THE UNIVERSITY OF TEXAS AT AUSTIN

TEXAS COMMISSION ON ENVIRONMENTAL QUALITY

AQRP

Air Quality Research Program

Annual Workshop
Pickle Research Campus
University of Texas, Austin
June 17 - 18, 2015

Project 14-016

Improved Land Cover and Emission Factor Inputs for Estimating Biogenic Isoprene and Monoterpene Emissions for Texas Air Quality Simulations

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Haofei Yu and Alex Guenther (PNNL)

Carsten Warneke and Joost de Gouw (NOAA CIRES)

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Project 14-016 - Improved Land Cover and Emission Factor Inputs for Estimating Biogenic Isoprene and Monoterpene Emissions for Texas Air Quality Simulations

Today:

- Improved land cover and emission factor inputs for MEGAN
- Constrained isoprene emissions using newly-available aircraft measurements from SAS 2013
  - Derived airborne isoprene fluxes from aircraft measurements using eddy covariance method and mass balance approach
  - Compared airborne isoprene fluxes with MEGAN/BEIS modeled emissions along aircraft flight tracks
  - Refined isoprene emissions factors using aircraft data
  - Compared CAMx-predicted isoprene with measured concentrations along flight tracks
- Further work/recommendations

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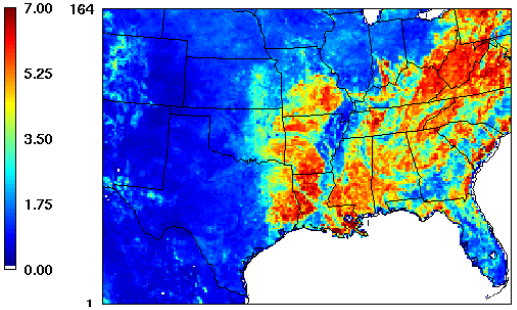
Development of High Resolution Land Cover Data for MEGAN Modeling

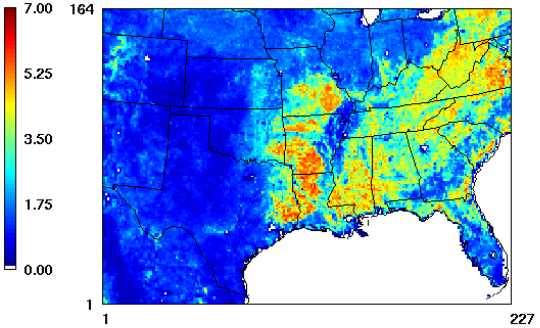
Default and Updated MEGAN LAIv

- 2013 8-day average LAI for all of North America from MODIS MCD15A2.005
- Applied maximum green vegetation fraction from USGS (also based on MODIS products)
- Spatial resolution of the LAIv data ~900m

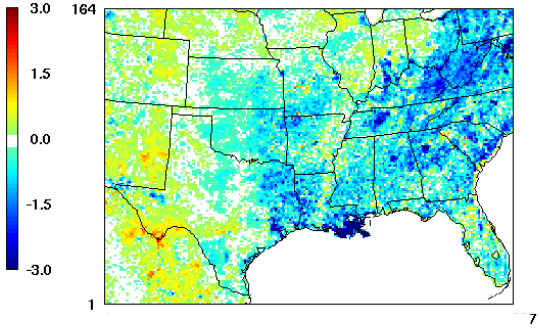
Default LAIv



Updated LAIv



Updated - Default LAIv



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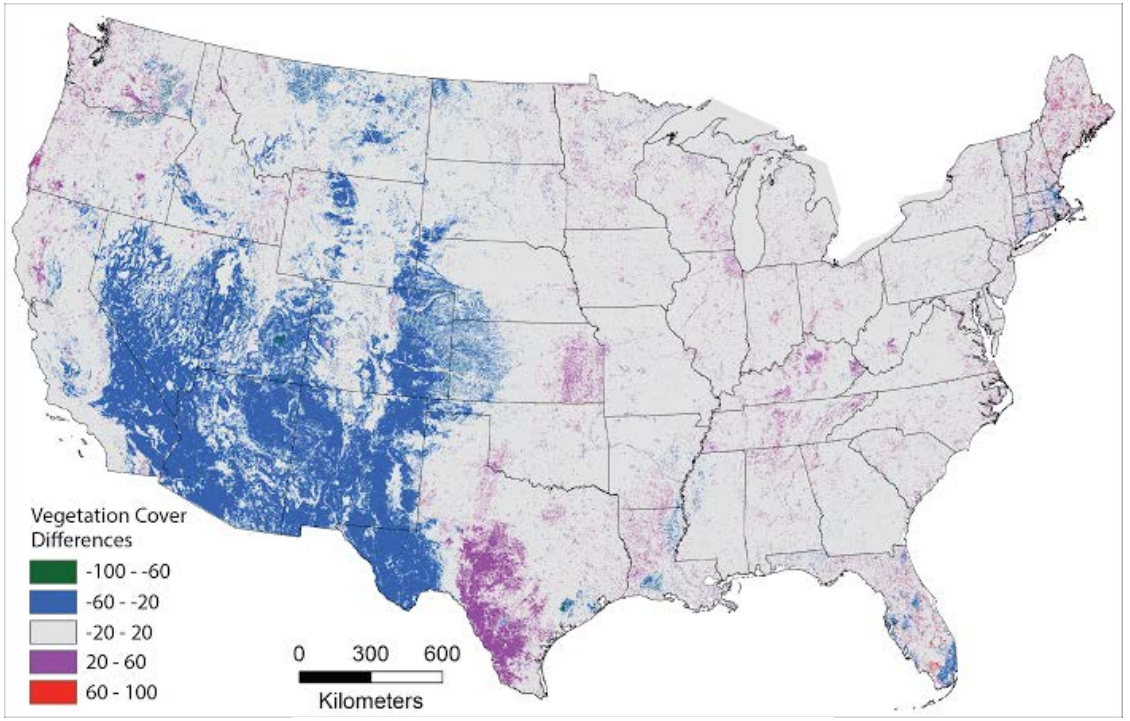
Development of High Resolution Land Cover Data for MEGAN Modeling

- An updated 30 meter PFT database was developed
- Based on ground survey, remote sensing and land surface model data products.
- v2015 based on more highly resolved LandFire EVT data

Differences in Total Vegetation Cover (PFT16v2015-PFT16v2011)



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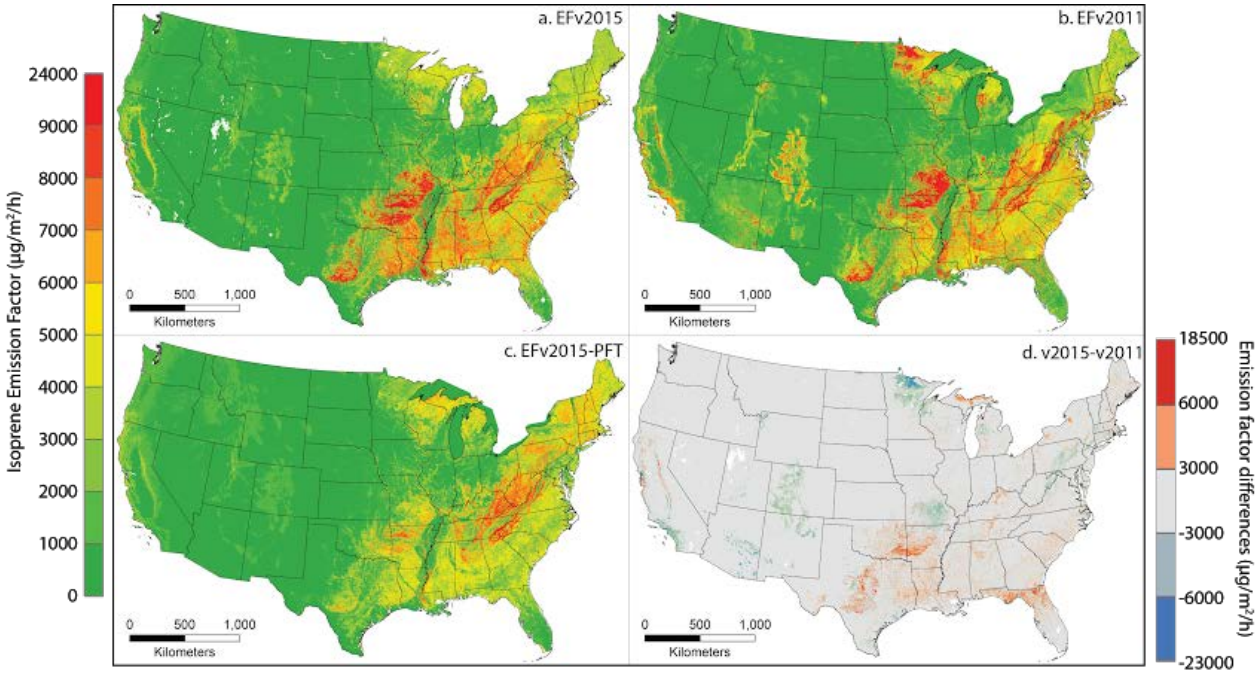
Development of New Emission Factor Data for MEGAN Modeling

- New high resolution (30 m) EF database based on PFT16v2015
- EFs based on LandFire EVTs and included spatially averaged surface flux data derived from aircraft observations
- Differences are mainly due to the LandFire EVT data – higher resolution than LC used to develop EFv2011 dataset

Isoprene Emission Factor Data



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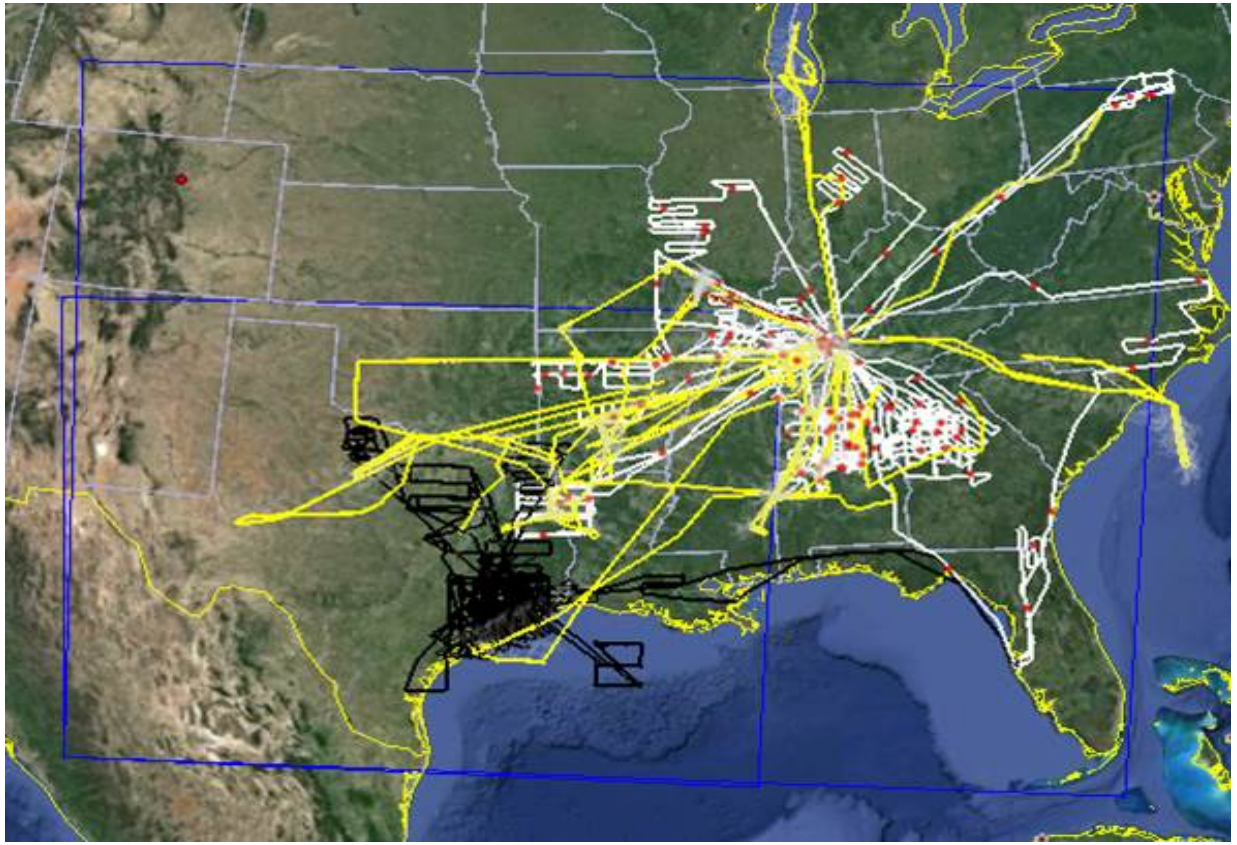
Constraining isoprene emissions using aircraft measurements from SAS 2013

Aircraft Flight Tracks



SAS C-130 (yellow), SAS P-3 (white), and TexAQS 2006 (black)

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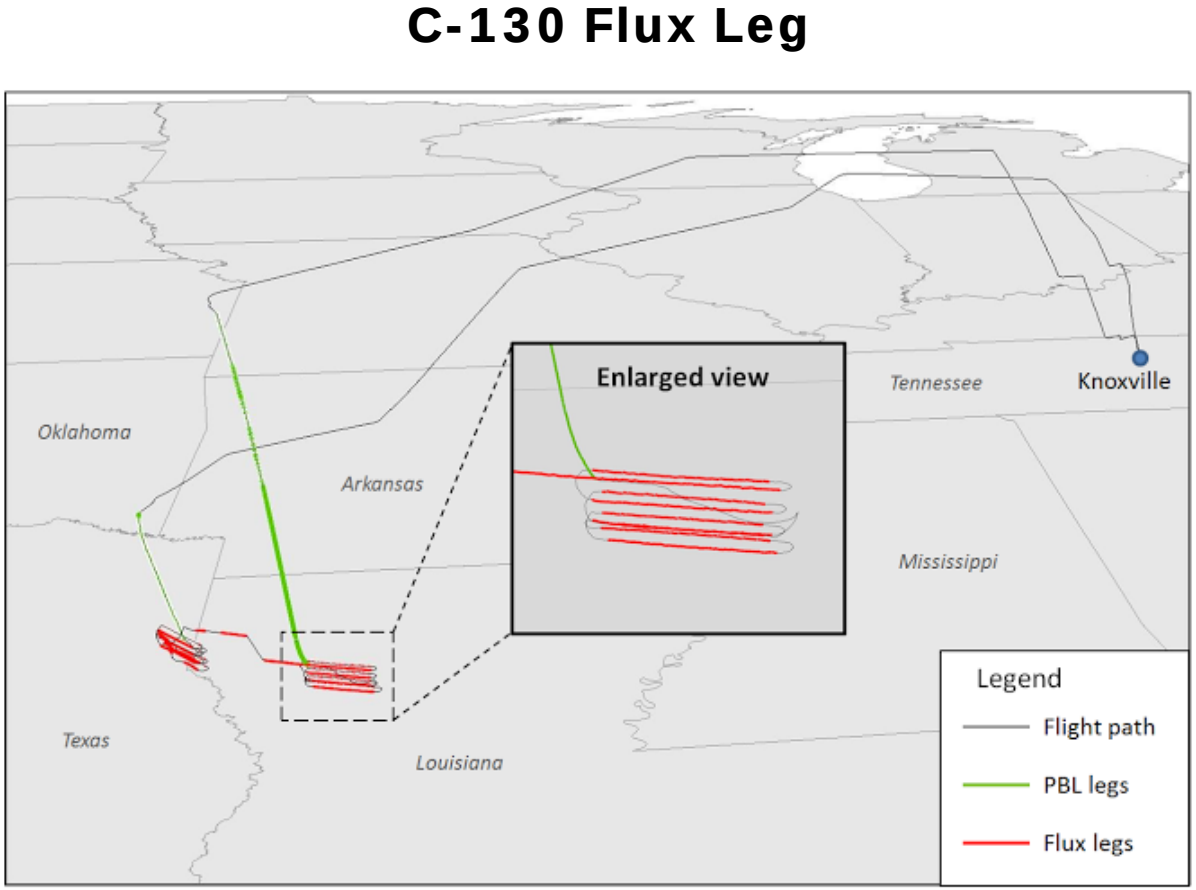
Isoprene Emission Fluxes from C-130 Aircraft Data

- Wavelet-based eddy-covariance approach
  - PTR-MS and turbulence measurements
- Applied for selected C-130 “racetracks” and transects
- Surface fluxes calculated using a vertical flux divergence correction method assuming linear relationship between fluxes at different altitudes.



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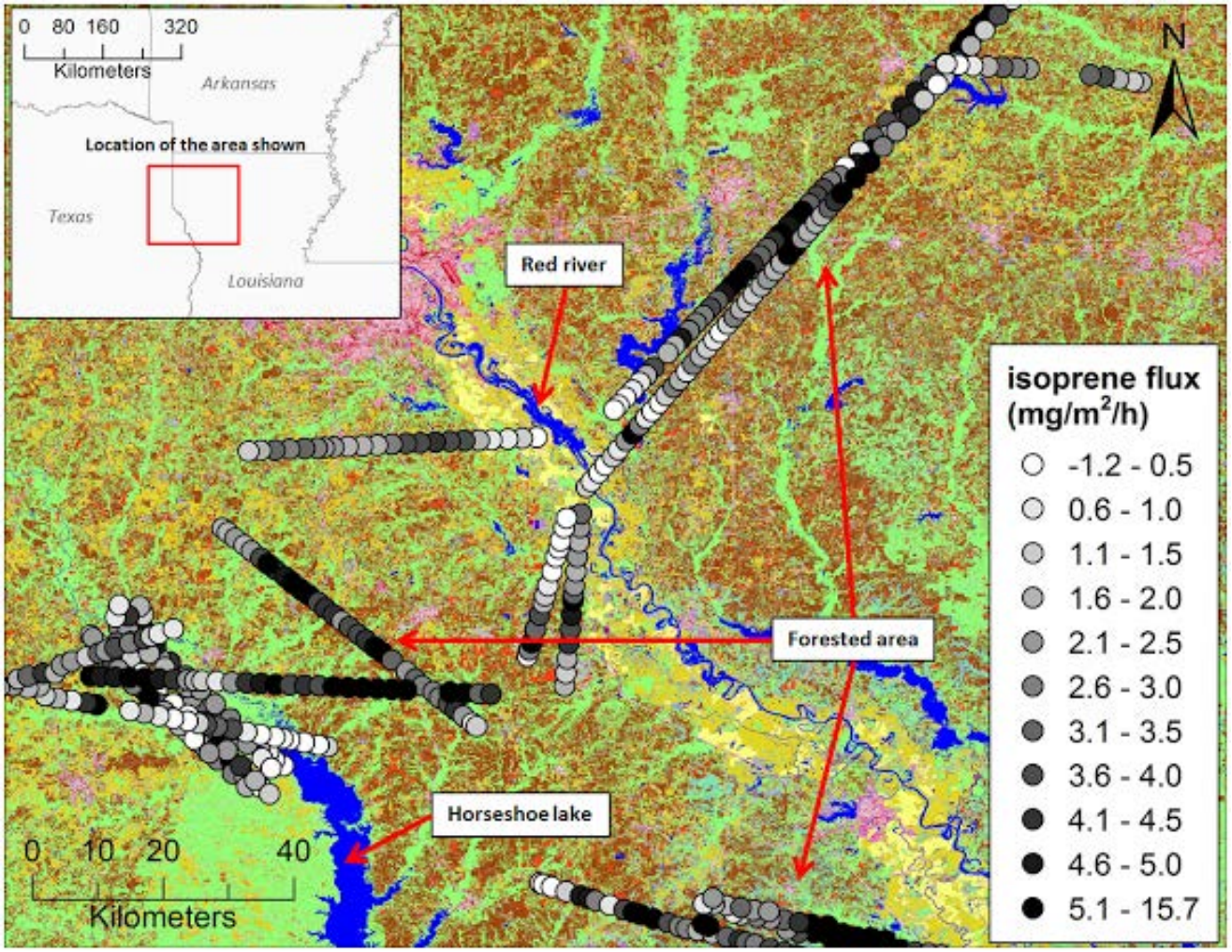
Isoprene Emission Fluxes from C-130 Aircraft Data

C-130 Isoprene Fluxes



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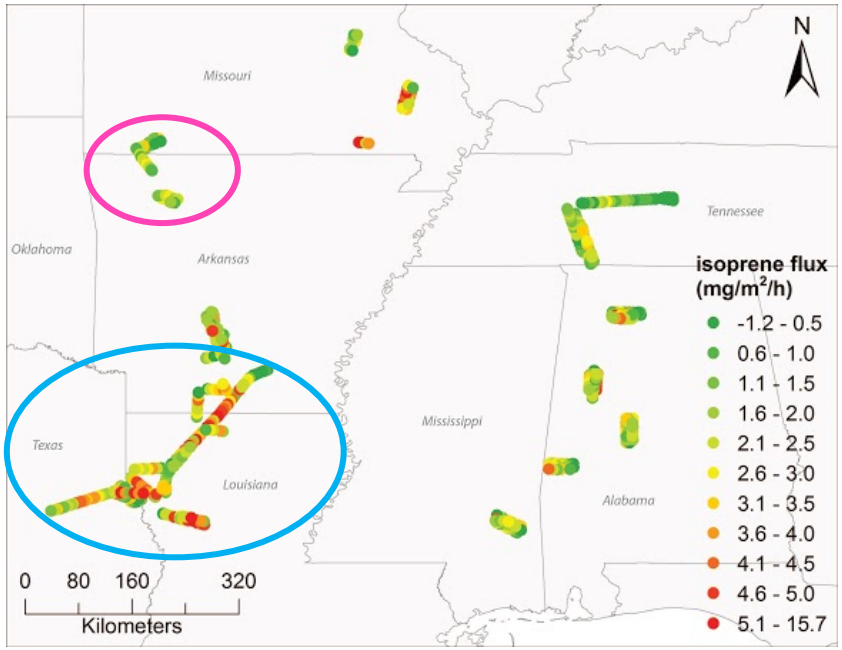
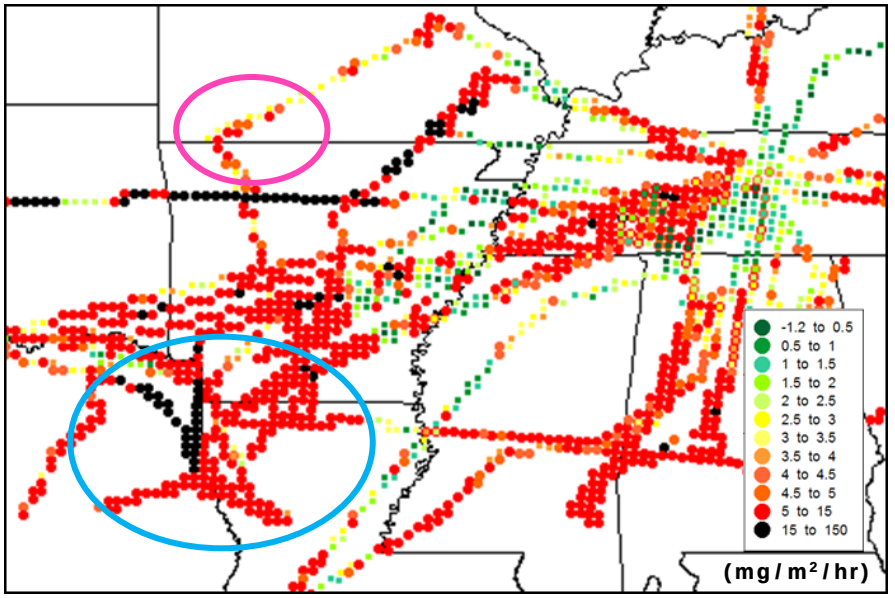
Isoprene Emission Fluxes from C-130 Aircraft Data

C-130 Airborne Isoprene Flux



MEGAN Isoprene Emissions



- Using default inputs, MEGAN isoprene fluxes are consistently higher than C-130 airborne fluxes

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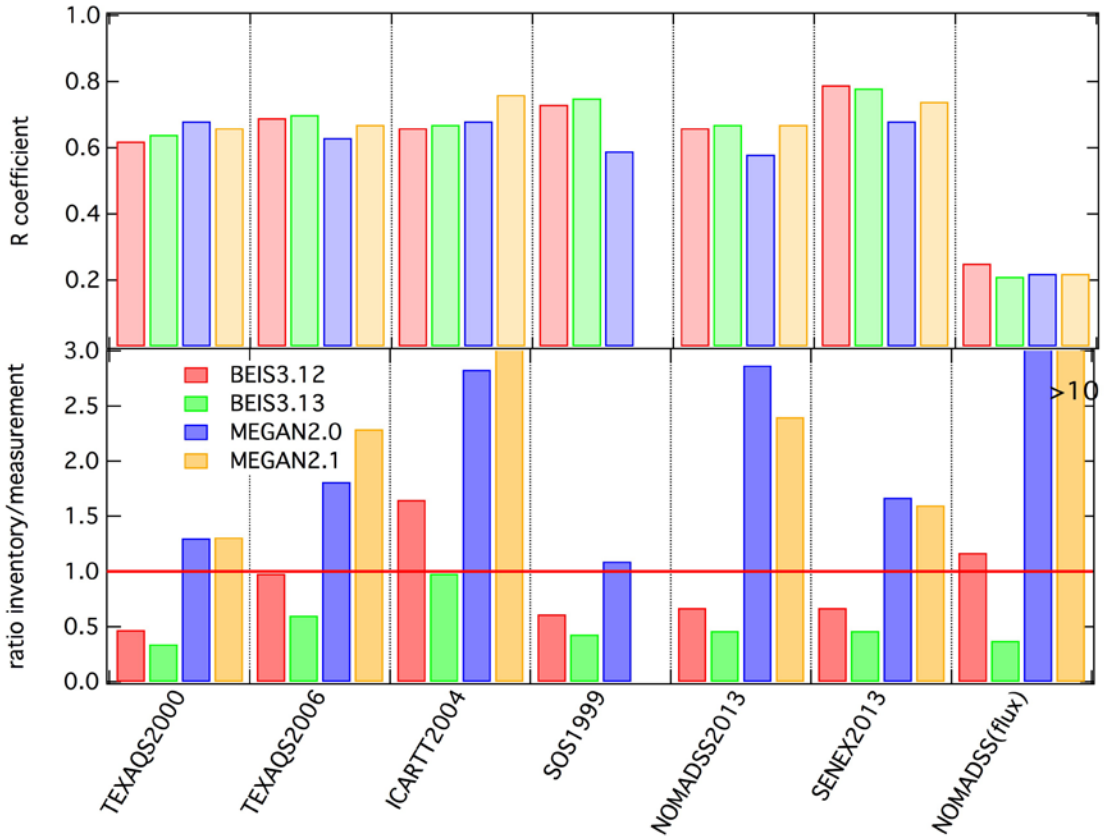
Isoprene Emission Fluxes from SAS P-3 Aircraft Data and Previous Studies

- Compared fluxes based on aircraft measurements and mass balance method with modeled fluxes
  - MEGAN v2.1 higher than fluxes inferred from measurements
  - BEIS lower
- Results consistent across most studies

Comparing Isoprene Fluxes Based on Measurements with Modeled Emissions



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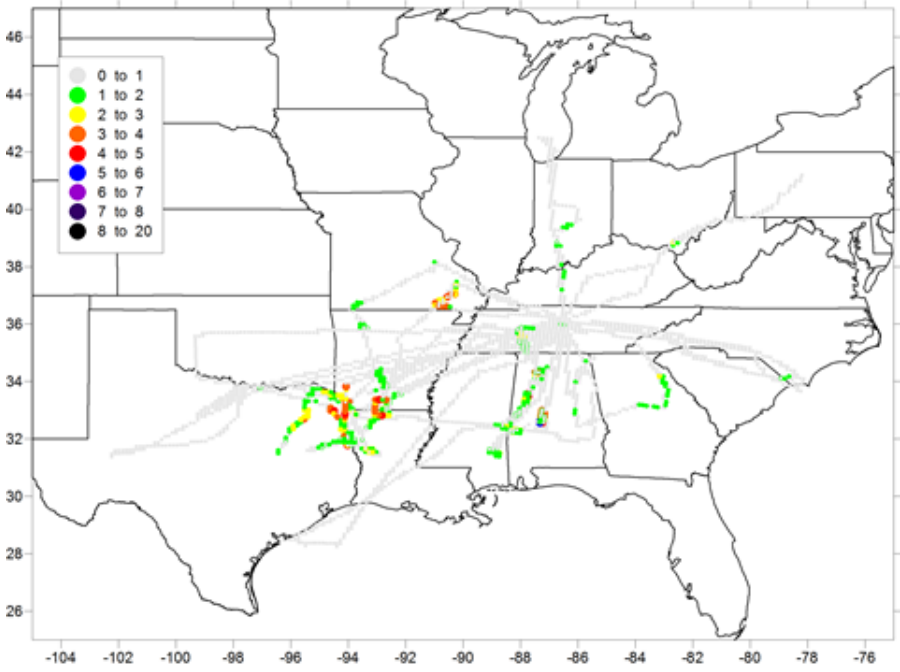
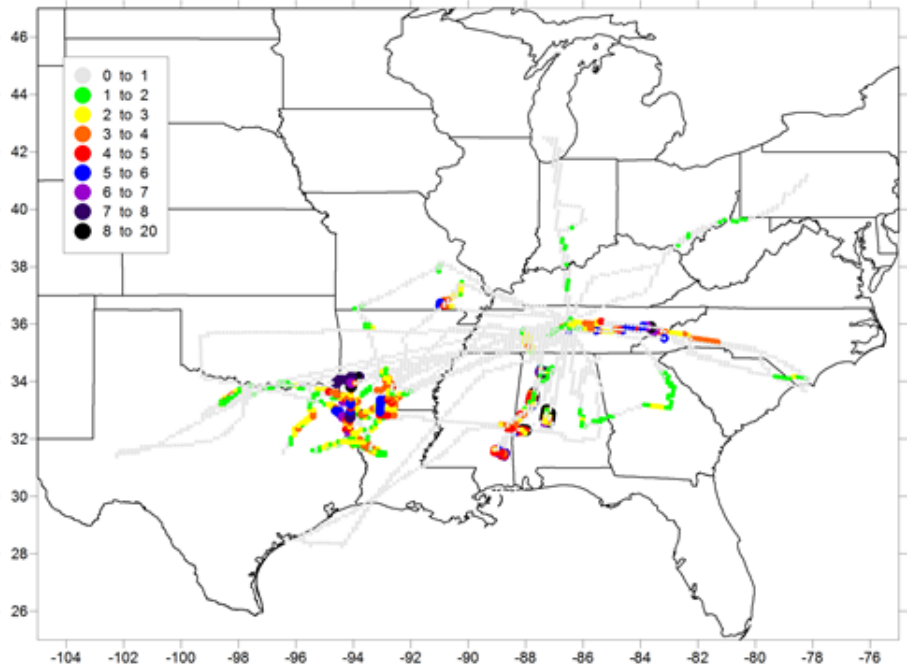
Modeled and Measured Isoprene along C-130 Flight Path

C-130 Measurements



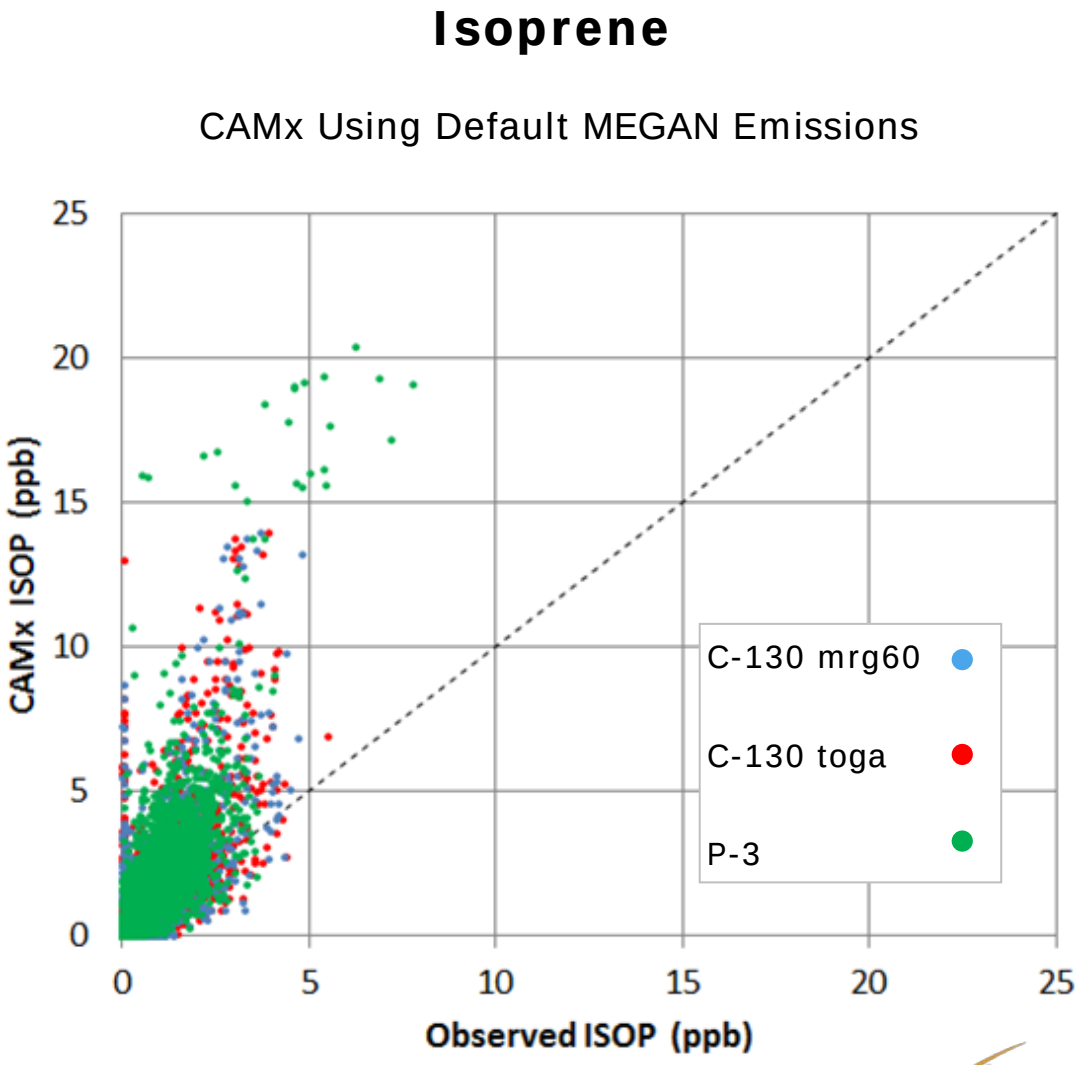
CAMx



- CAMx spatial patterns of high and low isoprene similar to those of C-130 observations
- Model consistently overestimates isoprene along the flight path

Modeled and Measured Isoprene along C-130 and P-3 Flight Paths

- CAMx modeled isoprene overestimated relative to C-130 and P-3 measurements
- NMB ranged from 83-113% for C-130 and P-3 datasets



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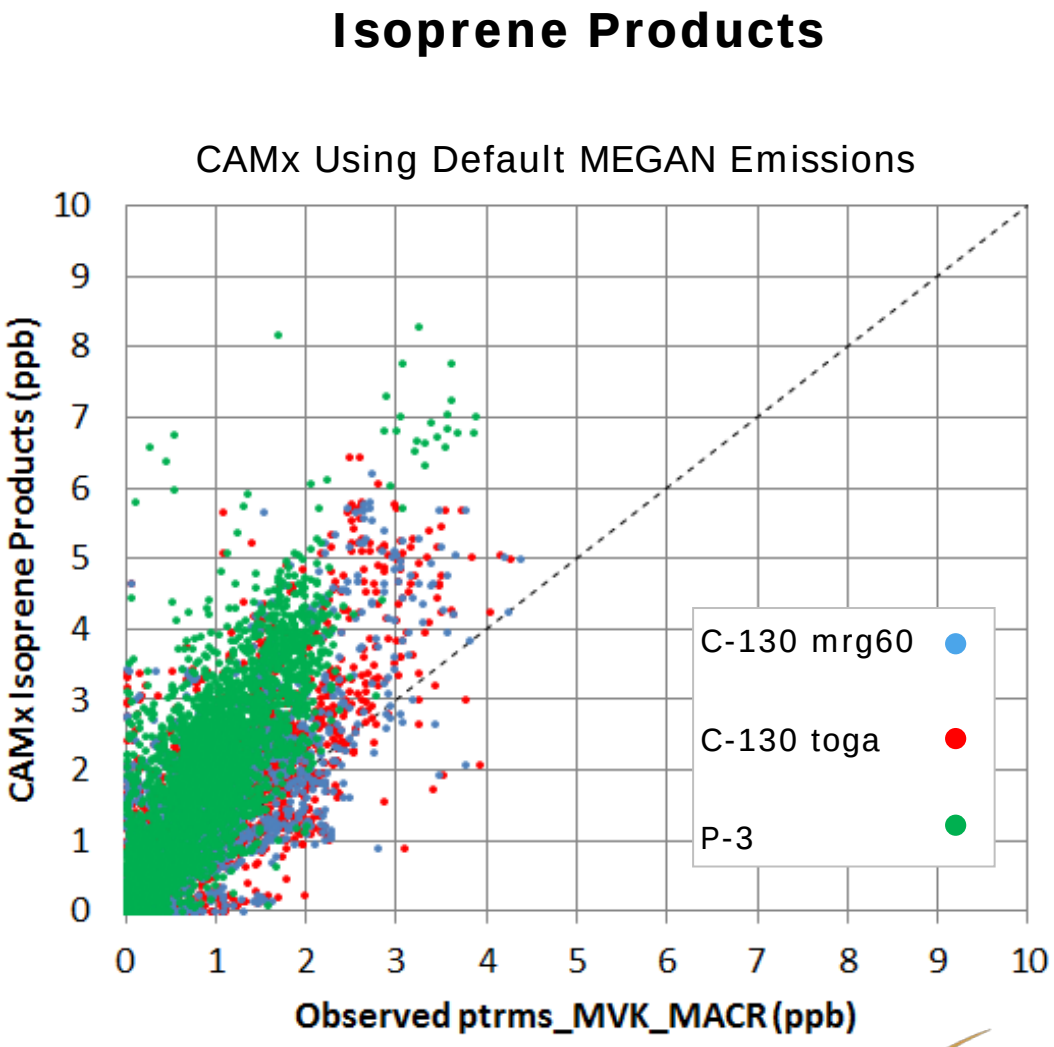
Modeled and Measured Isoprene Products along C-130 and P-3 Flight Paths

- CAMx modeled isoprene products overestimated relative to C-130 and P-3 measurements
- NMB ranged from 47-114% for C-130 and P3 datasets



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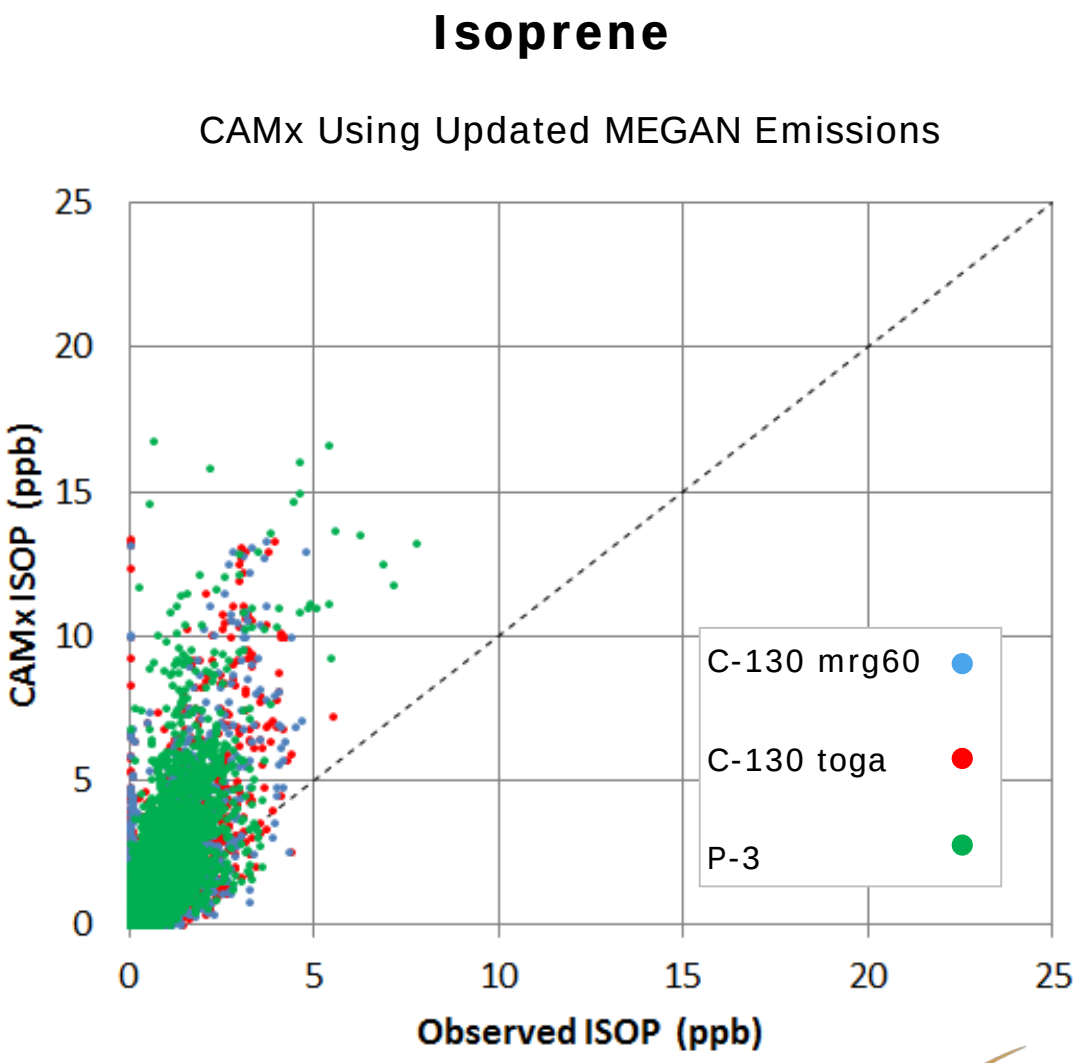
Modeled and Measured Isoprene along C-130 and P-3 Flight Paths

- MEGAN emissions used updated landcover and EF data
- CAMx modeled isoprene overestimated relative to C-130 and P-3 measurements
- NMB ranged from 102-132% for C-130 and P-3 datasets



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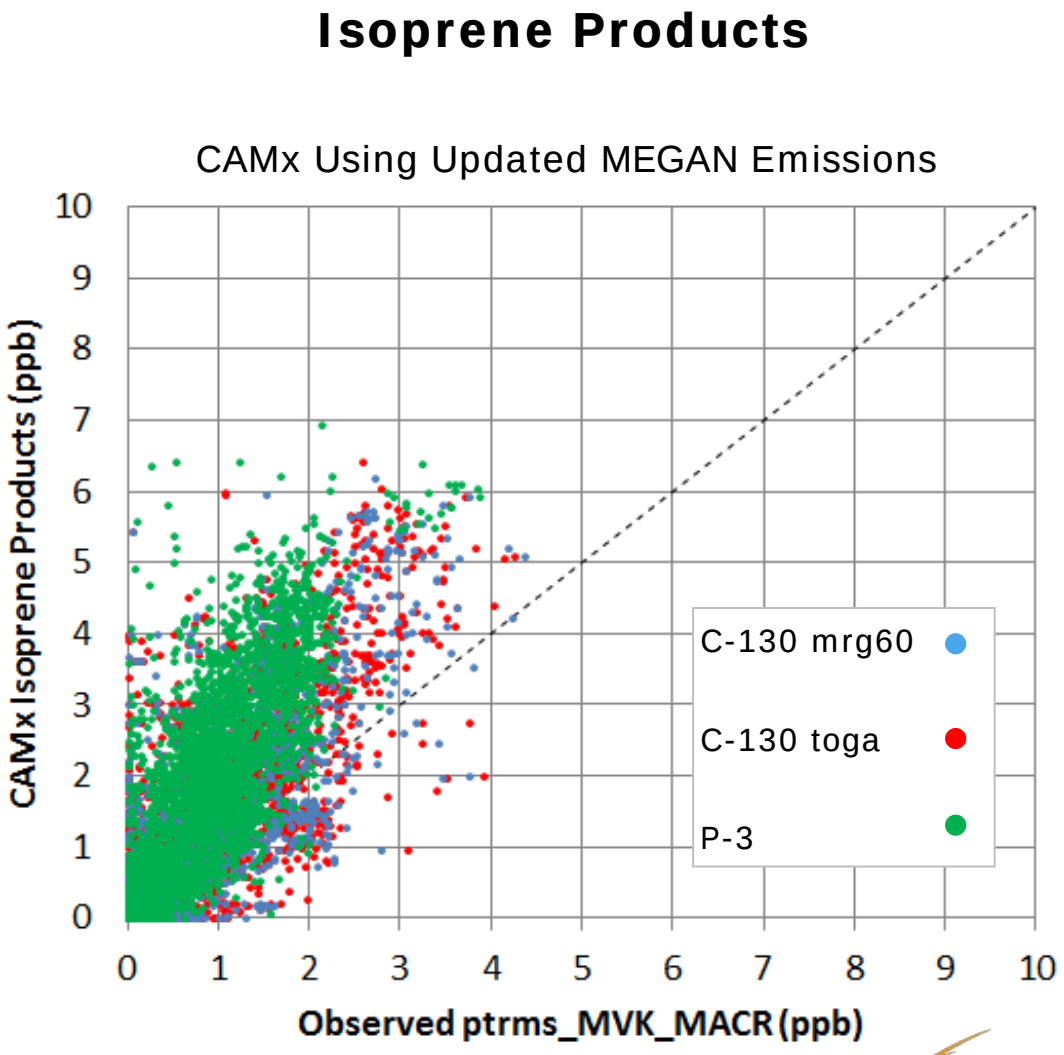
Modeled and Measured Isoprene Products along C-130 and P-3 Flight Paths

- MEGAN emissions used updated landcover and EF data
- CAMx modeled isoprene products overestimated relative to C-130 and P-3 measurements
- NMB ranged from 53-118% for C-130 and P3 datasets



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Modeled and Measured Isoprene Products along C-130 and P-3 Flight Paths

Understanding Differences in Modeled and Measured Isoprene Emissions and Concentrations

- Several factors may contribute to isoprene emission and concentration overestimates:
  - Isoprene emissions factor overestimate
  - Heterogeneity in landscape
  - PAR overestimate due to WRF model overestimate of downwelling solar radiation
  - OH underestimate

- Carried out sensitivity tests to investigate

Sensitivity Test: OH from Isoprene Degradation

- Test response to an isoprene mechanism that represents an upper limit on the production of OH from isoprene breakdown

- Altered the CB6r2 chemical mechanism to increase the production of OH
  - Follow mechanism of Peeters et al. (2013)
- Where standard CB6r2 produces one OH from isomerization, this scheme produces up to 5 OH

Changes to CB6r2 Chemical Mechanism

163	HPLD = OH + ISPD	Photolysis

Becomes:

163	HPLD = OH + HO2 + PCLD	Photolysis
217	PCLD = 2 OH + OKET	Photolysis (set J = 0.1 x JNO2)
218	PCLD + NO3 = HNO3 + ISPD	k = 6.00E-12 exp(-1860/T)
219	OKET + HO2 = CO + C2O3 + 2 OH	k = 1.0E-11
220	OKET = CO + C2O3	Photolysis (set J = MGLY)

PCLD has formula C5H5O4 and deposits like HPLD
OKET has formula C4H4O2 and deposits like HPLD

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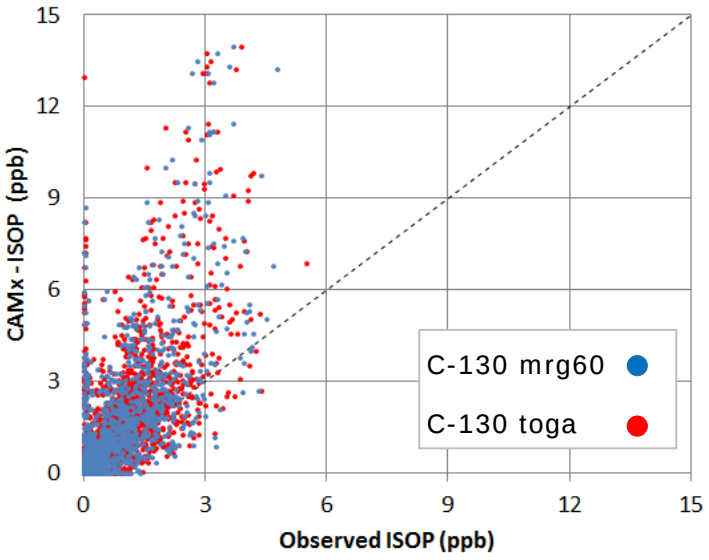
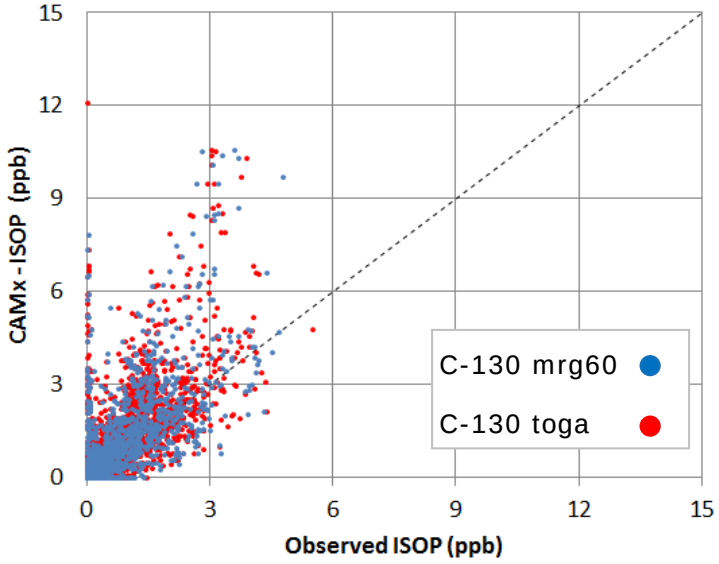
Sensitivity Test: OH from Isoprene Degradation

Isoprene

Base Run



OH Sensitivity Test



- Increasing OH from isoprene reduces but does not eliminate high bias
  - Mean normalized bias: 83%->43%
- Chemical mechanism is not the main factor contributing to modeled isoprene overestimates

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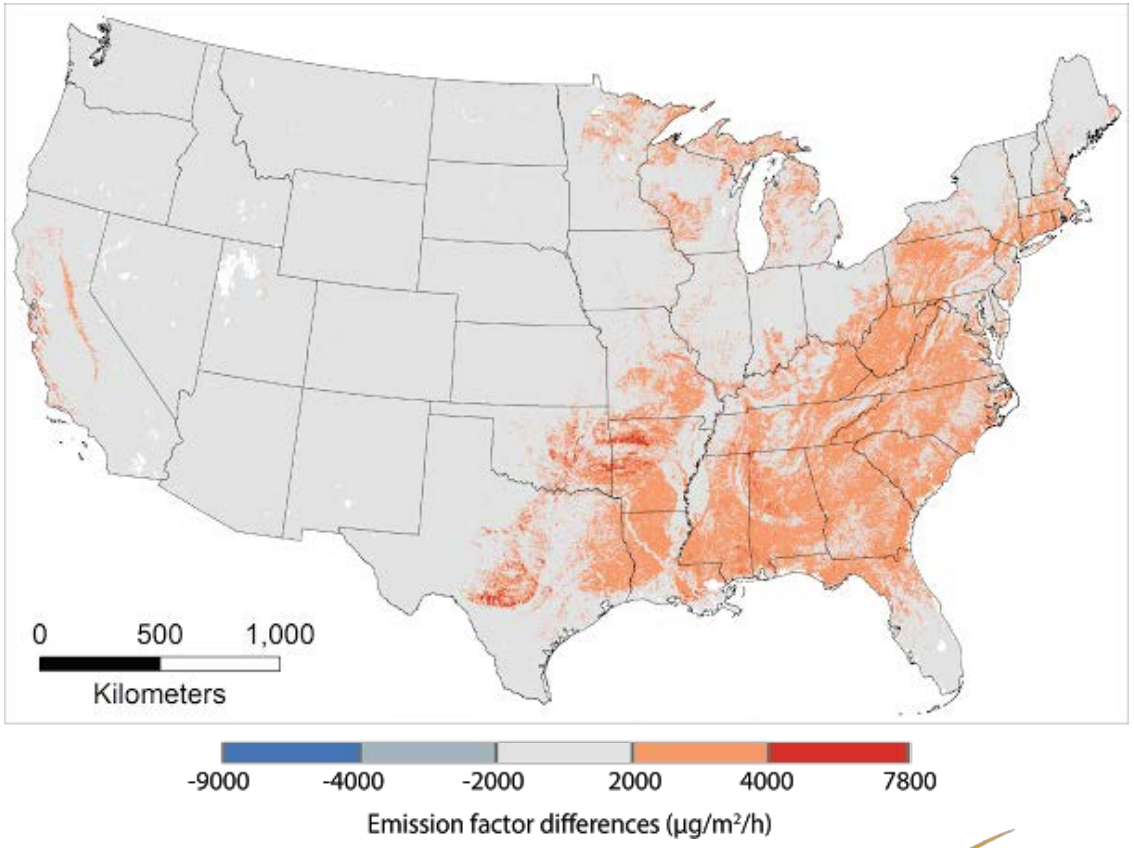
Sensitivity Test: Revised Emission Factor EF2015x

- Used relationships between vegetation cover types, EF calculated based on observations and LC to adjust emission factors for all vegetation types - including those not covered by aircraft observations
- Reduction in EFs
- Preliminary data

EF2015-EF2015x Difference Plot



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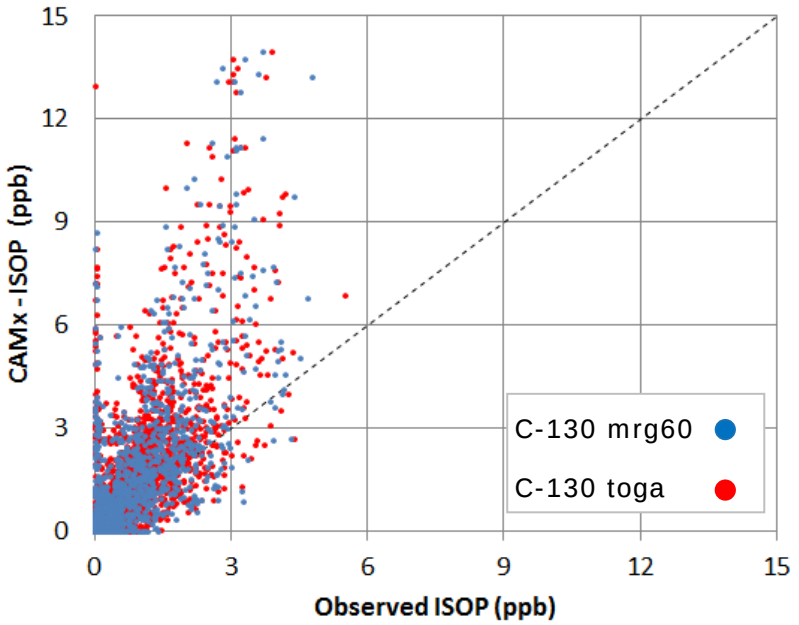
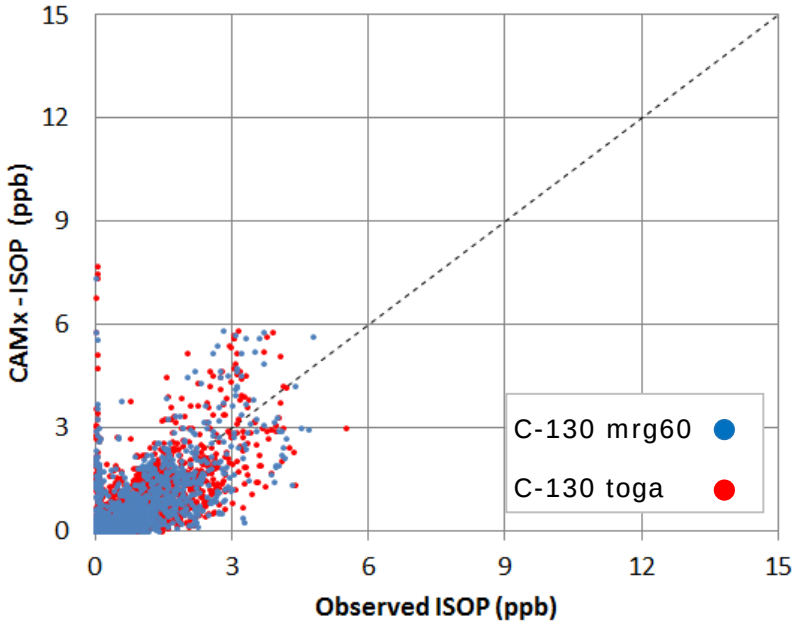
Sensitivity Test: Revised Emission Factor EF2015x

Isoprene

Base Run



EF2015x Sensitivity Test



- Isoprene bias reduced from ~ 84% to -16%
- Modeled MEGAN isoprene emissions and CAMx isoprene concentrations highly sensitive to change in emissions factor
- R^2 slightly lower in EF2015x run

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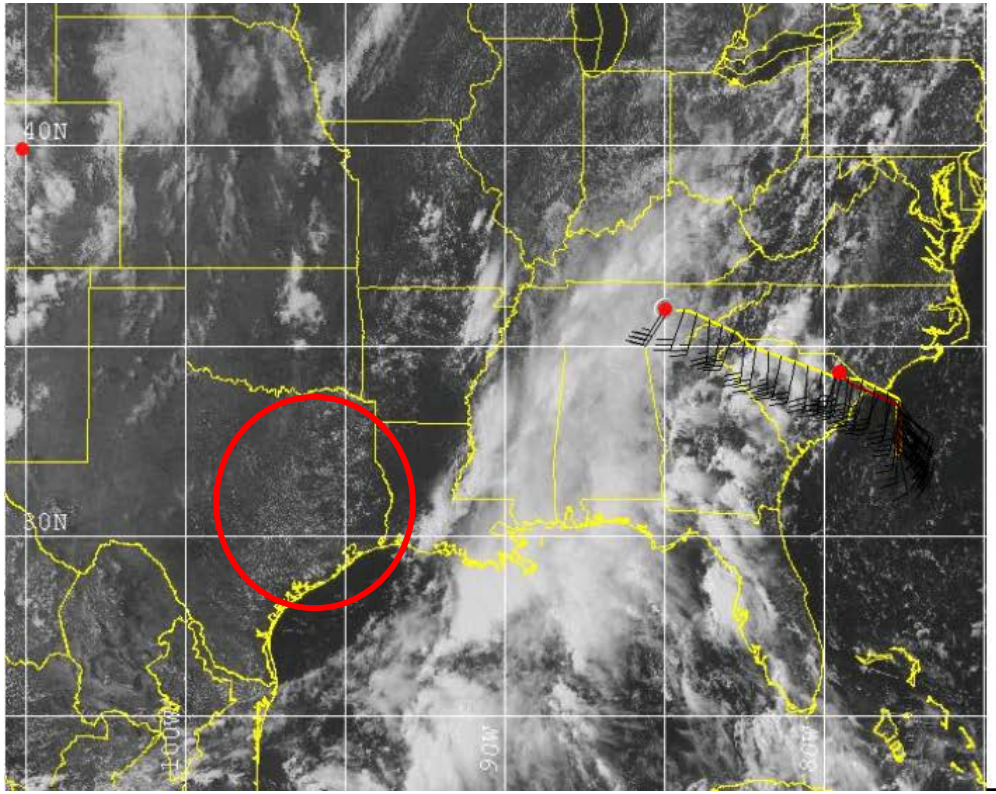
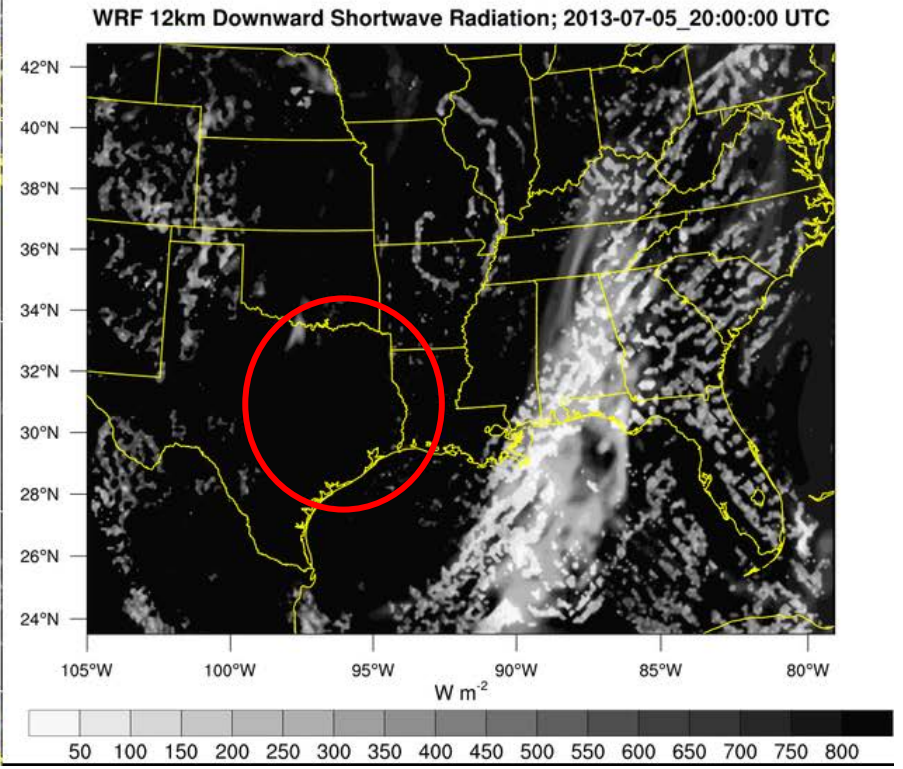
Other Sources of Error in MEGAN Emissions?

GOES Visible Image



WRF DSW Radiation



- WRF meteorological model supplies T and PAR to MEGAN
- WRF underestimates clouds, and therefore overestimates PAR
- How much bias does this introduce into MEGAN emission estimates?

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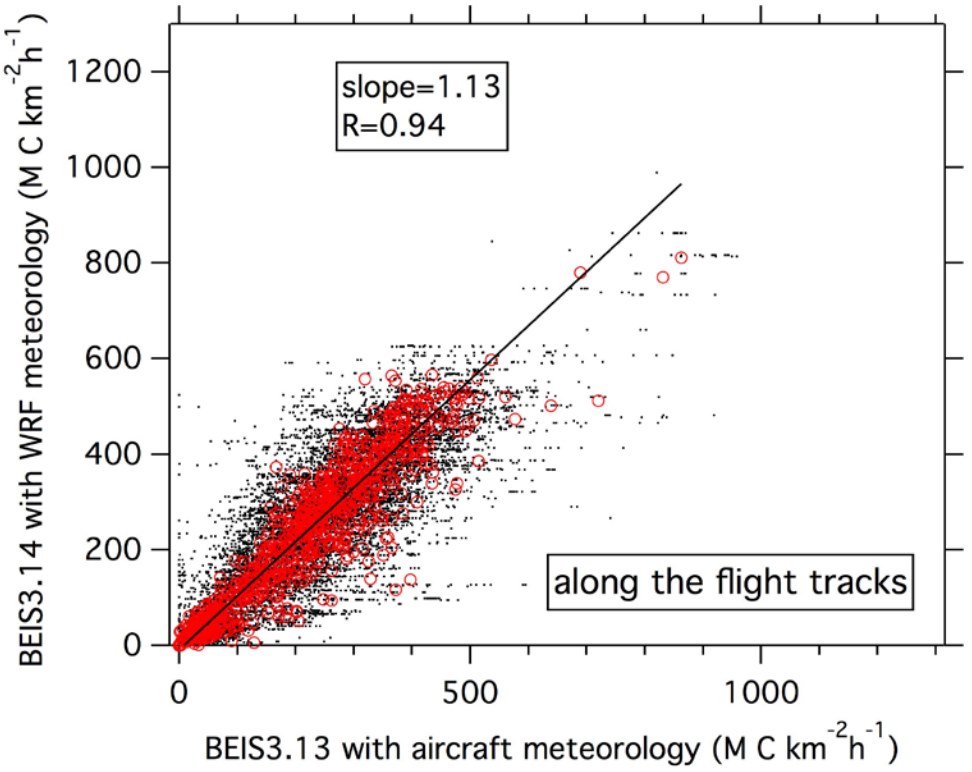
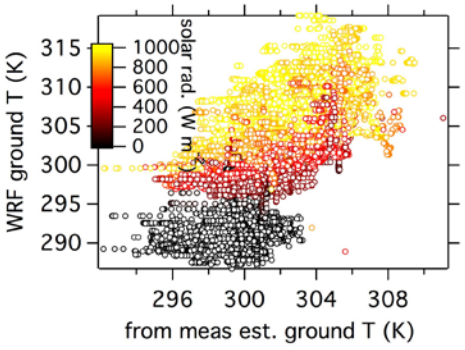
WRF-CHEM: ISOPRENE EMISSIONS ALONG FLIGHT TRACKS

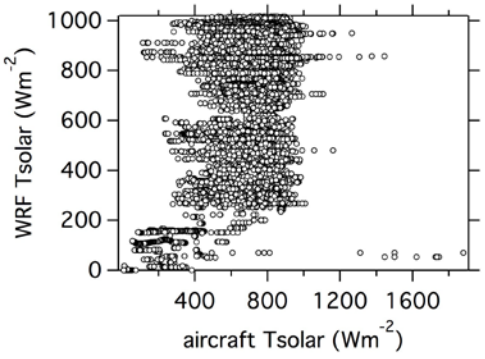


WRF-Chem:

- 12 km resolution
- NEI2011
- BEIS3.14

- BEIS3.14 Emissions: WRF-Chem agrees well with BEIS3.13 using aircraft data





- Ground temperature and solar radiation: WRF-Chem agrees reasonable with measurements

Model data provided by Stu McKeen (NOAA)

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Project 14-016

Summary:

- Newly-available aircraft measurements of isoprene, isoprene products and other species provided constraints on the biogenic emission inventory in southeast and Texas
  - Ruled out underestimate of OH in the isoprene chemical mechanism as a key factor in the CAMx isoprene concentration overestimate
- Update to MEGAN inventory using new high resolution LC data and EFv2015x improved agreement between isoprene emissions and airborne fluxes
  - CAMx-modeled isoprene and isoprene product concentrations agreed more closely with aircraft-measured concentrations

Project 14-016

Ongoing Work:

- Incorporate 1 m Texas urban data into land cover data
- Quantitative evaluation of errors in MEGAN emission estimates
  - Derive airborne fluxes using aircraft measurements of T, PAR

Recommendations for Future Work:

- Reconcile the substantial differences between leaf-scale, tower-scale and aircraft-scale emission estimates as well as comparisons to satellite based emission estimates
- There is evidence that other “unmeasured” compounds play an important role in atmospheric chemistry. New analytical techniques provide an opportunity for determining whether there are other important compounds and also for characterizing the contribution of these compounds.
- BVOC response to stress is an important but not well known component of emission models. Processes controlling BVOC emission response to stress should be quantified and evaluated with long-term above canopy flux measurements.

QUESTIONS?

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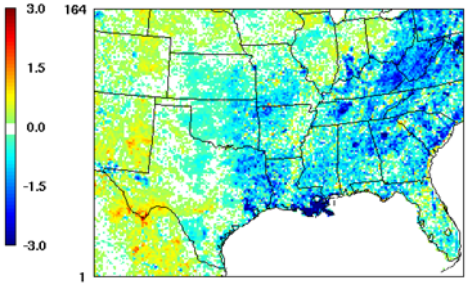
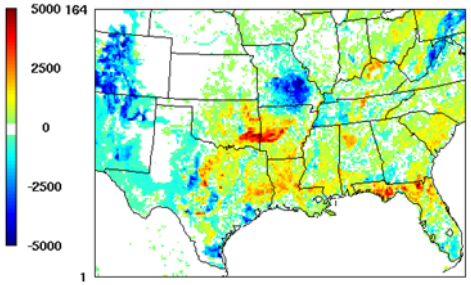
Episode Average LAIs Difference

Updated_v1 - Default



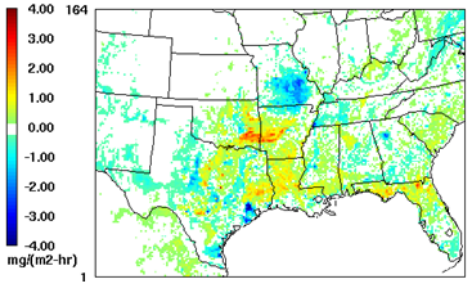
Isoprene EF Difference

Updated_v1 - Default



Isoprene Emissions Difference

Updated Emissions v1 - Default Emissions
Episode Average Emissions

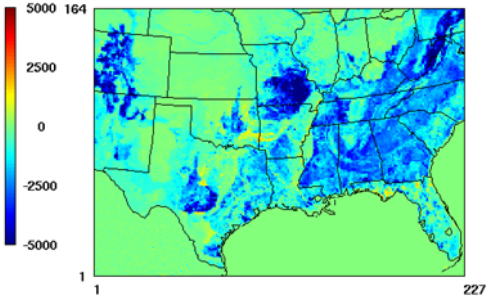


Episode Average LAIv Difference

Updated_v2-Updated_v1

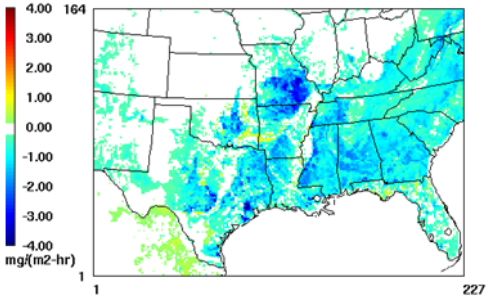
Isoprene EF Difference

Updated_v2 EF - Default EF



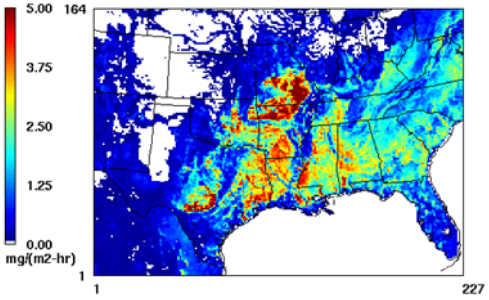
Isoprene Emissions Difference

Updated Emissions v2 - Default Emissions
Episode Average Emissions



MEGAN Episode Average Isoprene Emissions

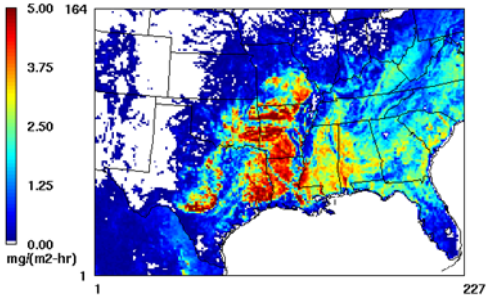
Default MEGAN Inputs



August 20,2003 0:00:00
Min= 0.00 at (81,1), Max= 8.80 at (76,48)

MEGAN Episode Average Isoprene Emissions

Updated_v1 MEGAN Inputs



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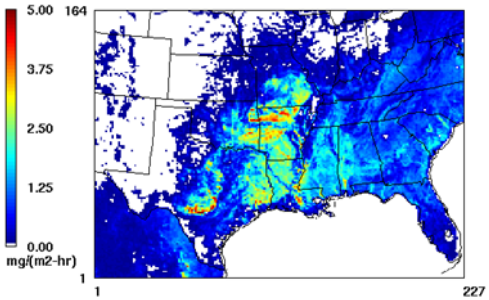
MEGAN Episode Average Isoprene Emissions

Updated_v2 MEGAN Inputs



August 21,2003 0:00:00
Min= 0.00 at (81,1), Max= 7.26 at (78,55)

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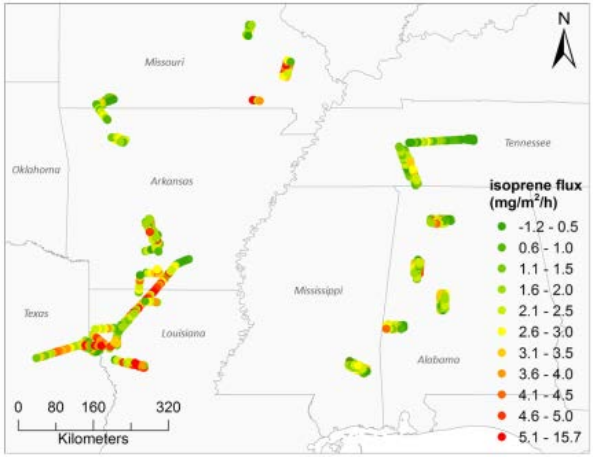
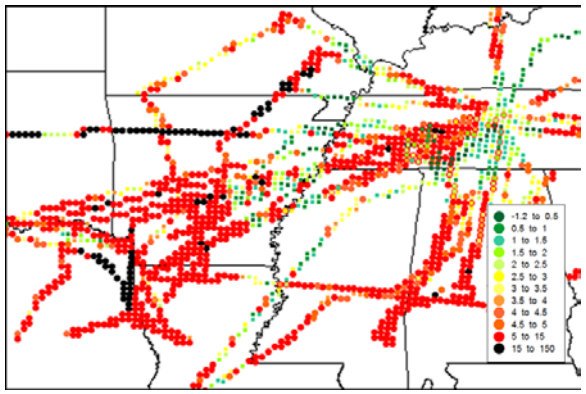
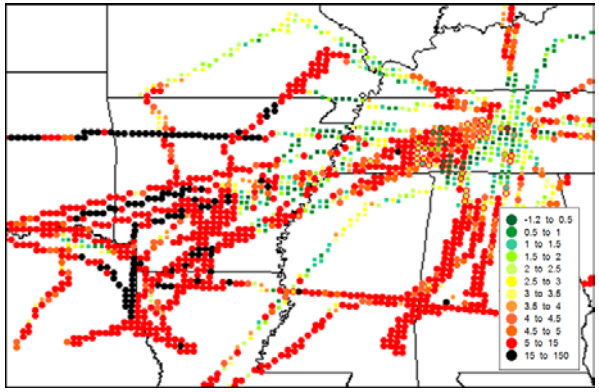
Isoprene Fluxes from Aircraft Data



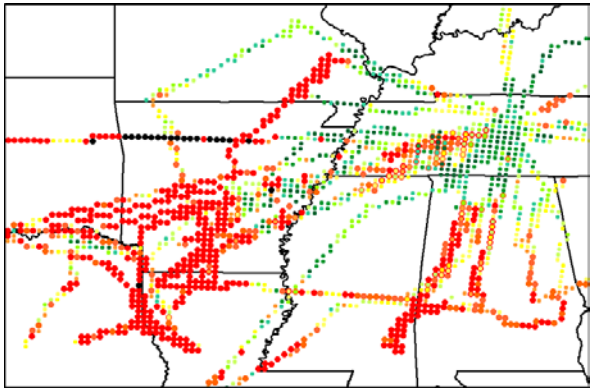
MEGAN ISOP Emissions (Default)



MEGAN ISOP Emissions (EFv2015)



MEGAN ISOP Emissions (EFv2015x)



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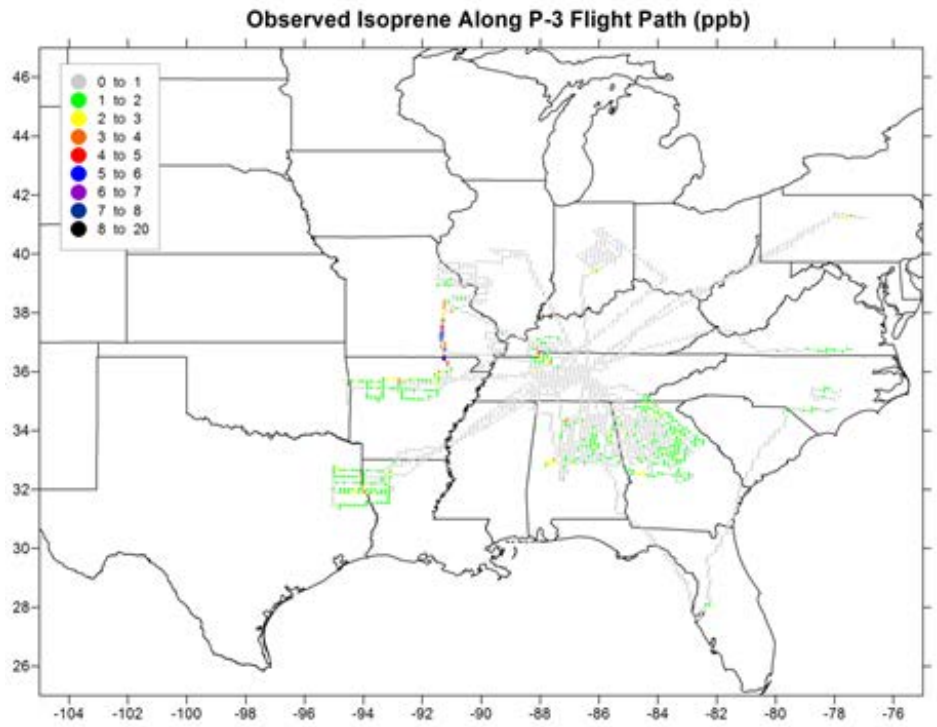
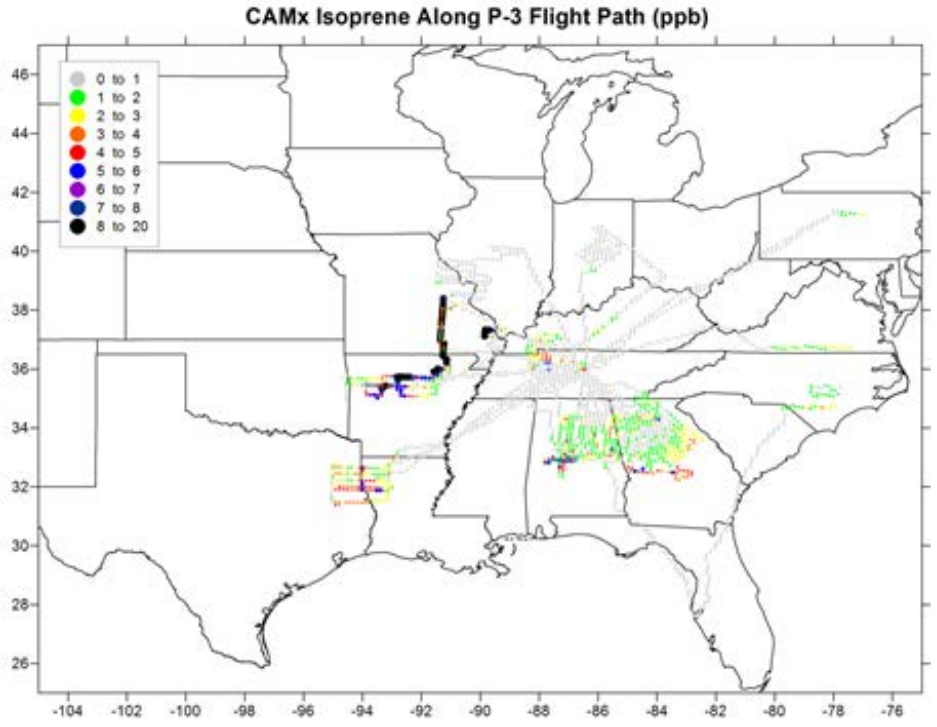
Modeled and Measured Isoprene along P-3 Flight Path

P-3 Measurements



CAMx



- CAMx spatial patterns of high and low isoprene similar to those of P-3 observations
- Model consistently overestimates isoprene along the flight path

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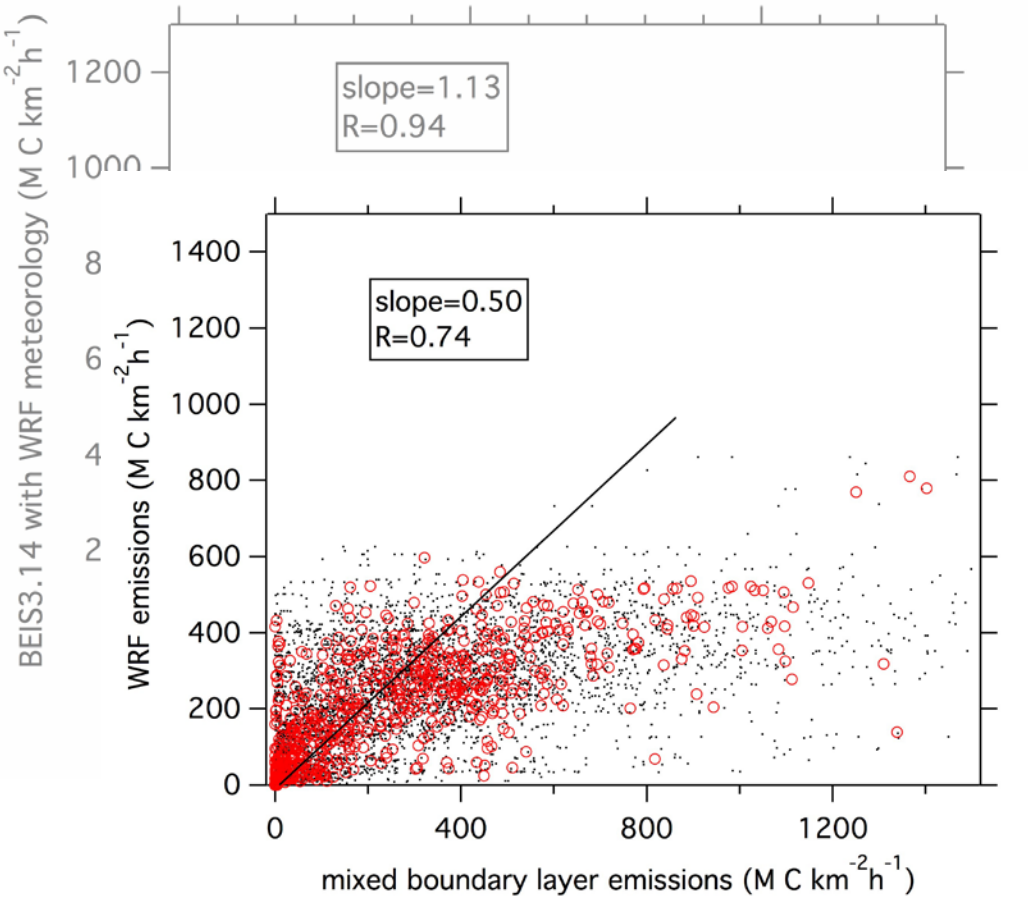
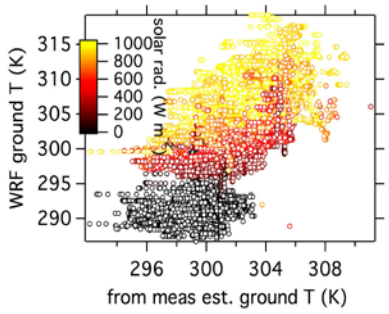
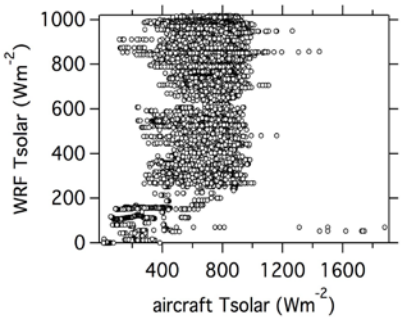
WRF-CHEM: ISOPRENE EMISSIONS ALONG FLIGHT TRACKS







WRF-Chem:

- 12 km resolution
- NEI2011
- BEIS3.14

- WRF Emissions lower than mixed boundary layer emissions from measurements

Model data provided by Stu McKeen (NOAA)