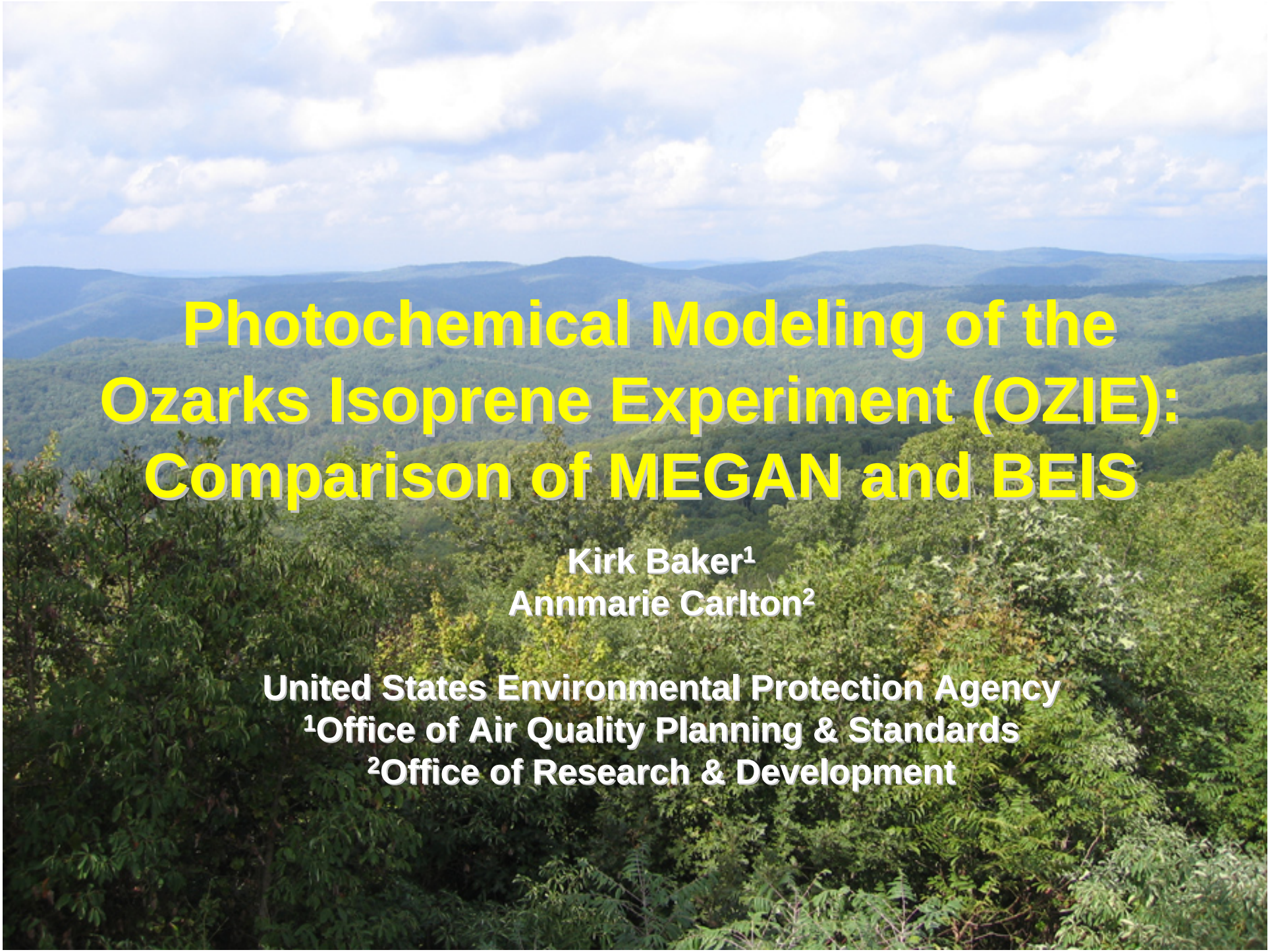

Photochemical Modeling of the Ozarks Isoprene Experiment (OZIE): Comparison of MEGAN and BEIS

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Background

- Biogenic VOC comprise approximately 75-80% of the North American annual 2005 VOC emission inventory
- Biogenic emissions largely a function of plant type, leaf area index, temperature, and solar radiation (PAR)
- Biogenic emissions for regional and global scale photochemical are typically developed from either MEGAN or BEIS
- Model of Emissions of Gases and Aerosols from Nature **(**MEGAN**)**
  - Currently developed by NCAR
- Biogenics Emission Inventory System **(**BEIS**)**
  - Currently developed by US EPA
- July 1998 OZarks Isoprene Experiment (OZIE) field study designed for evaluation of biogenic models

Motivation

- Which biogenic model should we use for upcoming regulatory modeling projects?
- Are one or both models acceptable for upcoming round of ozone and PM2.5 State Implementation Plans?
- Are there any significant issues related to routine regulatory application?

Project Background

- Compare MEGAN and BEIS isoprene and other biogenic VOC estimates to surface and upper air OZIE field study measurements

- Evaluate sensitivity of CMAQ predictions when using alternative biogenic emissions models for
  - Primary gas phase species: e.g., isoprene, monoterpenes
  - secondary species: e.g., O_3, $PM_{2.5}$, SOA
  - Primary and secondary: formaldehyde

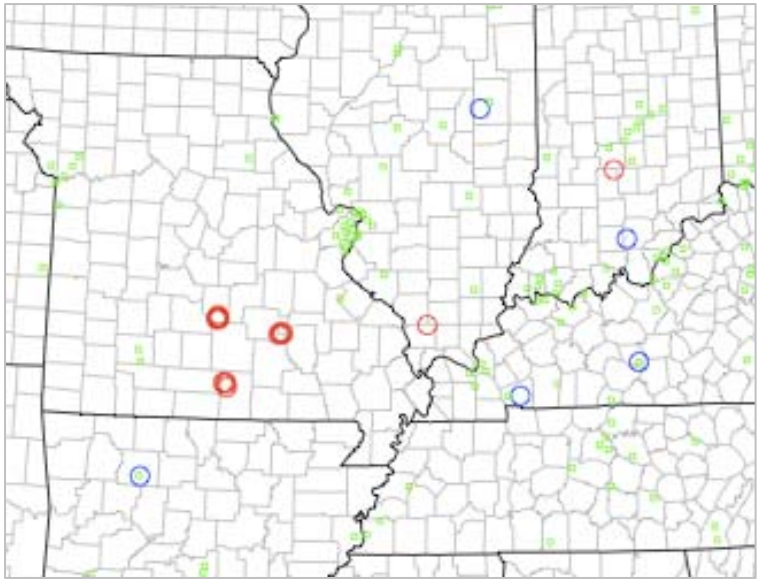
- Alternative source of solar radiation; what impact does this variable have on MEGAN and BEIS estimates? How well does WRF capture solar radiation?

- Examine the impact of grid resolution on biogenic emissions estimates; evaluate WRF performance at 12 and 4 km in a non-urban environment

Ozarks Isoprene Experiment: July 1998

Field Study Observations

- Surface
  - TNMOC, isoprene, a-pinene, b-pinene, formaldehyde, ozone
  - Solar radiation, soil temperature, wind speed, wind direction, temperature, relative humidity
- Balloon
  - Isoprene, a-pinene, b-pinene
- Aircraft (7 flights)
  - Ozone, isoprene, TNMOC, formaldehyde



Other Available Observation Data:

- AIRS (1-hr avg)
  - Ozone, NO2/NOX, PM10, Carbon monoxide
- CASTNET/IMPROVE (24-hr avg)
  - Speciated PM2.5
- FSL RAOB Springfield, MO
  - Temperature, wind vector
- U.S. Airways (DS472) (Hourly reported)
  - Temperature, mixing ratio, wind speed, wind direction

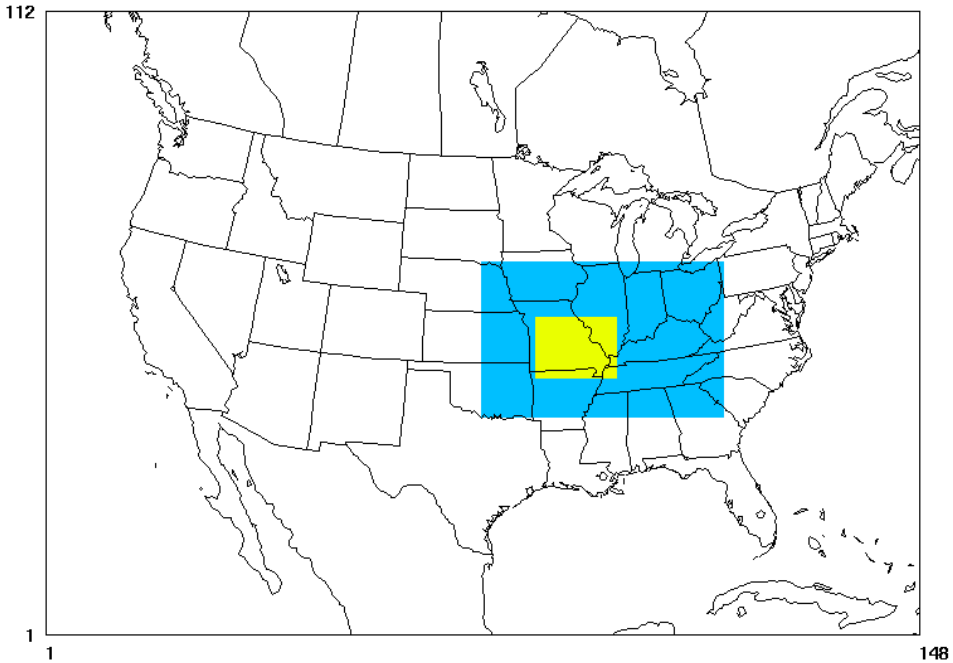
Modeling Overview

- Modeled June 15-July 31, 1998 episode

- CMAQ v4.7.1 (N2a)
- CB05 & AERO5

- WRF v3.1
- MCIP v3.4.1.1

- BEIS v3.14
- MEGAN v2.04
- 2001 v2 based anthropogenic emissions
- SMOKE inline emissions



- 36 km – continental US
- 12 km (blue)
- 4 km (yellow)

- 34 and 14 vertical layers

Meteorological Modeling

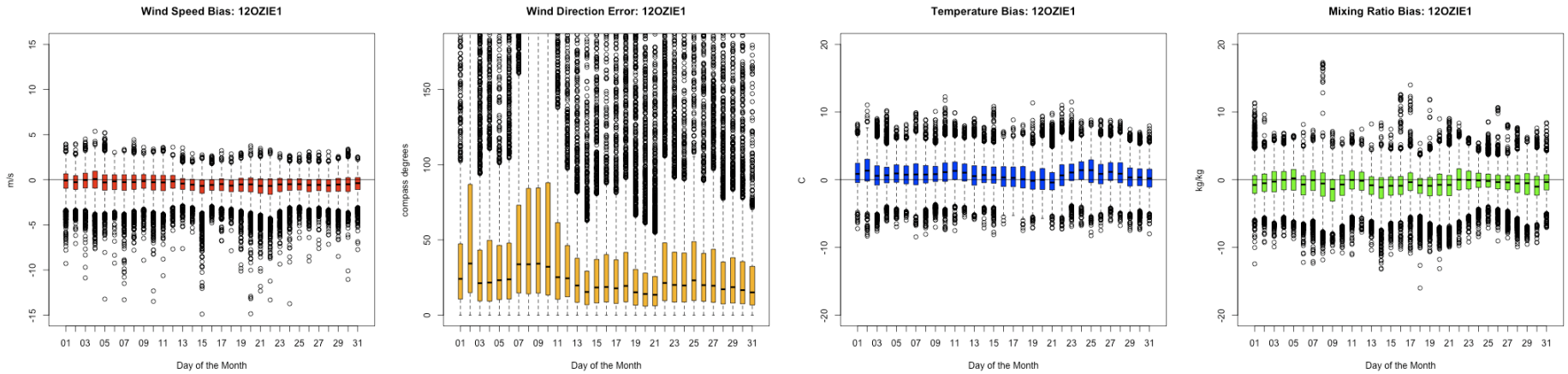
- **WRF version 3.1**
- Episode: June 15 to August 1, 1998
- North American Regional Reanalysis (NARR) input to 36 km domain
- NESTDOWN input to 12 and 4 km domains
- OBSGRID for soil nudging
- Soil moisture and temperature continued from one 5 day block to the next
- First 5 day block used average 2m temperature to initialize deep soil temperature

- Morrison double moment microphysics
- RRTMG longwave and shortwave radiation
- Pleim-Xiu land-surface and surface layer models
- ACM2 planetary boundary layer scheme
- Kain-Fritsch cumulus parameterization

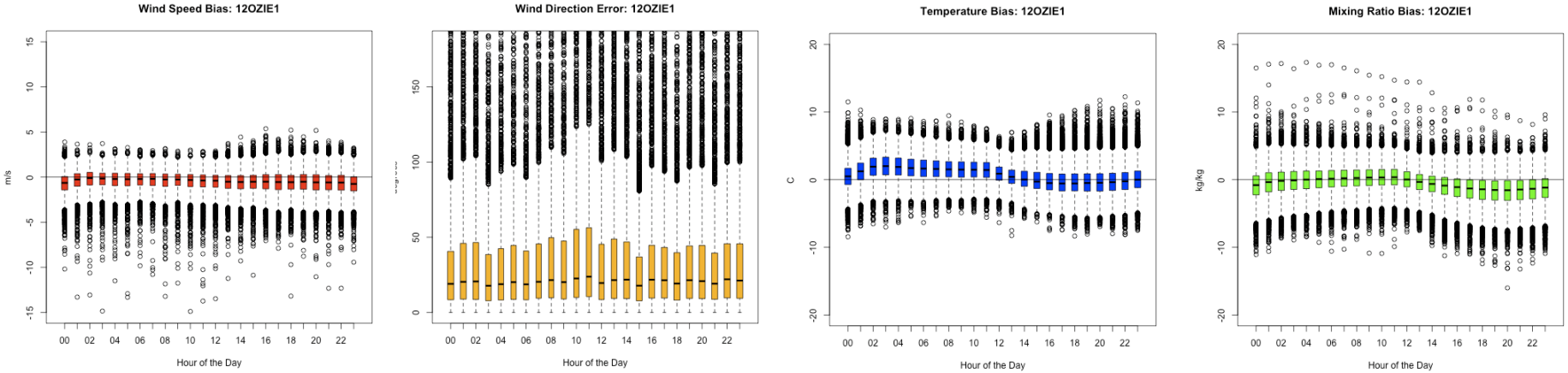
- Applied analysis nudging for winds above and below PBL
- Analysis nudging for temperature and moisture above PBL only

Meteorological Performance: All Sites in 12 km domain

Bias by day of the month

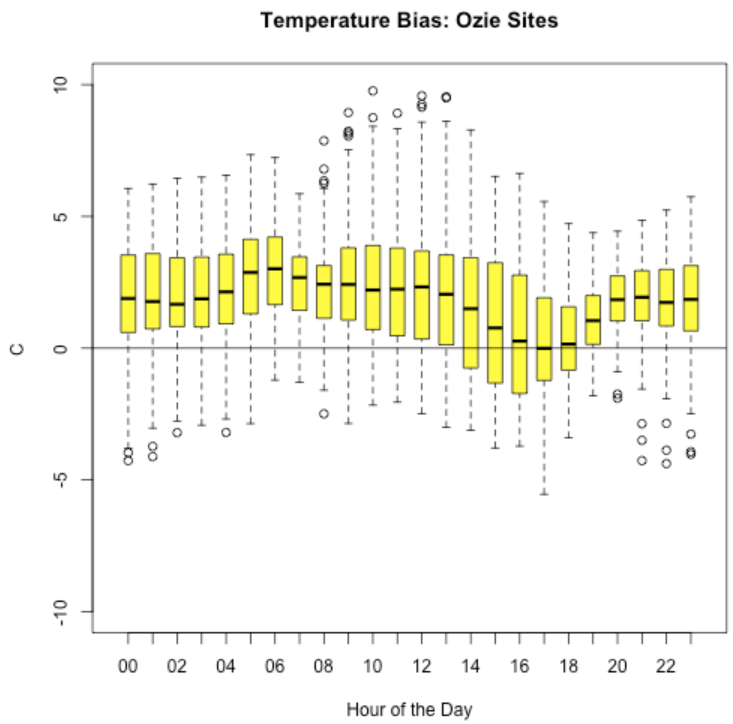


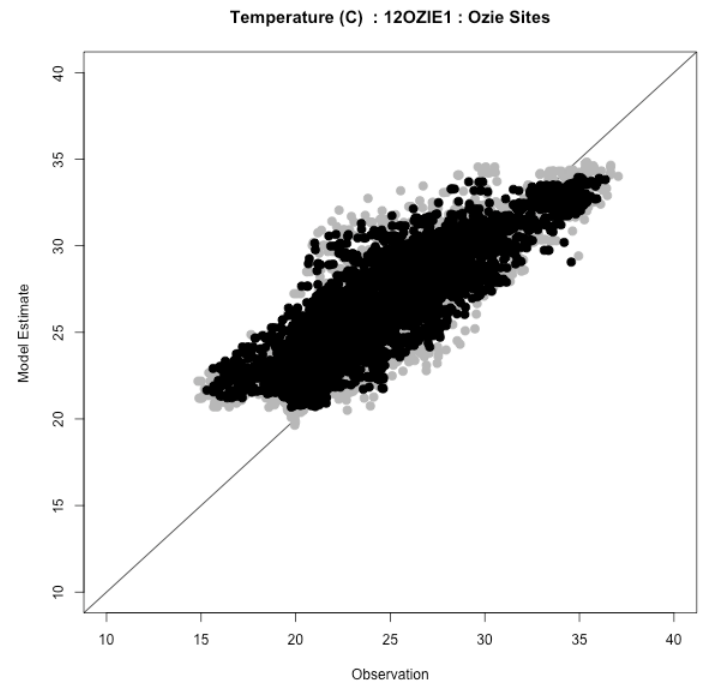
Bias by hour of the day



Temperature at OZIE Sites

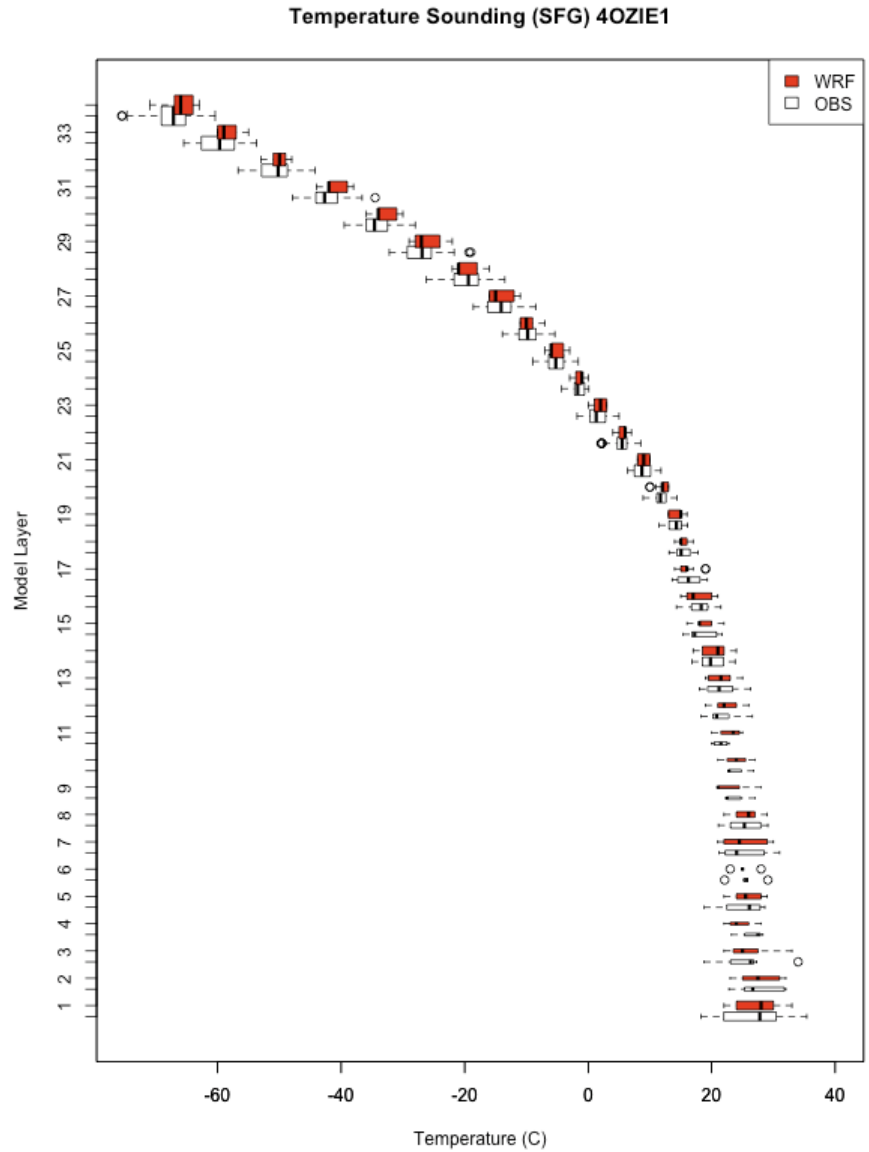
- Temperature and PAR drive biogenic model estimates
- General warm bias over all hours & days
- Underestimate the warmest temperatures





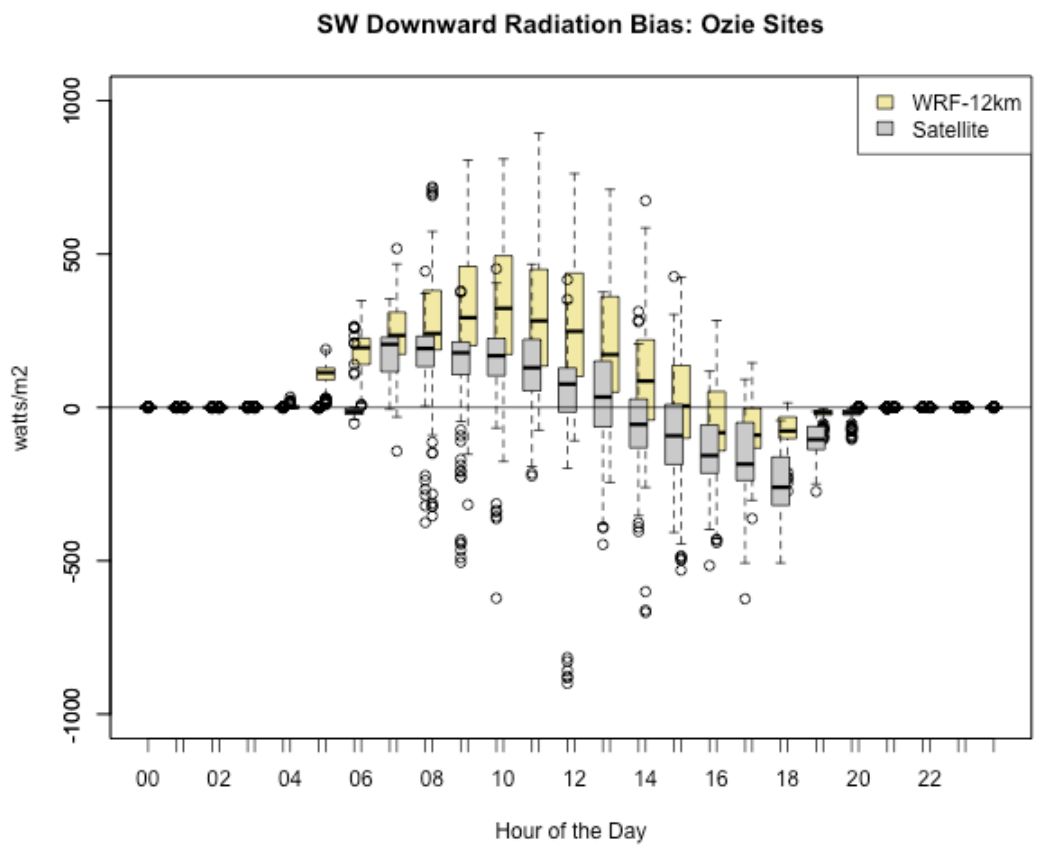
Vertical Temperature

- FSL RAOB soundings for July 1998
- 0Z and 12Z
- Springfield, MO
- Model estimates of temperature compare well to observations
- Warm bias in upper troposphere unlikely to have a noticeable impact on a one month simulation

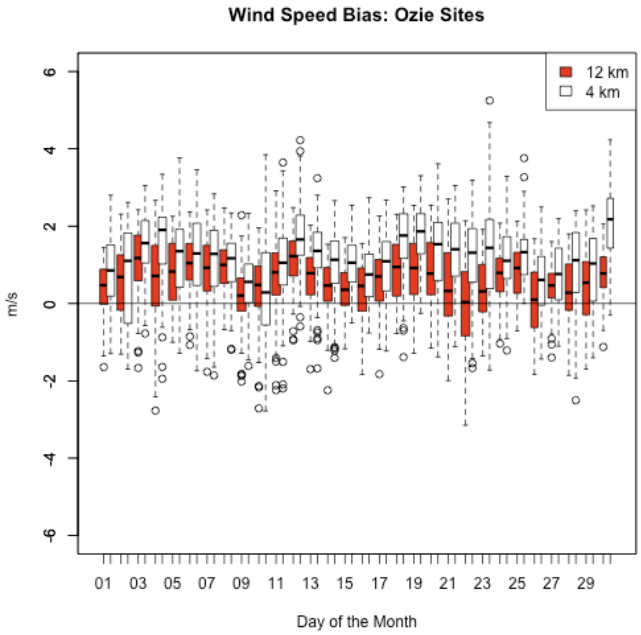


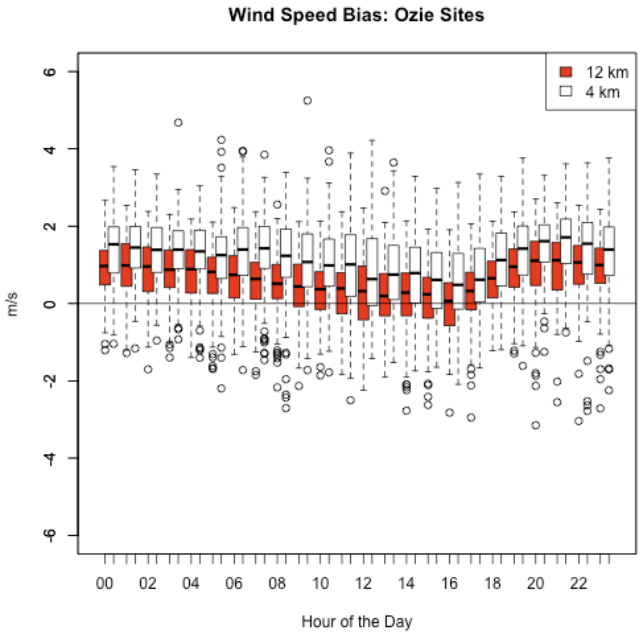
Solar Radiation at OZIE Sites

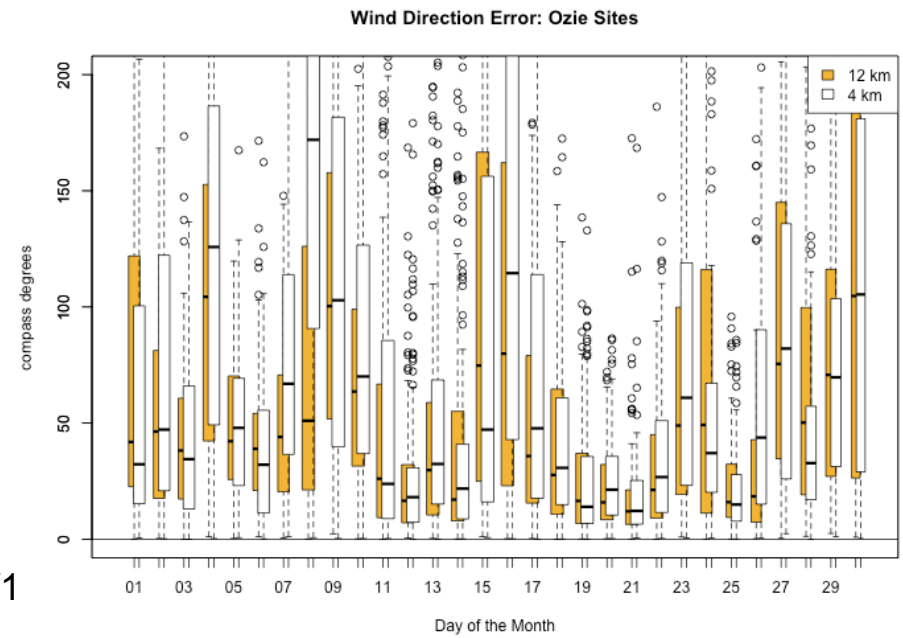
- Both methods tend to overestimate morning and early afternoon PAR and underestimate late evening PAR
- Satellite estimates compare better to ground observations

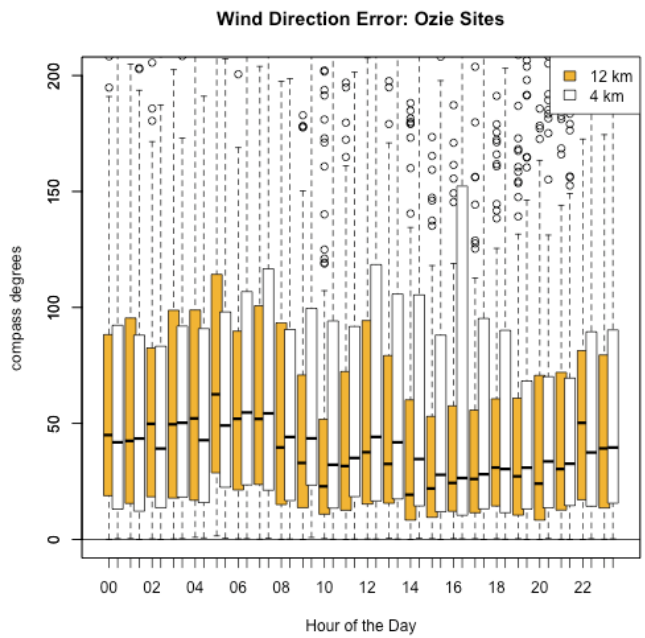


Wind Field

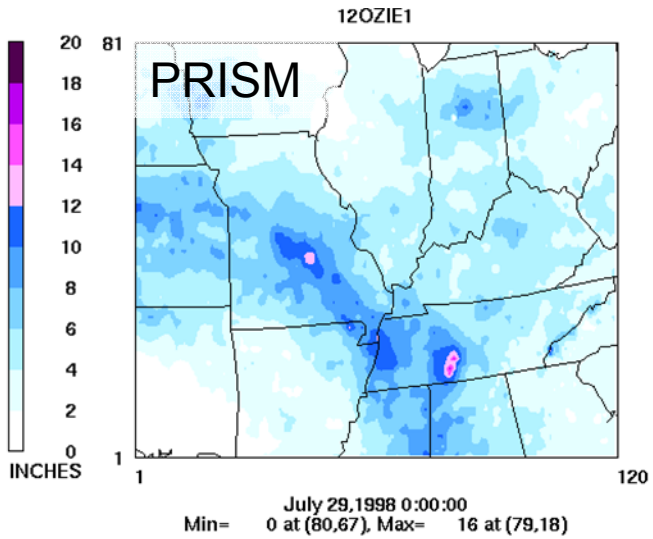

Wind Speed Bias: Ozie Sites
12 km
4 km
m/s
Day of the Month

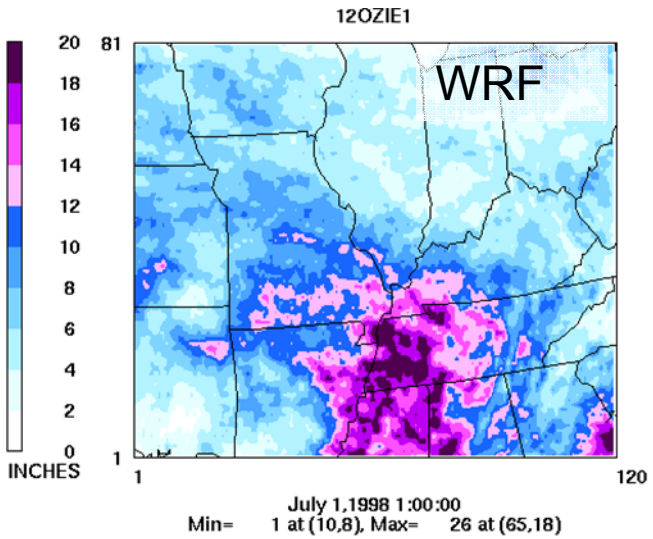

Wind Speed Bias: Ozie Sites
12 km
4 km
m/s
Hour of the Day

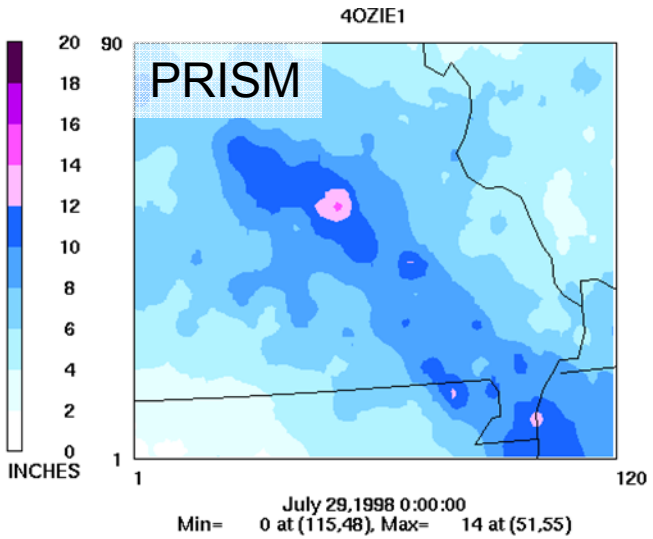

Wind Direction Error: Ozie Sites
12 km
4 km
compass degrees
Day of the Month

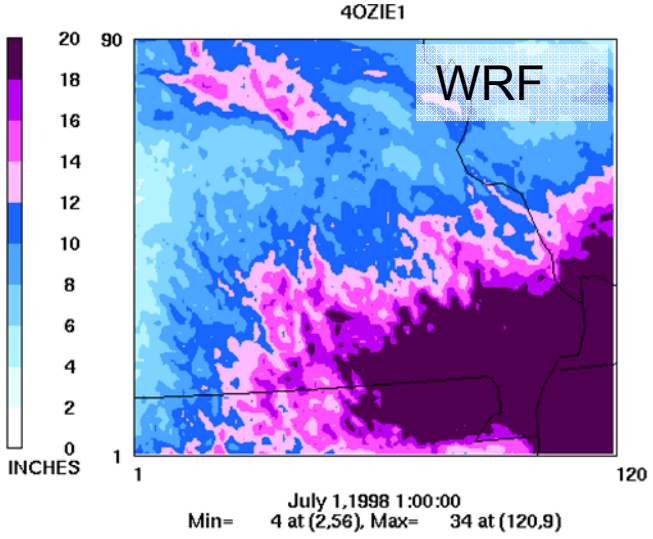

Wind Direction Error: Ozie Sites
12 km
4 km
compass degrees
Hour of the Day

Monthly Total Rainfall









Biogenic Modeling

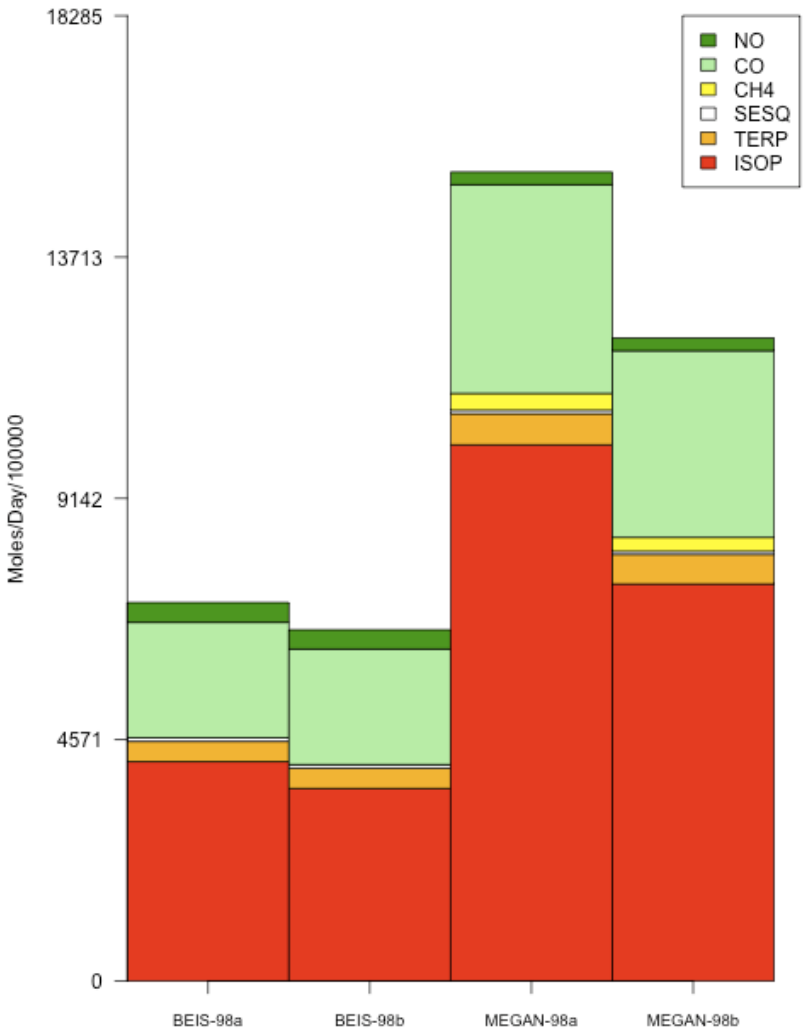
- BEIS v3.14 with BELD3 landuse
- MEGAN v2.04 with version 2.1 gridded emission factors obtained Oct 23, 2007
  - WRF 2 m temperature and WRF shortwave downward radiation (98a)
  - WRF 2 m temperature and satellite estimated photosynthetically activated radiation (98b)

- Photosynthetically activated radiation (PAR) is the visible light fraction of shortwave downward radiation

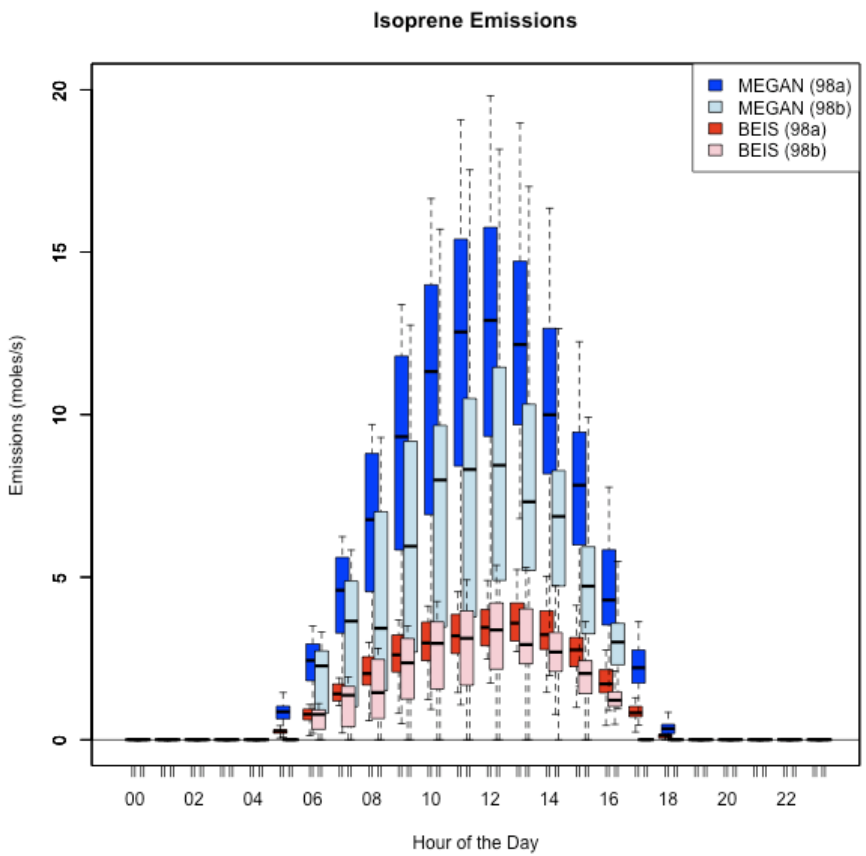
- Satellite photosynthetically activated radiation estimates taken from GEWEX Continental Scale International Project (GCIP) and GEWEX Americas Prediction Project (GAPP) Surface Radiation Budget (SRB) Data [http://www.atmos.umd.edu/~srb/gcip/cgi-bin/historic.cgi]
- Satellite PAR resolution 0.5 x 0.5 degrees and covers the continental United States
- Missing hours and days replaced by hourly monthly average satellite estimated PAR

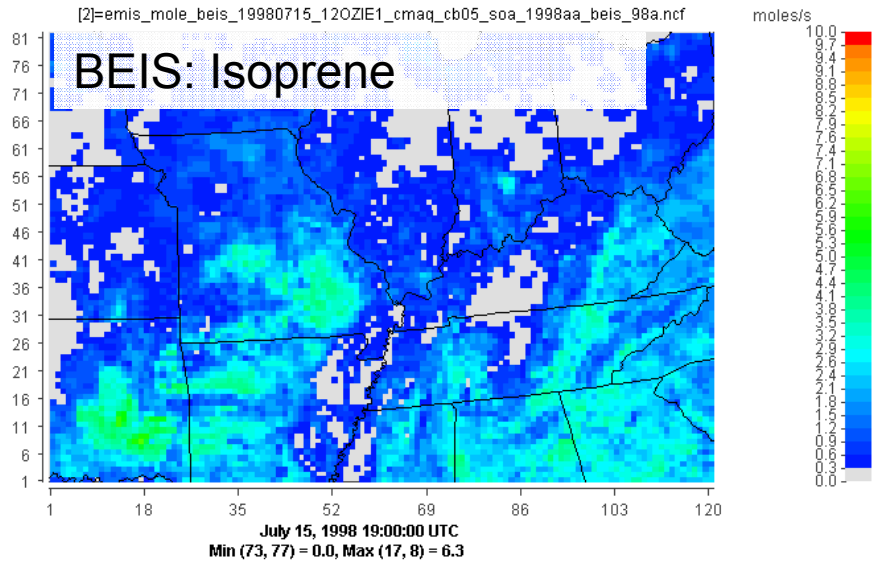
Biogenic Emissions

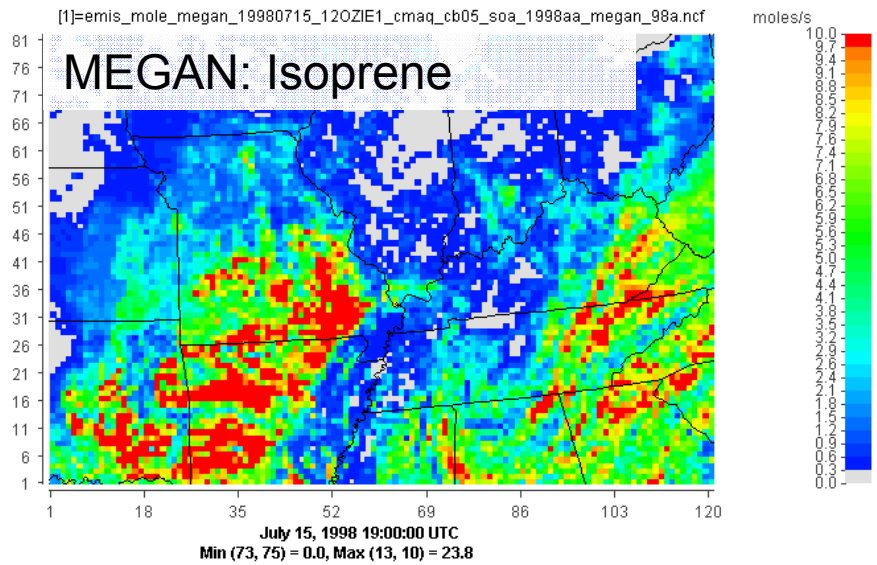
- Monthly domain (12OZIE1) total emissions
- MEGAN has substantially higher isoprene emissions and slightly higher terpene emissions
- Sesquiterpene emissions similar
- MEGAN has higher CO and methane; less NO



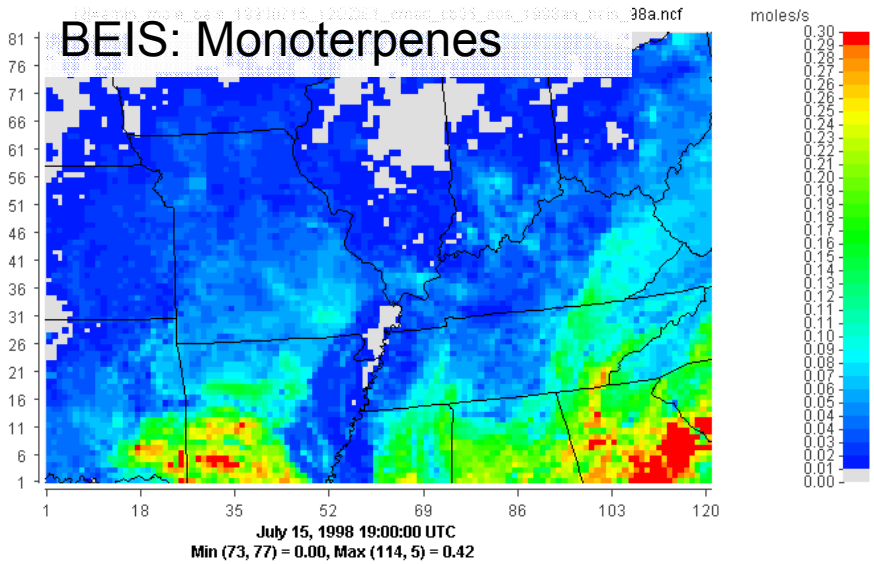
Isoprene Emissions

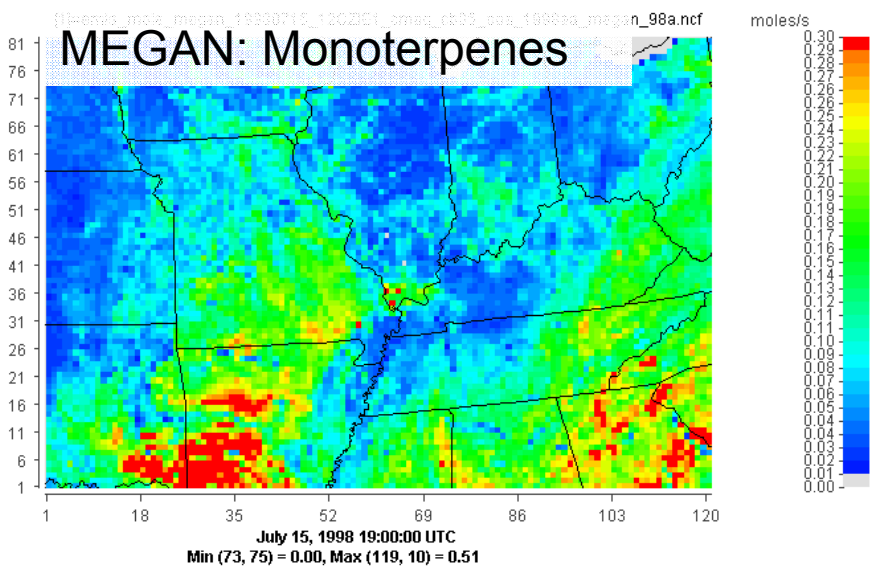


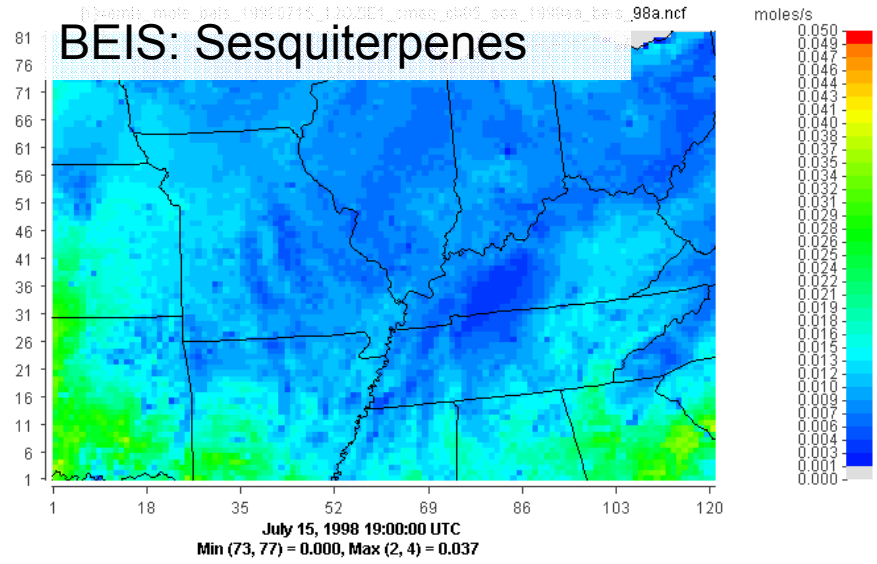


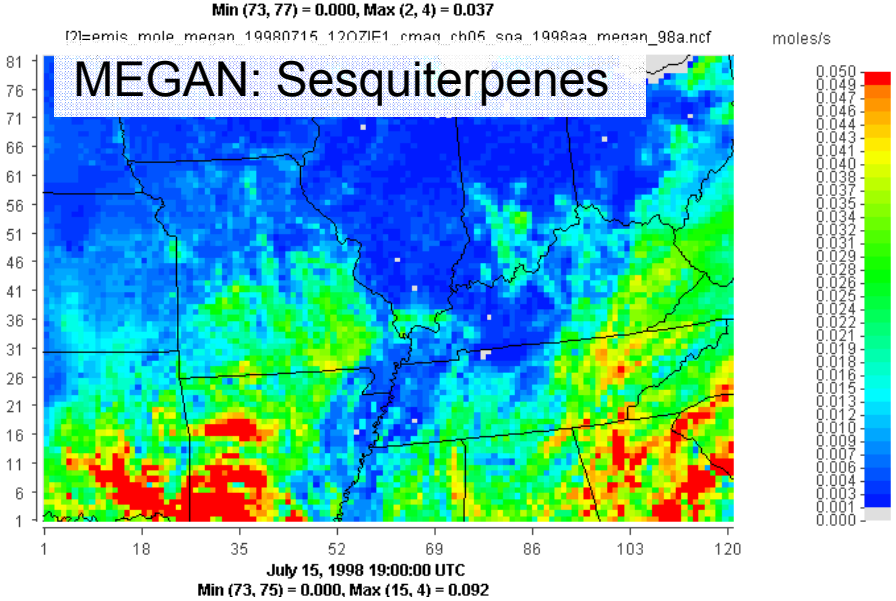


Monoterpenes & Sesquiterpenes

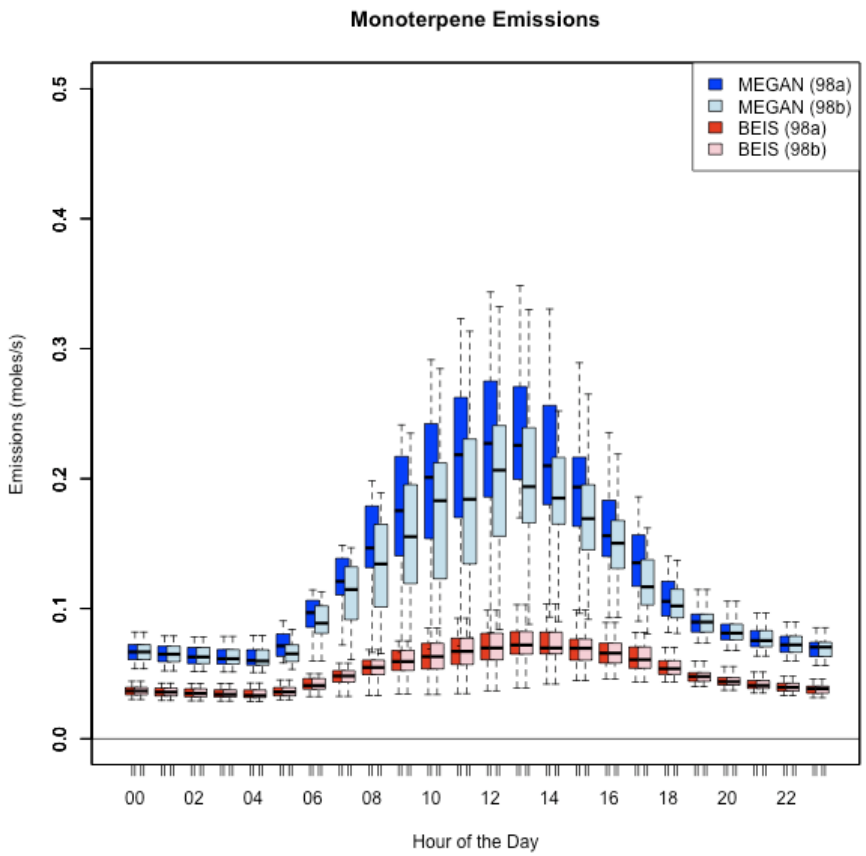


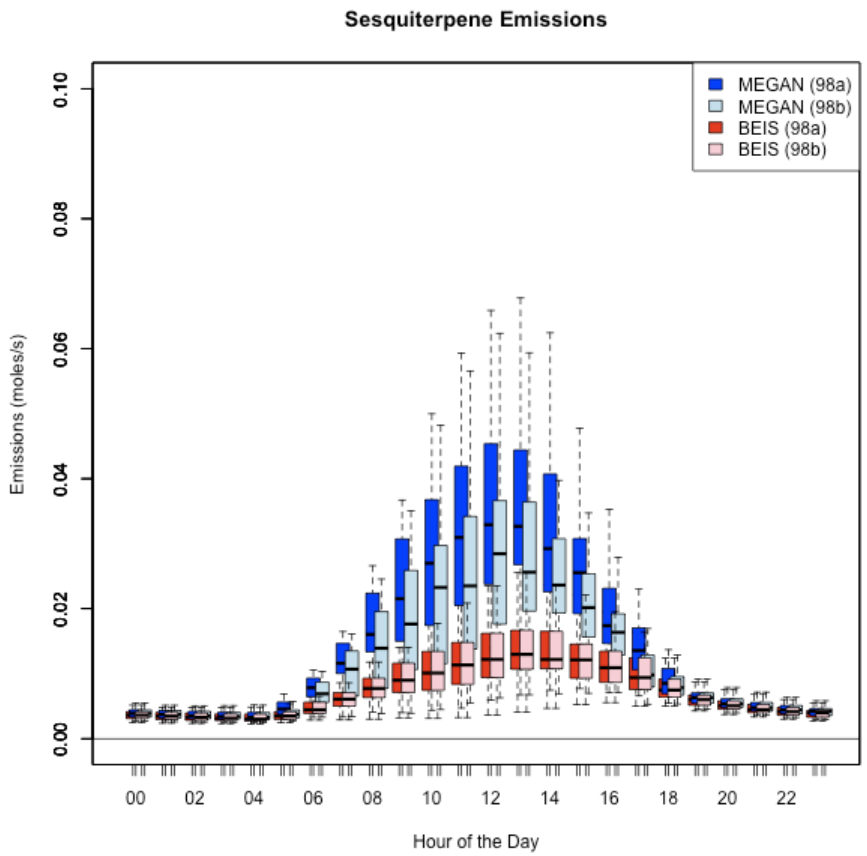






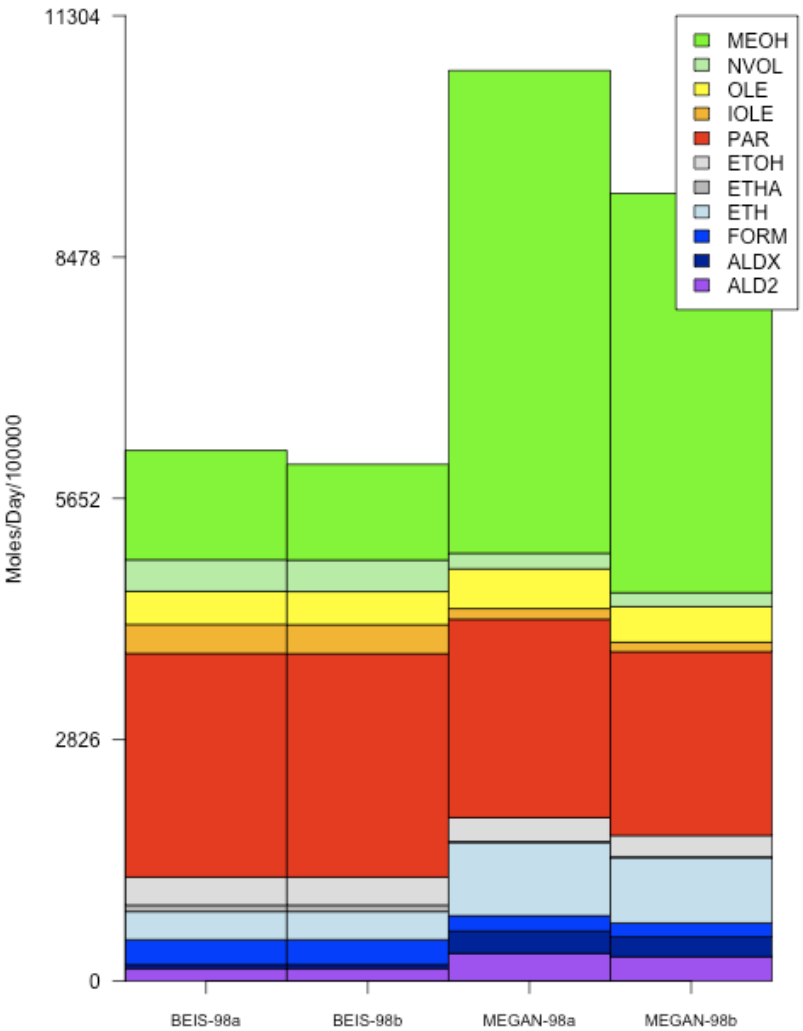
Monoterpenes & Sesquiterpenes



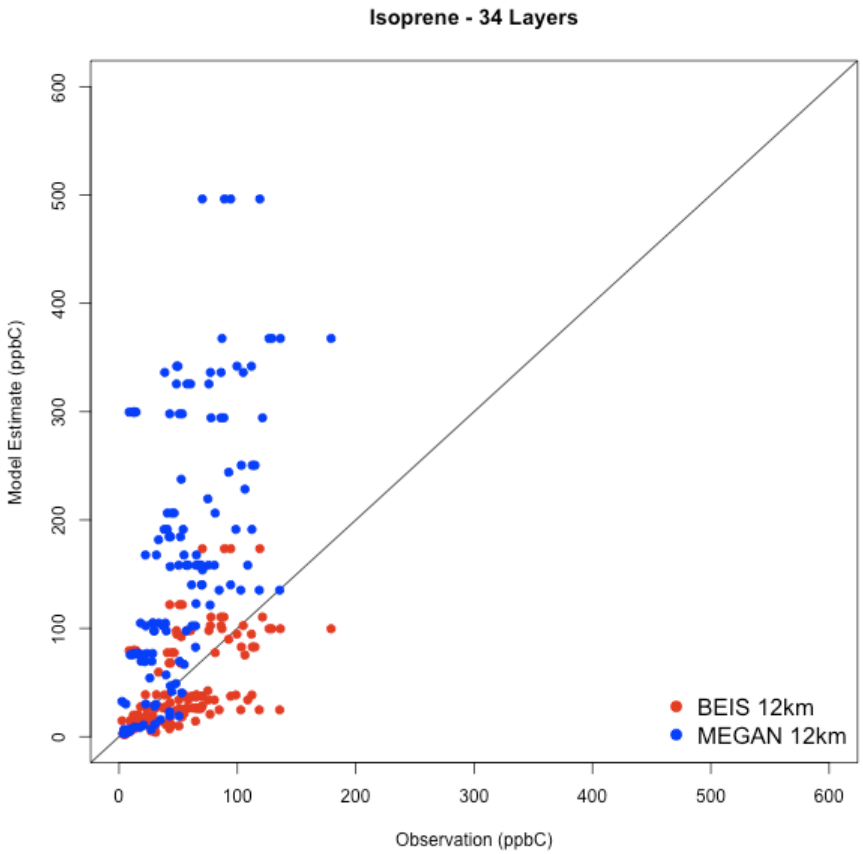


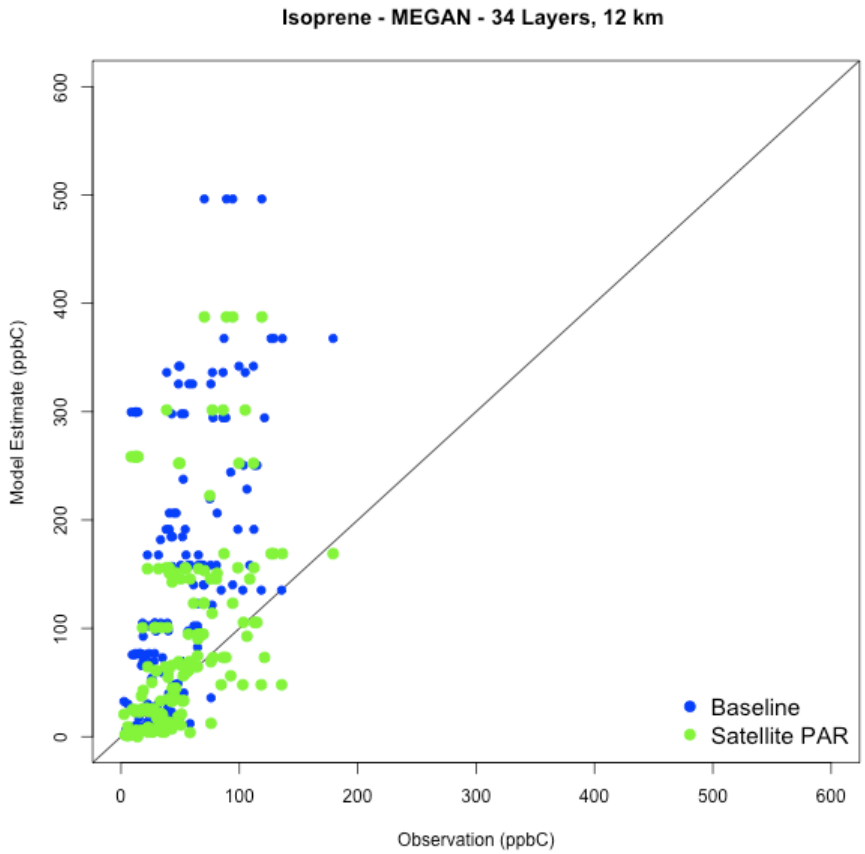
Biogenic Emissions

- MEGAN has more aldehyde and methanol emissions
- BEIS has more paraffin and olefin emissions
- Excluding methanol, OVOC totals similar but reactivity potential is different

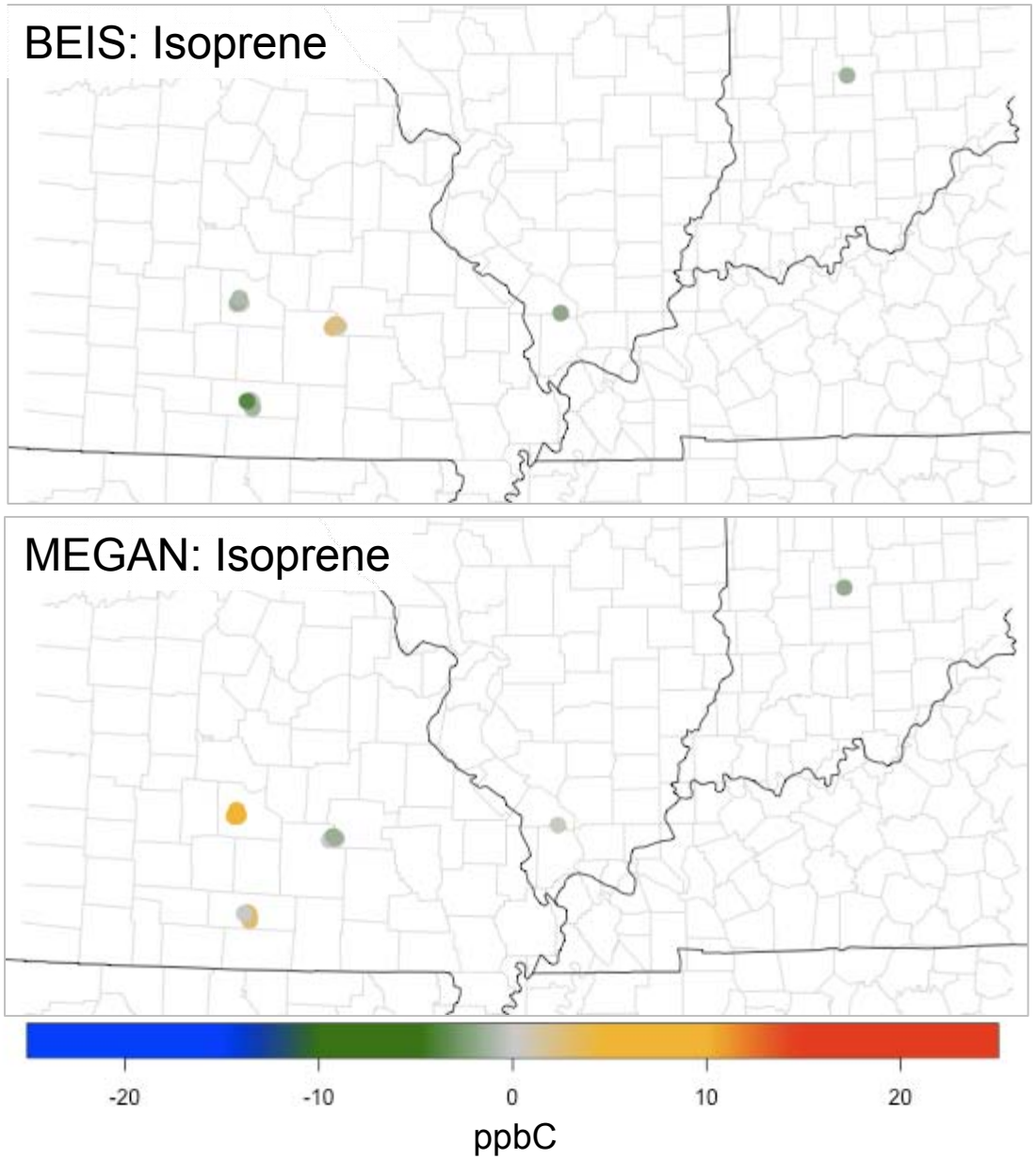


Isoprene Performance

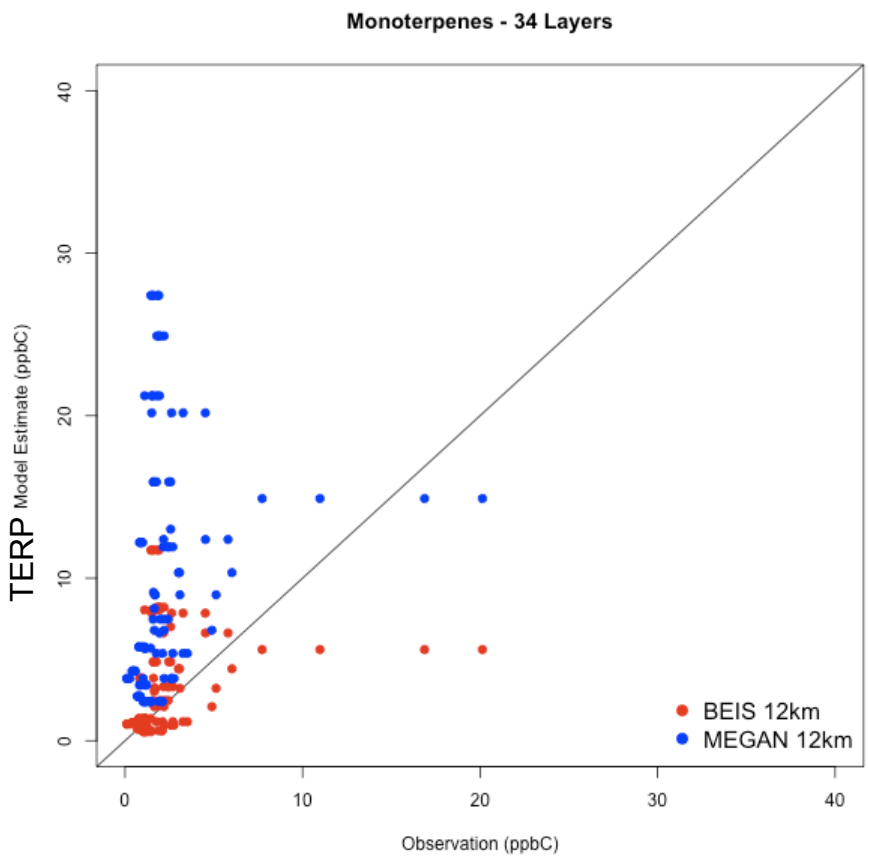




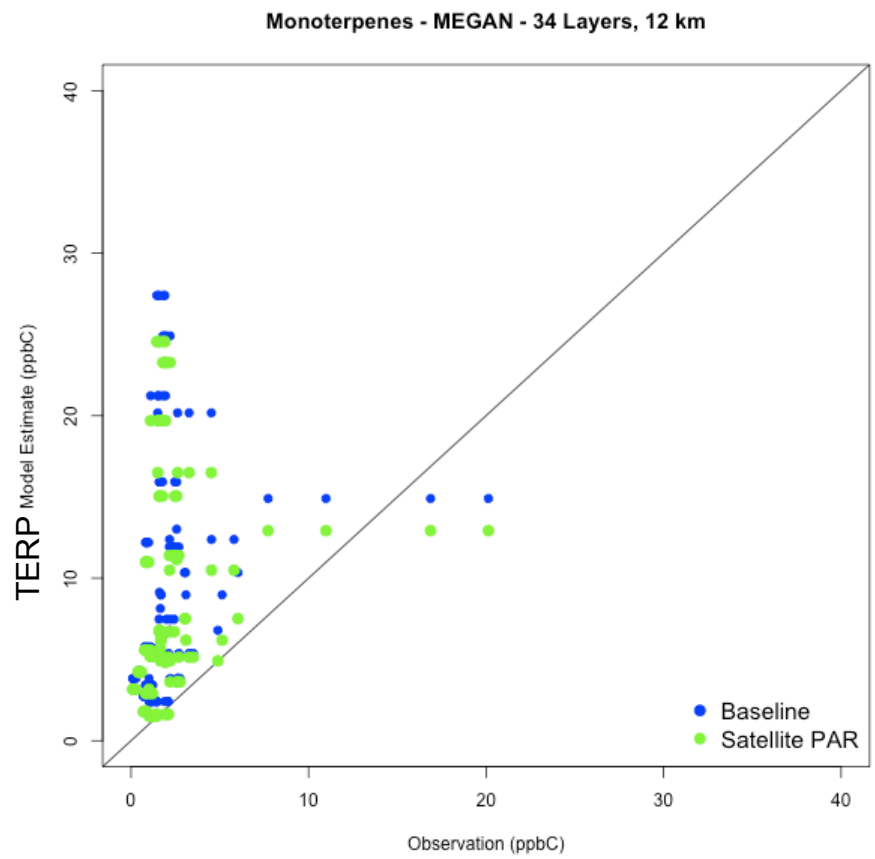
Isoprene Bias: July Episode



Monoterpene* Performance



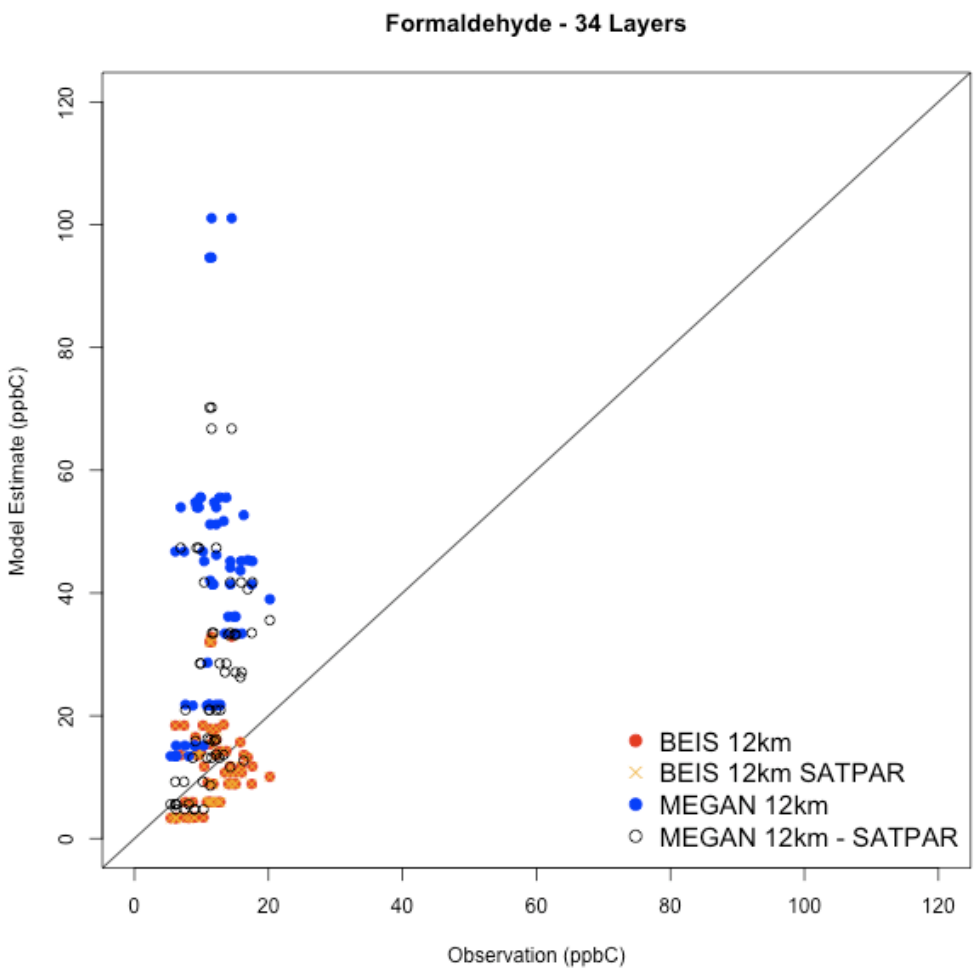
α-pinene + β-pinene



α-pinene + β-pinene

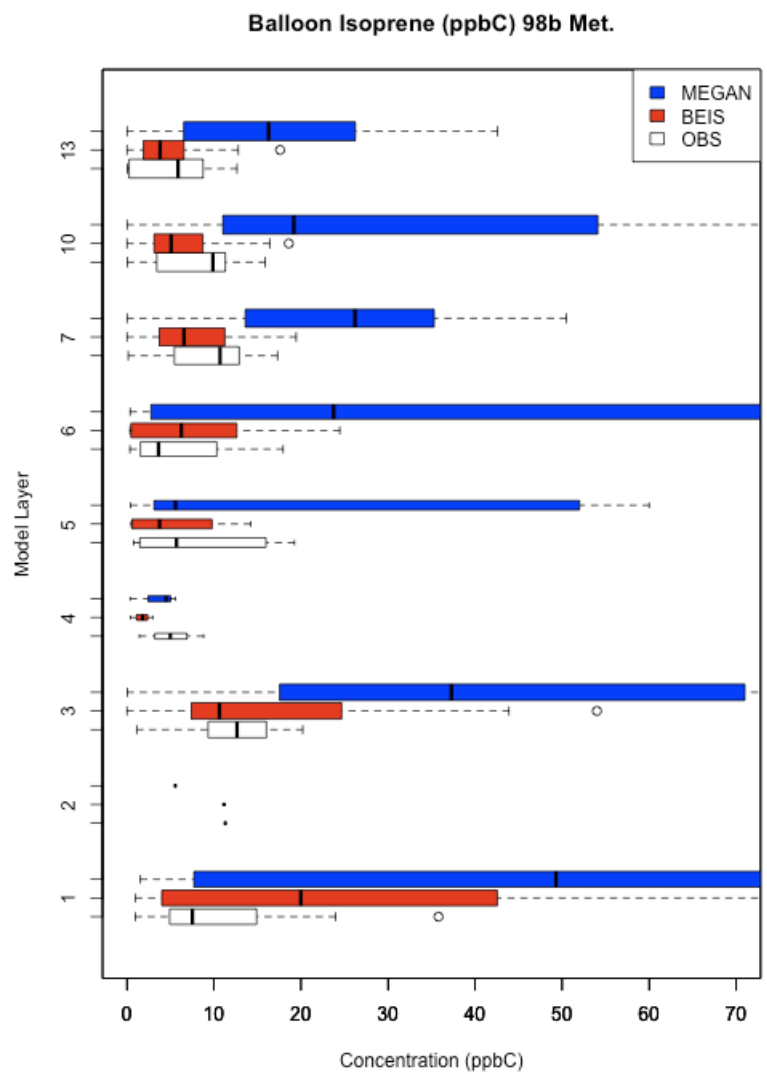
α-pinene + β-pinene are approx. 50 to 70% of total monoterpenes
(Sakulyanontvittaya et al, 2008)

Surface Formaldehyde Performance



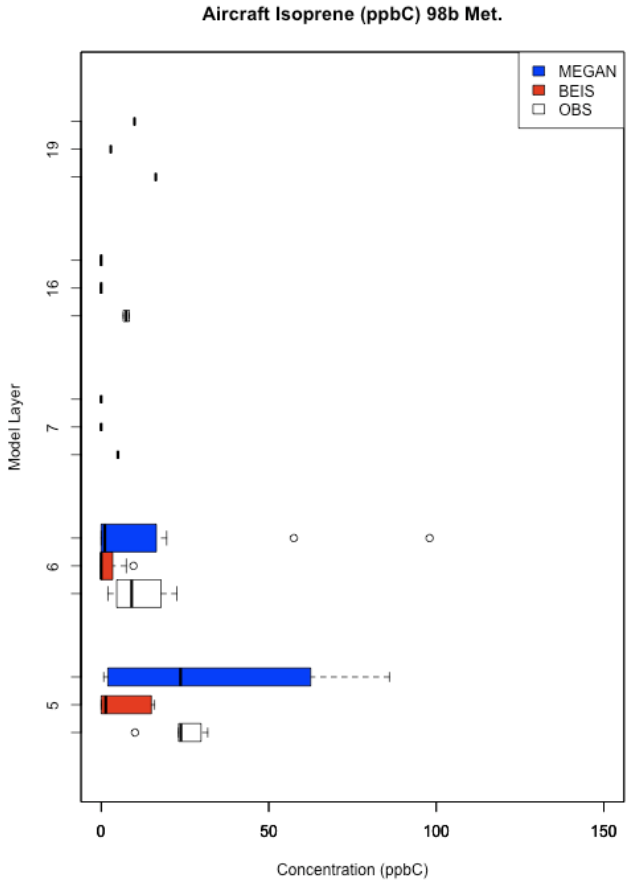
Balloon Measurements: Isoprene

- Model estimates compared to vertical balloon and aircraft measurements
- 98b meteorology (satellite PAR)
- Balloon: isoprene (right)

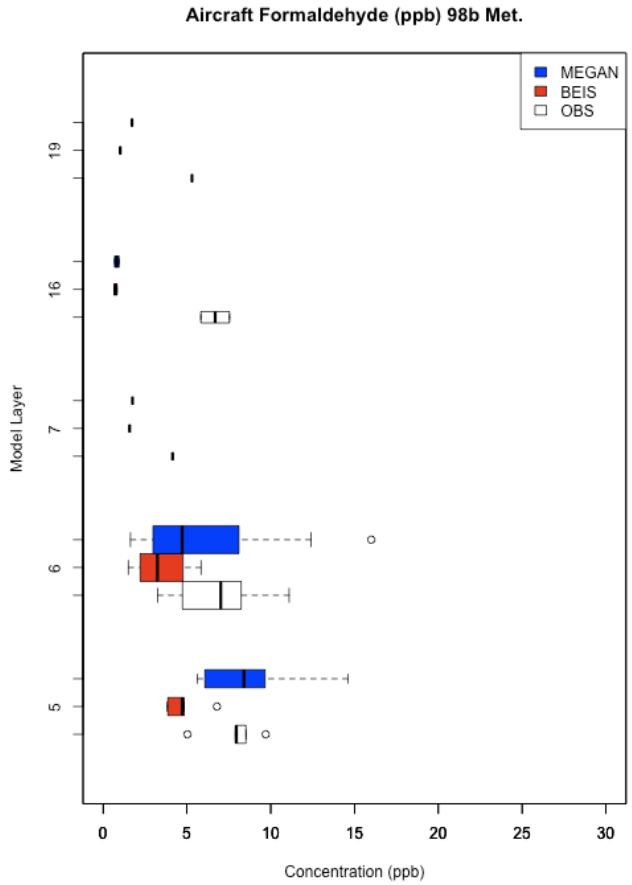


Aircraft Measurements

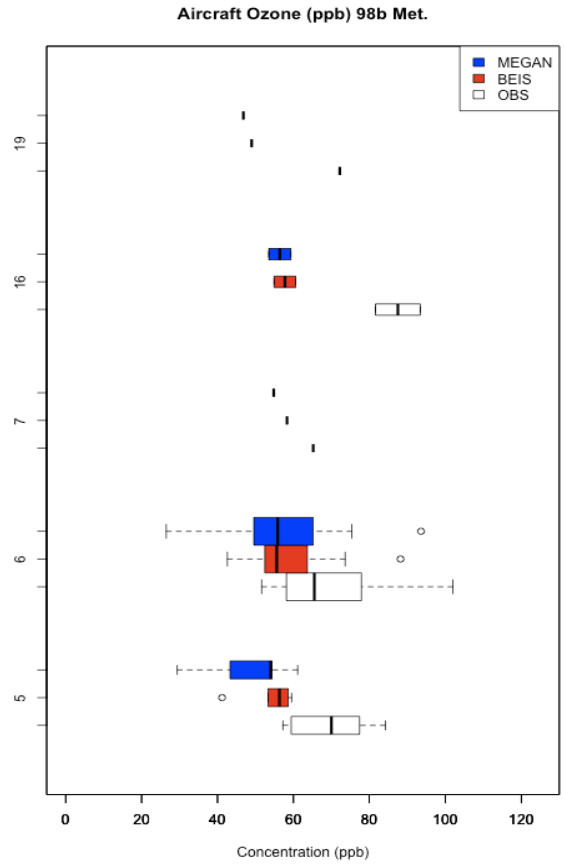
Isoprene



Formaldehyde

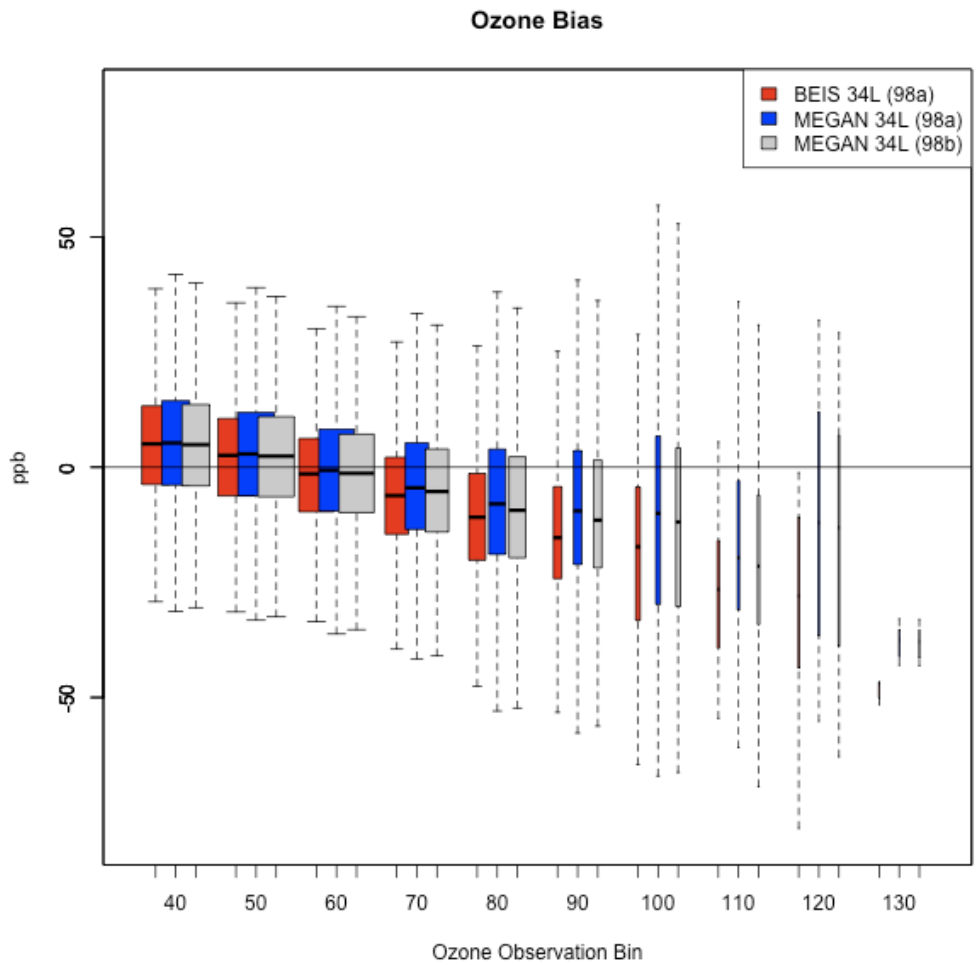


Ozone



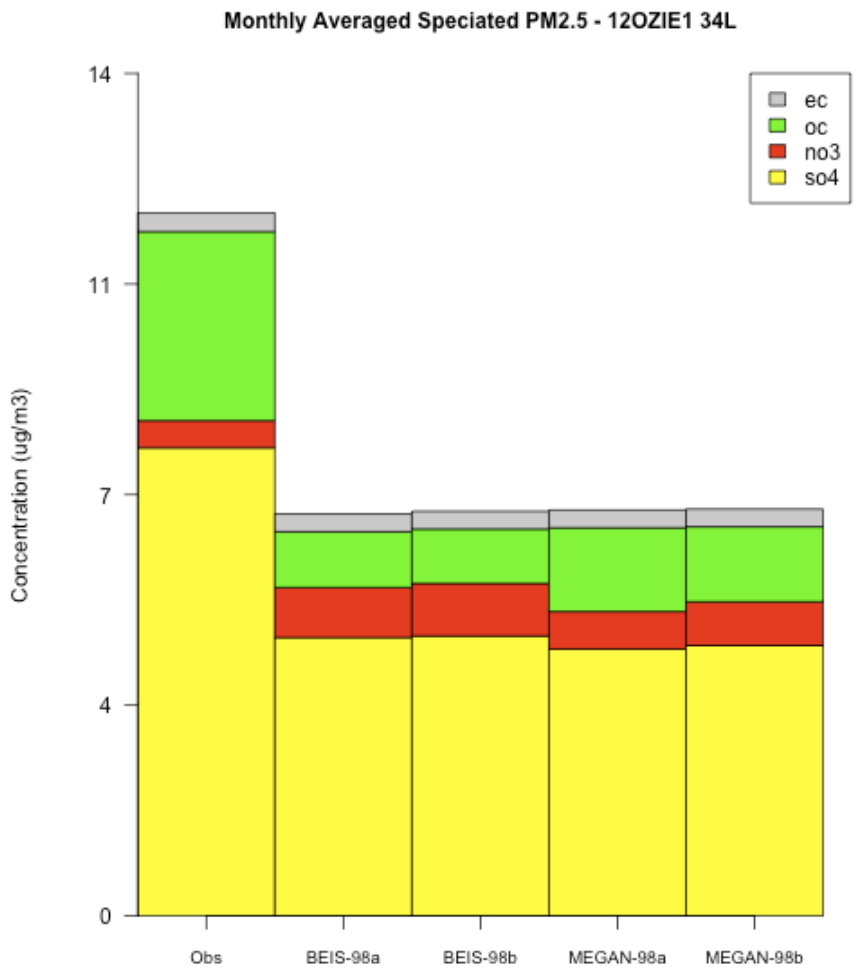
Model Performance: Ozone

- MEGAN tends to predict slightly higher regional ozone
- Satellite PAR MEGAN estimates result in slightly less ozone than using WRF PAR MEGAN

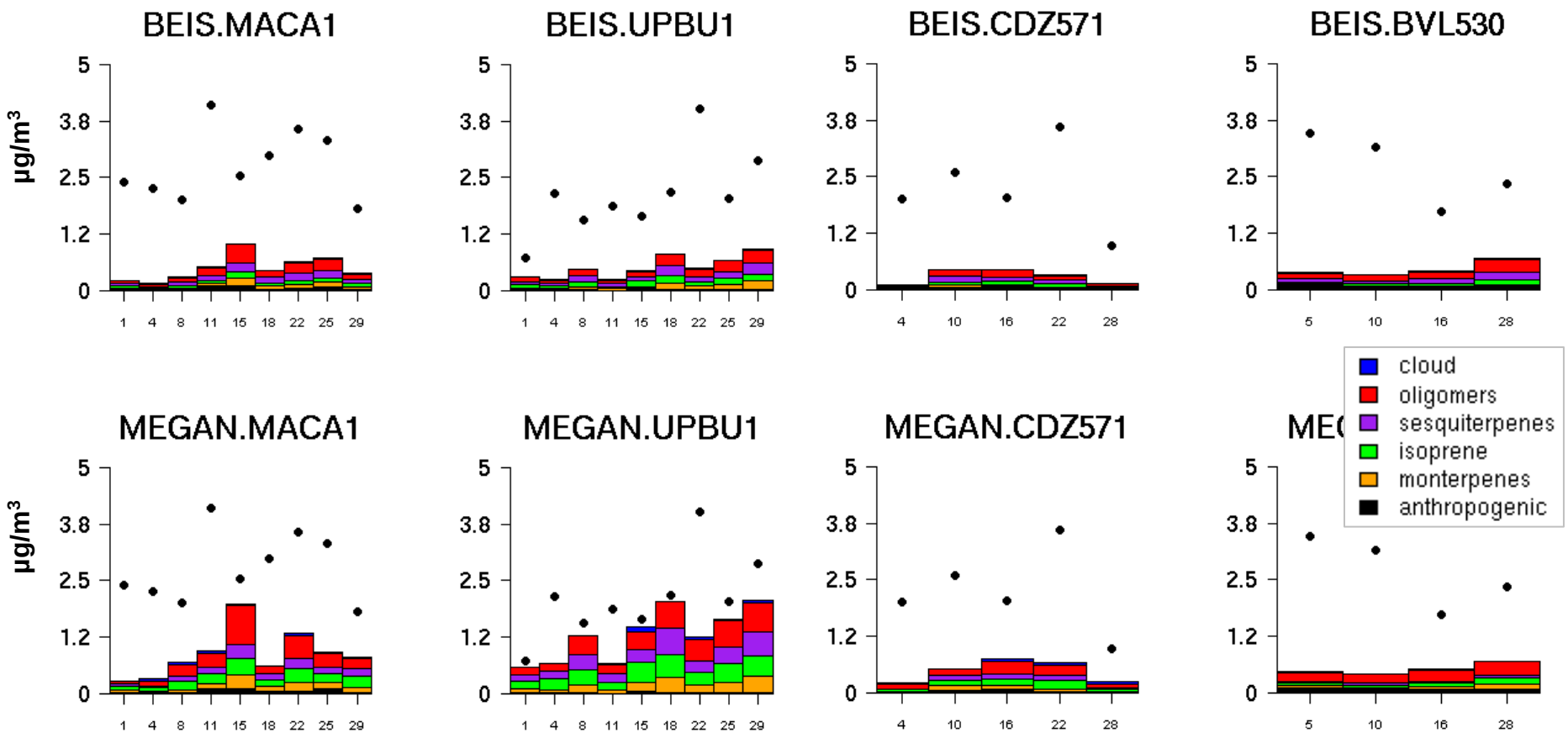


Model Performance: speciated PM2.5

- Similar PM2.5 performance using BEIS and MEGAN at rural speciated monitors
- Sulfate performance related to SO2 controls between 1998 and 2001
- More OC using MEGAN emissions



Daily CMAQ PM2.5 SOC Estimates

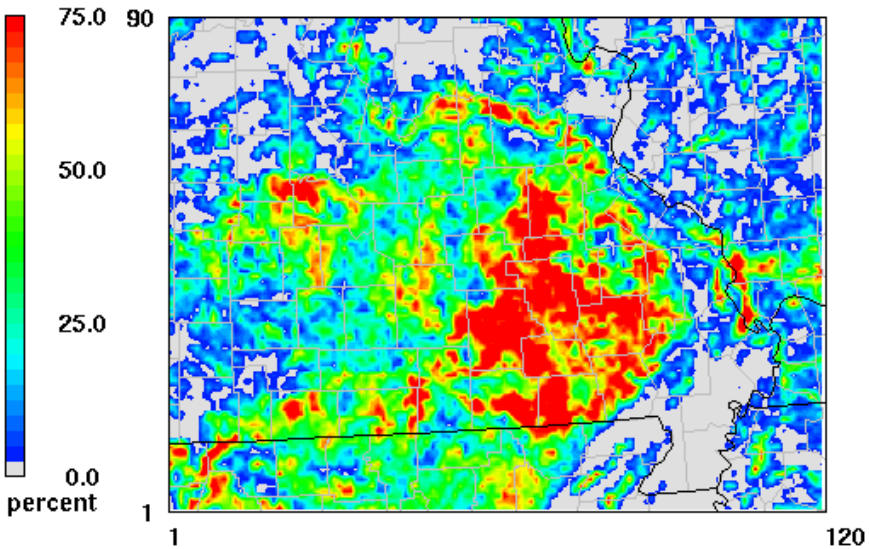


*semi-emipirical SOC estimates shown as dots and based on method described by Yu et al 2007

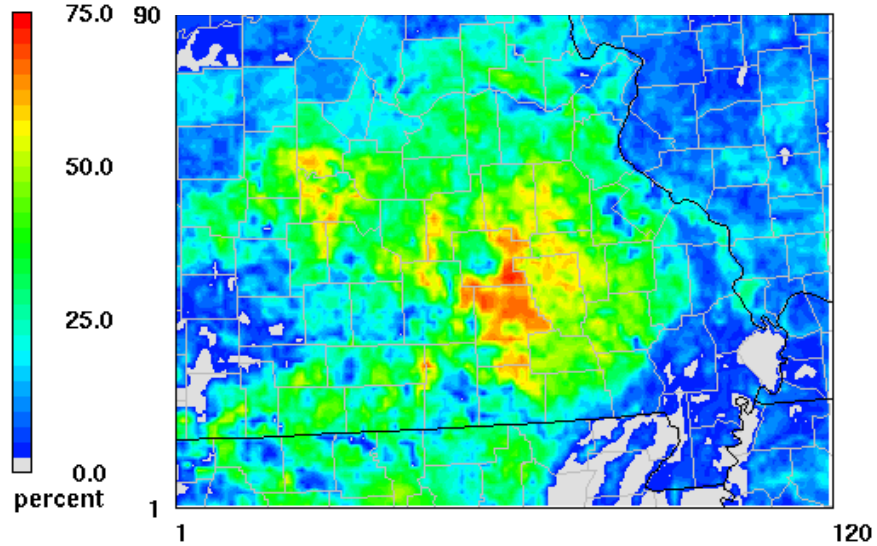
Landuse Information

- MEGAN uses MODIS landuse and plant species information to make gridded emission factors
- BEIS uses BELD3, a combination of plant species information and USGS landuse
- Different isoprene emission factors for high emitting species (top right) and USGS deciduous tree category (bottom right) in BEIS
- Difficult to differentiate plant coverage and emissions with MEGAN's gridded emission factor product (one plant functional type shown below)

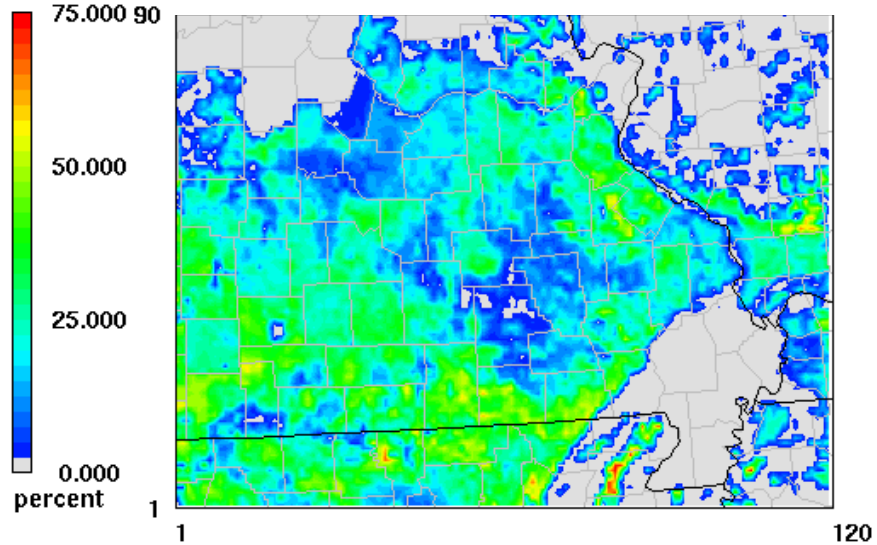
MEGAN: Broadleaf Trees



BELD3: Oak+Others

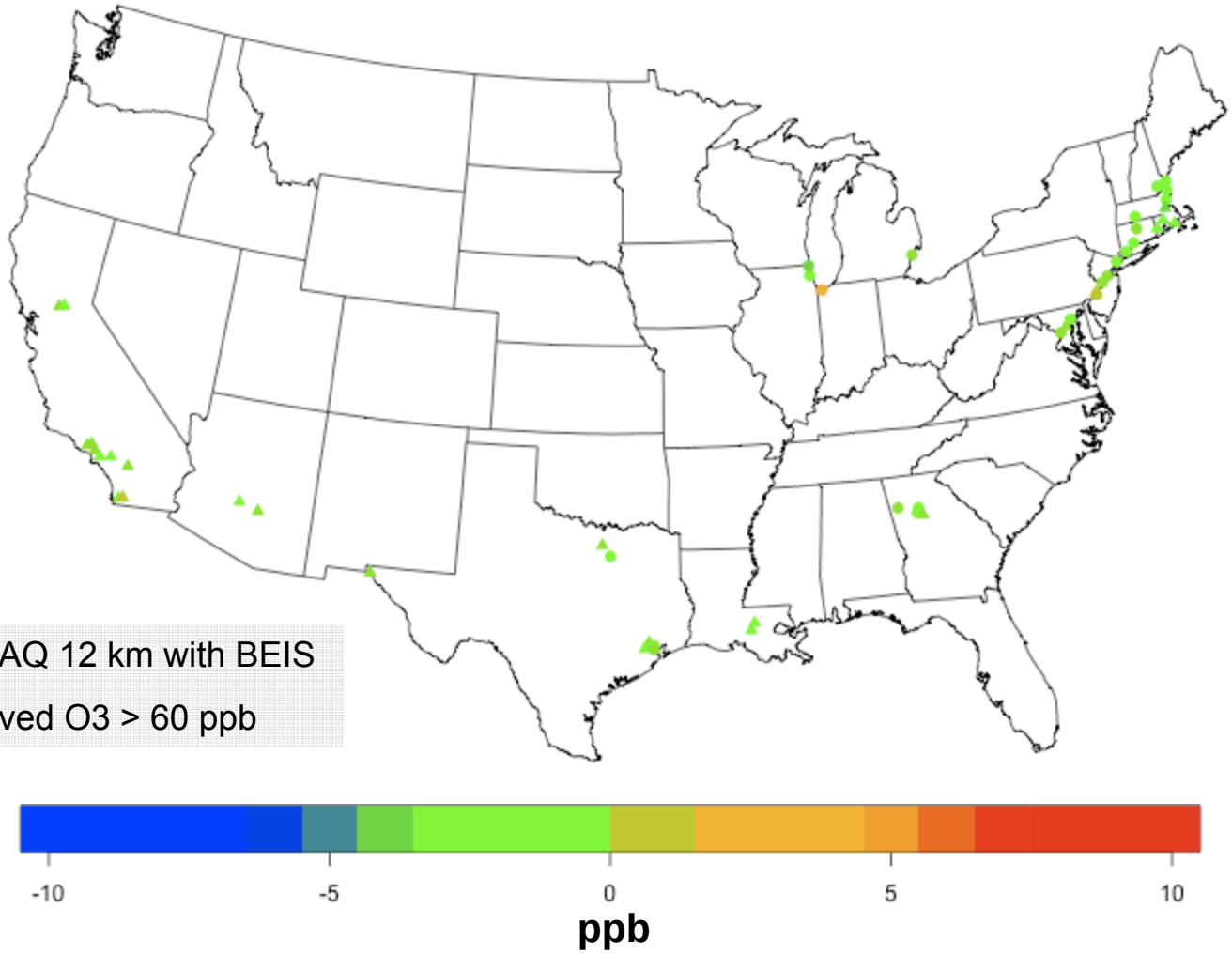


BELD3: USGS Deciduous Trees



**Others = Sycamore+Sweetgum+Willow+Populus*

Isoprene Bias: PAMS sites



- Annual 2002 CMAQ 12 km with BEIS
- Bias where observed O3 > 60 ppb

Conclusions

- CMAQ similarly estimates regional ozone and PM2.5 mass when using BEIS and MEGAN
  - Accept either for SIP modeling based on current state of chemical mechanisms
- SOA predictions are much higher with MEGAN than with BEIS, but CMAQ still under-predicts rural OC
- CMAQ/MEGAN tends to estimate higher concentrations of isoprene and monoterpenes than CMAQ/BEIS
- Similar regional O_3 estimates may be due to BEIS having higher emissions of reactive OVOC
- Differences in emissions estimates may diverge further in the future if differences are made to the gas phase chemical mechanisms.