense biological and chemical diversity of BVOC, and up to now this has been accomplished through a relatively opaque process. As a result, it has been nearly impossible to determine the basis for the various emission factors that are widely used for regulatory and scientific BVOC emission modeling.

Initial attempts to adopt a systematic approach for synthesizing BVOC emission data, e.g., Benjamin et al. 1996, led to unsatisfactory results due to limited data availability and because of unrepresentative measurements. For example, the Benjamin et al. isoprene emission factors for some California oak trees were set to extremely low values based on a single study, since that was the only study reporting emissions data for that species, consisting of one or a few measurements using a technique which did not provide representative emissions. While there are too few measurements, and many of those may be unrepresentative, for BVOC emissions from most plants, there is a growing need for a more flexible and transparent method for estimating BVOC emission factors. Ideally, this will be an approach will engage and guide the measurement community to provide suitable emissions data. As shown below, the Model of Emissions of Gases and Aerosols from Nature Emission Factor Processor (MEGAN-EFP) has been developed in response to this need. As shown below, the MEGAN-EFP can be successfully used to improve emission factors for well-studied compounds, as is currently the case for isoprene in the U.S., but there will be limited advances for other compounds until additional suitable measurements are made. It is hoped that the introduction of the MEGAN-EFP will be useful for developing measurement strategies for improving emission factor estimates of other BVOC. This can be accomplished by enabling users to determine what measurements went into each emission factor in order to identify the measurements that will lead to improvements by targeting the ecosystem components that dominate total emissions and are relatively understudied or based on conflicting results. This will also aid in assessments of uncertainties. Open source software and code were used to develop the database system which will be freely available to the regulatory and scientific communities. The database is expected to be expanded as a community effort that will improve the accuracy of widely available emission factors. The community will be engaged primarily through the MEGAN website (bai.ess.uci.edu/megan) and outreach activities such as the recent (August 2017) MEGAN training course at the University Nacional of Colombia (attended by more than 50 participants).

The MEGAN-EFP is built on the Python programming language as an open source program designed to be widely used by the regulatory and scientific communities. The approach enables users to generate the leaf level emission factor and light dependence data required to drive MEGAN3. While users can use the landcover input data available from global files available on the MEGAN3 website, the strength of this approach is that it provides a capability for users to process their own landcover and emissions data and assess the quality of the data available for representing BVOC emission factors in their region of interest. They can then consider improving these data, either through literature search or by making additional measurements, based on the MEGAN-EFP guidance on the most important plant species to target. Each emissions measurement is assigned a number from 0 to 4, called the J-rating, to indicate the quality of the data. A J-rating of 0 indicates the lowest quality including qualitative measurements and measurements conducted with methods that have high uncertainties and potentially strong bias. A J-rating of 4 is the highest quality data indicating methods that meet the recommendations of the BVOC emission measurement community (Niinemets et al. 2011). While we have made an initial framework for assigning other J-ratings, we recommend that the BVOC emission measurement community work together to develop an agreed on J-rating scheme. MEGAN-EFP allows users to choose to use all data or just measurements higher than a specified minimum J-value. In the following sections we refer to emission factors based on j=0 data, meaning data with J-rating of 0 or greater which results in using all data, and emission factors based on j=4, which means only data of the highest quality.

The MEGAN-EFP synthesizes leaf level plant trait data, including BVOC emission factors (EF), specific leaf area (SLA) and emission light dependence factor (LDF), with landcover data, including ecotype and growth-form fractions for each location in a modeling domain. Additional information required includes descriptions of biogenic compounds, emission classes, publication references, vegetation types, and canopy vertical distribution characteristics. The framework is illustrated in Figure 2-1. Instructions for running the code and details on the input files and variables are described in the MEGAN EFP user guide. The input data can be created from global files available on the MEGAN web site or can be created by the user.

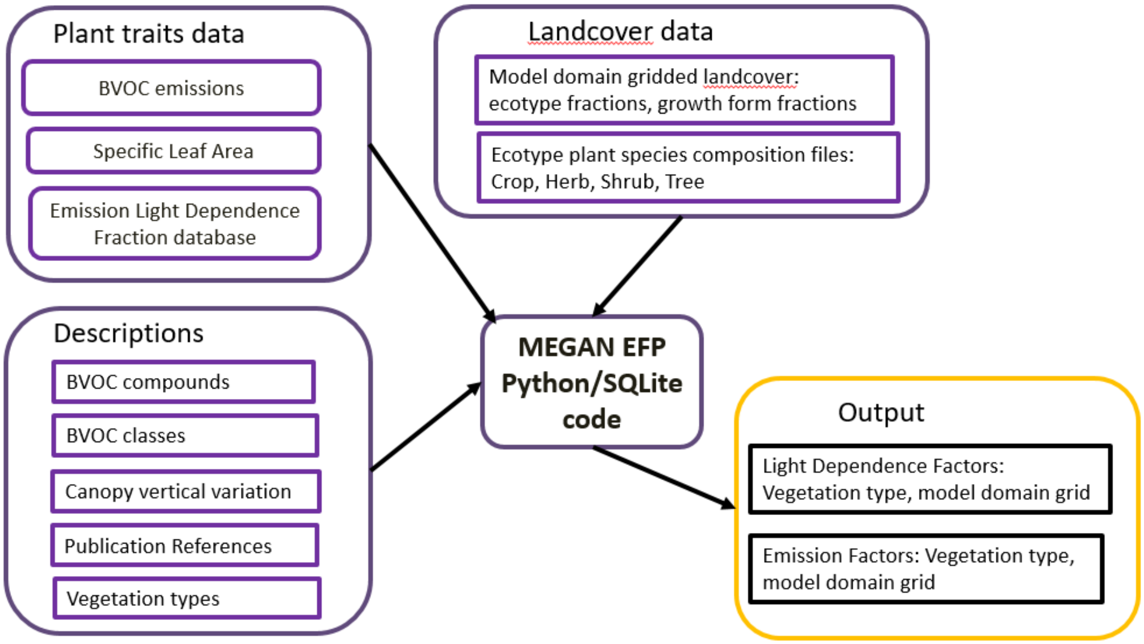


Figure 2-1. Schematic of the MEGAN-EFP input and output data.

A summary of each dataset associated with each of the three main input components is given in sections 2.2.1, 2.2.2, and 2.2.3.

2.2 Plant Traits Data

2.2.1 BVOC emissions data

The MEGAN-EFP currently includes over 10,000 biogenic emissions measurements from more than 200 studies. There are many other measurements published in the literature and the database will be extended in the future and is expected to guide and motivate new measurements that can fill gaps in the existing database.

About half of the isoprene and monoterpene emissions data in the MEGAN-EFP are from studies that were conducted during the decades between 1960 and 2000 and are referred to here as the Twentieth Century Emissions Database (TCED). The TCED is a synthesis of emissions measurements that include qualitative data, often only indicating whether a plant species emits or does not emit isoprene or total monoterpenes, or are highly uncertain and do not follow the protocols considered necessary to obtain high quality data as described by Niinemets et al. (2011). All TCED data are considered highly uncertain, and are assigned a J-value of 0. The TCED data are included in the MEGAN-EFP because in many cases they are the only data available for a plant genus or even an entire family. This is not surprising since if these earlier studies reported that some plant genera, such as maple, does not emit isoprene then later studies using high quality techniques (j=4) would be unlikely to consider it important to make or report measurements in these plants.

While there are more than 280 tree species in Texas and the surrounding region, defined here as 24° - 36° N latitude; 90° - 105° W longitude, just 10 species comprise about half of the total tree cover including three pines: *Pinus elliotii* (slash pine), *P. taeda* (loblolly pine), *P. echinata* (shortleaf pine), four oaks: *Quercus virginiana* (live oak), *Q. stellata* (post oak), *Q. nigra* (water oak), and *Q. falcata* (southern red oak) along with *Liquidambar styraciflua* (sweetgum), *Nyssa sylvatica* (black tupelo), and *Acer rubrum* (red maple). An additional 12 tree species comprise another 20% of total tree cover including additional pine, oak and gum species as well as *Taxodium* (bald cypress), *Juniperus* (juniper), *Liriodendron* (tuliptree), *Fraxinus* (ash), *Carya* (Hickory) and *Magnolia* species. Most of these species, and all of the genera, have been characterized by measurements included in the MEGAN-EFP. However, most of the measurements are low quality (J=0) data from the TCED. The exception is that there are high quality (J=4) isoprene emission measurements (Geron et al. [2001], Geron et al. [2016], Potosnak et al. [2014], Harley et al. [1996], Harley et al. [1997], Guenther et al. [1996], Lahr et al. [2015], Guenther et al. [2017]) available for most of the major isoprene emitters. The isoprene emission rates tend to be around 24 nmol/m^2/s for sweetgum and tupelo trees and around 34 nmol/m^2/s for oaks.

There are J=1 quality monoterpene emission data for three of the dominant species (loblolly pine, slash pine and red maple) reported by Yang et al. (2001), Kim et al. (2001), and Ortega et al. (2007). All of the other monoterpene data for trees in Texas and the surrounding region have a J-rating of zero indicating that monoterpene emissions are highly uncertain.

2.2.2 Specific Leaf Area (SLA) data

MEGAN3 emission factors are leaf-level emissions with a per area emission rate and units of nmol compound per m^2 leaf area per second. All high quality (J=4) BVOC emissions data include emissions reported on both per leaf area and per leaf mass basis so SLA (specific leaf area = leaf area per unit leaf mass) is not needed to calculate MEGAN3 emission factors. However, all of the TCED data, and many other J<4 measurements, are reported only as per-mass emissions, and so SLA (leaf per leaf mass) is required for converting these data to per-area emissions. Note that SLA is the inverse of specific leaf mass (leaf mass per unit leaf area) which is sometimes reported in the BVOC literature. We use SLA (cm^2 per gram) in MEGAN-EFP because this is more widely used by the plant trait community which has efforts underway to compile SLA measurements into global plant trait databases.

The MEGAN-EFP SLA database currently contains >180 measurements from >20 studies characterizing >160 plant species. The reported values range from 27 to 592 cm^2/g. The average SLA for the dominant isoprene emitting Texas trees (oaks, sweetgum and tupelos) is 81 cm^2/g for sun leaves. However, SLA is not constant within a canopy but typically decreases considerably from leaves in the top to the bottom of the canopy (Harley et al. 1997). The MEGAN-EFP SLA database includes an estimate of canopy position and adjusts the SLA to get a canopy average value. Accounting for this adjustment, the canopy average SLA for these isoprene emitters is about 95 cm^2/g.

The SLA data currently in the MEGAN-EFP represent only a small fraction of all plants. In order to calculate emissions of plants for which no SLA data are currently available, default SLA values are provided for each major plant type divisions.

2.2.3 Light Dependence Factor (LDF) Data

Earlier BVOC emission models assumed that isoprene emissions were completely light dependent while emissions of monoterpenes were totally independent of light. The discovery of light dependent emissions of some monoterpenes and sesquiterpenes led to the introduction of a light dependence factor in MEGAN2.1 that allowed all compounds to have both light-dependent and light-independent components defined by a light dependent fraction (LDF). This was implemented in MEGAN2.1 with an LDF that was constant for a given compound for all plant species. This was inconsistent with observations which indicate that LDF for a single compound can vary from 0 to 1 for various plant species. In particular, the LDF for some monoterpenes is close to 1 for some Mediterranean and most tropical trees but is relatively low for many temperate species including the dominant trees in Texas. MEGAN3 provides an approach to accurately represent LDF variations. However, it is currently limited by the lack of observations for populating the database. The LDF database currently includes relatively few measurements and LDF for most plants is set by default values for each plant division which still is an advancement over having a single value for all plants.

2.3 Landcover Data

The MEGAN-EFP requires three types of landcover data: the fraction of each ecotype, the fraction of each Growth Form, and the vegetation type relative composition for each combination of ecotype and growth form. Growth forms are limited to five types (angiosperm trees, gymnosperm trees, shrubs, forb/grass, crops) that can be relatively easily determined using satellite remote sensing and are available at high resolution (30 m to 1 km). The ecotypes can be based on any landcover scheme, including the default scheme provided in the MEGAN data portal or any other scheme developed by users. An example of the default MEGAN database is shown in Figure 2-2 with a 30 meter resolution landcover database identifying ecotype distributions and the fraction of each growth form. Each combination of ecotype and growth form is associated with a specific plant species composition that can characterize the distributions of individual plant species at 30 m resolution. The MEGAN-EFP database includes more than 42,500 vegetation types. This includes about 42,000 species and sub-species and about 500 landscape types. This approach provides the flexibility to assign emissions to landscape type (e.g., tropical rainforest) for locations where plant species distributions are unavailable. This will be the approach required for much of the world outside of the US where species composition data is unavailable.

Landcover data for the contiguous US is based on an updated version of the Yu et al. (2017) growth form and ecotype distribution data. MEGAN2.1 landcover data are used for Mexico and Canada. These landcover data are expected to work well for rural areas but may not be suitable for urban landscapes. Urban forest survey data that are available for Texas and other regions should be incorporated into the MEGAN3 landcover.

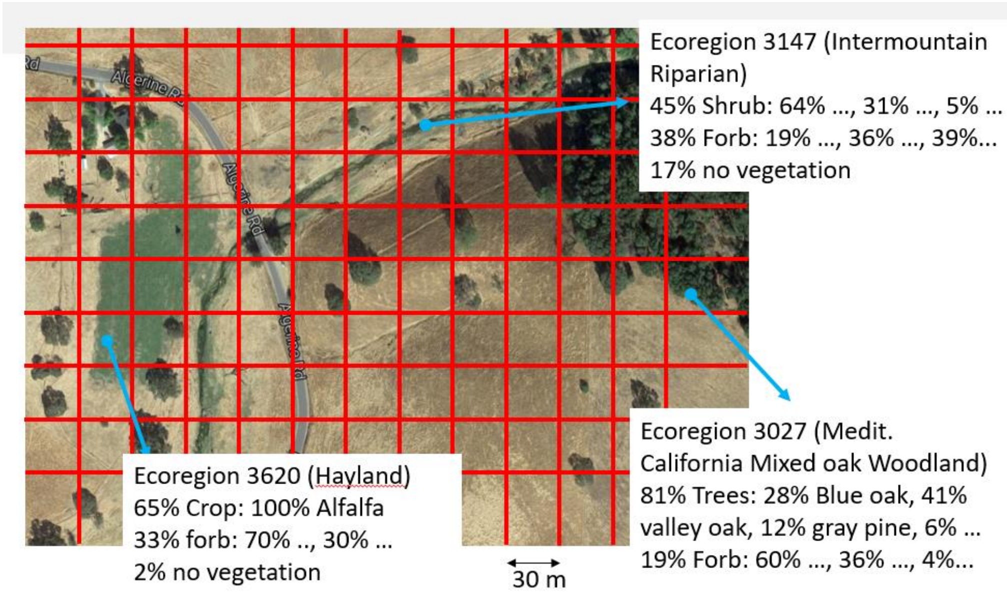


Figure 2-2. Image illustrating MEGAN-EFP landcover data used to characterize distributions of individual plant species.

2.3.1 Growth Form Cover Fraction

The MEGAN3 growth form data (fraction of gymnosperm tree, angiosperm tree, shrub, forb/grass, crop and non-vegetated) for the contiguous US are based on National Land Cover Data (NLCD) data with 30-m resolution as described by Yu et al (2017). The NLCD provides quantitative tree cover fraction. For the other growth forms, Yu et al. assigned estimated breakdowns based on the ecotype. Upcoming NLCD data will provide quantitative shrub and grass cover fractions that can be included in future MEGAN3 landcover.

2.3.2 Tree species composition

MEGAN 2.1 tree species composition was based primarily on field measurements at ~103,000 USFS Forest Inventory Analysis (FIA) measurement plots located in forests and woodlands across the US with some additional measurements for Texas woodlands that were not surveyed by FIA. The measurements were from the early 1990s or even earlier. Although there were more recent FIA data, the exact locations of the plots were not available due to privacy rules and so were not used. In addition to being outdated (i.e., describing composition of forests from more than two decades ago), MEGAN2.1 averaged the data over landscapes that were not homogeneous. The approach averaged FIA data over 967 ecoregions in the contiguous US using the level IV ecoregion scheme described by Omernik and Griffith (2014). Examples include ecoregions “21c: Crystalline Mid-Elevation Forests” covering extensive areas on the eastern side of the Southern Rocky mountains dominated by aspen, ponderosa pine, Douglas-fir, lodgepole pine and limber pine, “6b: Northern Sierran Foothills” along the west side of the Sierra Nevada Mountains with chaparral, oak and pine woodlands, and “35a: Tertiary Uplands, South Central Plains” known locally as the “piney woods that were historically oak and pine woods and are now extensively covered by pine plantations”. The number of FIA plots in each ecoregion ranged from 0 to 2,152. About 200 ecoregions had > 150 plots, ~275 had 25 to 149 plots, ~300 had 1 to 24 plots and ~200 ecoregions had no FIA plots. In general, the ecoregions with no or few plots have no or little tree cover. Average tree species composition was estimated for each of the 775 US ecoregions that had one or more FIA plots. This provided an average tree species composition over the spatial resolution of the ecoregions, typically tens of kilometers, but could not capture the heterogeneity at higher resolution within the ecoregions. For example, the tree species compositions estimated for ecoregion 21c (30% Ponderosa pine, 22% Douglas-fir, 15% aspen, 13% lodgepole pine, 4% Engelmann spruce, 16% comprised of another 15 tree species), ecoregion 6b (29% interior live oak, 28% blue oak, 11% Ponderosa pine, 11% gray pine, 7% canyon live oak, 6% California black oak, 3% willow, 5% comprised of 5 other tree species), and ecoregion 35a (36% loblolly pine, 14% sweetgum, 10% shortleaf pine, 6% southern red oak, 4% water oak, 4% post oak, 3% white oak, 3% comprised of 17 other oak species, 2% black tupelo and another 18% comprised of 61 other tree species) may be a reasonable representation of the ecosystem average composition, but the various landscapes within each ecoregion can differ dramatically. For example, ecoregion 21c has some landscapes that are almost pure Ponderosa pine while others are almost entirely aspen. Both ecoregion 6b and ecoregion 35a have some areas that are oak dominated while others are pine dominated.

To improve the representation of higher resolution spatial variability, and to introduce more recent FIA plot data, a new tree species composition database was developed using the LANDFIRE Existing Vegetation Type (EVT) landcover scheme and the LANDFIRE reference database plot data. The LANDFIRE landcover scheme includes 849 ecosystem types and uses 30-m satellite data, calibrated using field observations, to characterize high spatial resolution variability of US landscapes. For example, within Ecoregion 21c, there is a mosaic of EVT types including “3054: Southern Rocky Mountain Ponderosa Pine Woodland” dominated by 75% ponderosa pine, EVT “3061: Inter-Mountain Basins Aspen-Mixed Conifer Forest and Woodland” dominated by 42% aspen, 12% sub-alpine fir, and 10% douglas-fir, EVT “3011: Rocky Mountain Aspen Forest and Woodland” with 84% aspen, and EVT “3135: Inter-Mountain Basins Semi-Desert Grassland dominated by Juniper trees (44%). Within ecoregion 6b and ecoregion 35a are some EVT types dominated by oaks and others dominated by pine including pine plantations. The LANDFIRE reference database plot data are directly associated with the LANDFIRE vegetation types minimizing errors introduced in matching the plot data locations to the vegetation type.

2.3.3 Other Growth Form Species Composition

The US Natural Resources Conservation Services (NRCS) conducts soil surveys across the US with high spatial resolution. In addition to soil characteristics, some information on potential vegetation was included for a subset of soil map units and this information was used to define MEGANv2.1 grass and shrub species composition. Since these data are potential vegetation, rather than actual vegetation, some biases were introduced due to landcover change and invasive species in some regions. In addition, the grass and shrub data were missing in many regions. An assessment of the shrub and grass species composition indicated that these data were not representative of the actual grass and shrub distributions. There are very few emission measurements for shrub and grass species and those that are included in the emissions database have very little overlap with the NRCS shrub and grass species. For this reason, the available NRCS shrub and grass species composition data is not useful and so has not been included in the MEGAN3 landcover data. The NLCD is developing a shrub fraction and grass fraction product that is a substantial improvement. This will be integrated with accurate species composition data and incorporated into the MEGAN landcover when available, dependent upon funding. The NASS CROPLAND database does provide the data necessary for assigning crop species distributions but there are few emission measurements to combine with this crop data. The current MEGAN3 landcover data does not include the NASS crop data but this will be included in future efforts, dependent upon funding.

2.4 BVOC Emission Factor Database Deliverables

The python code, six landcover databases (ecotype and growth form distributions and four plant speciation databases), three measurement databases (EF, SLA, LDF), five descriptive databases and the user guide will be delivered directly to TCEQ and will be available to download for the rest of the community on the MEGAN Data Portal (bai.ess.uci.edu/megan). In addition, the data portal includes templates for the community to prepare data for submission to the database in a predefined format.

3.0 TASK 2: SYNTHESIS, RECONCILIATION AND CALCULATION OF ISOPRENE AND MONOTERPENE EMISSION FACTORS FOR TEXAS AND THE SURROUNDING REGION

3.1 BVOC emissions data

Less than half of all plant species emit substantial amounts of isoprene, but those that do emit isoprene emit at such high levels that isoprene is the dominant BVOC emission in most landscapes including many parts of Texas (Guenther et al., 2006). Monoterpene emission capacity is more widespread but enclosure measurements suggest that there is still considerable variation in the capacity of various plant species to emit. Low and high emitters can occur within the same plant family or even genera making the quantification of emission factor distributions a challenging task. However, since trees are the major source of terpenoid emissions from forest and woodland ecosystems, the task is simplified in regions such as East Texas where there are relatively few tree genera that dominate the contribution to the total terpenoid emission. We have compiled the observations available for assigning terpenoid emission factors in Texas and the surrounding region and reconciled those observations. We have also assessed the importance of each plant genera/species and ecoregion in Texas to determine the major gaps in knowledge of terpenoid emission from specific types of Texas vegetation.

Isoprene, monoterpene, SLA and LDF observations for Texas and the surrounding region have been compiled into the MEGAN-EFP system. This includes enclosure measurements and above canopy flux measurements. A J-value indicating measurement quality was assigned to each observation based on the number of measurements, the measurement approach and protocols used. Using the MEGAN-EFP with the compiled observations, a range of emission factor estimates were calculated including emission factors based on all data as well as emission factors based on a subset of these data (e.g., only high quality data). The resulting EF estimates can be used for sensitivity studies to consider how the uncertainty in BVOC emission factors impact air quality simulations. The emission factors have also been compared with those used in the BEIS and MEGAN2.1 and evaluated by comparison with results from different measurement approaches (e.g., enclosure, aircraft, tower fluxes).

Geron et al. (2001) showed that much of the reported variability among isoprene-emitting broadleaf tree species (e.g., *Quercus, Liquidambar, Nyssa, Populus, Salix*, and *Robinia* species) can be attributed to weather, plant physiology and the location of a leaf within the canopy rather than genetics. One implication of this finding is that the observations reported from many earlier studies, where these factors were not considered, are highly uncertain (low J value) for the purpose of assigning emission factors. This includes bias in estimates of light and temperature (Guenther et al. 2012), inconsistencies in canopy environment models that can result in differences of more than 35% (Guenther et al. 2006), unrepresentative measurements (Guenther et al. 1994), and other factors (Arneth et al. 2011). We have considered both differences in emission factors reported for similar techniques as well as differences in emission factors determined from measurements on various scales (enclosure, aircraft).

3.2 Isoprene Emissions Factors (EF)

BEIS3 and MEGAN2.1 both assume that all broadleaf trees that emit isoprene (e.g., oaks, poplars, sweetgum, sycamore) have a single EF. The same pool of emissions data was used to develop the single broadleaf tree isoprene EF for BEIS3 and MEGAN2.1 so it is somewhat surprising that the canopy EF is so different with a MEGAN2.1 canopy EF that is about 83% higher than the BEIS3 value. The major difference is not be the per mass EF but the SLA used to convert mass based EF measurements to canopy scale EF. BEIS3 assumes broadleaf trees have an SLA of 133 cm^2/g while MEGAN2.1 EF assumes that broadleaf tree SLA is 80 cm^2/g. After accounting for this 66% difference due to SLA, the MEGAN2.1 and BEIS3 isoprene emission factors agree within 13%. SLA varies considerably for different tree species and the use of a single SLA for all trees can result in significant errors. Our assessment of SLA measurements indicates that SLA of 10 most abundant Texas isoprene emitting tree species range from 65 cm/g (Quercus nigra) to 117 cm/g (Poplars) with an average value of 82 cm/g. This value is similar to the average SLA used for MEGAN2.1.

We have calculated “equivalent” leaf-level per-area ($nmol/m^2/s$) emission factors for BEIS3, MEGAN2.1 and for available leaf-level and aircraft flux data. As shown in Figure 3-1, most of the measurements fall between the values for BEIS3 (24 nmol/m2/s) and MEGAN2.1 (44 $nmol/m^2/s$). The BEIS3 value is similar to the average EF for all Texas isoprene emitters when all measurements, low and high quality, are used. When only higher quality data are used (J=4), the value for gums (Liquidambar and Nyssa species) is still close to this value but southeastern US oaks are about 40% higher. Aircraft based estimates of leaf level emission factors agree remarkably well with the higher quality (J=4) enclosure data. The southeastern US aircraft based EF is 18% lower than the value used for oaks by MEGAN2.1. Aircraft and enclosure based measurements of California oaks, however, are 45% higher than the MEGAN2.1 EF. This indicates the importance of assigning EF to individual species or at least regional values.

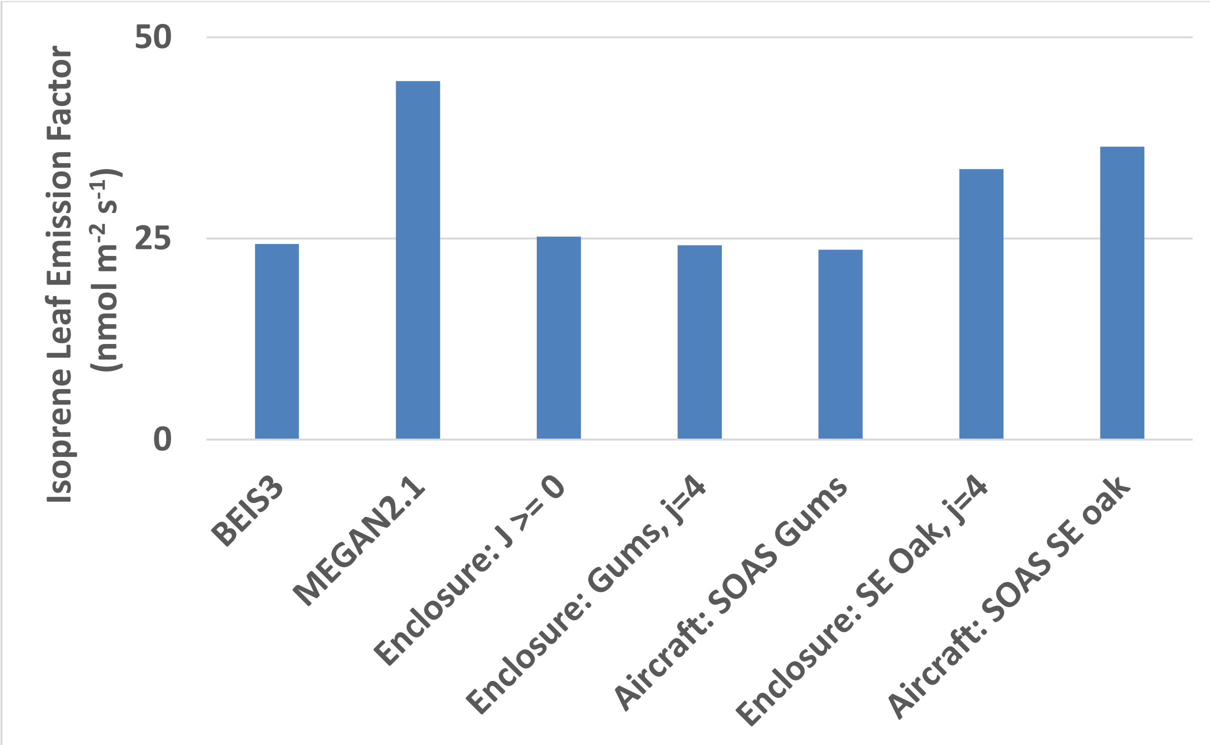


Figure 3-1. Isoprene emission factors for BEIS3, MEGAN2.1 and from enclosure and aircraft measurements.

3.3 Monoterpene Emission Factors

Unlike the single emission factor used for isoprene emitting trees, BEIS3 and MEGAN2.1 assign a range of values for monoterpene emitting plant species recognizing that most trees can emit some monoterpenes but some have more of a tendency to emit at high rates. The assignment of monoterpene emission factors is much more challenging than for isoprene due to the strong influence of stress on some monoterpene emissions. This leads to two issues that make it difficult to use enclosure measurement data to establish monoterpene emission factors: 1) various types of stress have a strong influence on monoterpene emission rates but this is not accounted for in emission rate studies, 2) the process of enclosing a leaf or branch can substantially increase the monoterpene emission rate from plants that have external monoterpene storage structures. The impact of the first issue (unknown stress levels) is that studies with only a few measurements are not likely to be representative of the population average. The individual selected for measurement could be much higher or lower than the population average if it happens to have a low or high level of stress. The impact of the second issue (enclosure disturbance) is expected to bias enclosure emission measurements by artificially increasing the measured emission rate. It has been argued that this can be overcome by placing the plant in an enclosure and then making measurements for several days afterwards (Ortega et al. 2008). However, there remains the possibility that this approach will underestimate emissions due to the loss of monoterpenes from the storage structures during the disturbance that occurs when the enclosure is placed on the plant. This “careful measurement" approach suggests that some plants previously thought to be high emitters, such as Eucalypts and Pines, may have much lower emissions than indicated by the EF used in current models. However, this suggestion does not agree with above canopy measurements that demonstrate that Eucalypt and Pine forests have substantial ambient monoterpene concentrations in the air within and above the canopies.

As discussed above, some of the lower quality (J=0) data are expected to have a bias towards overestimating monoterpene emissions and thus the use of these data, rather than just the highest quality (J=4) data, tends to result in higher monoterpene EF. In comparison with above canopy flux measurements, which minimize the errors due to the two issues discussed above, the higher quality enclosure data are similar for "high-emitters" such as pines but are low for other vegetation. This may indicate that the enclosure measurement approach has underestimated emissions from "low-emitters" by not including stressed vegetation.

The MEGAN-EFP approach can only work if there are enough suitable and reliable measurement data available for a BVOC emission from a specific plant type. Our assessment suggests that this is currently not the case for monoterpenes and other BVOC except for isoprene. At present, it is recommended that the above canopy aircraft flux measurements be used to assign monoterpene EF magnitude. We conclude that the existing monoterpene measurements cannot be used to establish accurate monoterpene EF and a substantial effort is needed to determine EF by applying a better measurement strategy for determining monoterpene emission factors.

3.4 Isoprene and Monoterpene Emission Factor Data Deliverables

Emission factors for isoprene, 5 monoterpene categories and 14 other emission categories have been calculated for 12 km and 36 km domains used for simulating BVOC emissions and air quality in Texas. Multiple emission factors datasets have been generated to demonstrate the range of values associated with the use of all observations or a subset of high quality data.

4.0 TASK 3: DEVELOPMENT OF MEGAN3

4.1 MEGAN3 Background

During the latter half of the twentieth century, BVOC emission estimates have progressed from a simple calculation based on a single measurement (Went, 1960) to compilations of enclosure measurements and regional landcover and weather data in the early 1980s (Zimmerman 1979; Winer 1982). The first EPA biogenic emission model, the Biogenic Emissions Inventory System (BEIS, Pierce and Waldruff, 1991) was adapted from the Lamb et al. (1987) approach developed for acid rain model simulations. The second version of the model (BEIS2), released in the mid-1990s, predicted dramatically higher (about a factor of five) estimates of isoprene emissions (Pierce et al. 1998) and differed in other aspects including leaf level emission algorithms, biomass densities, and landcover distributions. BEIS3 was developed in 2001 and designed for use with the Sparse Matrix Operational Kernel Emissions (SMOKE) emissions system for the Community Multiscale Air Quality (CMAQ) modeling system. BEISv3.6.1 is the latest version and has two main updates: the use of leaf temperature instead of ambient temperature and a new landcover database (Biogenic Emissions Landuse Database, version 4; BELD4). The MEGAN model, developed as a collaborative effort between USEPA and the NSF sponsored National Center for Atmospheric Research (NCAR), was based on BEIS3. It was built to be more flexible and is widely used for scientific studies as well as regulatory activities in nations around the world. The MEGAN2.1 update was released in 2011 and included additional compounds, source types, and emission processes (Guenther et al. 2012). We describe here a new version, MEGAN3, that includes the updates and enhancements illustrated in Figure 4-1 and described below.

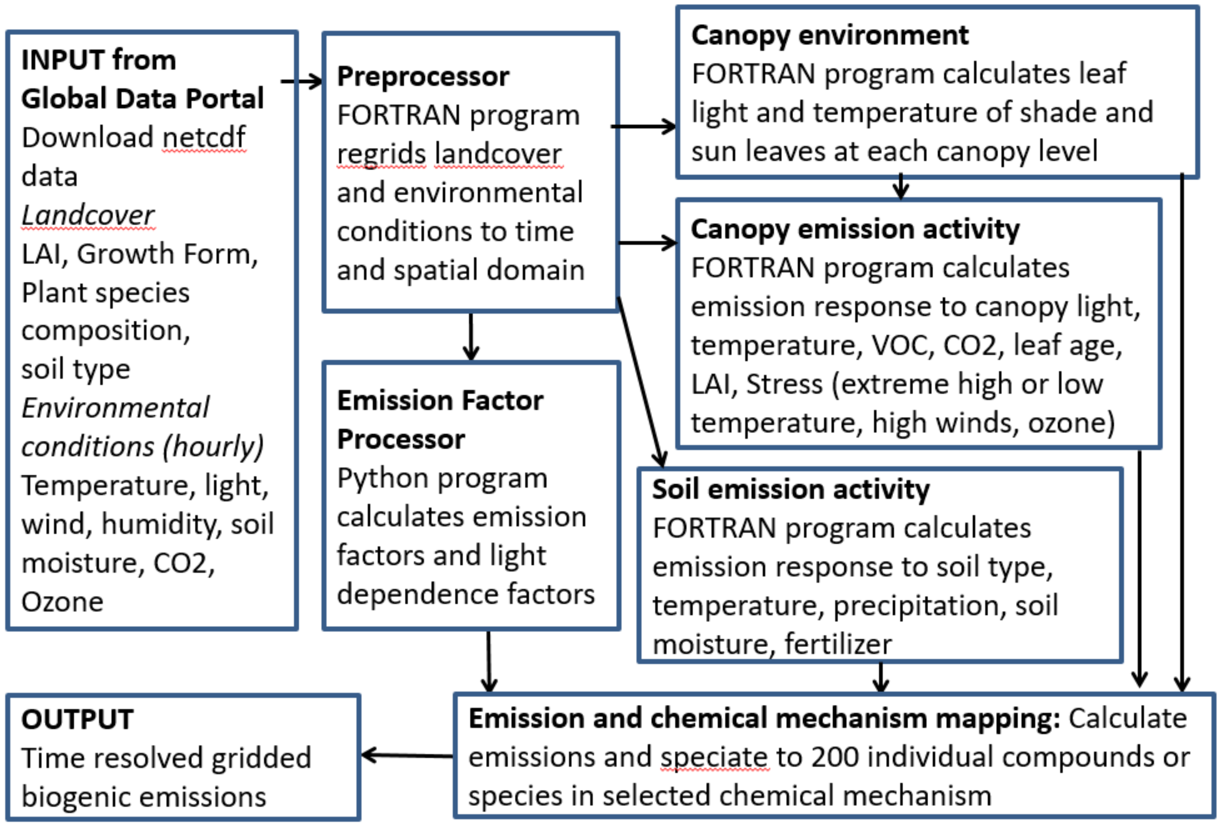


Figure 4-1. Schematic of MEGAN3 framework.

4.2 MEGAN3 Canopy Environment Model

While some BVOC emission models assume that vegetation canopies act as a "big leaf", it has been shown that explicit simulation of canopy environment, especially solar radiation distributions on sun and shade leaves at different canopy depths, can have a substantial impact on predicted emissions, mainly for light dependent compounds such as isoprene and should be included as a component of BVOC emission models (Keenan et al. 2011). We have continued the development of the MEGAN canopy environment model with the addition of three new procedures that improve the representation of canopy processes. Each of the three procedures can impact predicted isoprene emissions by about 15 to 20%. However, since two of the processes cause a decrease and one causes an increase, the overall impact is a relatively modest (15 to 20%) decrease. In addition to the improvements to the canopy model, we have restructured the MEGAN program so that it can easily be driven by the results of other canopy environment models providing more flexibility for users so that they can evaluate the use of other canopy environment models.

4.2.1 Leaf Energy Balance

Leaf temperature can differ considerably from air temperature with some studies reporting differences of 5K or more. Since some leaves in the canopy are warmer than air while others are colder than air, the canopy average may not differ greatly but there may still be substantial differences in predicted emissions since the response functions are non-linear and there is a strong correlation between emission capacity, light and temperature. The leaf energy balance simulated by MEGAN considers all of the major energy components (e.g., absorbed and emitted radiation, convection, transpiration). One of these components is the infrared radiation exchange between a sun leaf (exposed to the sky) and the atmosphere. The MEGAN2.1 canopy environment model underestimated the net loss of infrared radiation to the sky and so overpredicted the temperature of sun leaves by about 1K. Since sun leaves are the major source of isoprene emission from the canopy, a 1K overestimation in leaf temperature can result in about a 15% overestimation in emission. The exact impact of this change depends on the specific environmental conditions and canopy characteristics and so will differ for locations and seasons.

4.2.2 Canopy Gaps (Transparency)

MEGAN2.1 combines satellite based estimates of vegetation cover fraction and Leaf Area Index (LAI) to estimate the LAI of vegetation covered surfaces, referred to as LAIv. For example, if a location has an LAI of 3 m^2/m^2 and a vegetation cover fraction of 0.5 then the LAIv will be 6 m^2/m^2. When vegetation cover fraction is significantly less than 1, the use of LAIv, instead of LAI, to drive the canopy environment model results in a significant difference in the simulated light environment with a larger fraction of shaded leaves at low light levels. Because isoprene is emitted at considerably lower rates from shaded leaves, the higher LAIv resulting from a decrease in vegetation cover, for a given LAI, results in a decrease in isoprene emission. The satellite-based vegetation cover fraction data used to drive MEGAN are representative of total crown cover as shown in Figure 4-2. Typically, some fraction of the total crown cover contains gaps without foliage resulting in sunlight that reaches the ground surface and so is unavailable for stimulating isoprene emission. Figure 4-2 illustrates this gap fraction within the crown area, called transparency. Just as the presence of bare ground outside of the canopy cover results in a higher LAI for vegetation covered surfaces, the presence of gaps (transparency) within the canopy cover results in the total LAI being higher over the remaining canopy. A canopy transparency factor was introduced into the MEGAN canopy environment model with canopy transparency values assigned to each growth form type. The resulting increase in LAIv is associated with a decrease in isoprene emission of about 15%. Emissions of most monoterpenes and other compounds that are primarily light independent are relatively unaffected by the addition of the transparency factor in the canopy environment model.

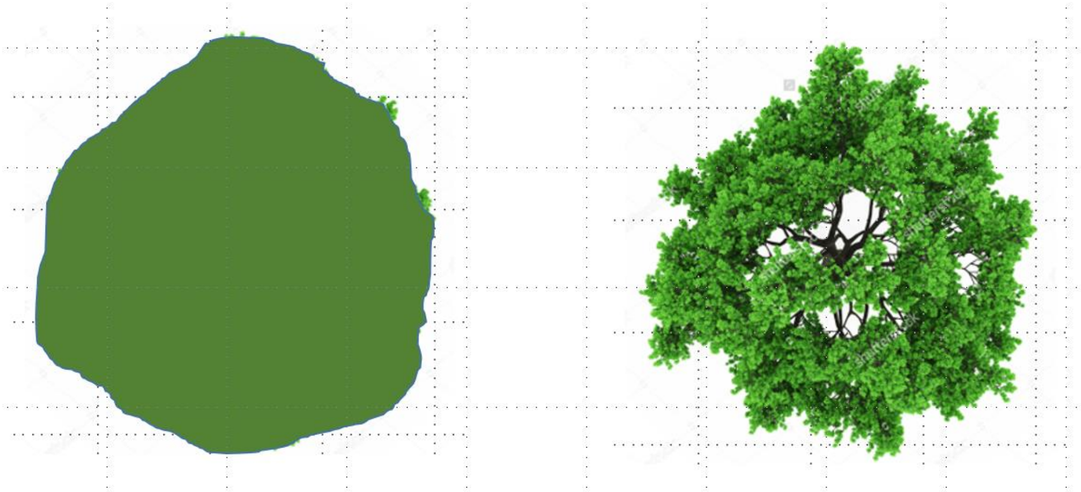


Figure 4-2. Downward looking view of a tree canopy illustrating total canopy cover area (left) and gaps within the canopy associated with transparency (right).

4.2.3 Emission Capacity Decrease with Canopy Depth

Plant leaf traits vary considerably throughout a tree canopy with leaves near the top and edge of the canopy exposed to high light conditions having higher specific leaf area, nitrogen content, photosynthetic capacity and isoprene emission capacity. MEGAN2.1 provided an approach for simulating within canopy variation in isoprene emission capacity by calculating the past light and temperature conditions for sun and shade leaves at each canopy depth and modifying the parameters in the isoprene light and temperature response algorithms. This approach assumes that leaves can be classified as either sun or shade leaves but in reality the growth environment of leaves is a gradient from full sun to full shade. MEGAN3 employs a simpler approach that recognizes that emission capacity decreases with canopy depth and uses the comprehensive study of Niinemets et al. (2010) to parameterize the decrease in isoprene emission capacity with canopy depth. Niinemets et al. investigated the within canopy isoprene emission variation in *Quercus, Populus* and *Salix* species and found that isoprene emission capacity varied more than other plants traits including structural, chemical and photosynthetic rate properties. The inclusion of the canopy depth algorithm in MEGAN results in about a 16% increase in isoprene emission.

4.3 Emission Activity Response Algorithms

4.3.1 Stress Induced Emissions

Recent studies have shown that environmental stress from extreme weather (drought, winds, temperature) and air pollution (ozone) can induce emissions of compounds that are not otherwise emitted (e.g., C6 oxygenated VOC, benzenoid VOC, ocimene and other terpenoids) and substantially modify emission rates of other VOC (e.g., a-pinene and other monoterpenes) but there have been no attempts to explicitly include stress BVOC in emission model estimates. For example, Kaser et al. (2013) concluded that a severe storm caused a 40% increase in monthly total monoterpene emissions from a western U.S. pine plantation. BVOC emissions induced by ozone and other air pollution stress were estimated to increase total BVOC emissions in the Beijing region by about 65% (Ghirardo et al. 2016). Ozone reactions with diterpenes on leaf surfaces have recently been suggested as an important unaccounted source of BVOC emissions into the atmosphere (Jud et al. 2016).

We have created a framework in MEGAN3 for including BVOC emissions induced by extreme weather and air pollution stress. Simple response functions have been implemented based on recent observations characterizing BVOC emission response to extreme weather (high and low temperatures and high winds) and pollution events as an initial approach for incorporating stress induced emissions into BVOC emission models.

Both chilling and heat stress can elevate biogenic VOC emissions from plants (Ding et al. 2002) by a factor of 5 or more (Emmerson et al. 2016, Karl et al. 2008). Plants tend to have a temperature optimum of around 25 °C with a range of 20 to 30 °C considered to be nonstressful while temperatures below 10 °C or above 40 °C are typical for inducing stress accompanied by BVOC emission. We expect temperature thresholds to differ among plants with, for example, tropical plants being more susceptible to cold temperature stress and plants from mild climates being more susceptible to high temperatures (Kleist et al. 2012). We have established a simple framework to introduce stress induced emissions and assess their potential importance. For this initial assessment, we have set the threshold temperatures at 10 °C for chilling stress and 40 °C for heat stress. A factor of five increase in emissions has been implemented for 4 emission categories including stress induced monoterpenes (e.g., ocimene), sesquiterpenes (e.g., farnescene, longifolene), and stress compounds (e.g., linalool). Additional research will be required to better quantify these emissions if this initial implementation indicates that BVOC emissions in response to chilling or heating stress make a significant contribution to total BVOC emissions.

Mechanical damage to plants, such as damage and wounding caused by high winds, can dramatically increase emissions of some induced BVOC and some stored BVOC by an order of magnitude or more (Juuti et al. 1990) and this increase can persist for days. We have used the whole canopy flux observations of Kaser et al. (2013) to establish a wind speed threshold and the increase associated with BVOC emission response to high winds. This includes monoterpenes and sesquiterpenes that are stored within plant leaves and other tissues.

For several decades, it has been known that short-term exposure to high levels of ozone can induce emissions of stress BVOC including various benzenoid and C6 oxygenated compounds (Heiden et al. 1999, 2003). In addition, it is now clear that ozone oxidizes semivolatile compounds found on the surface of leaves (waxes, terpenoids) producing volatile products that are emitted into the atmosphere (Jud et al. 2016). More recently it has been shown that plants growing in a polluted environment emit various stress BVOC at substantial rates whereas plants growing in unpolluted environments do not emit detectable amounts of these stress BVOC (Ghirardo et al. 2016). We have implemented a threshold algorithm intended to simulate stress BVOC emissions at the level reported by Ghirardo et al. (2016) for polluted regions. Polluted regions are identified using the W126 ozone exposure index, a seasonal statistic that reflects the seasonal cumulative exposure of plants to ozone.

4.3.2 Stress Suppression of BVOC Emissions

Extended periods of stress will ultimately shut down the plant photosynthetic mechanisms responsible for the uptake of carbon and production of BVOC substrates. This has clearly been demonstrated for isoprene response to extended drought. A simple threshold algorithm was implemented in the Community Earth System Model / Community Land Model (CESM/CLM) version of MEGAN2.1 to account for the reduction in isoprene emission that occurs when soil moisture nears the wilting point where plants cannot pull water out of the soil. The algorithm was not included in the released version of the MEGAN2.1 stand-alone FORTRAN code because many users did not have soil moisture data available. The simple threshold algorithm has now been included in the MEGAN3 standalone FORTRAN code. In addition, users are given the option of using soil moisture activity factors calculated by a new MEGAN3 algorithm that has been implemented in CESM/CLM. This algorithm simulates the response of isoprene emission to drought and other stress based on two plant physiological parameters: BTRAN and VCmax. BTRAN (transpiration beta factor) indicates soil water stress as a linear function based on the amount of soil moisture available to a plant. VCmax is the maximum rate of carboxylation indicating the ability of a plant to convert CO_2 into the carbon substrates for BVOC production.

4.3.3 BVOC Response to Past Temperature, Light, CO_2 and Bidirectional Exchange

MEGAN2.1 calculates light (Photosynthetic Photon Flux Density, PPFD) and temperature on sun and shade leaves at each of five canopy depths. The past 24 hour and past 240 hour PPFD and temperature were tracked for each of these ten canopy components and used to drive the PPFD and temperature isoprene response algorithms that account for the impact of past PPFD and temperature conditions on current emissions. This assumed that canopy leaves fall into shade or sun categories but in reality most leaves spend at least part of the day exposed to the sun and the remainder as shade leaves. Also, this algorithm required assigning a standard past 24 hour and 240 hour PPFD and temperature condition to each canopy component but accurate estimates are difficult to obtain on regional to global scales. MEGAN3 accounts for the past PPFD and temperature conditions using canopy scale PPFD and temperature which greatly simplifies the implementation of this response. The tendency for the lower canopy to have lower emissions is accounted for in MEGAN3 using the algorithm described in Section 4.2.3.

MEGAN2.1 included two algorithms that were not called in the released version of the standalone code: 1) an algorithm simulating the response of isoprene to CO_2 concentration and 2) an algorithm simulating the response of bidirectional exchange compounds to increasing LAI. Both of these algorithms are now implemented in MEGAN3. The isoprene response to CO_2 accounts for the substantial decrease of isoprene with an increase in CO_2 but this only has an impact with simulations of future or past scenarios. The algorithm is described by Heald et al. (2009) and predicts that the increase in isoprene with higher temperatures predicted for the year 2100 could be completely offset by the decrease associated with higher CO_2.

The canopy scale emission of most compounds increase with increasing LAI. Exceptions to this behavior are compounds, such as ethanol and acetaldehyde that are emitted from sun leaves and consumed by shade leaves (Jardine et al. 2008). Thus total canopy emissions decrease, rather than increase, with increasing canopy LAI. The MEGAN3 algorithm simulates this behavior with a simple algorithm.

4.3.4 Light Dependence Fraction (LDF) Variations

The use of variable emission traits (i.e. different parameters) allows MEGAN to account for differences among plant types. MEGAN2.1 had only one emission trait, the emission factor, which could be specified for individual vegetation types. MEGAN3 adds the capability of adding information on light dependence fraction (LDF) for each vegetation type. This allows simulation of the considerable variation that has been observed in emission measurement studies. For example, α-pinene emissions from tropical forest trees are almost entirely light dependent while only a small part of the α -pinene emission from temperate forest trees is light dependent. We have implemented this approach in MEGAN3 by including LDF data in the MEGAN-EFP along with emission factors. The framework is flexible so that additional plant emission traits can be added in the future.

4.4 Compounds, Emission Categories and Mapping to Chemical Schemes

Recent studies have revealed additional BVOC that are emitted from vegetation but previously were not included in the list of 150 species included in MEGANv2.1. As illustrated in Figure 4-3, the total number of compounds has been extended to 200 but the number of categories that are used for calculating emissions is the same. This results in computational requirements that are similar.

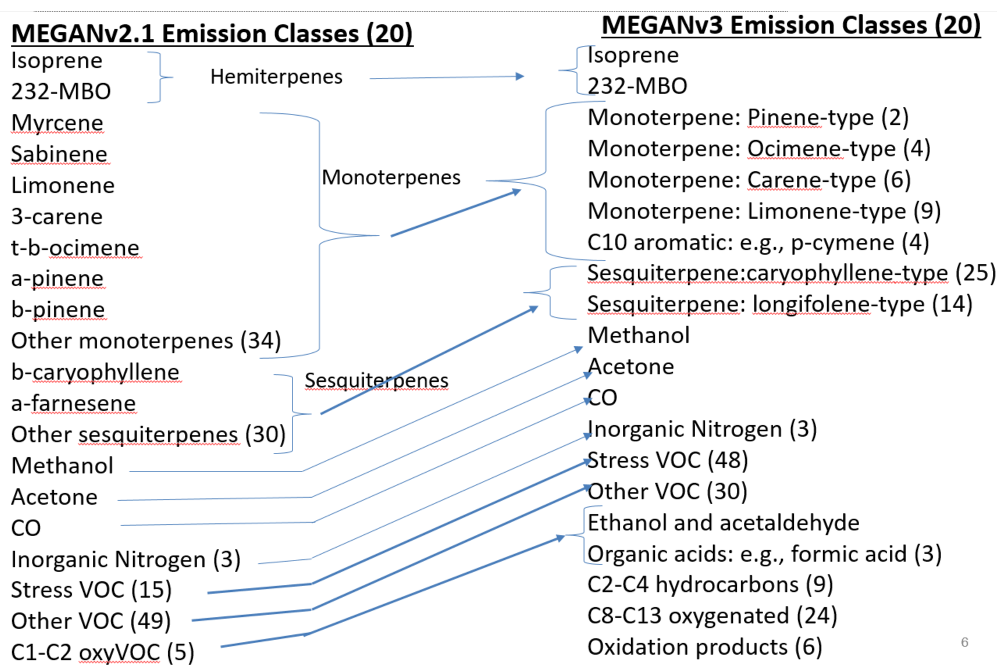


Figure 4-3. Comparison of MEGAN2.1 and MEGAN3 compounds and compound classes.

One of the differences illustrated in Figure 4-3 that MEGAN3 does not include any individual monoterpenes or sesquiterpenes but places them all in categories based on their emission processes and chemical characteristics (e.g., reactivity). This reduces the number of categories while losing very little information. MEGAN3 includes several new categories including light hydrocarbons and oxidation products and adds 33 compounds to the “stress VOC” category.

4.5 MEGAN Code Improvements

The MEGAN code was improved by eliminating several errors and by generally improving the code structure to clarify the code and make it easier to follow in order to facilitate future flexibility and updates. For example, the canopy environment model and the soil emission activity module were placed in separate modules and some variables were renamed to clarify their purpose. In addition, some unused code was removed. Most of the errors had little or no impact on estimated emissions. One exception was an error in code associated with calculating the MEGAN2.1 soil NO emissions.

MEGAN (version 2.1) includes two key soil NOx emission calculation subroutines:

1. “EMPROC” calculates soil NOx emission activity factors which adjust basal emission rates in response to temperature, precipitation, fertilizer stimulation, and other factors.

2. “MGN2MECH” combines the soil NOx emission activity factors with basal NOx emission rates to generate final NOx emission rates for a given grid cell and hour.

A coding error associated with the soil NOx emission calculation was found in the “MGN2MECH” calculation step. This error appears in four lines of original source code listed below:

a. Line 639 and 655 estimate grid cell-adjusted NOx emission rates outside of the growing season:

Line 639: tmper(nmpsp,C,R) = inper(INO,C,R) * EF(INO,C,R) * CFNOG(C,R) * TMO2 / TMO1* n2no

Line 655: tmper(nmpsp,C,R) = inper(INO,C,R) * CFNOG(C,R) * TMO3* n2no

b. Line 682 and 698 estimate grid cell-adjusted NOx emission rates in the growing season:

Line 682: tmper(nmpsp,C,R) = inper(INO,C,R) * EF(INO,C,R) *TMO2 / TMO1* n2no

Line 698: tmper(nmpsp,C,R) = inper(INO,C,R) * TMO3* n2no

In the original source code, the “inper” variable (in red text above) was incorporated into the calculation of final soil NOx emission rates “tmper”. However, “inper” represents the emission activity factors for biogenic VOCs and should not be applied to soil NOx. Adjustment factors for soil NOx emissions are already represented by the “CFNOG”, “TMO2”, and/or “TMO3” term (in green text above).

In MEGAN3, calculation of the soil NO emission activity factor is pulled out of the previous "EMPROC" subroutine and a new subroutine "MEGSEA" is added to only deal with soil NO emission activity factor. In this subroutine, the soil NO emission activity factor – GAMNO – is calculated as below:

a. For non-growing season, GAMNO is just CFNOG (emission activity factor for grass)

Line 433: GAMNO(I,J) = CFNOG(I,J)

b. For growing season, GAMNO is canopy type weighted average of CFNOG and CFNO (emission activity factor for crops):

Line 438:

```
TMO1 = 0.

        TMO2 = 0.

        DO I_CT = 1,5 'for all canopy types except crops, use CFNOG

          TMO1 = TMO1 + CTF(I_CT,I,J)

          TMO2 = TMO2 + CTF(I_CT,I,J) * CFNOG(I,J)

        ENDDO

        ! CFNO for crops

        TMO1 = TMO1 + CTF(6,I,J)

        TMO2 = TMO2 + CTF(6,I,J) * CFNO(I,J)

        IF (TMO1 .EQ. 0.0) THEN

           GAMNO(I,J) = 0.0

        ELSE

           GAMNO(I,J) = TMO2 / TMO1

        ENDIF
```

In the final "MGN2MECH" step, this "GAMNO" is directly multiplied with the basal NOx emission rate to get the real emission rate.

Line 599: tmper(nmpsp,:,:) = GAMNO(:,:) * EF(INO,:,:)

```
&                        * effs_all(nmpsp)
```

4.6 MEGAN3 Deliverables

The MEGAN3 FORTRAN code and the updated documentation and user's guide will be delivered directly to TCEQ and will be available to download for the rest of the community on the MEGAN Data Portal (bai.ess.uci.edu/megan).

5.0 MEGAN EVALUATION AND SENSITIVITY STUDY

Once the development of MEGAN3 was completed, we investigated MEGAN3 model sensitivity and evaluated emission and ambient concentration estimates using surface and aircraft observations. We prepared a best estimate emission inventory using the MEGAN-EFP and the MEGAN3 model as well as two additional sensitivity test emission inventories and compared them to an inventory prepared using MEGAN v2.1. We evaluated all of the inventories against aircraft flux data from the 2013 Southeast Atmosphere Study (SAS) and then used them as inputs to a photochemical model.

5.1 Modeling Strategy

All MEGAN biogenic emission inventories were prepared using Weather Research and Forecasting (WRF; Skamarock et al. 2008) meteorological model data developed during AQRP Project 14-016 (Yu et al. 2015). Emission inventories encompassed the June 1-July 15, 2013 period, which coincides with the SAS C-130 and P-3 aircraft campaigns. We prepared three sets of model-ready MEGAN3 biogenic emissions using three sets of emission factors: (1) emission factors from MEGAN-EFP using high quality (J=4) data (2) emission factors from the MEGAN-EFP system including lower quality (J≥0) data (3) emission factors from MEGAN-EFP using high quality (J=4) data but without stress induced emissions. We used the MEGAN2.1 model-ready emissions developed for AQRP Project 14-016 project for comparison with the three MEGAN3 inventories. For all of the MEGAN emission inventories, we compared modeled and measured BVOC fluxes along the aircraft flight tracks.

The Comprehensive Air quality Model with Extensions (CAMx; Ramboll Environ 2017) version 6.40 with IEEE compile flag was used to model fluxes and atmospheric concentrations of BVOCs. We ran the CAMx model for the June 1-July 15, 2013 period separately using each of the three MEGAN3 inventories as well as the MEGANv2.1 inventory. For each CAMx run, we compared modeled and measured concentrations of BVOCs and other species along the aircraft flight tracks. The latest CB6r4 chemical mechanism was used in the CAMx modeling. We used 2013 MOZART boundary conditions with a patch applied as described in the TCEQ Near-Real Time Ozone Model platform (Johnson et al. 2016). All other CAMx inputs were drawn from the AQRP Project 14-016 2013 modeling platform.

The modeling domain consists of a 36 km continental-scale grid and a nested 12 km grid (Figure 5-1). The regional 12 km grid covers Texas and surrounding states so that it contains nearly all of the overland flight tracks of the NCAR C-130 and NOAA P-3 made during June-July 2013. The vertical structure of the CAMx model is shown in Figure 5-2. CAMx was run from June 1-July 15, 2013 to simulate the period when C-130 and P-3 aircraft data are available. A two-week spinup period leading up to June 1 was modeled to remove the influence of the model initial conditions.

The Weather Research and Forecasting (WRF) (Skamarock et al., 2008) meteorological model was used in hindcast mode to develop the meteorological fields required for input to the MEGAN biogenic emissions modeling as well as to the photochemical model. The WRF model configuration is shown in Table 5-1. The WRF domains are slightly larger than the CAMx domains shown in Figure 5-1 and the vertical structure of the WRF model is shown in Figure 5-2. The WRF model was run for the period April-October, 2013.

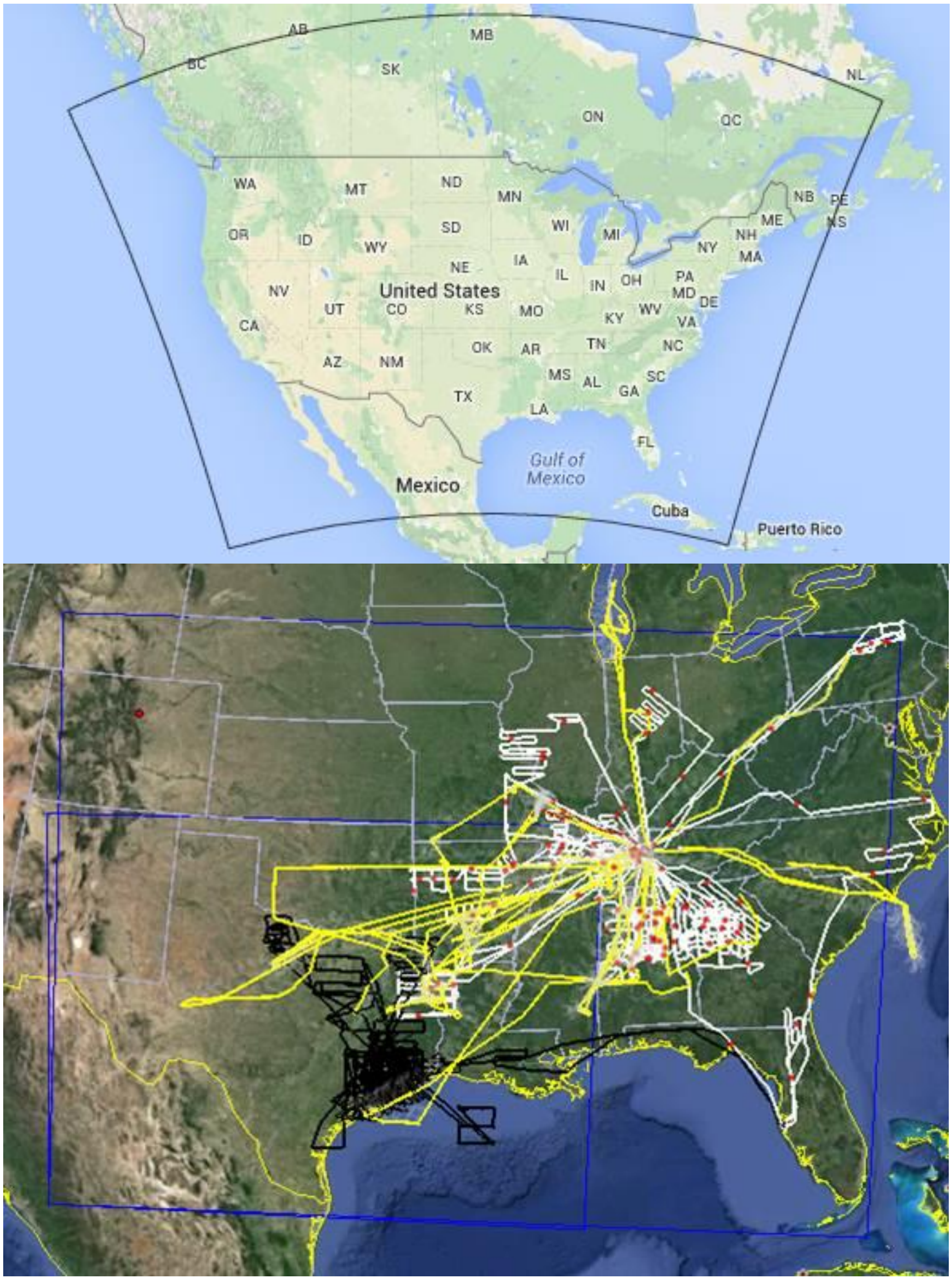
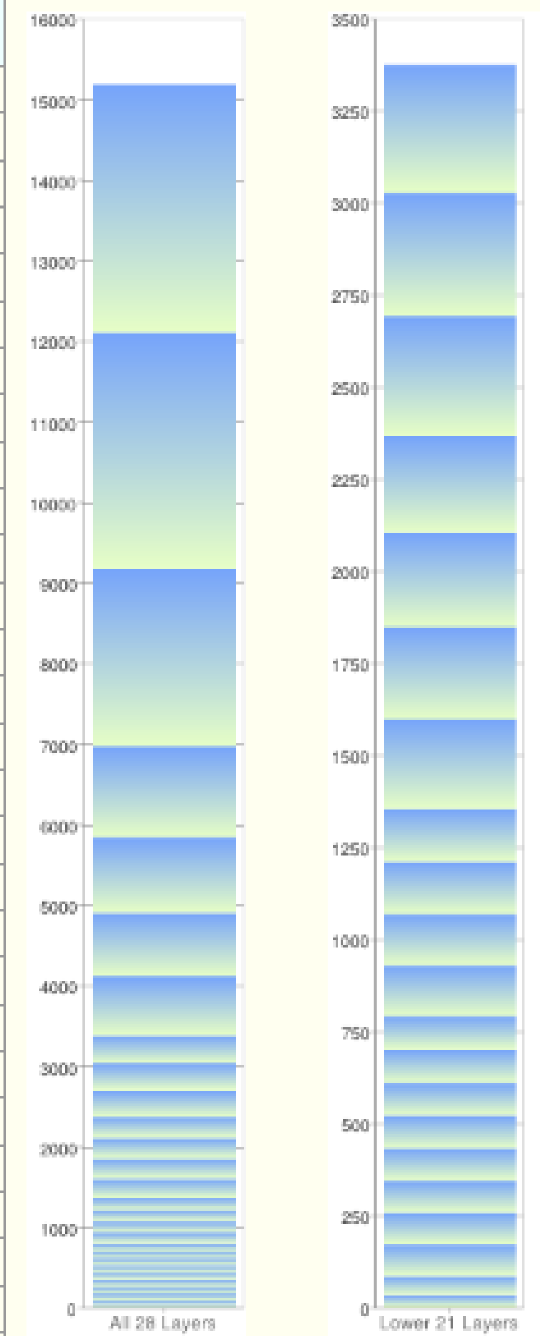


Figure 5-1. Upper panel: 36 km continental-scale CAMx modeling grid. Lower panel: 12 km CAMx modeling grid and aircraft flight paths. Aircraft flight paths: SAS C-130 (yellow), SAS P-3 (white), and TexAQS 2006 (black). TCEQ 12 km grid extent (smaller blue domain), and expanded 12 km grid (larger blue domain) used in this project.

Vertical Layer Structure

Corresponding WRF Layer	Layer Top (m AGL)	CAMx Layer	Layer Center (m AGL)	Thickness (m)
38	15179.1	28	13637.9	3082.5
36	12096.6	27	10631.6	2930.0
32	9166.6	26	8063.8	2205.7
29	6960.9	25	6398.4	1125.0
27	5835.9	24	5367.0	937.9
25	4898.0	23	4502.2	791.6
23	4106.4	22	3739.9	733.0
21	3373.5	21	3199.9	347.2
20	3026.3	20	2858.3	335.9
19	2690.4	19	2528.3	324.3
18	2366.1	18	2234.7	262.8
17	2103.3	17	1975.2	256.2
16	1847.2	16	1722.2	249.9
15	1597.3	15	1475.3	243.9
14	1353.4	14	1281.6	143.6
13	1209.8	13	1139.0	141.6
12	1068.2	12	998.3	139.7
11	928.5	11	859.5	137.8
10	790.6	10	745.2	90.9
9	699.7	9	654.7	90.1
8	609.7	8	565.0	89.3
7	520.3	7	476.1	88.5
6	431.8	6	387.9	87.8
5	344.0	5	300.5	87.1
4	256.9	4	213.8	86.3
3	170.6	3	127.8	85.6
2	85.0	2	59.4	51.0
1	33.9	1	17.0	33.9



AGL - Above Ground Level.

Figure 5-2. WRF and CAMx layer structure. TCEQ figure [1].

[1] http://www.tceq.texas.gov/airquality/airmod/data/domain

Table 5-1. WRF model configuration.

	AQRP Biogenics WRF Run Configuration
WRF version	3.6
Horizontal Resolution	36/12 km
Microphysics	WSM6
Longwave Radiation	RRTMG
Shortwave Radiation	RRTMG
Surface Layer Physics	MM5 similarity
LSM	Noah
PBL scheme	Yonsei University (YSU)
Cumulus parameterization	Kain-Fritsch
Boundary and Initial Conditions Data Source	12 km NAM analysis
Analysis Nudging Coefficients (s^{-1})	36/12 km grids
Winds	$3x10^{-4}$
Temperature	$3x10^{-4}$ (above BL only)
Mixing Ratio	$3x10^{-4}$ (above BL only)
Observation Nudging Coefficients (s^{-1})	36/12 km grids:
Winds	None
Temperature	None
Mixing Ratio	None
Miscellaneous Notes	Using KF-RRTMG interaction which feeds back subgrid cloud information to radiation scheme (36/12 km grids)

5.2 WRF Model Performance Evaluation

During AQRP Project 14-016, we evaluated the performance of the WRF model in reproducing observed weather at the surface and aloft. A graphical and statistical evaluation of model performance was carried out for winds, temperatures, humidity, the placement of frontal boundaries, and the intensity of precipitation, clouds and downward solar radiation at the Earth's surface. Output from the 12 km WRF modeling domain was compared against meteorological observations from the TCEQ's Continuous Air Monitoring Stations (CAMS), airport meteorological monitoring sites (ds472 data set), analyzed precipitation fields and satellite imagery.

The WRF model performance in simulating surface meteorology, large scale synoptic features, precipitation and clouds is typical of summer US WRF applications at 12 km resolution. Wind, temperature and humidity performance was generally within standard performance benchmarks except at sites located offshore or along the coast. These areas may be influenced by sea breeze circulations that are not well-resolved at 12 km model resolution.

The most important finding of the WRF model performance evaluation from the point of the MEGAN emissions modeling is the overestimate of downward shortwave radiation at the surface. This will likely produce a high bias in photosynthetically active radiation (PAR) and temperature used as input to MEGAN and can impart a high bias to the modeled terpenoid emission estimates. The MEGAN emissions and the CAMx photochemical modeling that relies upon it should be viewed with this WRF model bias in mind.

5.3 MEGAN Emissions Modeling

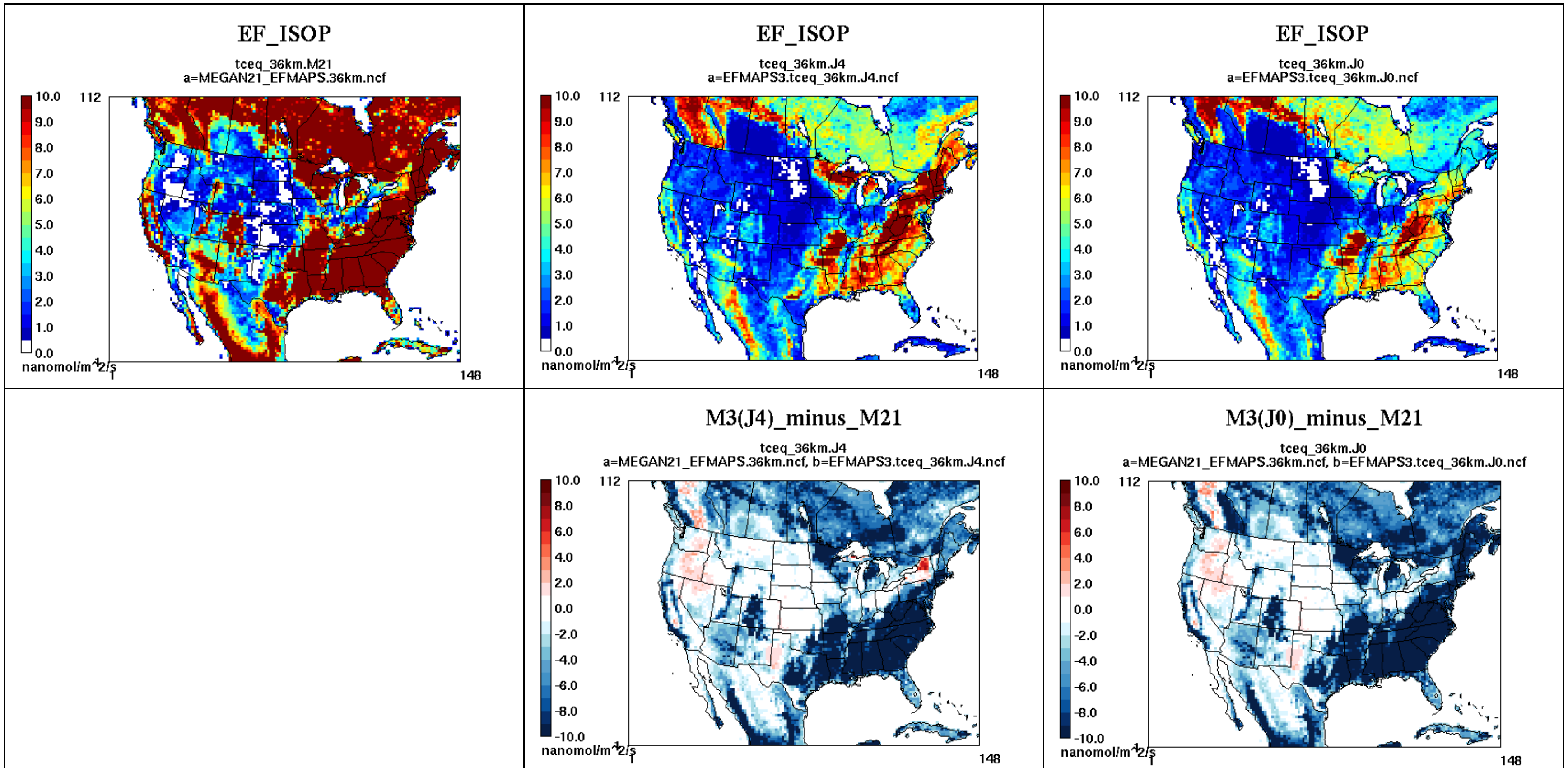
5.3.1 MEGAN Modeling Configuration and Inputs

WRF model output data was used in the development of biogenic emission inventories for the June 1-July 15, 2013 period. The MEGAN model requires information about temperature, soil moisture and solar radiation from the meteorological model. WRF model output was formatted for use by MEGAN through application of the EPA's MCIP (Meteorology-Chemistry Interface Processor) processor. PAR data, an important input driving the MEGAN light dependency algorithm, can be derived from satellite observations or from predicted solar radiation from WRF/MCIP. However, satellite PAR observations were not available for the year 2013. Instead, we used solar radiation from WRF/MCIP with a solar radiation-to-PAR conversion factor of 0.45 (Sakulyanontvittaya et al., 2012).

The MEGAN-EFP system was used to develop emission factor database with different minimum quality ratings threshold of measurement data. As discussed in Sections 2 and 3, The MEGAN-EFP synthesizes leaf level plant trait data, including BVOC emission factors (EF), specific leaf area (SLA) and emission light dependence factor (LDF), with landcover data, including ecotype and growth form fractions for each location in a modeling domain, and descriptions of biogenic compounds, emission classes, publications, vegetation types, and canopy vertical distribution characteristics.

5.3.2 Results of Emission Factor Database Development

Figure 5-3 shows MEGAN2.1 and MEGAN3 isoprene emission factors for the contiguous U.S. and the differences between the MEGAN2.1 and MEGAN3 datasets. MEGAN3 isoprene emission factors using both higher and lower quality data are generally lower than MEGAN2.1 across the continental U.S. with some exceptions. For example, the MEGAN3 using J=4 database has higher emission factor in parts of western states and northern portion of New York as compared to MEGAN2.1. There are large reductions in the isoprene emission factor across East Texas and the southeastern US. The higher MEGAN3 emission factors in some cases may occur because MEGAN2.1 (and BEIS) have just one emission factor for all broadleaf trees that emit isoprene whereas, with the MEGAN3-EFP, MEGAN3 can have different emission factors for individual species, so a tree species that occurs in New York could have an especially high emission rate. The high isoprene emission in the northeastern US for the J=4 database is also due to the complete lack of high quality (J=4) emissions data for trees that don't emit isoprene. As a result, these non-emitting trees are assigned the average value for all trees which is a moderate isoprene emission rate. This issue was minimized for Texas and the southeastern US by assigning a J=4 isoprene emission rate of zero for all of the non-emitting isoprene trees in this region. This approach should be extended to including other regions including the northeastern US.



MEGAN2.1	MEGAN3 using J=4	MEGAN3 using J=0

Figure 5-3. MEGAN2.1, MEGAN3 using J=4, MEGAN3 using J>=0 isoprene emission factors in nanomoles (m^2-hr)$^{-1}$ for the contiguous U.S. and the differences between the MEGAN2.1 and MEGAN3 emission factor database. Note that MEGAN2.1 uses canopy scale emission factors which must be converted, using a canopy environment model, to an equivalent leaf scale emission factor for comparison.

5.3.3 Comparison of Default and Updated MEGAN Emissions

Figure 5-4 and Figure 5-5 compare domain-wide and state-wide isoprene (ISOP) emissions in the MEGAN2.1 and the three MEGAN3 scenario emission inventories for the 36 km continental-scale modeling grid (upper panel of Figure 5-1) and the 12 km grid (lower panel of Figure 5-1). On both grids, domain-wide isoprene totals decrease in going from the MEGAN2.1 to the three MEGAN3 inventories. On the 12 km grid, the difference in emissions among the three MEGAN3 inventories is relatively small (25%), while there is a much larger decrease (up to -49%) in going from MEGAN2.1 to MEGAN3 inventories. The breakdown by state shows that the decreases are not uniform in the MEGAN3 inventories; there are large decreases in isoprene emissions in Texas, Georgia and Missouri, but decreases in Arkansas, Louisiana and Oklahoma are small. In the MEGAN3 inventories, there are decreases in isoprene emissions relative to the MEGAN2.1 emission inventory for all states.

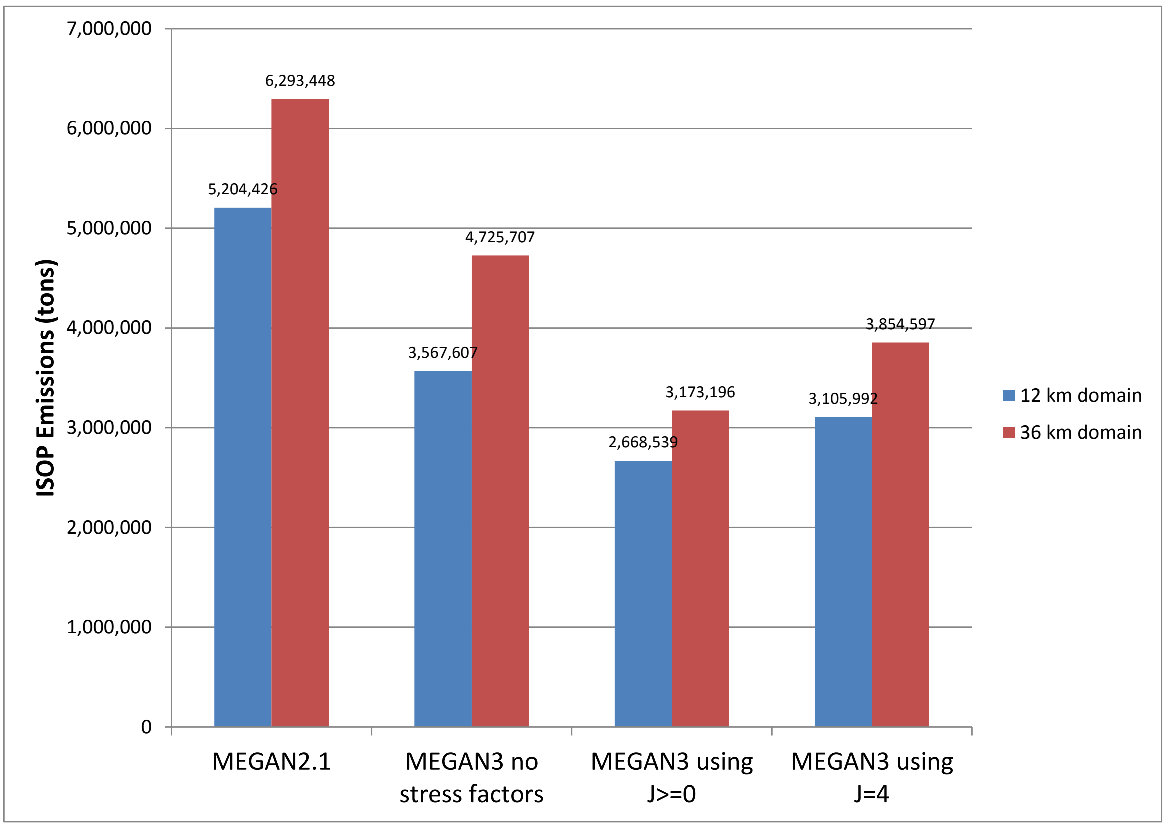


Figure 5-4. MEGAN isoprene (ISOP) emissions for the MEGAN2.1 and MEGAN3 scenario emission inventories: domain wide isoprene emissions in the 12 km and 36 km modeling domains for the modeling episode.

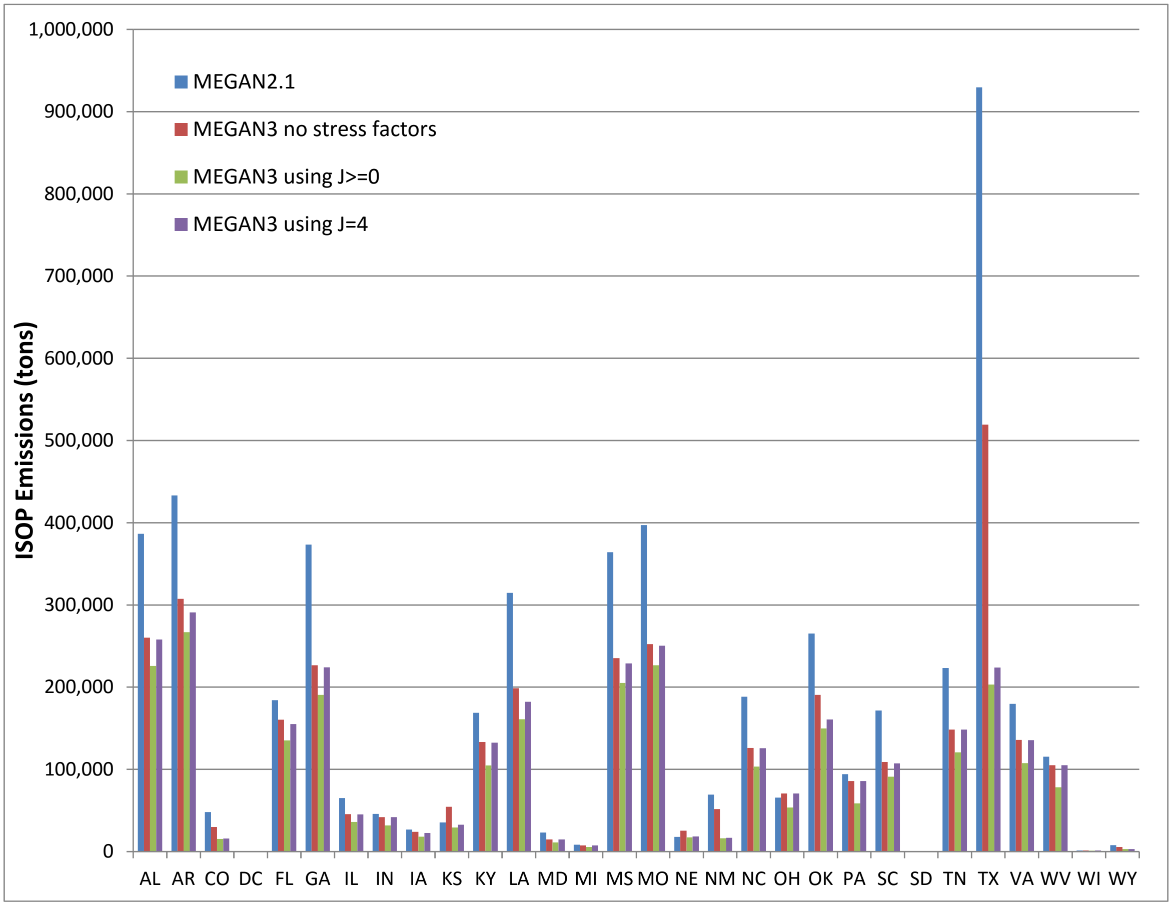


Figure 5-5. MEGAN isoprene (ISOP) emissions for the MEGAN2.1 and MEGAN3 scenario emission inventories: isoprene emission totals by state within the 12 km domain for the MEGAN2.1 and MEGAN3 scenario inventories.

Figure 5-6 summarizes the episode average differences between isoprene emission inventories developed with MEGAN2.1 and MEGAN3 using J=4. The largest reductions in isoprene emissions occurred in areas with high isoprene emissions in MEGAN v2.1: over the Edwards Plateau in Texas, over Northeast Texas and Louisiana and in Northern Arkansas and Southern Missouri.

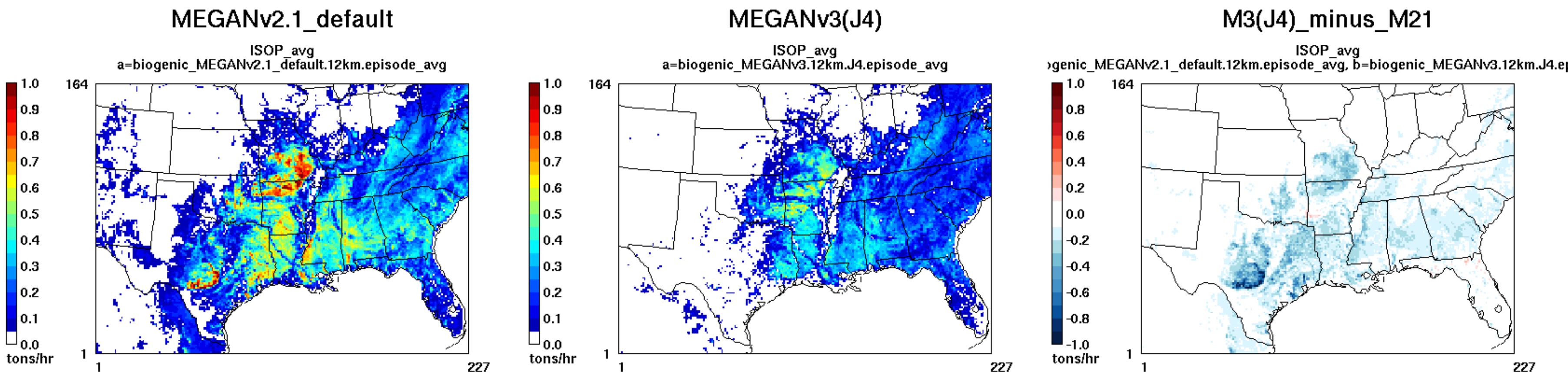


Figure 5-6. Comparison of isoprene emissions for MEGAN2.1 and MEGAN3 using J=4 emission inventories. Left: episode average MEGAN2.1 isoprene emissions. Middle: episode average MEGAN3 using J=4 isoprene emissions. Right: difference in episode average isoprene emissions (MEGAN3 (using J=4) – MEGAN2.1)).

The mapping approach of MEGAN compounds to model species of each condensed chemical mechanism was reviewed and updated in the MEGAN3 model. A table showing the mapping of MEGAN3 compounds to model species of supported chemical mechanisms is given in Appendix B. In the MEGAN3 inventory, all MEGAN terpene compounds were mapped to the lumped terpene(s) species available in each condensed mechanism. The MEGAN3 species mapping approach improved upon mappings used in earlier MEGAN models where terpenes were mapped to other model species of condensed mechanism. In the MEGAN3 inventory, monoterpene emissions decrease domain-wide for both the 36 km and 12 km grids (Figure 5-7). The largest reductions in monoterpene emissions occurred in areas with high emissions in MEGAN v2.1: East Texas, Southern Arkansas/Northern Louisiana, and Northern Florida (Figure 5-8).

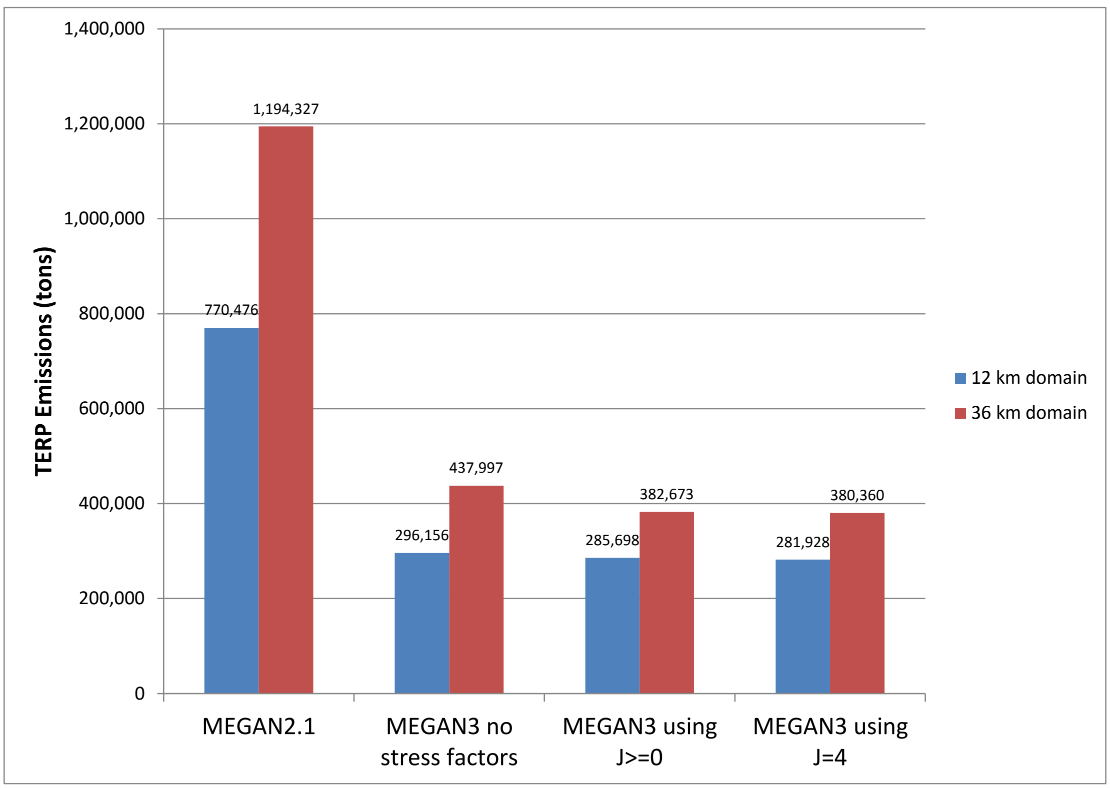


Figure 5-7. MEGAN monoterpene (TERP) emissions for the MEGAN2.1 and MEGAN3 scenario emission inventories. Domain wide isoprene emissions in the 12 km and 36 km modeling domains for the modeling episode.

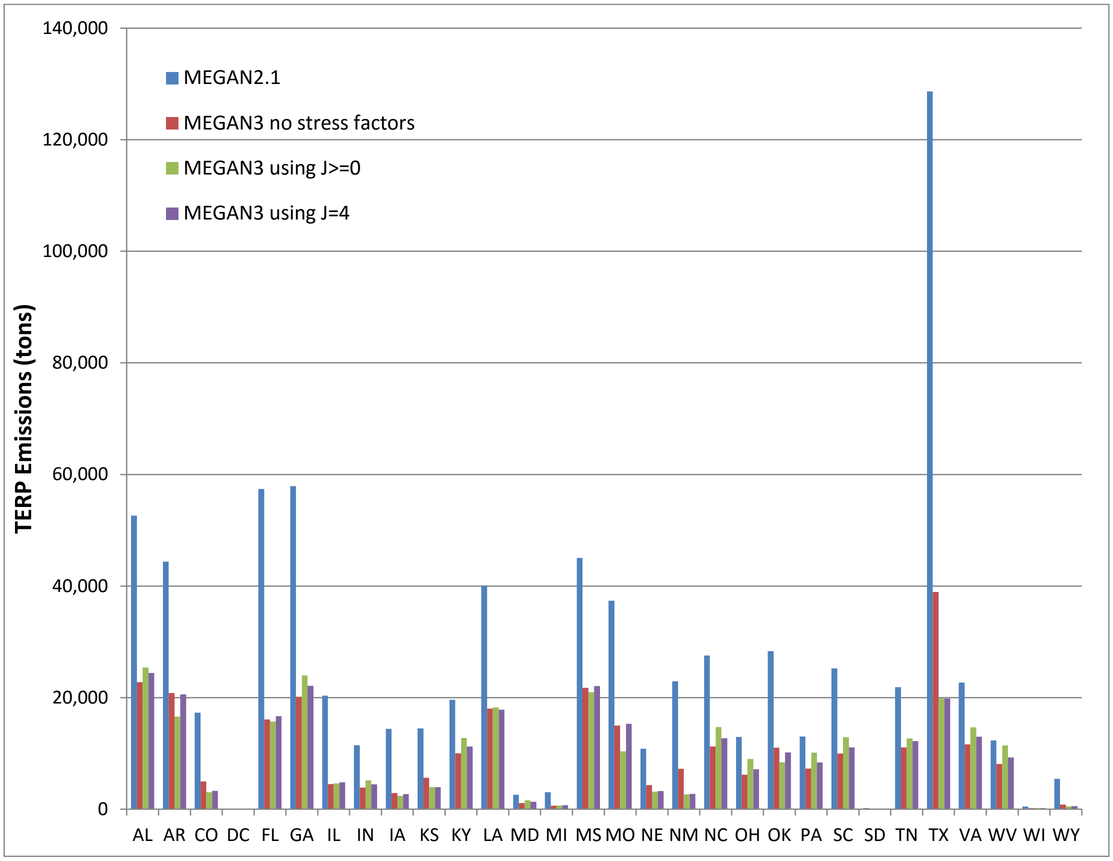


Figure 5-8. MEGAN monoterpene (TERP) emissions for the MEGAN2.1 and MEGAN3 scenario emission inventories. Isoprene emission totals by state within the 12 km domain for the MEGAN2.1 and MEGAN3 scenario inventories.

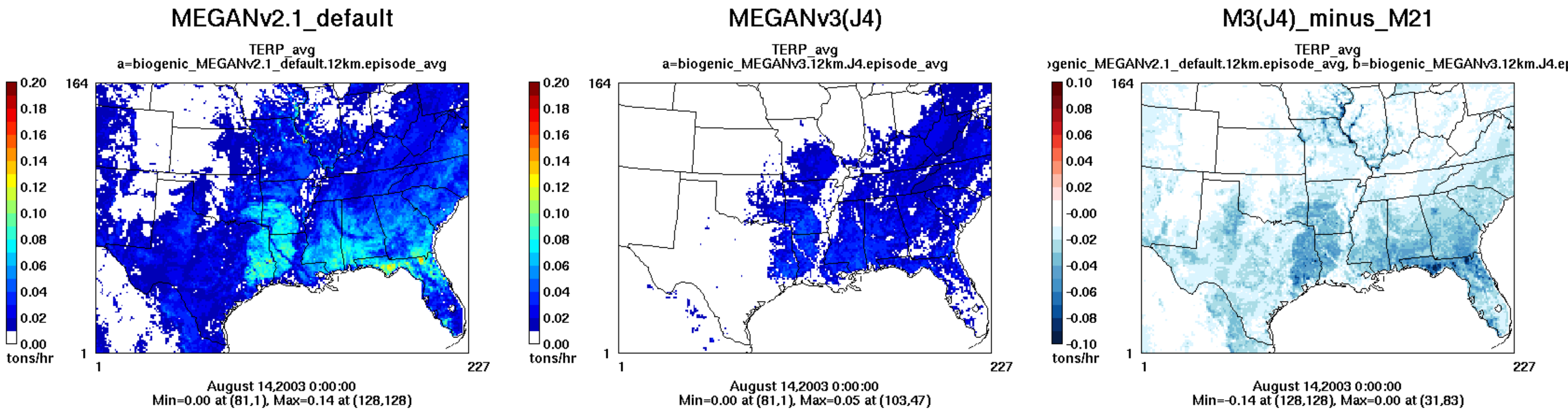


Figure 5-9. Comparison of monoterpene emissions for MEGAN2.1 and MEGAN3 using J=4 emission inventories. Left: episode average MEGAN2.1 isoprene emissions. Middle: episode average MEGAN3 using J=4 isoprene emissions. Right: difference in episode average isoprene emissions (MEGAN3 (using J=4) – MEGAN2.1)).

5.3.4 Comparison of MEGAN Emissions and Airborne Emission Fluxes

We extracted MEGAN emissions along the C-130 flight segments for the following emission inventories: MEGAN2.1, MEGAN3 using J=4, MEGAN3 using J≥0 and MEGAN3 using J=4 but without stress induced factors. The MEGAN emissions were paired in space and time with the aircraft data. Figure 5-10 shows the isoprene comparison for all the emission inventories. In the MEGAN2.1 inventory, isoprene emissions are higher than fluxes derived from aircraft measurements for most of the racetrack flight segments. In the MEGAN3 J=4 emission inventory, isoprene fluxes are generally lower along the racetrack segments than for MEGAN v2.1 and show improved agreement with the aircraft fluxes. Along the racetrack segments in southern Missouri along the Texas-Louisiana border, isoprene is reduced in the MEGAN3 inventories relative to MEGAN v2.1 and agreement with the aircraft data is improved in MEGAN3. The same is true for the Mississippi and Alabama racetrack segments. MEGAN3 isoprene emission estimates generally agree with the aircraft fluxes with some locations where MEGAN3 values are larger than the aircraft fluxes, including racetrack segments in Mississippi and Georgia, and others regions where MEGAN3 values are lower. Differences between the two MEGAN3 inventories are relatively small.

Monoterpene emissions for the MEGAN2.1 and MEGAN3 inventories are compared to airborne flux data in Figure 5-11. There is a widespread reduction in monoterpene emissions in the MEGAN3 inventories relative to MEGAN v2.1. The MEGAN3 inventories estimate lower monoterpene emissions than the aircraft fluxes over large portions of all of the racetrack segments.

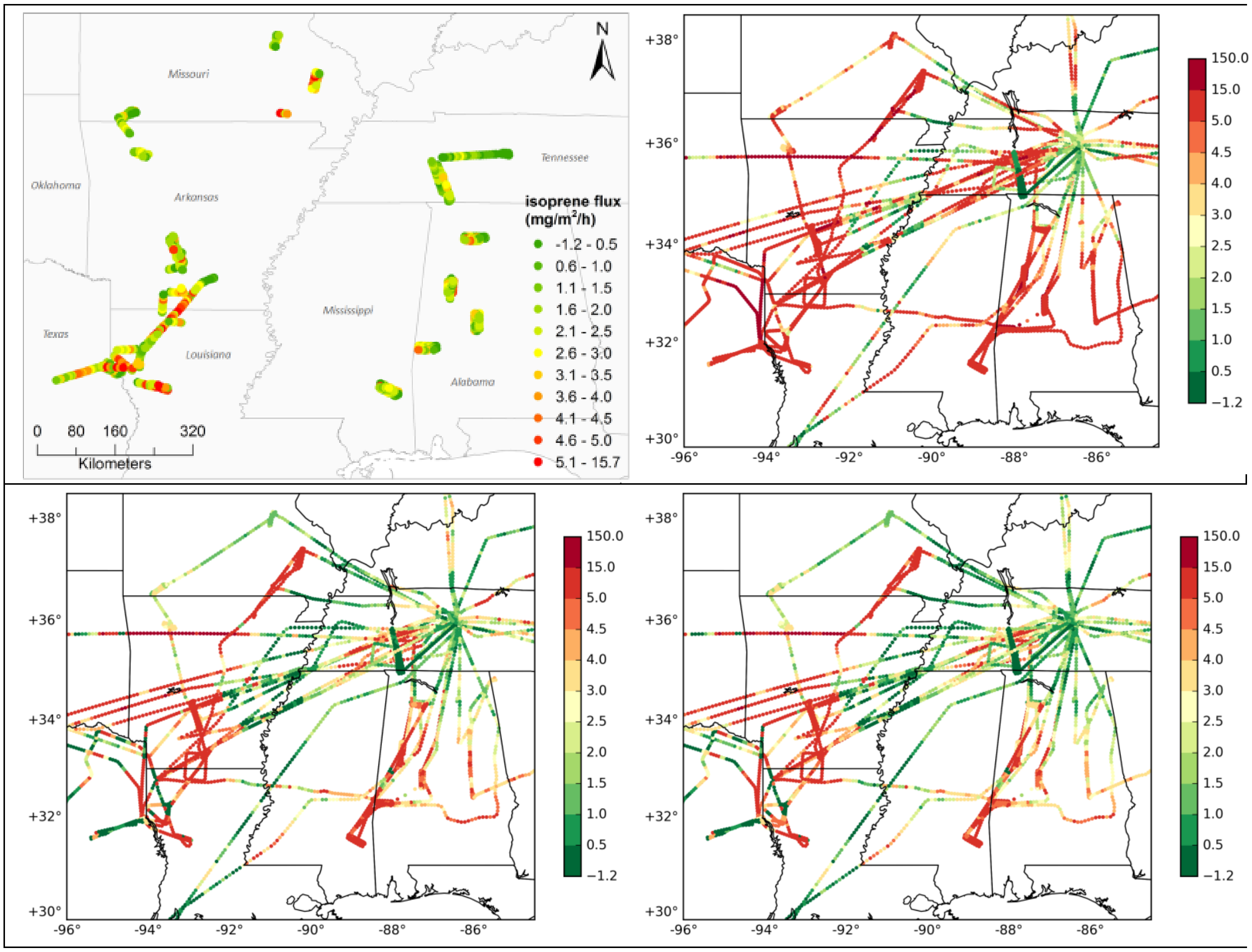


Figure 5-10. Isoprene fluxes derived from airborne data for C-130 racetrack flight segments (upper left) and MEGAN v2.1 isoprene emissions along all C-130 flight tracks for the default (upper right), MEGAN v3_J4 isoprene (lower left) and MEGAN v3_J0 (lower right) emission inventories. Units are mg (m^2-hr)$^{-1}$ for all panels.

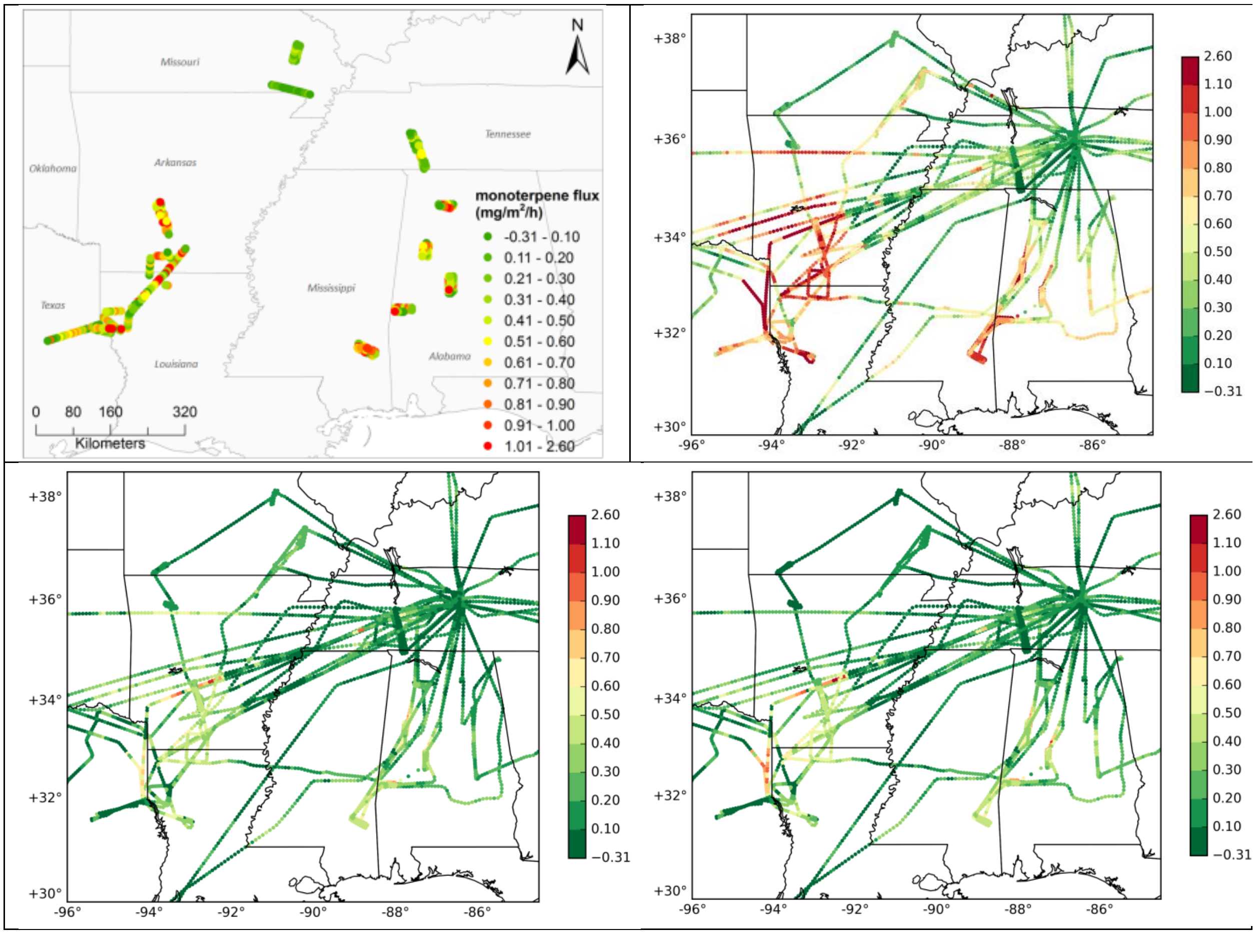


Figure 5-11. Monoterpene fluxes derived from airborne data for C-130 racetrack flight segments (upper left) and MEGAN v2.1 monoterpene emissions along all C-130 flight tracks for the default (upper right), MEGAN v3_J4 (lower left) and MEGAN v3_J0 (lower right) emission inventories. Units are mg (m^2-hr)$^{-1}$ for all panels.

Table 5-2 and Table 5-3 compare the aircraft EF with MEGAN3 EF. The aircraft EF were calculated using direct eddy covariance measurements and response factors calculated using NLDAS solar radiation and temperature. Table 5-2 compares average values for LANDFIRE ecoregions (existing vegetation types, EVT) and Table 5-3 compares the average value for each racetrack sampling region. As we discuss in the report for AQRP Project 14-016, relating aircraft measurements to specific ecoregion EVT values is challenging due to uncertainties in the aircraft flux footprint. Comparison between racetrack sampling regions is also complicated since the racetrack if typically an area of about 24 km x 6 km and here is being compared to the value for the 36 km grid that it falls within. This is not a very direct comparison since the landscape is fairly heterogeneous as can be seen by the comparison between the forest cover in the 36 km grid and the forest cover of the racetrack. In most cases, we expect a bias towards a higher forest fraction for the racetracks, since we chose those locations to target forest landscapes, which may result in the aircraft measurements having higher values than the model.

The EVT and racetrack results agree remarkably well providing some confidence in this evaluation. MEGAN3 isoprene fluxes using j=4 are 10% lower than the aircraft fluxes (9% for EVT comparison and 10% for racetrack comparison) and the MEGAN3 isoprene fluxes using j=0 are 21% lower than the aircraft fluxes. For total monoterpene fluxes, MEGAN3 using j=4 is 30% higher than the aircraft fluxes (17% for EVT comparison and 44% for racetrack comparison) and MEGAN3 using j=0 is 4% higher. These results demonstrate that the MEGAN3 emission estimates, with either j=4 or j=0, agree within the uncertainties (Yu et al. 2017) of the aircraft flux measurements.

Table 5-2. LANDFIRE Existing Vegetation Type (EVT) ecoregion descriptions including leaf area index (LAI, m2 m-2) and tree cover (%). Number of aircraft measurements (N), and emission factors (mg m-2 h-1) based on aircraft direct eddy covariance flux measurements (AEF), MEGAN3 using J=0 (M3J0), MEGAN3 using J=4 (M3J4) are shown for both isoprene and total monoterpenes. Statistics were not calculated if the number of measurements was less than 20 (indicated by dash).

EVT		Dominant		% Tree	Isoprene Emission Factors				Total Monoterpene Emission Factors			
ID	Description	Trees	LAI	Cover	N	AEF	M3J0	M3J4	N	AEF	M3J0	M3J4
3194	Ruderal upland- treed	Pine	4.98	81	247	3.9	4.09	4.62	187	0.66	0.79	0.94
3304	Ozark-Ouachita Oaks	Oak	5.13	75.8	261	9.78	6.4	6.74	71	0.42	0.41	0.8
3305	Interior Plateau Oaks	Oak	4.21	68.3	193	5.43	3.28	4.08	111	0.48	0.47	0.62
3307	Gulf Upland hardwoods	Pine/Oak	3.78	68.4	23	7.48	4.63	5.17	24	0.6	0.6	0.82
3317	Allegheny Oaks	Oak	4.94	93.5	65	8.64	4.97	6.67	25	1.16	0.67	0.91
3321	Southcentral forest	Oak	5.11	95.7	69	5.27	4.44	6.31	54	0.7	0.69	0.86
3349	E. Gulf Pine woods	Pine	4.64	88.8	115	1.89	3.27	3.81	116	0.98	0.78	0.97
3371	W. Gulf Pine forest	Pine	5.29	81.5	43	3.5	2.96	3.28	18	-	-	-
3473	Gulf Floodplain	Pine/Oak	5.17	79.5	131	5.62	3.32	4.1	71	0.66	0.57	0.72
3474	Gulf Riparian woods	Pine/Oak	4.95	84.3	23	3.89	3.53	4.61	14	-	-	-
3535	Southeast tree plantations	Pine	5.17	78.9	600	3.22	3.12	3.86	445	0.67	0.78	0.89
3997	Pasture and Hayland	Pine/Oak	3.23	48.9	84	3.05	2.51	2.84	64	0.63	0.54	0.63

Table 5-3. Racetrack measurement region descriptions including leaf area index (LAI, m2 m-2) and tree cover (%) within the aircraft measurement footprint and the MEGAN3 model domain location. The MEGAN3 statistics are averaged over a 36 km x 36 km area while the aircraft racetracks are averaged over regions of ~ 24km x ~6km. Number of aircraft measurements (N), and emission factors (mg m-2 h-1) based on aircraft direct eddy covariance flux measurements (AEF), MEGAN3 using J=0 (M3J0), MEGAN3 using J=4 (M3J4) are shown for both isoprene and total monoterpenes. A dash indicates that statistics were not calculated because the number of measurements was less than 20.

							Isoprene Statistics				Total Monoterpene Statistics			
Name	Location	Lat/Lon	Dominant Tree	LAI	Aircraft Footprint Tree Cover	MEGAN Footprint Tree Cover	N	AEF	M3J0	M3J4	N	AEF	M3J0	M3J4
RT 1	N. Alabama	34.3/87.3	Pine/Oak	4.99	94.3	65.2	140	6.72	5.21	6.48	80	0.86	0.71	0.93
RT 2	Texas	31.9/94.0	Pine/Oak	4.49	68.4	52.4	98	3.21	3.48	3.93	34	0.46	0.8	0.89
RT 3	Louisiana	31.6/93.3	Pine	5.21	84.7	59	68	7.36	3.68	4.14	0	-	-	-
RT 4	N. Missouri	38.0/91.0	Oak	5.39	67.5	73.5	29	15.4	8.47	8.87	0	-	-	-
RT 5	W. Missouri	36.7/93.8	Oak	5.3	80	38.2	51	8.96	3.95	4.4	0	-	-	-
RT 6	N. Arkansas	35.9/93.5	Oak	5	88.2	76.1	48	12.1	8.64	9.05	0	-	-	-
RT 7	S. Arkansas	34.1/92.8	Pine	5.45	80.1	57.8	239	2.94	3.96	4.42	157	0.72	0.86	0.97
RT 8	C. Alabama	33.4/87.8	Pine/Oak	4.88	81.9	70.8	99	4.61	5.12	5.62	62	0.78	0.93	1.08
RT 9	SOAS	32.8/87.3	Pine/Oak	5.11	79.6	72.1	127	3.82	4.97	5.51	107	0.61	0.96	1.09

Name	Location	Lat/Lon	Dominant Tree	LAI	Aircraft Footprint Tree Cover	MEGAN Footprint Tree Cover	Isoprene Statistics				Total Monoterpene Statistics			
							N	AEF	M3J0	M3J4	N	AEF	M3J0	M3J4
RT 10	S. Alabama	32.3/88.9	Pine	5.41	86.4	61.5	98	2.33	4.2	4.63	93	0.72	0.89	1
RT 11	Mississippi	31.5/88.9	Pine	4.76	88.5	69	147	2.03	3.98	4.42	147	0.9	0.93	1.08
RT 12	W. Missouri	37.3/90.3	Oak	4.95	65.6	69.8	55	6.81	7.92	8.32	48	0.47	0.4	0.91
RT 13	Tennessee	35.0/87.9	Oak	4.17	72.3	45.5	123	5.64	3.45	3.89	113	0.47	0.55	0.68

5.3.5 Comparison of MEGAN Runtimes

We evaluated the time required to run the MEGAN3 model and compared it with the time required to run MEGANv2.1. Table 5-4 shows the results of the run time comparison between MEGAN2.1 and MEGAN3 based on time stamps of the model output files. Times are for MEGAN runs on the 12 km domain (Figure 5-1) for the period May 25- July 17, 2013 (54 days). The MEGAN3 run time is approximately half that of MEGAN2.1 for the same domain and modeling episode. It should be noted that the run times below are only for running major MEGAN steps and do not include time for preparation of input data (i.e. EFP or prepmegan4cmaq).

Table 5-4. Comparison of MEGAN run times.

MEGANv2.10		MEGAN3	
Subroutines	**Running time**	**Subroutines**	**Running time**
MET2MGN	13 min	MET2MGN	13 min (same as MEGANv2.10)
EMPROC	140 min	DAYMET	< 5 min
		MEGSEA	2 min
		MEGCAN	23 min
		MEGVEA	23 min
MGN2MECH	21 min	MGN2MECH	15 min
Total	**~ 174 min**	**Total**	**~ 80 min**

5.3.6 Summary of MEGAN3 Modeling

Overall, MEGAN3 isoprene emission estimates agree more closely with the aircraft derived fluxes than the MEGAN v2.1 isoprene emissions. MEGAN2.1 isoprene emissions have a high bias while the MEGAN3 inventories have a small (10%) negative bias. For monoterpenes, the MEGAN3 emission estimates are generally in better agreement with the aircraft fluxes in comparison to MEGAN v2.1. For both isoprene and monoterpenes, differences among the MEGAN3 emission inventories are relatively small compared with the differences between MEGAN3 and MEGAN v2.1 emissions.

The comparison between MEGAN emissions and the airborne fluxes is affected by the use of different meteorological data (WRF and NLDAS) in preparing the Model emission flux estimates. The MEGAN EF shown in tables 5-2 and 5-3 do not require any temperature and solar radiation data but the aircraft EF estimates used NLDAS data to derive an EF from the direct flux measurement. The aircraft fluxes shown in Figure 5-10 and Figure 5-11 are a direct flux measurement, and so do not require any temperature and solar radiation data to derive a flux, but the model estimates shown in these figures used WRF data to calculate emission responses to temperature and solar radiation. In the AQRP 14-016 BVOC project, it was noted that there are differences of ~37% between airborne emission factors developed using WRF and NLDAS data and concluded that the NLDAS values were more accurate. The MEGAN2.1 isoprene emission estimates shown in Figure 5-10 and Figure 5-11 would be lower if NLDAS data were used and would have shown better agreement with the airborne fluxes.

5.4 CAMx Modeling

5.4.1 CAMx Model Configuration

The modeling platform developed by Johnson et al., (2013) and used in AQRP Project 14-016 was used in this study to simulate June 1-July 15, 2013. This period encompassed all of the SAS C-130 and P-3 flights. To model the July and September, 2013 episodes, we developed meteorological inputs for CAMx by running the WRF model in hindcast mode as described in Yu et al. (2015). The WRF outputs were converted into CAMx model-ready inputs using the WRFCAMx preprocessor v4.3 with YSU vertical diffusivity (Kv). The Kv landuse patch was applied up to 100 m and the Kv cloud patch was also applied.

2012 day-of-week specific anthropogenic emissions were provided by the TCEQ. The 2012 emission inventory was augmented by the TCEQ with 2013 oil and gas emissions for the State of Texas. Electric generating unit emissions were typical ozone season day averages for 2012. 2013 day-specific FINN wildfire emissions (Wiedinmyer et al., 2012) were used and the fire emission modeling is described in Kemball-Cook et al. (2014).

The Zhang dry deposition scheme was used. Photolysis rates files were generated using O3MAP 2012 monthly averages from 1 degree TOMS satellite ozone column data. Land use/land cover inputs were generated using the USGS 24-category dataset and monthly LAI data from MODIS satellite were used.

Boundary conditions for the 36 km grid were developed from Near Real Time MOZART-4/MOPITT chemical forecasts from NCAR (http://web3.acd.ucar.edu/acresp/forecast). Chemical forecasts are run each day using MOZART-4, driven by GEOS-5 meteorology and including the standard (100 species) chemical mechanism (Emmons et al., 2010). We performed a flat 10 ppb ozone reduction and applied a set of caps to ozone precursors and other key species (Table 5-5) in all 36 km grid cells located over the Gulf of Mexico and Atlantic Ocean (red boundary cells in Figure 5-12) in order to reduce potential high bias in ozone transported onshore. We apply an additional 5 ppb ozone reduction over all remaining 36 km grid cells outside of the Gulf of Mexico and Atlantic Ocean (blue boundary cells in Figure 5-12).The boundary condition caps are summarized in Table 5-5.

Table 5-5. Maximum concentration limits for ozone precursors applied to the 36 km boundary condition grid cells across the Gulf of Mexico, Caribbean Sea, and Atlantic Ocean south of Cape Hatteras. These boundary grid cells are shown as red in Figure 5-12.

Species	Description	Max. Concentration (ppb)
NO2	Nitrogen dioxide	0.05
CO	Carbon monoxide	150.0
N2O5	Dinitrogen pentoxide	0.001
HNO3	Nitric acid	0.25
PNA	Peroxynitric acid	0.001
H2O2	Hydrogen peroxide	0.5
NTR	Organic nitrates	0.01
FORM	Formaldehyde	0.25
ALD2	Acetaldehyde	0.05
ALDX	Propionaldehyde and higher aldehydes	0.02
PAR	Paraffin carbon bond (C-C)	1.0
OLE	Terminal olefin carbon bond (R-C=C)	0.01
ETHA	Ethane	1.0
MEPX	Methylhydroperoxide	0.1
PAN	Peroxyacetyl Nitrate	0.01
PANX	C3 and higher peroxyacyl nitrate	0.001
INTR	Organic nitrates from ISO2 reaction with NO	0.001
ISOP	Isoprene	0.1
ISPD	Isoprene product (lumped methacrolein, methyl vinyl ketone, etc.)	0.1
TERP	Monoterpenes	0.05
ISP	Isoprene (SOA chemistry)	0.1
TRP	Monoterpenes (SOA chemistry)	0.05
TOL	Toluene and other monoalkyl aromatics	0.02
XYL	Xylene and other polyalkyl aromatics	0.01
SO2	Sulfur dioxide	0.1
PRPA	Propane	0.5
ACET	Acetone	0.25
KET	Ketone carbon bond (C=O)	0.05
BENZ	Benzene	0.1

•

36 km grid

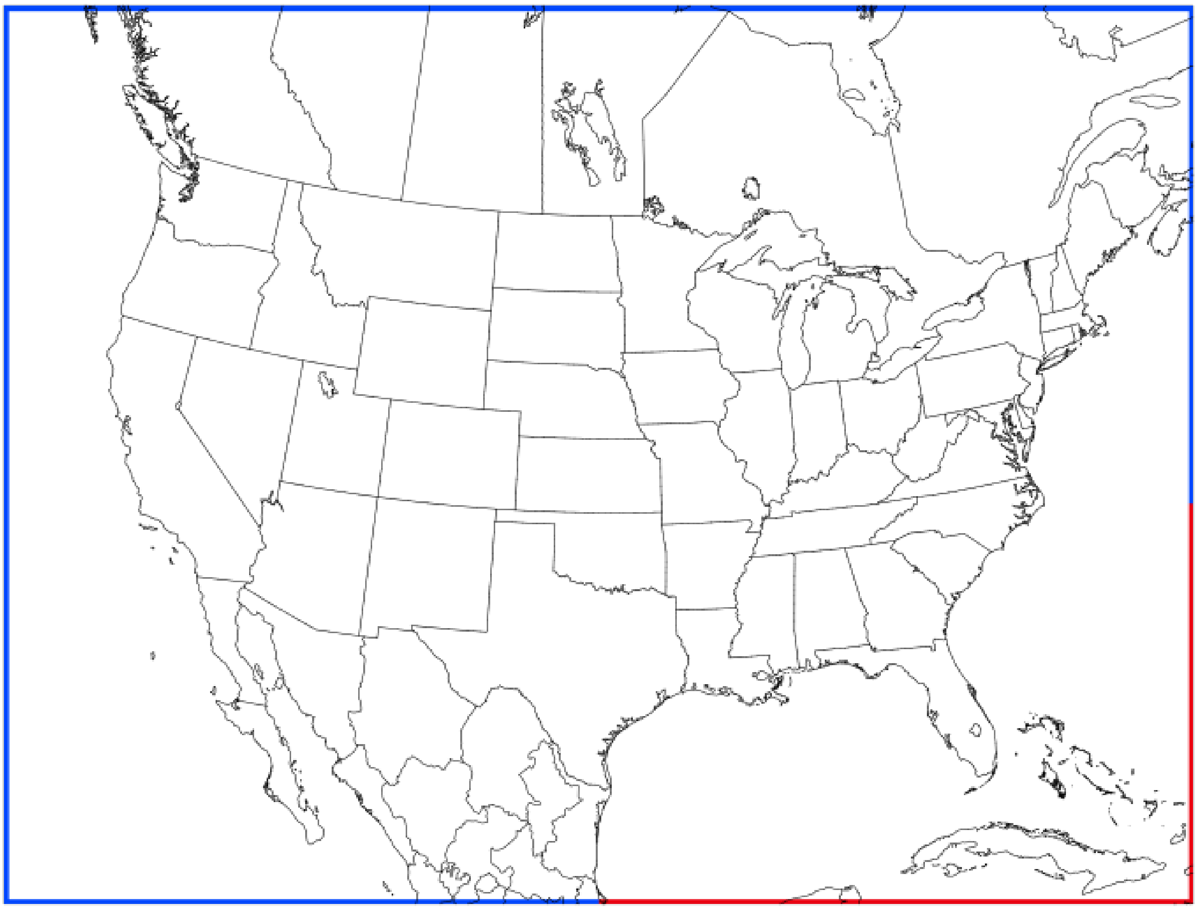


Figure 5-12. Map of CAMx 36 km modeling domain showing the cells where the two boundary condition patches were applied. A flat 10 ppb ozone reduction and ozone precursor caps were applied over the Gulf of Mexico and Atlantic Ocean boundary cells (red) and a flat 5 ppb ozone reduction was applied over the remaining boundary cells (blue).

The CB6r4 chemical mechanism (Yarwood et al., 2012) was used in the CAMx modeling. CB6r4 combines a condensed set of reactions involving ocean-borne inorganic iodine with a temperature- and pressure-dependent organic nitrate branching ratio. CB6r4 is supported by an in-line iodine emissions parameterization that computes inorganic iodine emissions caused by ozone deposition to seawater. CB6r4 also adds pseudo-heterogeneous hydrolysis of isoprene-derived organic nitrate (INTR). Aerosol uptake of organic nitrate followed by particle-phase hydrolysis to HNO_3 formation can be an important pathway for loss of atmospheric NOx (Hildebrandt Ruiz and Yarwood, 2013; Jacobs et al., 2014; Fisher et al., 2016). CB6r4 assumes the same lifetime (1 hour) against particle-phase hydrolysis of INTR as Fisher et al. (2016). Partitioning of organic nitrate into particle phase is modeled using a two-product parameterization based on ambient measurement data (Rollins et al., 2013). As with earlier versions of the CB6 chemical mechanism, CB6r4 contains an explicit hydroperoxyaldehyde

(HPLD) product and the lumped isoprene product species ISPD represents methyl vinyl ketone (MVK), methacrolein (MACR) and similar products.

We made the following simulations of the June 1-July 15, 2013 period with CAMx:

1. CAMx with MEGAN v2.1 emissions developed with default inputs (CAMx_MEGAN2.1)
2. CAMx with MEGAN3 with emission factors from MEGAN-EFP using high quality (J=4) data (CAMx_MEGAN3_J4)
3. CAMx with MEGAN3 with emission factors from MEGAN-EFP using lower quality (J=0) data (CAMx_MEGAN3_J0)
4. Emission factors from MEGAN-EFP using high quality (J=4) data but without stress induced factors (CAMx_MEGAN3_nostress)

First, we describe the model performance evaluation method for ground level ozone and provide an overview of the results of the evaluation of the four CAMx runs. More information on the surface ozone evaluation is given in Appendix C. In the remainder of Section 5, we focus on the evaluation of the base run and sensitivity tests against C-130 and P-3 aircraft data from the 2013 SAS Study.

5.4.2 CAMx Model Performance Evaluation Method

We evaluated the four CAMx runs against ground level ozone observations from Clean Air Status and Trends Network (CASTNET) sites for stations within the 12 km grid and outside of Texas. The CASTNET monitors are located in rural areas and this is appropriate considering the model's relatively coarse horizontal resolution. U.S. CASTNET sites are shown in Figure 5-13. We used data from the subset of these stations that had monitoring data available for the June 1-July 15, 2013 modeling period. We also evaluated ozone at rural locations in Texas using ozone measurements from TCEQ Continuous Air Monitoring Stations (CAMS). To evaluate the model's performance in simulating ground level ozone, we prepared time series of hourly observed and modeled ozone for each station for the June 1-July 15, 2013 model run. We also evaluated model performance for 8-hour average ozone against two statistical metrics. The statistical metric used in this model performance evaluation is the normalized mean bias (NMB), defined as

$$NMB = \frac{\sum_{i=1}^{N}(P_i - O_i)}{\sum_{i=1}^{N} O_i}$$

where P_i and O_i are the predicted and observed values (O_i,P_i) paired in space and time and N is the number of observed/modeled data pairs. The NMB shows whether a modeled quantity such as ozone is under- or over-predicted on average, compared with observations.

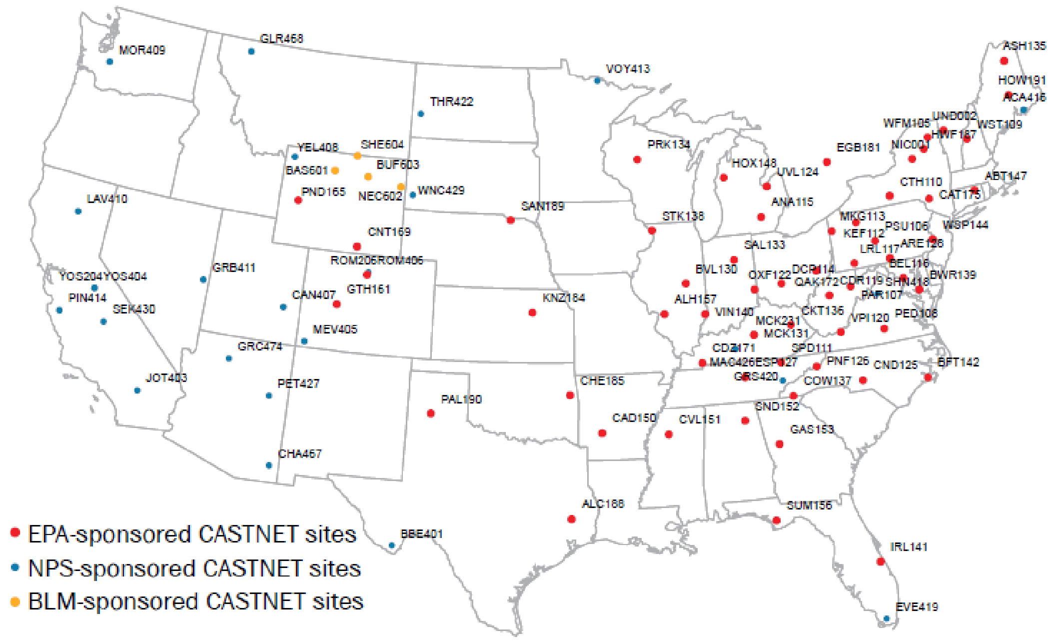


Figure 5-13. Location of CASTNet monitoring sites. EPA figure[2].

[2] http://epa.gov/castnet/javaweb/docs/CASTNET_Factsheet_2013.pdf

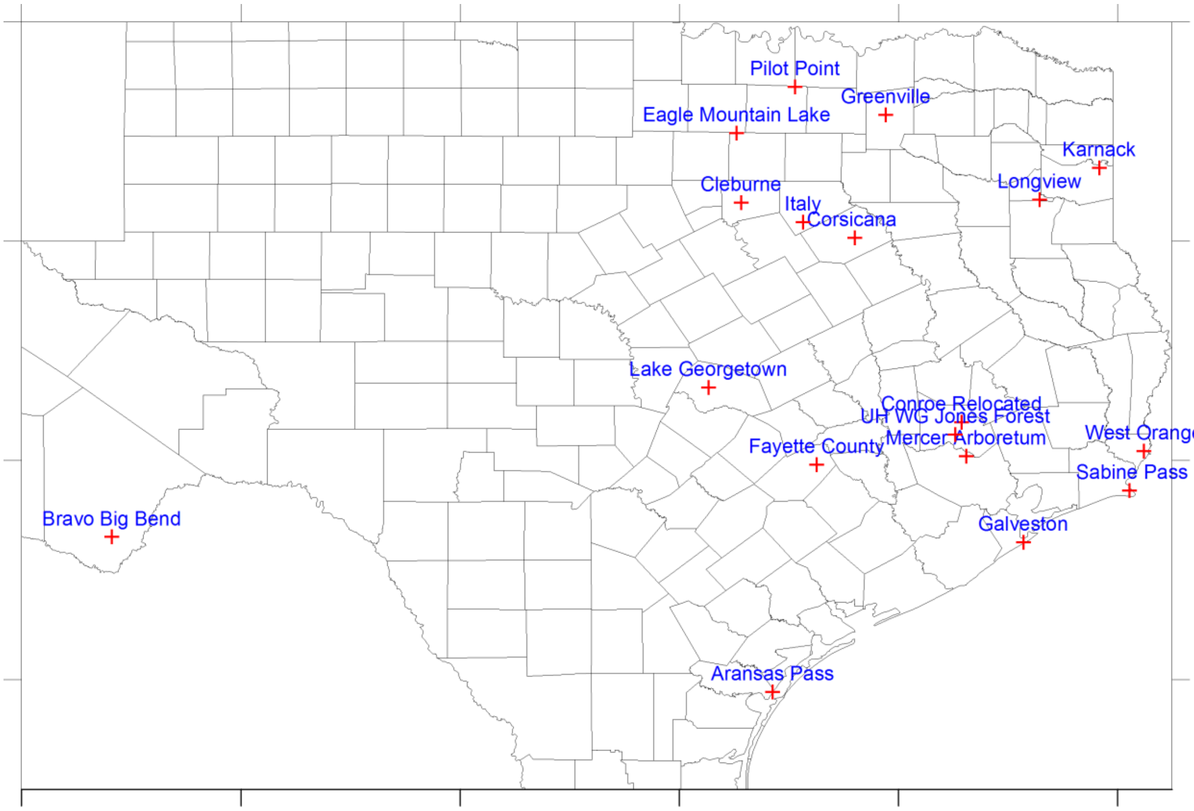


Figure 5-14. TCEQ CAMS monitoring sites used in the model performance evaluation.

5.4.3 CAMx Performance Evaluation Results

5.4.3.1 Comparison with Surface Observations

The hourly ozone time series and daily bias statistics for the CAMx evaluation against observed ozone at CASTNET and CAMS stations are shown in Appendix C and are summarized below. The model performance evaluation for surface ozone at Texas CAMS sites showed the following:

- CAMx model performance was reasonably good at rural/suburban sites in north and central Texas (e.g. Pilot Point, Cleburne). The model captured much of the variability in observed ozone on weekly and daily timescales and no persistent positive or negative bias.
- CAMx has a general high bias for ozone at coastal sites and sites near the eastern border of Texas.
- Ozone was generally lower in the CAMx_MEGAN3 runs than in the CAMx_MEGAN2.1 run. The effect of changing biogenic inventories on surface ozone performance for most inland Texas sites was mixed. For days where the model overestimated ozone, the CAMx_MEGAN3 runs simulated observed ozone more accurately than the CAMx_MEGAN2.1 run, while on days where the model underestimated ozone the CAMx_MEGAN2.1 simulation was closer to observations.
- Differences among the three CAMx_MEGAN3 simulations were relatively small compared with differences between the CAMx_MEGAN3 and CAMx_MEGAN2.1 simulations.

- Of the three CAMx_MEGAN3 simulations, the CAMx_MEGAN3_nostress simulation generally had the highest ozone.
- At CAMS sites in the Houston-Galveston-Brazoria area, there was a large (up to 20 ppb) reduction in ozone in the CAMx_MEGAN3 runs relative to the CAMx_MEGAN2.1 runs. The effect of this reduction was to improve agreement with observations because these reductions frequently happened on days where the CAMx_MEGAN2.1 run had a high bias relative to observed ozone. Model performance at Mercer Arboretum (Figure 5-15) was typical of Houston-Galveston-Brazoria monitors. Many sites, including Mercer Arboretum as well as Sabine Pass and Galveston, had periods of extremely high bias where ozone was overestimated during periods of onshore flow (e.g. June 22-24 in Figure 5-15). The MOZART model boundary conditions are day-specific and are capped to reduce ozone but a high bias for ozone remains. The CAMx overestimates at coastal sites may also reflect the WRF model's difficulty in simulating near surface winds at coastal sites at 12 km resolution.

The model performance evaluation for surface ozone at CASTNet sites showed the following:

- At most CASTNet sites in the southeast, the CAMx model had periods of both high bias and low bias. For example, at the Great Smoky National Park CASTNet site in Tennessee (GRS 420; Figure 5-16) the model has a period of high bias from July 3-7 but greatly underestimates ozone during June 28-30.
- The high bias was most pronounced at coastal sites such as IRL141 and SUM156 in Florida, which had consistent overestimates of ozone. These overestimates sometimes occurred during periods of onshore flow and may be related to bias in the CAMx 36 km grid boundary conditions.
- As for the Texas monitors, ozone at the CASTNet sites was generally lower in the CAMx_MEGAN3 runs than in the CAMx_MEGAN2.1 run and differences among the three CAMx_MEGAN3 simulations were relatively small compared with differences between the CAMx_MEGAN3 and CAMx_MEGAN2.1 simulations.
- Also similar to the Texas sites, the CASTNet evaluation showed that of the three CAMx_MEGAN3 simulations, the CAMx_MEGAN3_nostress simulation generally had the highest ozone.

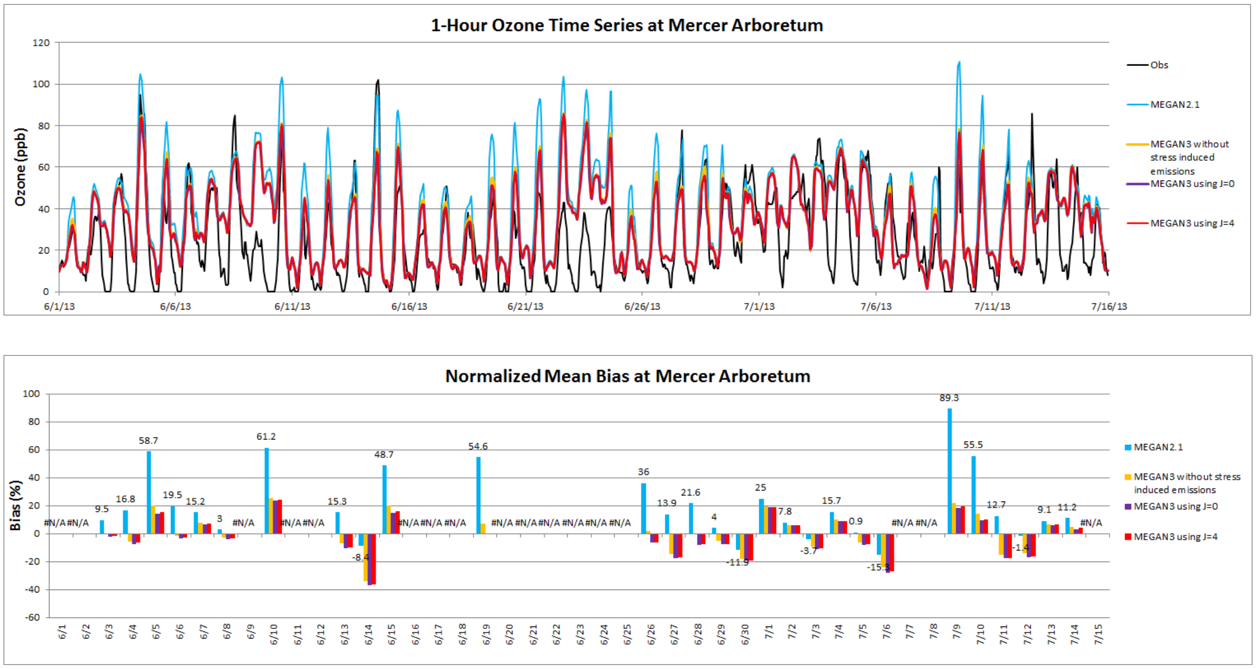


Figure 5-15. 1-hour ozone time series (upper panel) and normalized mean bias (lower panel) for the Mercer Arboretum (CAMS 557) monitor in the Houston area. NMB was not calculated on days when observed daily maximum 8-hour ozone was < 40 ppb and these days are indicated by #N/A.

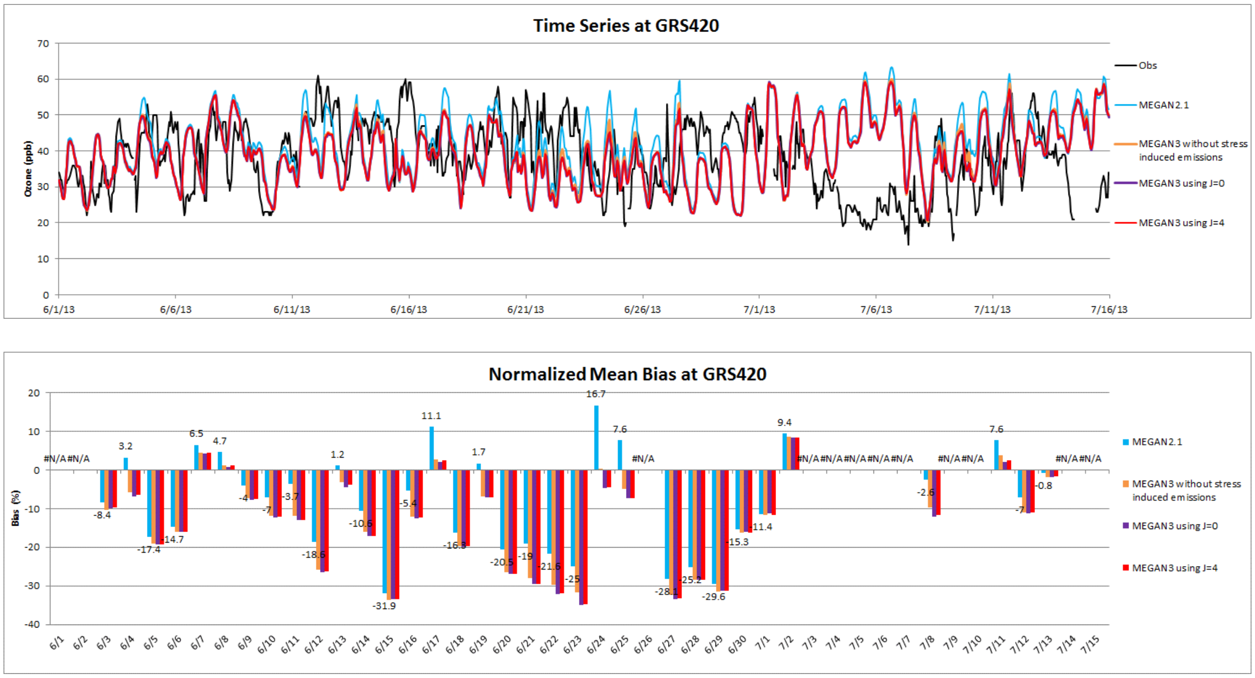


Figure 5-16. 1-hour ozone time series (upper panel) and normalized mean bias (lower panel) for the Great Smoky Mountain CASTNet site in Tennessee. NMB was not calculated on days when observed daily maximum 8-hour ozone was < 40 ppb and these days are indicated by #N/A.

5.4.3.2 Comparison with SAS C-130 and P-3 Aircraft Data

We evaluated the CAMx simulations against C-130 and P-3 aircraft observations paired in time and space. Two datasets were available for the C-130 flights. These two merged datasets combine observations from the different instruments on the aircraft to a common time base. The first dataset, mrg60, combines the data to a 1-minute time base. The time listed in the data set is the mid-point of the 1-minute average and any measurement that occurred within or overlapped the 1 minute period is included in the average and is weighted accordingly[3]. The TOGA dataset is averaged to the 2 minute time period of the Trace Organic Gas Analyzer (TOGA). The TOGA is a fast online Gas Chromatograph/Mass Spectrometer (GC/MS) that measures VOCs and other species with a measurement frequency of approximately one 30s sample every 2 minutes[4]. We compared the mrg60 and TOGA datasets to the CAMx output. The P-3 data were reported as 1 minute averages. Measured species and measurement methods used aboard the P-3 and C-130 for species analyzed in this study are shown in Table 5-6 and Table 5-7.

Table 5-6. P-3 species and measurement methods[5].

Species	Technique	Data ID
Airborne Cavity Enhanced Spectrometer (NO_2 and glyoxal)	Airborne Cavity Enhanced Spectrometer	ACES
Nitrogen Oxide, Nitrogen Dioxide, Ozone (O_3), Nitrogen Trioxide (NO_3), Dinitrogen Pentoxide (N_2O_5)	Cavity ring-down spectrometer.	CaRDS
Carbon Monoxide (CO)	Vacuum UV resonance fluorescence	CO
HNO_3, HCOOH, HONO	Chemical Ionization Mass Spectrometry (CIMS).	HNO3HCOOH
Nitric Oxide (NO)	NO/O3 Chemiluminescence.	NO
Nitrogen Dioxide (NO_2)	Photolysis and NO/O3 Chemiluminescence.	NO2
Total Reactive Nitrogen Oxides (NOy)	Au Converter and NO/O3 Chemiluminescence.	NOy
Ozone (O_3)	Chemiluminescence.	O3
Peroxyacyl Nitrates (PANs)	Chemical Ionization Mass Spectrometer (CIMS).	PANs
Sulfur Dioxide (SO_2)	Pulsed UV fluorescence.	SO2

[3] https://www2.acd.ucar.edu/campaigns/nomadss
[4] http://data.eol.ucar.edu/datafile/nph-get/373.023/Hornbrook_TOGA_VOC_Analyzer_readme.pdf
[5] http://www.esrl.noaa.gov/csd/groups/csd7/measurements/dataui/

Species	Technique	Data ID
Various VOCs using PTR-MS	Proton Transfer Reaction Mass Spectrometer (PTRMS).	VOCsPTRMS
Various VOCs using whole air sampler (WAS) (SENEX 2013 P-3)	Whole air sampler and post-flight gas chromatograph.	VOCsiWAS2

Table 5-7. C-130 Species and measurement methods[6].

CU CIMS: OH, H_2SO_4, sCIs
In Situ Chemiluminescence: NO, NO_2, O_3 Data
NSF/NCAR C-130 HONO Particulate Nitrate and Nitric Acid Data
Proton Transfer Reaction Mass Spectrometer (PTR-MS) Data
Trace Organic Gas Analyzer (TOGA) VOC Analyzer Data

5.4.4 Comparison of CAMx Simulations Using MEGAN v2.1 and MEGAN3 Base Case Biogenic Emissions against SAS Aircraft Measurements

The upper and lower panels of Figure 5-17 compare measured and modeled isoprene concentrations along the aircraft flight tracks for the C-130 mrg60 and P-3 data, respectively. In the CAMx CB6r4 chemical mechanism, isoprene is represented explicitly by the species ISOP. Isoprene was measured via PTR-MS on both aircraft. With both MEGAN v2.1 and MEGAN3 emissions, CAMx shows patterns of higher and lower isoprene that are similar to the aircraft observations. For example, both the modeled and the measured isoprene are relatively high in the region that includes northeast Texas, northwest Louisiana and southwestern Arkansas. Both observed and CAMx modeled isoprene show hot spots in southeastern Missouri, northern Alabama and northern Georgia. Areas of lower isoprene occur in the model and measurements in northern Indiana, northern Mississippi, South Carolina, northeastern Kentucky and central Texas.

CAMx_MEGAN2.1 generally overestimates isoprene where observed isoprene has its largest values (northeast Texas, northwest Louisiana, Arkansas, southeast Missouri, and western Alabama) and underestimates isoprene where C-130 observed values are relatively low (e.g. western Tennessee and Kentucky). Agreement with the P-3 observations is better for lower values of isoprene. In the CAMx_MEGAN3_J4 simulation, isoprene concentrations are lower than in the CAMx_MEGAN2.1 simulation in the areas of highest observed isoprene. Over areas with high observed isoprene in Northeast Texas, Arkansas, Georgia and Alabama, the CAMx_MEGAN3_J4 simulation agrees more closely with the aircraft measurements. Like the CAMx_MEGAN2.1 simulation, the CAMx_MEGAN3_J4 run underestimates isoprene where C-

[6] http://data.eol.ucar.edu/master_list/?project=SAS

130 observed values are low, but shows better agreement with lower isoprene values measured aboard the P-3.

The scatter plots in Figure 5-18 and Figure 5-19 show all (observed, modeled) isoprene data pairs from the C-130 and P-3 flights. Both the C-130 mrg60 and TOGA data sets are shown in Figure 5-18. Coefficient of determination (r^2) values range between 0.4 and 0.6 for CAMx and the three aircraft datasets, consistent with the overall agreement in spatial patterns between observed and modeled isoprene. CAMx_MEGAN2.1 has a pronounced high bias for isoprene relative to all three data sets, with NMB ranging from 76-117%. This high bias is eliminated in the CAMx_MEGAN3_J4 run, which has a low bias ranging from -7% to -34%. The magnitude of the isoprene NMB and NME is substantially lower in CAMx_MEGAN3_J4 than in CAMx_MEGAN 2.1. The value of r^2 is lower in CAMx_MEGAN3_J4 than in CAMx_MEGAN v2.1.

The comparison of CAMx modeled and measured isoprene reaction products is shown in Figure 5-20 and Figure 5-21. In CAMx, isoprene products are represented by the sum of ISPD and HPLD. The CB6r4 species ISPD represents isoprene products and includes lumped methacrolein (MACR) and methyl vinyl ketone (MVK). HPLD represents hydroperoxyaldehydes. The PTR-MS instrument does not distinguish MACR, MVK and HPALD and the total isoprene product measurement from the PTR-MS instrument is shown.

Figure 5-20 and Figure 5-21 indicate that CAMx_MEGAN2.1 overestimates isoprene reaction products along the flight track for both aircraft, and this is consistent with the isoprene overestimates shown in Figure 5-19. The bias for isoprene products is smaller than for isoprene, which implies that the chemical aging of isoprene is too slow in CAMx. It is possible that OH from isoprene could be biased low, or a high bias for isoprene could be slowing oxidation by consuming OH.

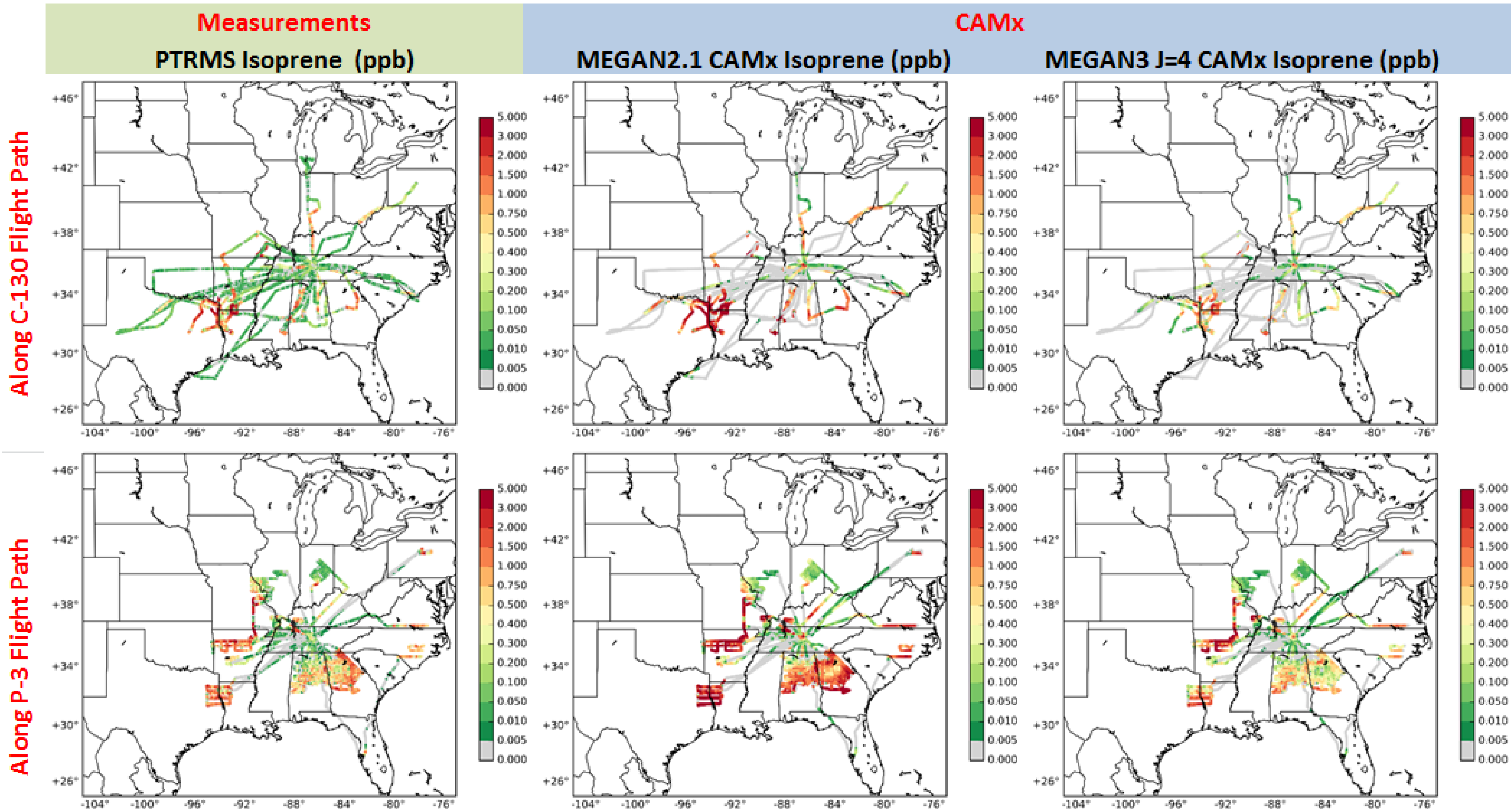


Figure 5-17. Measured and modeled isoprene along the C-130 (upper panels) and P-3 (lower panels) flight tracks for the June 1-July 15, 2013 period. Aircraft measurements are shown in the left panels. Center panels show CAMx_MEGAN2.1 modeled concentrations and right panels show concentrations for CAMx_MEGAN3_J4 simulation.

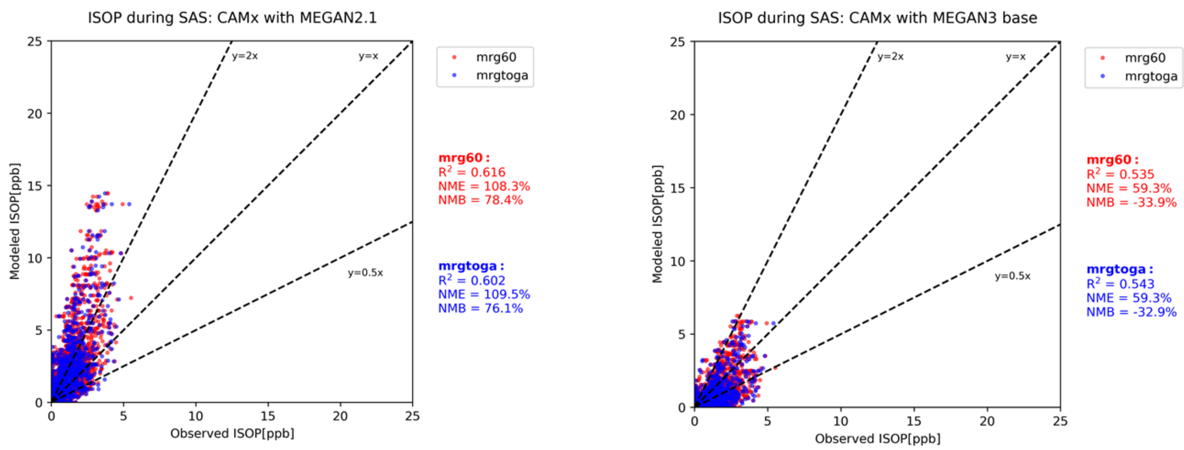


Figure 5-18. Measured and modeled isoprene along the C-130 flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

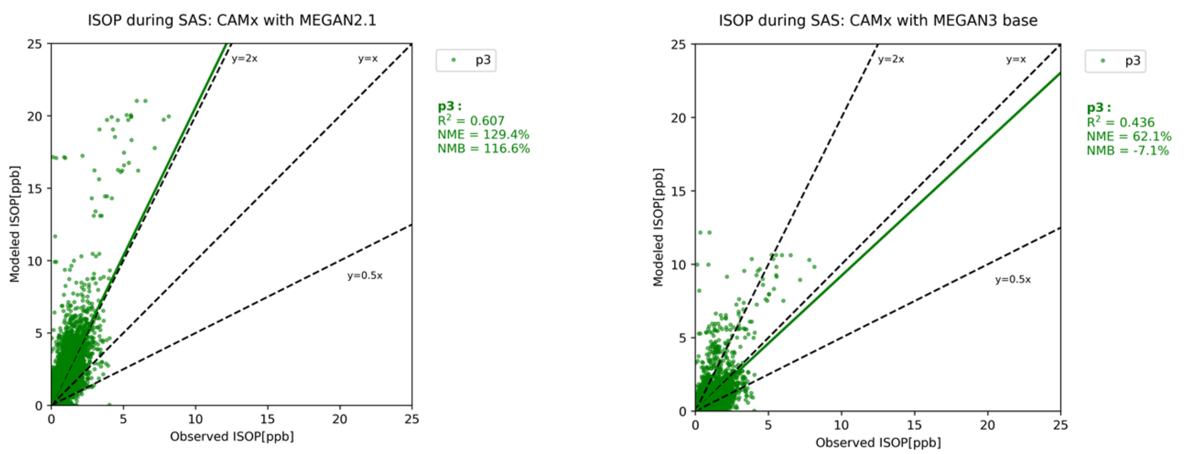


Figure 5-19. Measured and modeled isoprene along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

As for isoprene, the magnitude of the NMB and NME is substantially lower in CAMx_MEGAN3_J4 than CAMx_MEGAN 2.1. There is a shift from a high bias in CAMx_MEGAN2.1 to a low bias with far smaller magnitude in CAMx_MEGAN3_J4 and a lower r^2 in CAMx_MEGAN3_J4 than in CAMx_MEGAN v2.1.

The upper and lower panels of Figure 5-22 compare measured and modeled monoterpene concentrations along the aircraft flight tracks for the C-130 mrg60 and P-3 data, respectively. Scatterplots in Figure 5-23 and Figure 5-24 compare the modeled and measured sum of monoterpenes along the C-130 and P-3 flight tracks, respectively. Values of r^2 are lower for monoterpenes than for isoprene, and mismatches between modeled and measured values are more pronounced in the C-130 measurements than in the P-3 measurements. Examples of this can be seen in the C-130 flight tracks along the northern border of West Virginia and through central Oklahoma and Indiana.

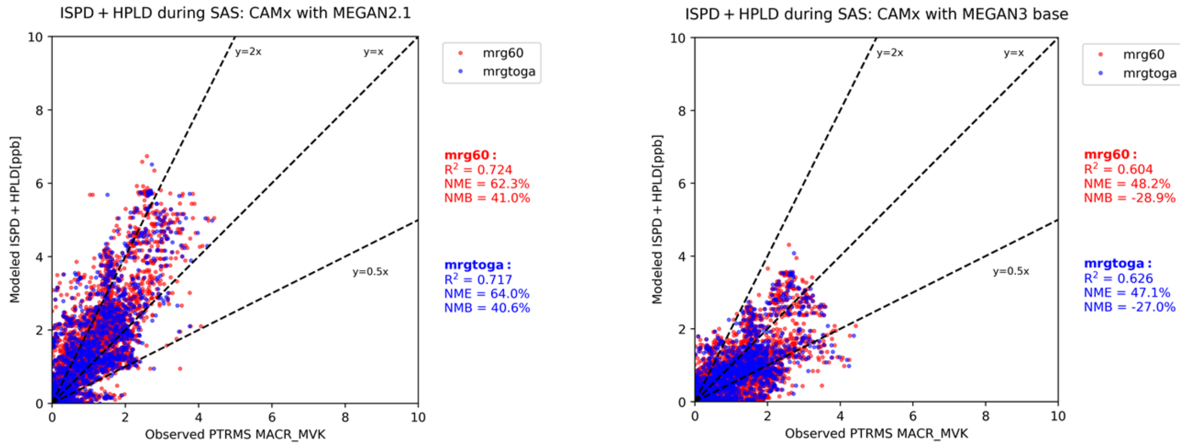


Figure 5-20. Measured and modeled isoprene products along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

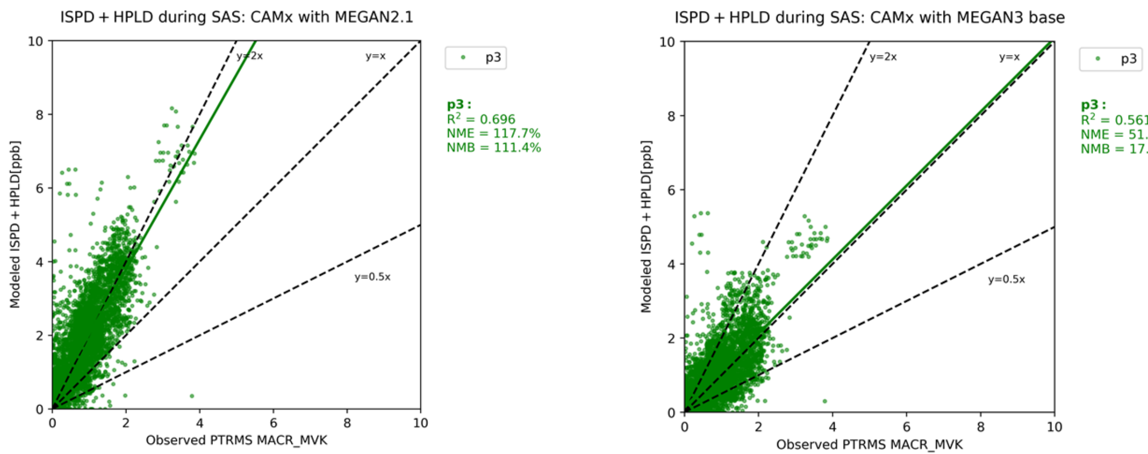


Figure 5-21. Measured and modeled isoprene products along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

The negative values of NMB indicate that CAMx monoterpene concentrations are generally less than the observed concentrations. The magnitude of the NMB and NME is higher for the CAMx_MEGAN3_J4 simulation than for the CAMx_MEGAN 2.1, indicating that the existing low bias for monoterpenes becomes more pronounced in CAMx_MEGAN3_J4. The spatial plots show that the CAMx_MEGAN3_J4 run shows large decreases in monoterpene concentrations in areas where observed monoterpene concentrations are largest, such as Northeast Texas, Northern Louisiana, southern Arkansas, and Georgia; in these regions, the CAMx_MEGAN2.1 agrees more closely with aircraft measurements than CAMx_MEGAN3_J4. r^2 is lower for CAMx_MEGAN3_J4 than for CAMx_MEGAN v2.1.

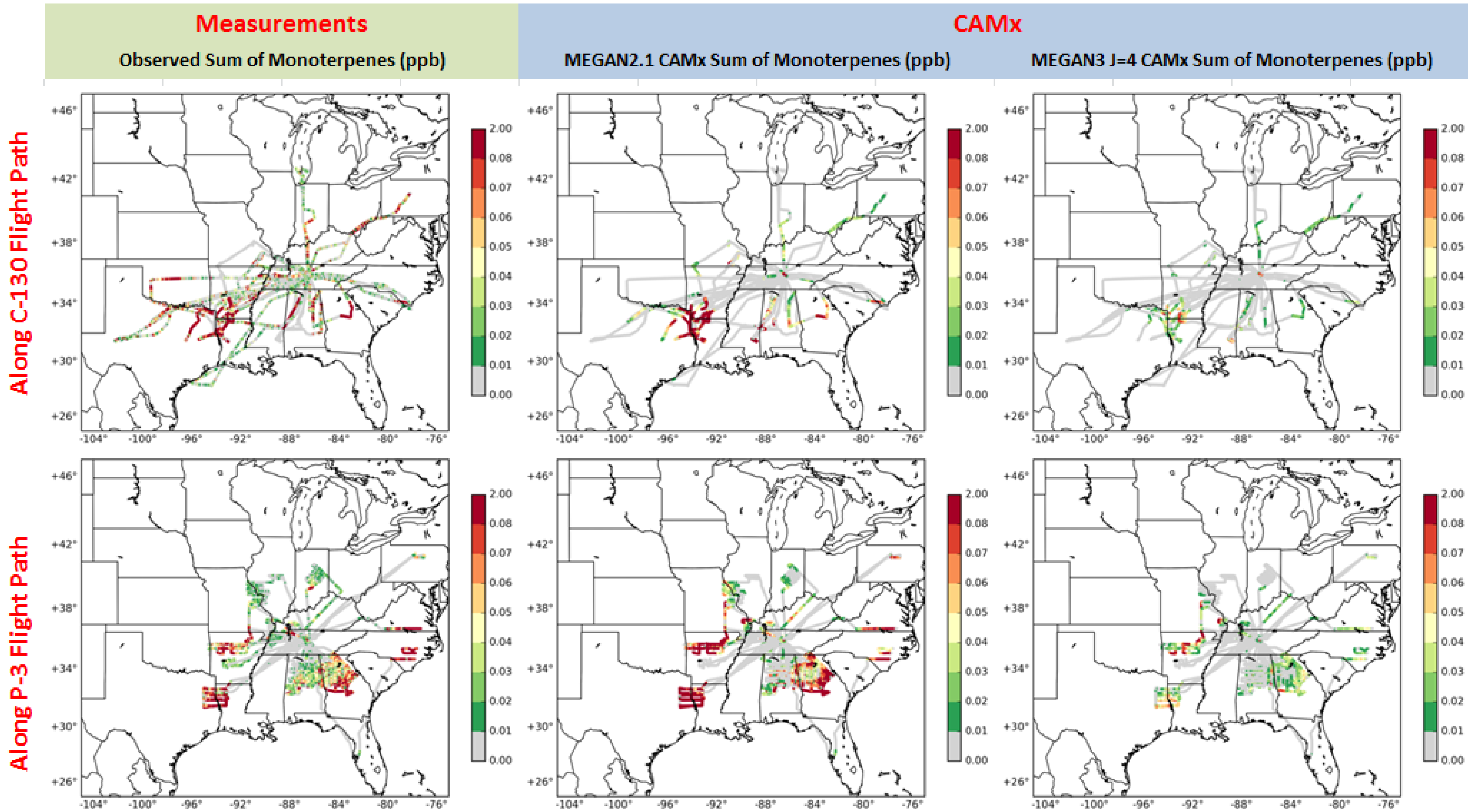


Figure 5-22. Measured and modeled monoterpenes along the C-130 (upper panels) and P-3 (lower panels) flight tracks for the June 1-July 15, 2013 period. Aircraft measurements are shown in the left panels. Center panels show CAMx_MEGAN2.1 modeled concentrations and right panels show concentrations for CAMx_MEGAN3_J4 simulation.

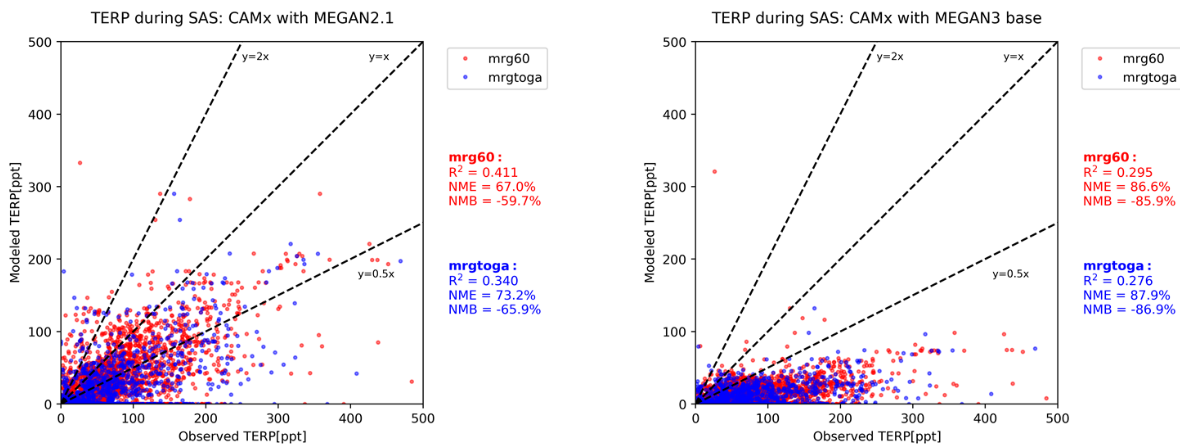


Figure 5-23. Measured and modeled sum of monoterpenes along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

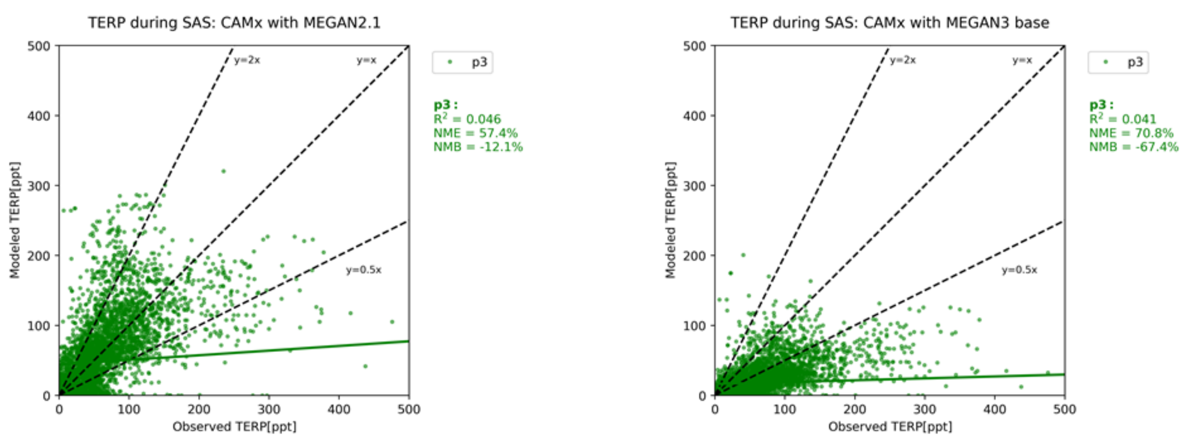


Figure 5-24. Measured and modeled sum of monoterpenes along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

Figure 5-25 compare measured and modeled ozone along the aircraft flight tracks. CAMx bias for ozone is small (|NMB|<10%) along both flight tracks. r^2 values are low with all values less than 0.18. The use of regression statistics may be inappropriate here because ozone is a relatively long-lived species with a regional background and the positive bias may be partly caused by error in the transported background due to model boundary conditions (i.e., an offset that shows up in the intercept). This is consistent with the dramatic overestimates of ozone seen in the CAMx surface performance evaluation at coastal sites during periods of onshore winds. A high bias due to boundary conditions may result from using boundary conditions that reflect a bias in the global model used to develop them.

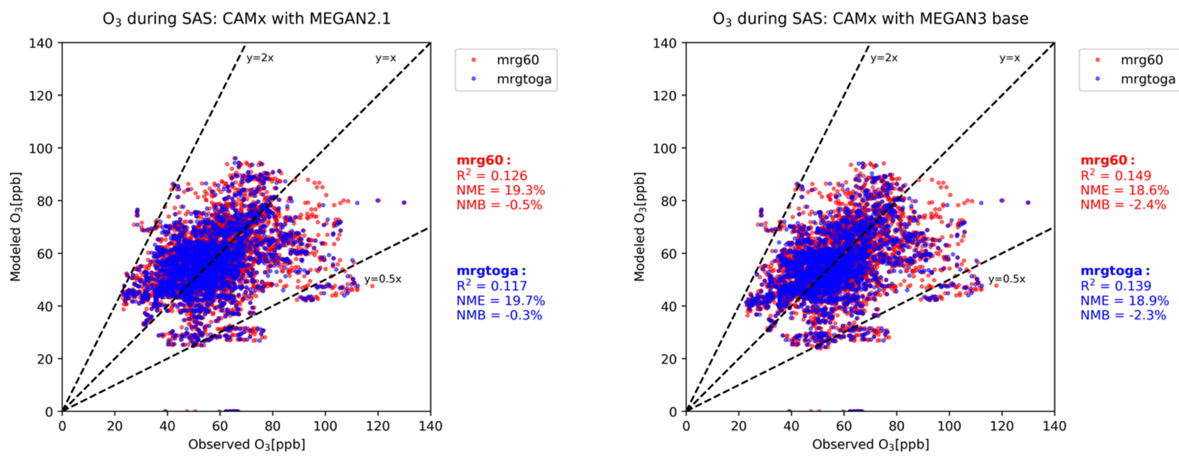


Figure 5-25. Measured and modeled ozone along the C-130 and P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

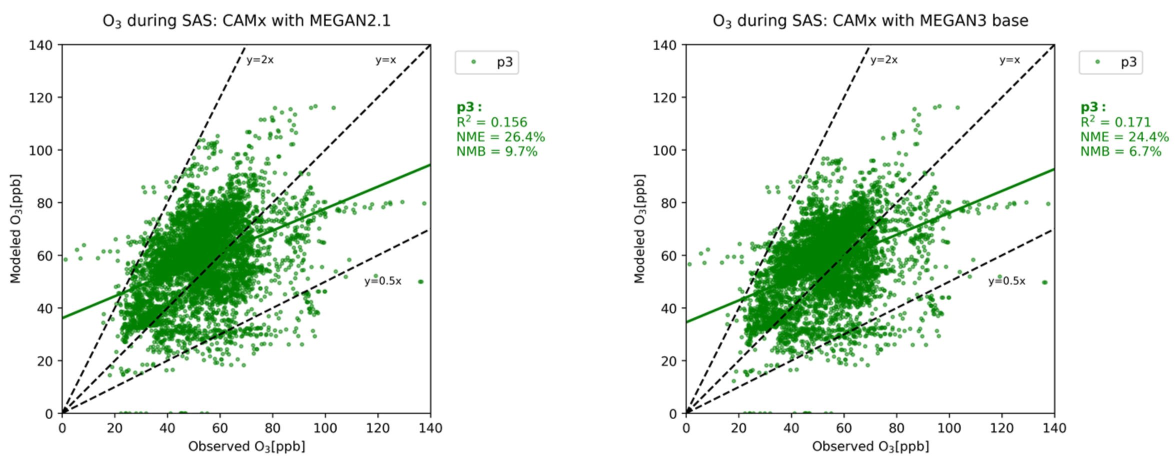


Figure 5-26. Measured and modeled ozone along the C-130 and P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

CAMx model performance for OH is shown in Figure 5-27. OH was not available for all C-130 flights, and was not measured aboard the P-3. CAMx_MEGAN3_J4 shows improved performance for OH relative to CAMx_MEGAN 2.1. The magnitude of the NMB is lower in CAMx_MEGAN3_J4 and R^2, while small in both runs, increases from 0.1 in CAMx_MEGAN2.1 to 0.2 in CAMx_MEGAN 2.1.

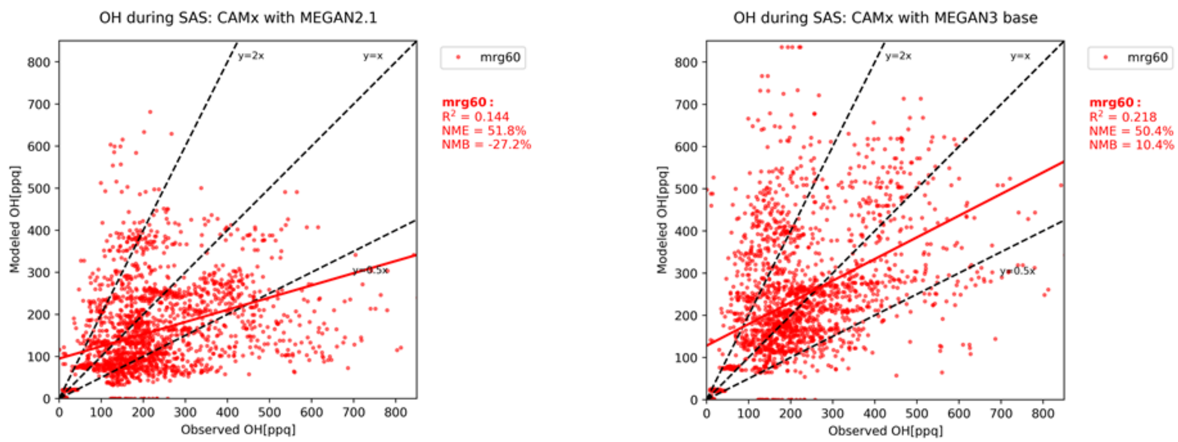


Figure 5-27. Measured and modeled OH along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period. OH measurements were not available for the P-3 flight tracks for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

Comparison of modeled and measured formaldehyde (HCHO) along the C-130 and P-3 flight tracks (Figure 5-28 and Figure 5-29). In both CAMx runs, measurements and modeled values are well-correlated ($r^2 > 0.8$). The NMB and NME have larger magnitude in CAMx_MEGAN3_J4 than in CAMx_MEGAN 2.1. For both the C-130 and P-3 data sets, the low bias in CAMx_MEGAN 2.1 becomes larger in CAMx_MEGAN3. Observed outliers are from a small set of days. For example, all values of measured formaldehyde > 10 ppb were from the July 2 flight. All measured values > 8.4 ppb are from either the July 2 or June 12 flight.

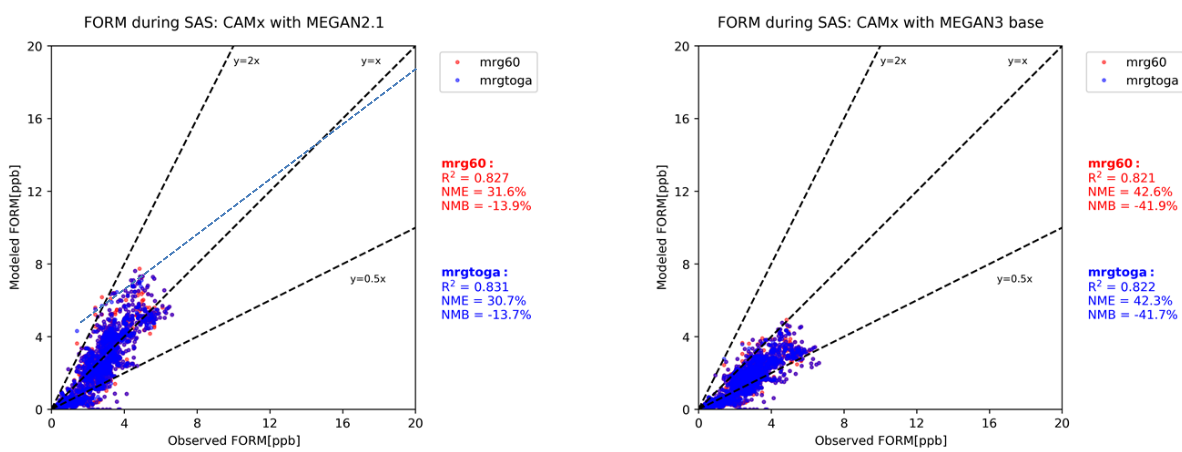


Figure 5-28. Measured and modeled formaldehyde along the C-130 (right panel) aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

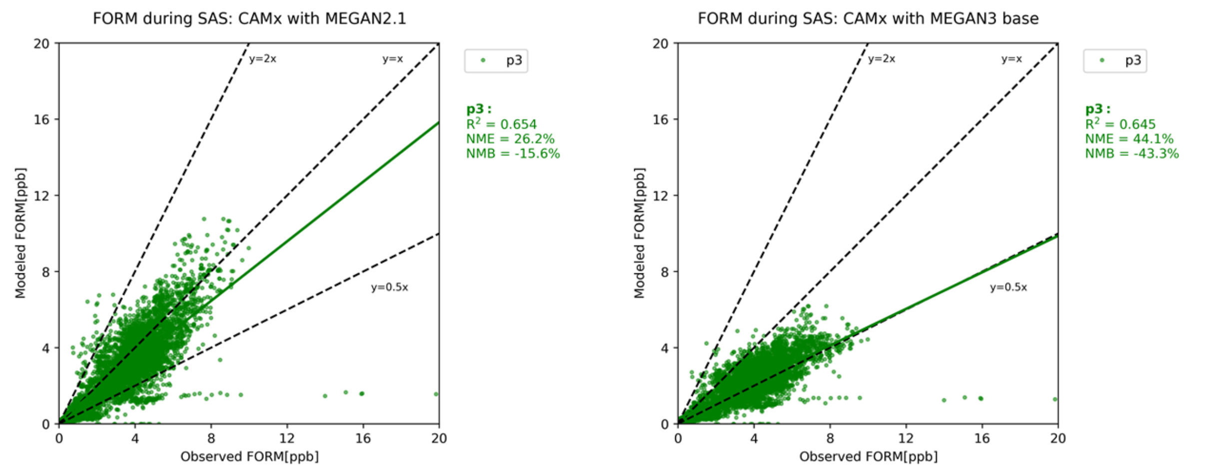


Figure 5-29. Measured and modeled formaldehyde along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

For acetaldehyde, evaluation against C-130 and P-3 measurements shows differing performance against different data sets (Figure 5-30 and Figure 5-31). Figure 5-30 indicates a much higher correlation with C-130 data (r^2 of 0.4 vs 0.04) in CAMx_MEGAN3_J4 than CAMx_MEGAN 2.1. NMB and NME have smaller magnitude in CAMx_MEGAN3_J4 than in CAMx_MEGAN 2.1. Against the C-130 data, both CAMx simulations have a low bias.

Evaluation against the P-3 data shows that the magnitude of the NMB is comparable in the CAMx_MEGAN3_J4 and CAMx_MEGAN 2.1 runs, but the bias shifts sign with a high bias in CAMx_MEGAN 2.1 and low bias in CAMx_MEGAN3_J4. The NME is smaller in CAMx_MEGAN3 than in CAMx_MEGAN v2.1. The value of r^2 is lower in the CAMx_MEGAN3_J4 run.

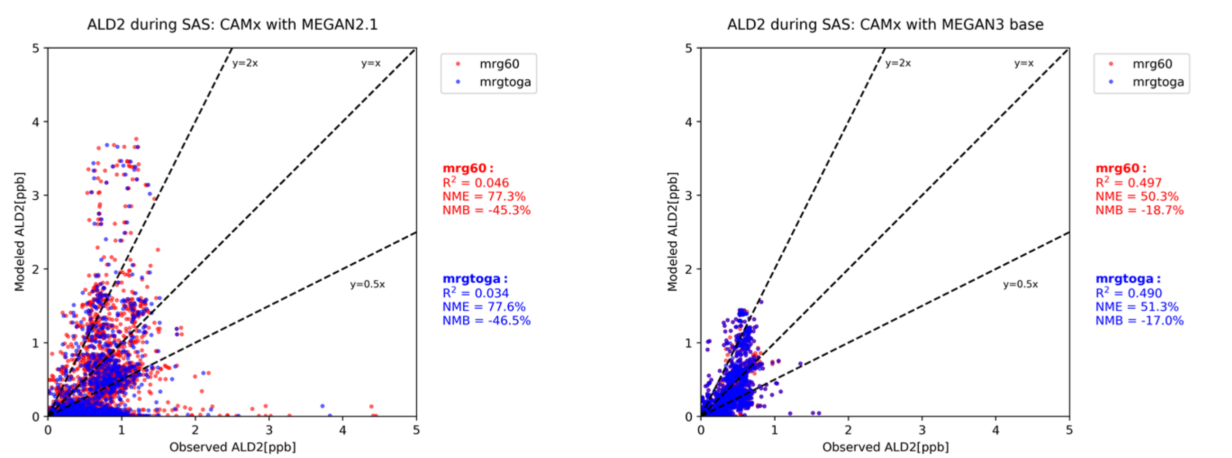


Figure 5-30. Measured and modeled acetaldehyde along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

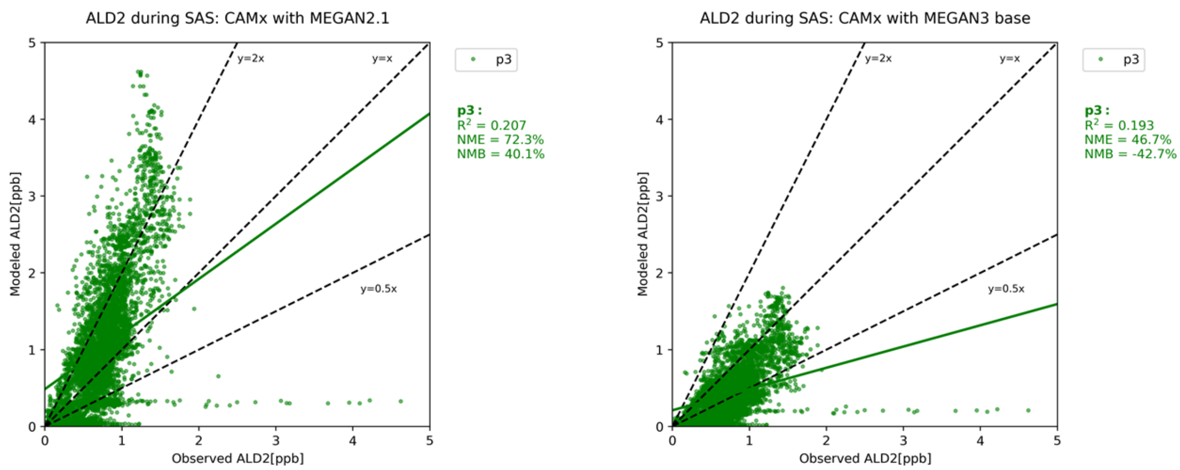


Figure 5-31. Measured and modeled acetaldehyde along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

CAMx_MEGAN2.1 underestimates both methanol and acetone along C-130 and P-3 flight tracks (Figure 5-32-Figure 5-35). The low bias becomes more pronounced in the CAMx_MEGAN3_J4 run. R^2 values are greater than 0.5 for both runs for methanol and greater than 0.4 for acetone. For acetone and methanol, the magnitudes of the NMB and NME are higher in the CAMx_MEGAN3_J4 simulation than in the CAMx_MEGAN 2.1 run.

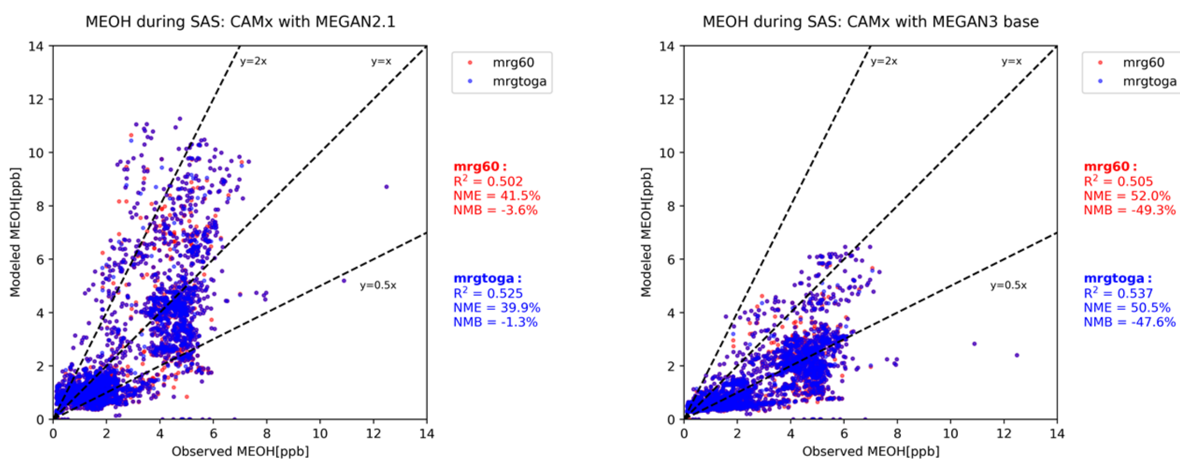


Figure 5-32. Measured and modeled methanol along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

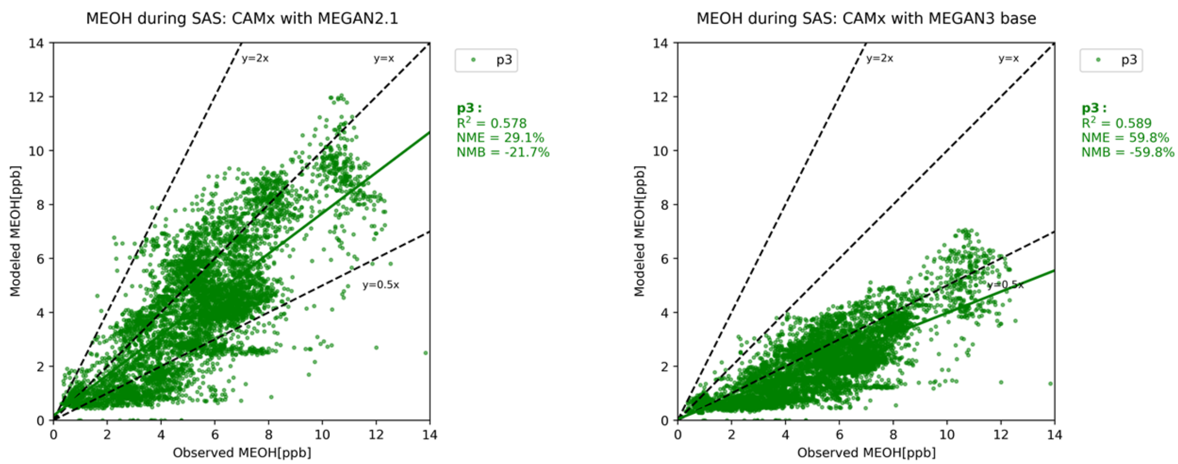


Figure 5-33. Measured and modeled methanol along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

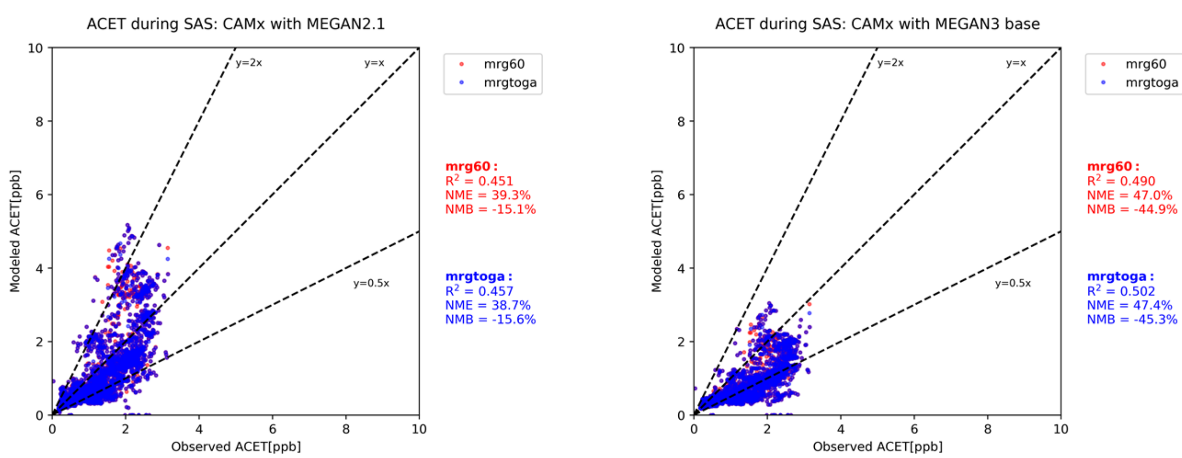


Figure 5-34. Measured and modeled acetone along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

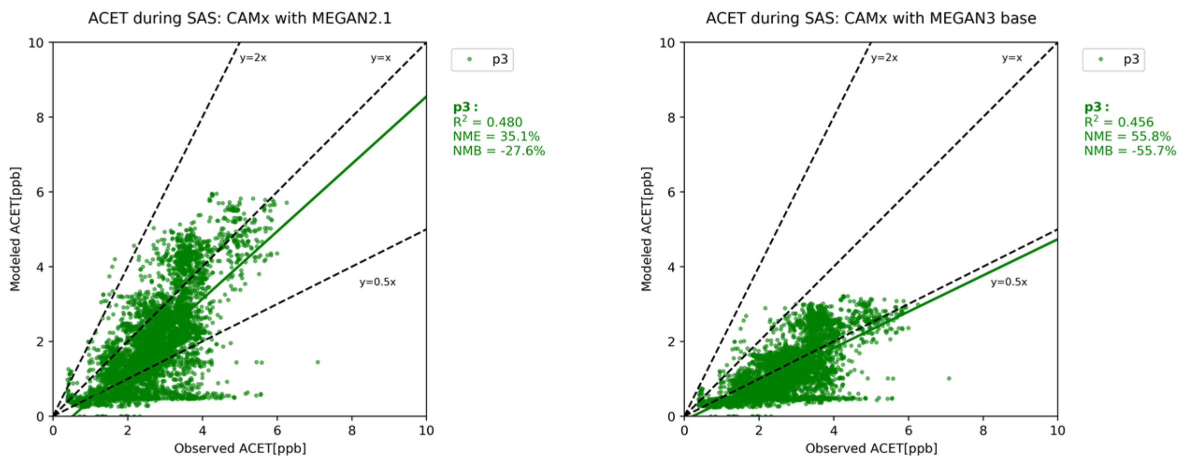


Figure 5-35. Measured and modeled acetone along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

Figure 5-36 and Figure 5-37 compare modeled and measured NO_2 for the C-130 and P-3 aircraft data, respectively. Both aircraft were most often in low NOx ($NO_2 < 0.5$ ppb) environments, although plumes containing higher values were encountered. Agreement with CAMx is reasonably good for values of $NO_2 < 0.5$ ppb, but the figures indicate that the aircraft encountered NOx plumes that were not captured by the model, which has horizontal resolution of 12 km. The CAMx_MEGAN2.1 and CAMx_MEGAN3_J4 runs show very similar performance for NO_2 as expected.

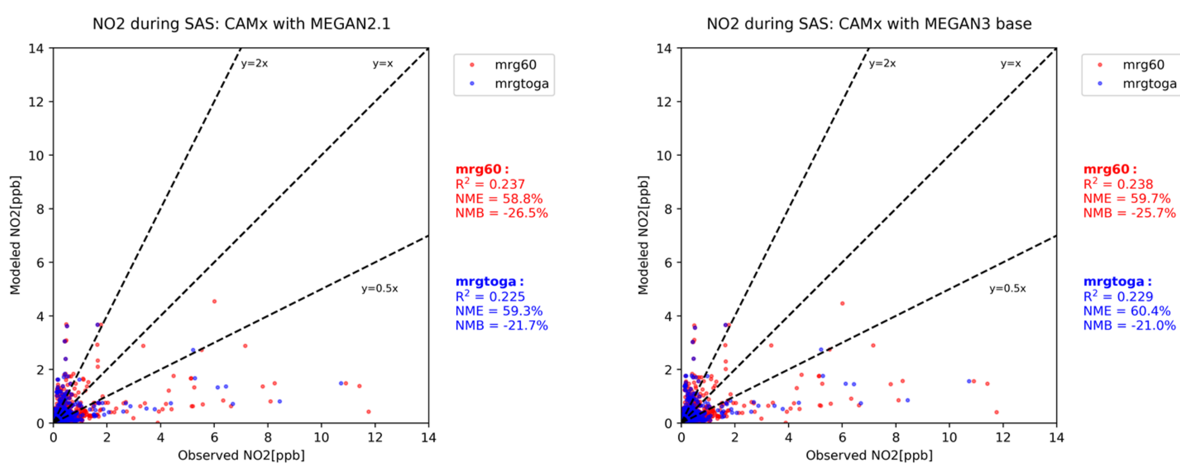
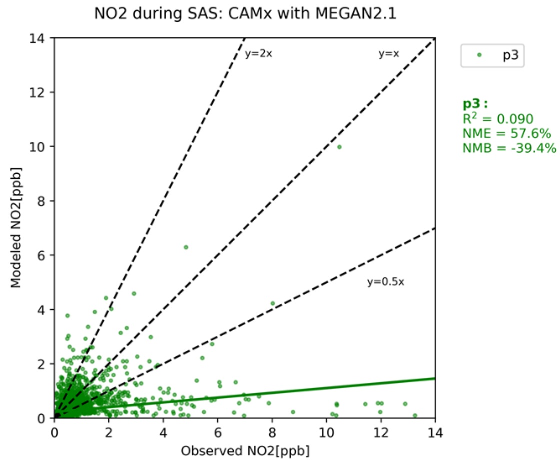


Figure 5-36. Measured and modeled NO_2 along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.



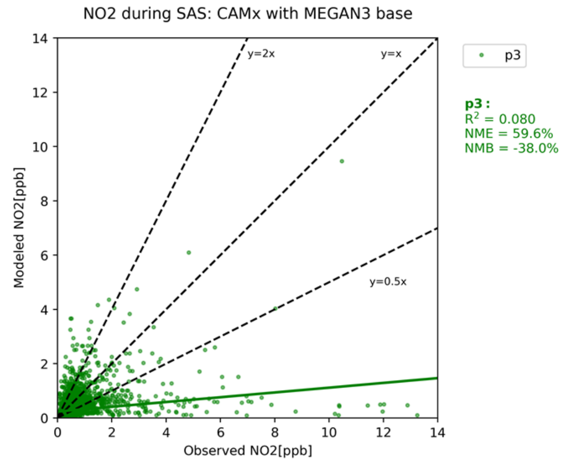


Figure 5-37. Measured and modeled NO_2 along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx_MEGAN2.1 (left) and CAMx_MEGAN3 (right) runs.

5.4.5 MEGAN3 Sensitivity Tests

We compared the results of the three CAMx simulations running with MEGAN3 emission inventories using different J values and without stress induced emissions (CAMx_MEGAN3_J4; CAMx_MEGAN3_J0 and CAMx_MEGAN3_nostress). The results of the comparisons are shown in Figure 5-38 through Figure 5-48. The scatterplots for isoprene (Figure 5-38, Figure 5-39) show that the CAMx_MEGAN3_nostress run has the smallest magnitude NMB and NME overall and that there is little difference in r^2 among the CAMx_MEGAN3 sensitivity runs. Figure 5-40 indicates that the spatial patterns of isoprene concentrations are similar in the three runs.

For isoprene products (Figure 5-41, Figure 5-42), all CAMx_MEGAN3 runs have a low bias when compared against the C-130 data and mixed results for bias when compared against the P-3 measurements. CAMx_MEGAN3_nostress has the smallest NMB for all data sets and the smallest NME for the C-130 measurements. Among the MEGAN3 sensitivity runs, there is little difference in r^2 values.

For monoterpenes (Figure 5-43 through Figure 5-45) and ozone (Figure 5-46, Figure 5-47), the performance of the three CAMx_MEGAN3 simulations in simulating the aircraft data was very similar.

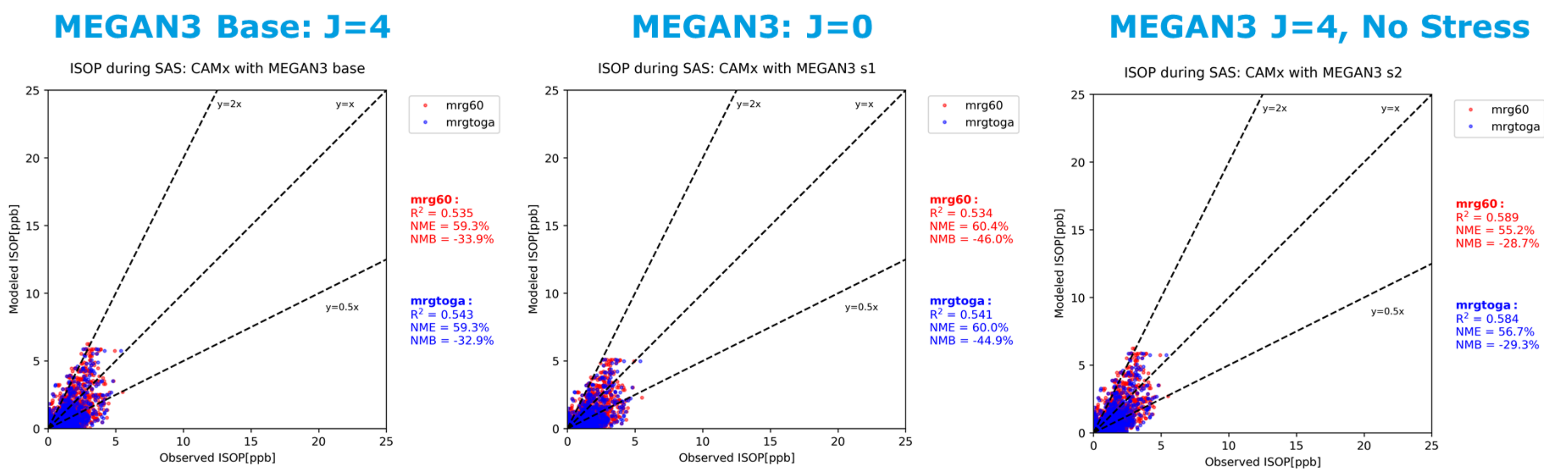


Figure 5-38. Measured and modeled isoprene along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

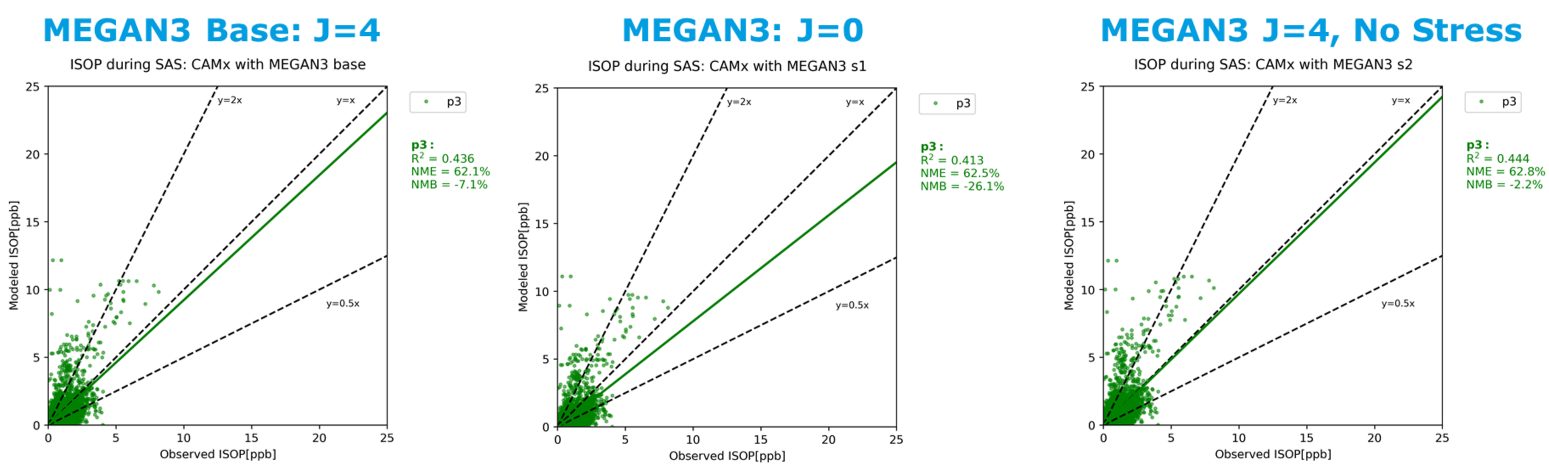


Figure 5-39. Measured and modeled isoprene along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

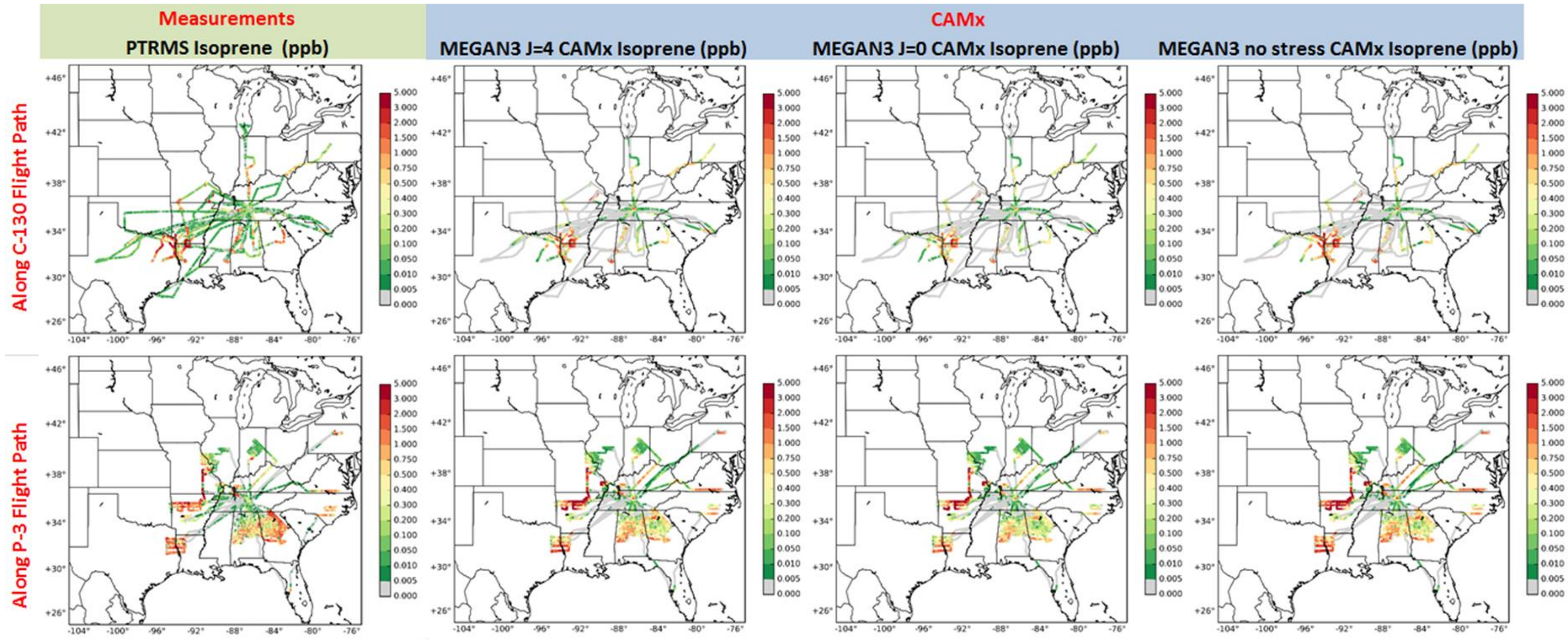


Figure 5-40. Measured and modeled isoprene along the C-130 (upper panels) and P-3 (lower panels) flight tracks for the June 1-July 15, 2013 period. Aircraft measurements are shown in the left panels. The three right-most panels show modeled concentrations for the three CAMx_MEGAN3 simulations.

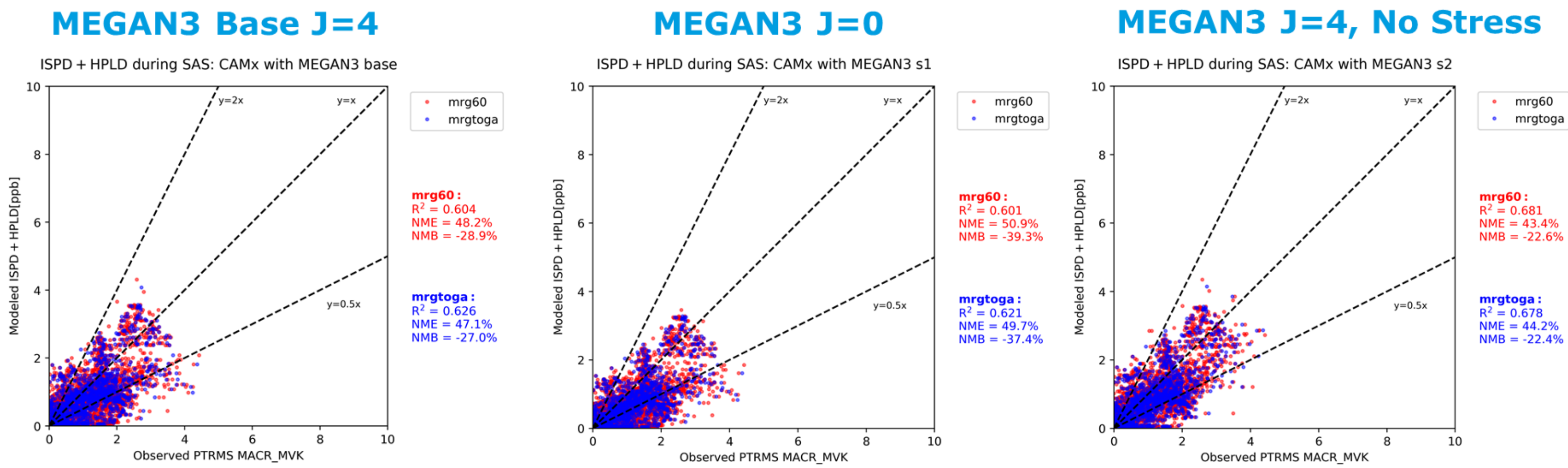


Figure 5-41. Measured and modeled isoprene products along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

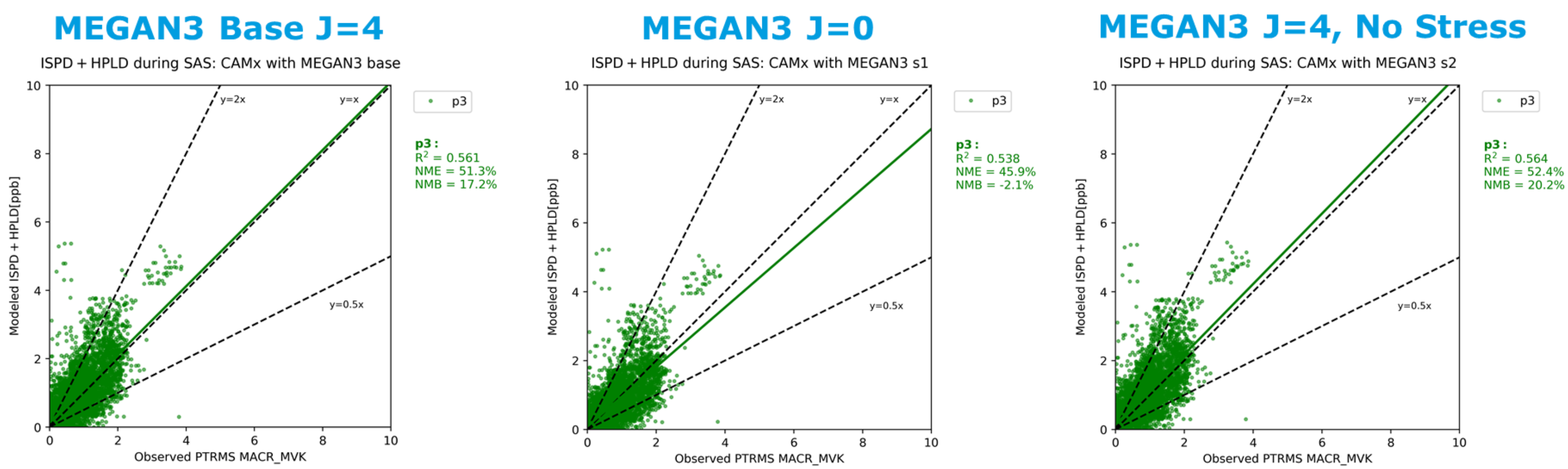


Figure 5-42. Measured and modeled isoprene products along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

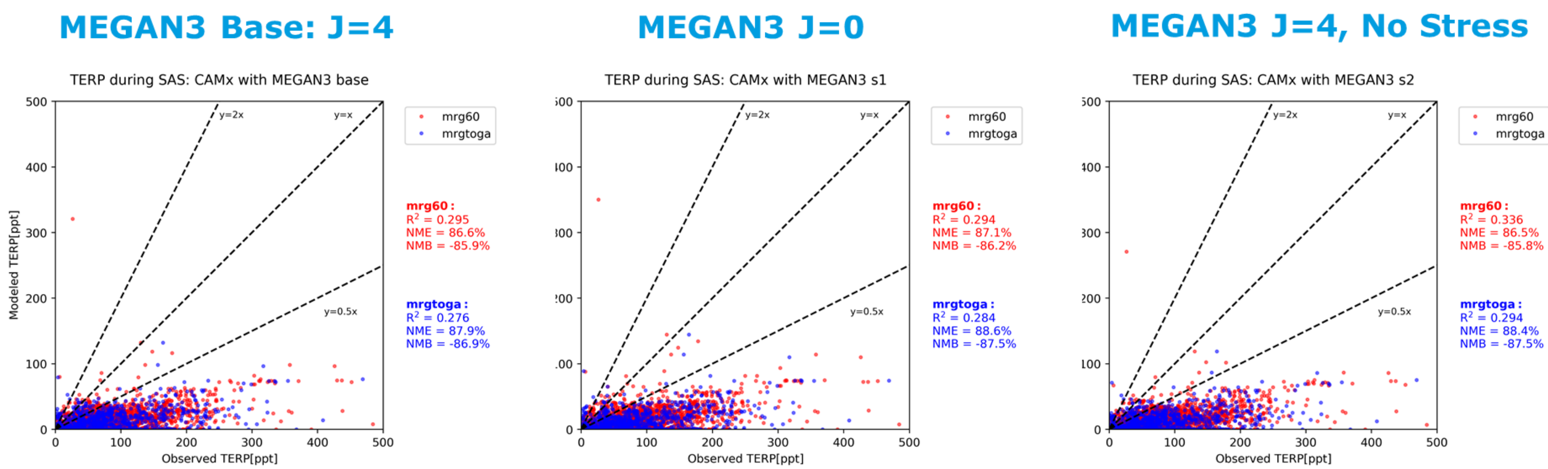


Figure 5-43. Measured and modeled monoterpenes along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

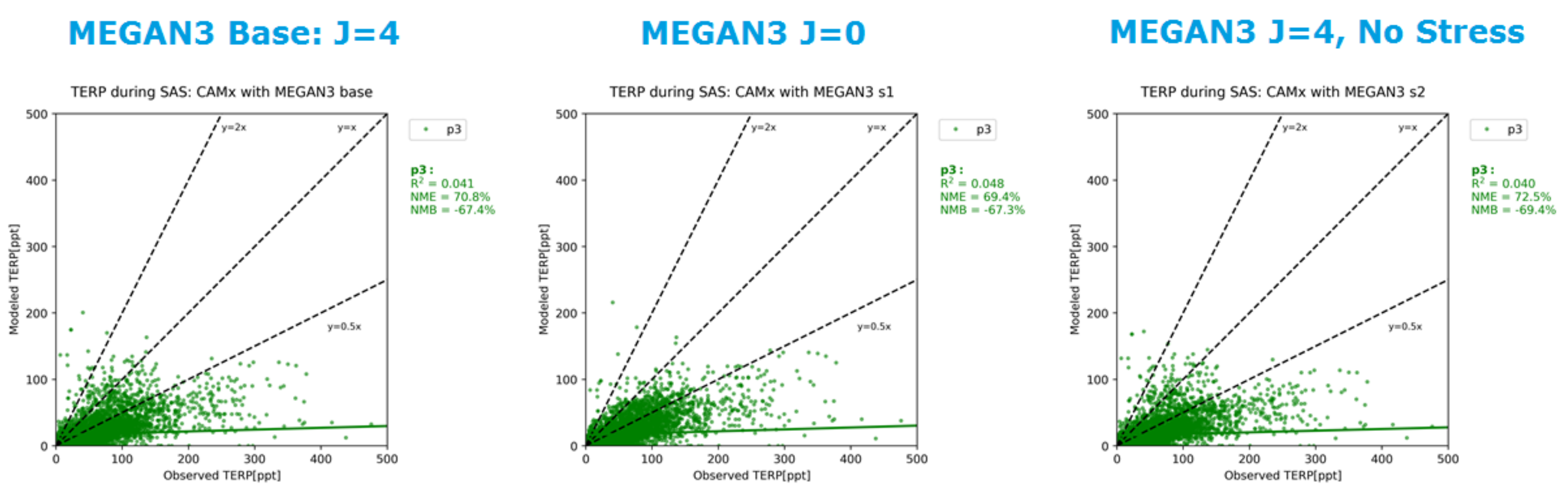


Figure 5-44. Measured and modeled monoterpenes along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

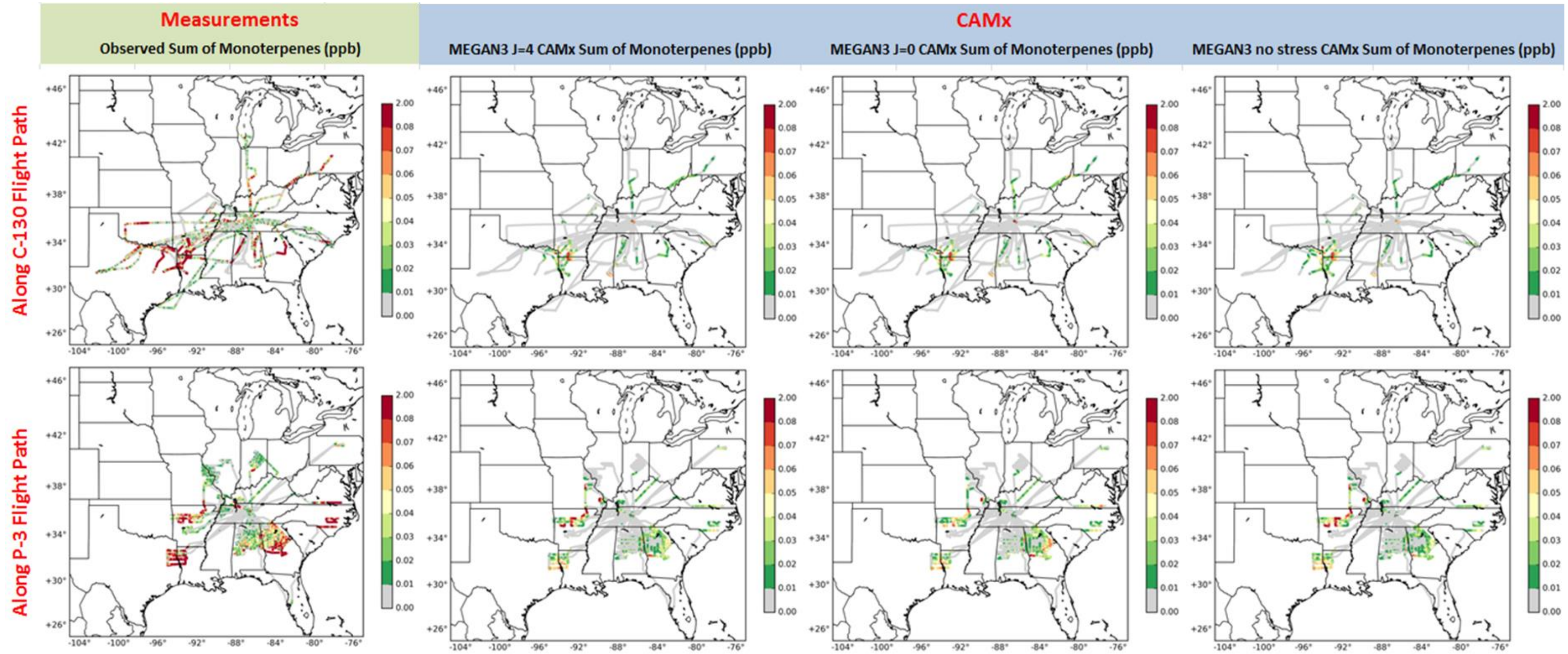


Figure 5-45. Measured and modeled sum of monoterpenes along the C-130 (upper panels) and P-3 (lower panels) flight tracks for the June 1-July 15, 2013 period. Aircraft measurements are shown in the left panels. The three right-most panels show modeled concentrations for the three CAMx_MEGAN3 simulations.

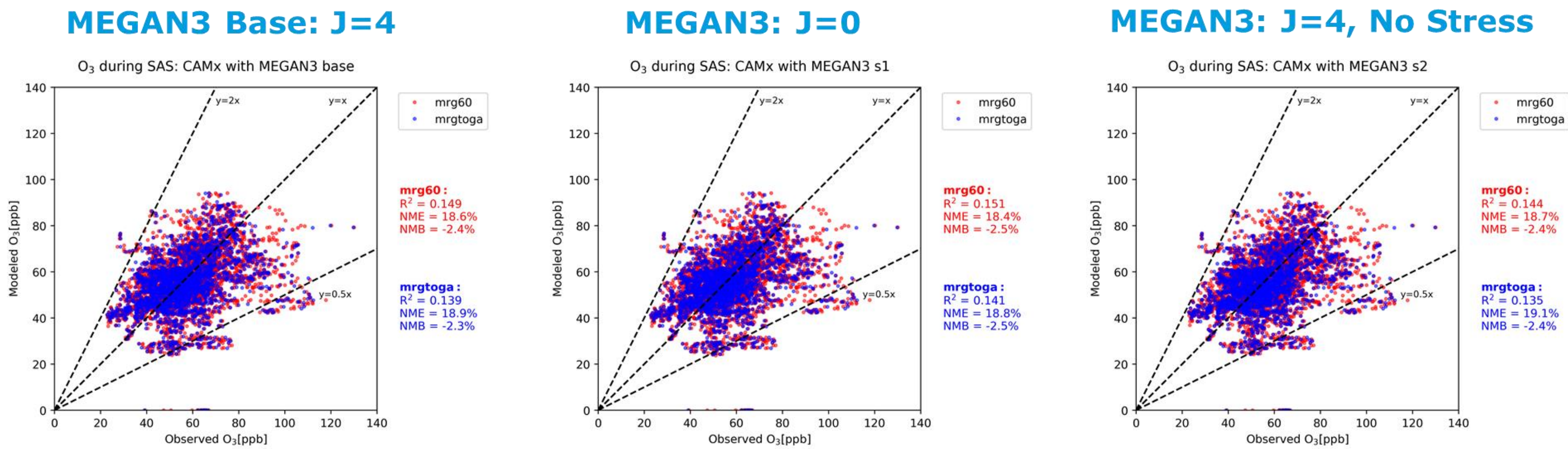


Figure 5-46. Measured and modeled ozone along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

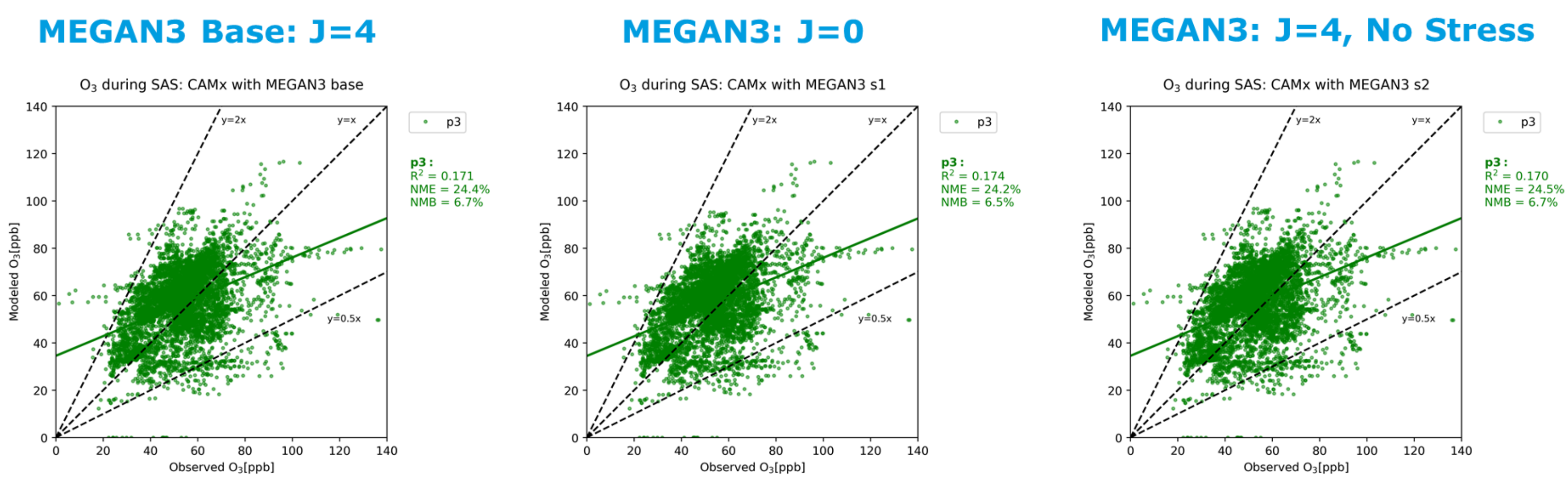


Figure 5-47. Measured and modeled ozone along the P-3 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

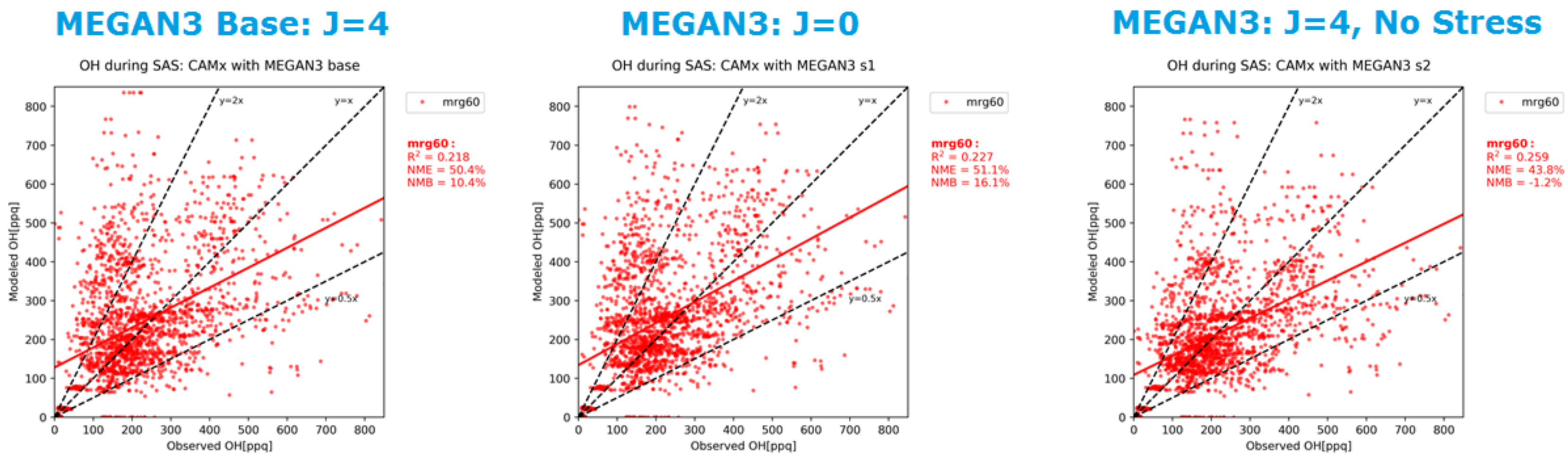


Figure 5-48. Measured and modeled OH along the C-130 aircraft flight tracks for the June 1-July 15, 2013 period for the CAMx runs with MEGAN3 with J=4 (left), MEGAN3 with J=0 (center) and MEGAN3 with J=4 and no stress-induced emissions.

5.4.6 Summary of CAMx Modeling

CAMx model performance using biogenic emissions developed with MEGAN v2.1 and with MEGAN3 is summarized in Figure 5-49 through Figure 5-52, which indicate how the episode average NMB varied among the different CAMx runs as the model results were compared to measurements made aboard the C-130 and P-3 aircraft. The high bias for isoprene and isoprene products in CAMx_MEGAN v2.1 is greatly reduced in all of the CAMx_MEGAN3 runs. The CAMx_MEGAN3 runs all have a low bias which is smaller in magnitude than the CAMx_MEGAN v2.1 bias. The CAMx_MEGAN3_nostress run was the best performing CAMx run for isoprene. Overall, CAMx showed improved performance in simulating aircraft isoprene concentration measurements using MEGAN3 relative to MEGAN v2.1. This is reasonable given that MEGAN3 shows improved performance in simulating aircraft isoprene flux measurements relative to MEGAN v2.1.

There was a widespread reduction in monoterpene emissions in MEGAN3 relative to MEGAN v2.1. The existing low bias in CAMx simulation of monoterpenes in CAMx_MEGAN2.1 became more pronounced in CAMx_MEGAN3. CAMx ozone and OH performance was similar using MEGANv2.1 and MEGAN3 and differences among the MEGAN3 sensitivity tests were relatively small.

The best overall performance for the subset of species (isoprene, isoprene products, sum of monoterpenes, ozone, OH) occurred in the CAMx_MEGAN3_nostress run. The NMB for ozone was nearly unchanged across all CAMx runs, which indicates that modeled ozone along the aircraft flight track was not sensitive to changes in the specification of the biogenic emissions. Modeled ozone shows periods of both underestimates and overestimates that are caused by other processes, which are currently not well understood.

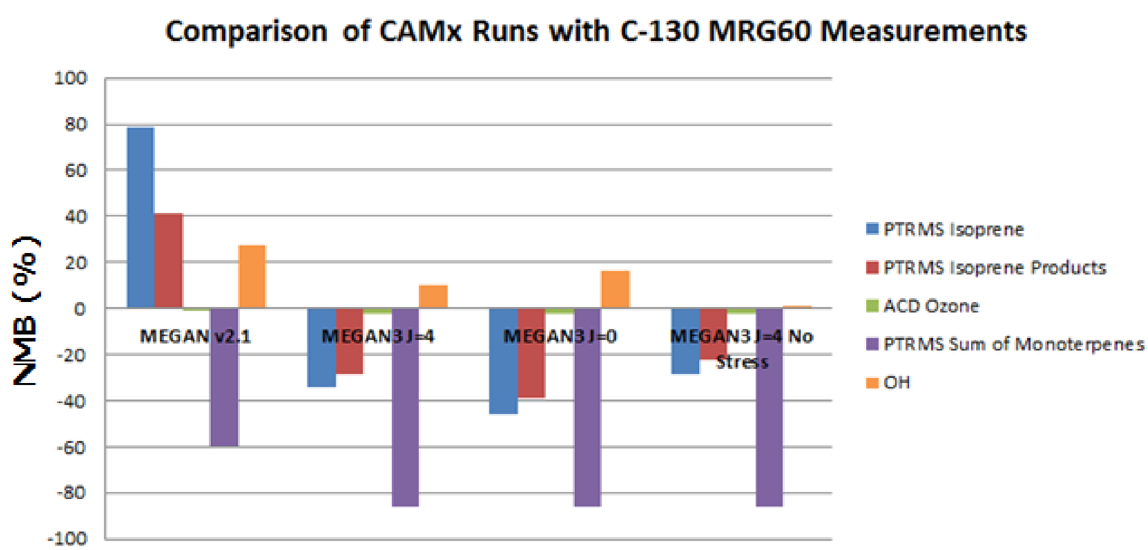


Figure 5-49. Summary of variation of NMB for the CAMx simulations running with MEGAN v2.1 and MEGAN3 when model results were compared to C-130 measurements for a subset of key species. ACD indicates measurements made via chemiluminescence detection.

Species	Normalized Mean Bias (%)			
	MEGANv2.1	MEGANv3.0 Base	MEGANv3.0	MEGANv3.0
		J=4	J=0	J=4, No Stress Emissions
PTRMS Isoprene	78.4	-33.9	-46.0	-28.7
PTRMS Isoprene Products	41.0	-28.9	-39.3	-22.6
ACD Ozone	-0.5	-2.4	-2.5	-2.4
PTRMS Sum of Monoterpenes	-59.7	-85.9	-86.2	-85.8
OH	27.2	10.4	16.1	1.2
TOGA Formaldehyde	-13.9	-41.9	-45.2	-39.7
PTRMS Methanol	-43.3	-71.4	-71.8	-68.2
TOGA Methanol	-3.6	-49.3	-50.0	-45.3
TOGA Acetone	-15.1	-44.9	-47.3	-42.6
TOGA Benzene	-36.5	-41.6	-42.4	-40.7
Zhou HNO3	179.4	187.6	193.0	183.5
ACD NO2	-26.5	-25.7	-24.6	-26.6
ACD NO	-24.0	-14.4	-11.8	-16.9
TOGA Acetaldehyde	104.4	-18.7	-23.1	-12.1
PTRMS acetaldehyde	-45.3	-77.2	-79.0	-74.5
TOGA Propane	-61.2	-61.4	-61.8	-60.5

\|NMB\| < \|NMB of MEGAN v2.1\|

\|NMB\| > \|NMB of MEGAN v2.1\|

Figure 5-50. Summary of variation of NMB for the CAMx running with MEGAN v2.1 and MEGAN3 when model results were compared to C-130 mrg60 measurements. ACD indicates species measurement made via chemiluminescence detection.

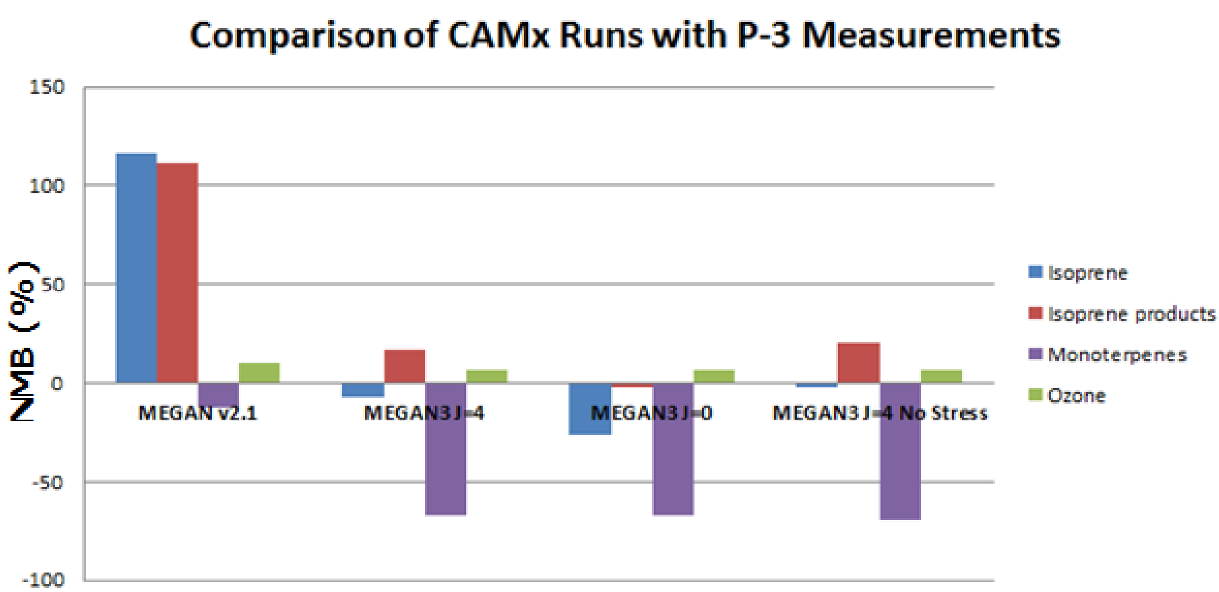


Figure 5-51. Summary of variation of NMB for the CAMx simulations running with MEGAN v2.1, MEGAN3 and the two MEGAN3 and sensitivity tests when model results were compared to P-3 measurements.

Species	Normalized Mean Bias (%)			
	MEGANv2.1	MEGANv3.0 Base	MEGANv3.0	MEGANv3.0
		J=4	J=0	J=4, No Stress Emissions
isoprene	116.6	-7.1	-26.1	-2.2
isoprene products	111.4	17.2	-2.1	20.2
monoterpenes	-12.1	-67.4	-67.3	-69.4
Ozone	9.7	6.7	6.5	6.7
Ozone_CaRDS	14.1	11.0	10.8	11.0
NO2_ACES	-25.2	-23.4	-22.1	-23.1
NO_CaRDS	-83.7	-81.3	-80.5	-81.3
NO2_CaRDS	-42.4	-41.0	-40.0	-41.0
NO3	128.9	203.9	269.8	206.4
N2O5	-66.8	-57.5	-49.2	-57.0
CO	-4.2	-12.4	-13.4	-11.6
HCHO	-15.6	-43.3	-47.5	-42.3
HNO3	-2.6	-1.7	0.0	-1.8
HONO	-90.3	-83.8	-82.1	-84.1
NO	-34.3	-23.9	-20.5	-24.5
NO2	-39.4	-38.0	-37.0	-38.0
NOy	-5.2	-13.1	-13.3	-12.8
PAN	31.8	1.6	-3.1	2.9
SO2	14.9	9.4	8.1	9.9
methanol	-21.7	-59.8	-60.4	-57.2
acetaldehyde	40.1	-42.7	-47.3	-40.1
acetone	-27.6	-55.7	-58.5	-54.5
benzene	-46.3	-51.0	-52.0	-50.5

|NMB| < |NMB of MEGAN v2.1|

|NMB| > |NMB of MEGAN v2.1|

Figure 5-52. Summary of variation of NMB for the CAMx simulations running with MEGAN v2.1 and MEGAN3 when model results were compared to P-3 measurements. ACES indicates measurements made with airborne cavity enhanced spectrometer. CARDS indicates measurements made with cavity ringdown absorption spectrometer. ACD indicates measurements made via chemiluminescence detection.

5.5 MEGAN3 and CAMx Modeling Data Deliverables

The MEGAN3 and CAMx modeling databases will be compiled and delivered to the AQRP Project Manager at the conclusion of the project. This includes all MEGAN inputs and modeling files and all CAMx modeling files and evaluation of MEGAN and CAMx model results against ambient data

6.0 CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

Below, we provide a summary of findings of this study.

6.1 Summary of Findings

- BEIS3 and MEGAN2.1 isoprene emission factors are based on enclosure measurements made from the 1970s/80s (identifying non-emitters) to the early 1990s (characterizing isoprene emitters). Both models use a single EF for all broadleaf trees that emit isoprene. The BEIS3 and MEGAN2.1 EF differ primarily because there is a 66% difference in the Specific Leaf Area used to convert leaf mass to leaf area. An estimate of SLA is required when using older EF measurement data but not for measurements that follow current EF measurement protocols (Niinemets et al. 2011).
- Although more than 280 tree species occur in Texas and the surrounding region, just 22 tree species, including many pine and oak species, comprise 70% of total tree crown cover. Ten of these trees are known to be isoprene emitters and together are estimated to contribute about 75% of the total isoprene emission. Almost all (>94%) of the total isoprene emission is from trees in just three genera: *Quercus* (oaks), *Liquidambar* (sweetgum), and *Nyssa* (gum). The top 50 isoprene emitting tree species include one species of *Liquidambar*, two *Nyssa* species, and more than 40 *Quercus* species.
- High quality (J-rating of 4; Niinemets et al. protocols) isoprene enclosure measurements are available for at least one species from each of the three dominant isoprene-emitting Texas tree genera. These measurements indicate that Texas isoprene emitting trees can be grouped into two categories: Gum (*Liquidambar* and *Nyssa* species) trees with a canopy-average leaf-level EF of ~24 nmol m^{-2} s^{-1} and oak (*Quercus*) trees with a canopy-average leaf-level EF of ~35 nmol m^{-2} s^{-1}. These leaf-level EF agree remarkably well (within 10%) with aircraft based isoprene EF estimated for Texas and southeastern US forests dominated by sweetgum and oak, respectively.
- An issue with basing EF only on high quality (j=4) emissions data is that there are no reported high quality isoprene measurements on trees known to be non-emitters (e.g., pine, hickory). As a result, these non-emitting trees are assigned a non-zero isoprene emission rate (average of all trees in a family or division). To avoid this bias, known non-emitting families that occur in Texas and the surrounding region were assigned a zero isoprene emission rate with a J-rating of 4.
- High quality (J-rating of 4) monoterpene emission enclosure measurements are relatively difficult (compared to isoprene measurements) to make due to the presence of specialized storage structures and stress induced emissions. As a result, there are very few of these measurements. At present, there are no high quality monoterpene enclosure emission data (J-rating =4) for any Texas tree species. There have been only a few recent measurements on Texas tree species since the 1990s (J-rating=1) and nearly all of the available Texas monoterpene data are classified with a J-rating of 0. Above canopy flux estimates can be used to constrain monoterpene EF but, due to the large number of emitting genera, it is difficult to deconvolute a canopy scale monoterpene flux to the individual tree types.

- The flexible landcover scheme developed for the MEGAN-EFP can integrate high resolution satellite data with available ground surveys of species composition and can be updated with user provided landcover data.
- Isoprene emission estimates for shrub and savannah regions, such as the Edwards plateau in Texas, have relatively high uncertainties due to the lack of reliable data for assigning moderate-sized woody plants to shrub or tree growth-forms. In addition, there is a need for better species composition data for shrubs.
- Each of the three improvements to the MEGAN canopy environment model can change isoprene emissions by about 15 to 20%. Two of these changes (leaf temperature model and light transparency factor) decrease emissions while one (emission capacity variation with canopy depth) increases emissions. As a result of these offsetting effects, the net impact of the revised canopy environment model tends to be a decrease in isoprene emissions of about 20%.
- The MEGAN3 monoterpene and sesquiterpene categorization scheme can better represent terpenoid emission categories without adding complexity. The 50 additional compounds are mostly stress induced emissions that will be important only under stress conditions.
- Reduced soil moisture can have a major impact on isoprene emission and probably on other light dependent biogenic VOC emissions. The simple algorithm used in MEGAN2.1 can adequately represent the isoprene drought response but only if accurate soil moisture and wilting point data are available. This was not the case for the WRF simulation used for this study but the new MEGAN3 approach enables users to calculate a more accurate drought response off-line using a mechanistic land surface model.
- Stress-induced emissions (e.g. by ozone, low temperature, high temperature, high winds) can greatly (factor of 5) increase emissions of some BVOC but there are few observations available for parameterizing this behaviour. The current approach is highly simplified and designed to be relatively conservative so that emissions are impacted only with the most extreme events.
- MEGAN3 shows improved performance in simulating aircraft isoprene and monoterpene flux measurements relative to MEGAN v2.1
- CAMx surface ozone tends to be lower with MEGAN3 in comparison to MEGAN2.1

6.2 Recommendations for Future Work

- High quality measurements of monoterpene emission factors should be conducted to characterize the dominant Texas vegetation. Emission factors for isoprene, including low or zero emissions, and other compounds, including sesquiterpenes and stress compounds, could be estimated by the same study.
- The oaks are a diverse genus and include some European species that do not emit isoprene. The isoprene EF of more of the dominant Texas oaks, including the savannah and shrub oaks that are relatively understudied, should be investigated with high quality measurements to quantify any within-genera variation.

- High quality measurements of isoprene emissions should be used to characterize at least one species in all dominant genera of Texas trees in order to identify non-emitters. If these measurements are not available then existing data, even low quality data that identifies plants as non-emitters should be used to assign a zero isoprene emission rate to these plants.
- The MEGAN3 stress-induced emission algorithms should be used to investigate the sensitivity of air quality model results for cases where stress events are suspected of impacting emissions. If these indicate air quality simulations are sensitive to stress-induced emissions, then additional studies should be conducted to improve the current parameterizations.
- The sensitivity of Texas air quality to soil NO emissions should be investigated. If determined to be important, improved crop landcover and nitrogen fertilizer rate distributions should be incorporated into the MEGAN emission factor processor.
- Sub grid scale heterogeneity of highly reactive VOC may be important for quantifying ozone and PM and for effective comparisons of modelled VOC concentrations with TCEQ auto-GC data and should be investigated with field measurements of ambient concentrations and emission sources.
- BVOC concentrations in shrub and savannah regions, such as the Edwards plateau, should be measured to determine if these regions are a significant source of terpenoid emissions. If they are, then improved landcover and emissions data should be obtained for these landscapes along with an improved canopy environment model and canopy depth emission algorithm suitable for open canopies.
- MEGAN3 is a new tool for estimating emissions of isoprene, monoterpene, and other biogenic emissions in Texas that allows use of the most accurate input data, emission factors and response functions. While the MEGAN3 framework is completed and the model is fully functional, there are additional input data processing tasks that are urgently needed. This includes MEGAN-EFP landcover and emissions data especially non-tree landcover and compounds other than isoprene and monoterpenes.

7.0 AUDITS OF DATA QUALITY

During this study, we performed Quality Assurance/Quality Control (QA/QC) procedures to ensure that all data and products generated are of known and acceptable quality. QA/QC procedures were performed in accordance with the Category III Quality Assurance Project Plan (QAPP) that was completed at the beginning of the study. In a Category III Project, data audits must be performed for at least 10% of the data sets and a report of QA findings must be given in the final report (this document). A technical systems audit is not required. In Section 7, we report on the findings of our QA audits during this project.

7.1 Aircraft Data

100% of the aircraft data used in this study have undergone extensive QA/QC by the research groups who collected the data during the SAS Study. The NOAA and PNNL teams reviewed more than 10% of the aircraft data for quality assurance purposes before we performed the analysis presented in Section 5. Aircraft data were evaluated against the quality metrics outlined in the QAPP for AQRP Project 14-016 and were found to be of acceptable quality.

7.2 MEGAN Emissions Modeling Data

The MEGAN3 model was run by Ramboll Environ using emission factors from the MEGAN-EFP system and Weather Research and Forecasting (WRF; Skamarock et al. 2008) meteorological model data developed during AQRP Project 14-016 (Yu et al. 2015). We prepared three sets of model-ready MEGAN3 biogenic emissions using three sets of emission factors: (1) emission factors from MEGAN-EFP using high quality (J=4) data (2) emission factors from MEGAN-EFP system including lower quality (J≥0) data (3) emission factors from MEGAN-EFP using high quality (J=4) data but without stress induced emissions. The Ramboll Environ team member who performed the MEGAN modeling documented steps taken to obtain and process the MEGAN inputs, file paths to all inputs and outputs, and provided a brief summary of the results. Once the MEGAN modeling was completed, a Ramboll Environ team member who had not performed the MEGAN modeling reviewed the modeling scripts for accuracy and then reviewed the model outputs. For the ISOP and TERP species, model outputs for 10% of the episode days were reviewed using the PAVE visualization tool for completeness and compared with observations as reported in this document. We also summarized and reviewed episode average emissions by state and prepared MEGAN3 emissions difference plots against MEGAN v2.1. In addition to the episode average, we compared midday average (e.g., noon) values in a plot because it would be informative to compare midday average values, which were calculated as an average of hours 11:00-13:00 (CST), for the MEGAN3 scenarios and MEGAN v2.1. All data were examined for values that were outliers or otherwise unreasonable and none were found. For other MEGAN output species such as SQT, NO, MEOH and FORM, model outputs for 10% of the episode days were reviewed using the PAVE visualization tool for completeness and consistency with episode averages as well as the range of modeled values-no comparisons with observations were made. The MEGAN output data were determined to be correctly developed and complete and therefore suitable for the purposes of this study.

7.3 WRF Meteorological Modeling Data

The WRF model run output was evaluated against observed winds, temperatures, humidity and precipitation for all hours for 100% of episode days to ensure that the model had been run correctly and provided a reasonable simulation of atmospheric conditions during the modeling period. The model output data were evaluated against the quality metrics described in the QAPP. This evaluation is described in Yu et al. (2015) and is described briefly in Section 5 of this report. A Ramboll Environ team member who did not perform the WRF modeling reviewed the WRF model scripts to ensure that the model had been run correctly. The WRF modeling was determined to have been carried out correctly and the model results to be suitable for use in the MEGAN emissions modeling and the CAMx air quality modeling.

7.4 CAMx Modeling Data

All CAMx runs were evaluated against aircraft and surface measurements to ensure that the model had been run correctly and provided a reasonable simulation of the chemical species of interest in this study. This evaluation is described in Section 5 and in Yu et al. (2015). Additional QA/QC checks were performed to ensure that the modeling was performed correctly. A member of the research team who did not conduct the modeling or air quality model input data processing reviewed animations of the model-ready emissions for NO, NO2, ISOP, and TERP using PAVE for 10% of the episode days. Spatial patterns of emissions were reviewed and the reasonableness of emissions values was assessed. No outliers or missing data were found and the emissions inputs were deemed acceptable for use in the CAMx modeling.

A member of the Ramboll Environ team who did not conduct the modeling or air quality model input data processing reviewed all CAMx modeling and post-processing scripts for accuracy as well as consistency among the Base Run and sensitivity tests. For 10 % of episode days, CAMx output for each hour of the day was reviewed using PAVE animations for the following species: O3, NO2, TERP, SQT, ISOP, FORM, ACET, ALD2, BENZ, CO, MEOH, HNO3, PAN and SO2. The modeling outputs were determined to be of acceptable quality and suitable for use in this study.

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