Next steps for improving Texas biogenic VOC and NO emission estimates

AQRP 18-005

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Next steps for improving Texas biogenic VOC and NO emission estimates

AQRP 18-005

- **Texas BVOC emission factor measurements**
- **MEGAN model improvements (MEGAN3.1)**
- **Sensitivity study**
- **Key Points**
- **Recommendations for future work**

Task 1. Texas BVOC emission factor measurements

Deliverables

Databases

- Isoprene emission factor database. Ancillary data includes leaf thickness, slope and aspect, chlorophyll, LAI depth, canopy %, daily solar radiation, photosynthesis, stomatal conductance, photosynthetic efficiency.
- Speciated terpenoid emission factor database. Ancillary data includes stress compounds, photosynthesis, stomatal conductance, growth environment.
- Crop BVOC emission database.

Isoprene emission factors

2 Licor 6400 gas exchange systems with on-site GCMS analysis on Rice campus in June 2019

Acknowledgment: Thanks to Rob Griffin (Rice), Jimmy Flynn, Yuxuan Wang, Yunsoo Choi (UH) and their teams

Texas 2019
Leaf-level isoprene emission factors (Canopy Average)

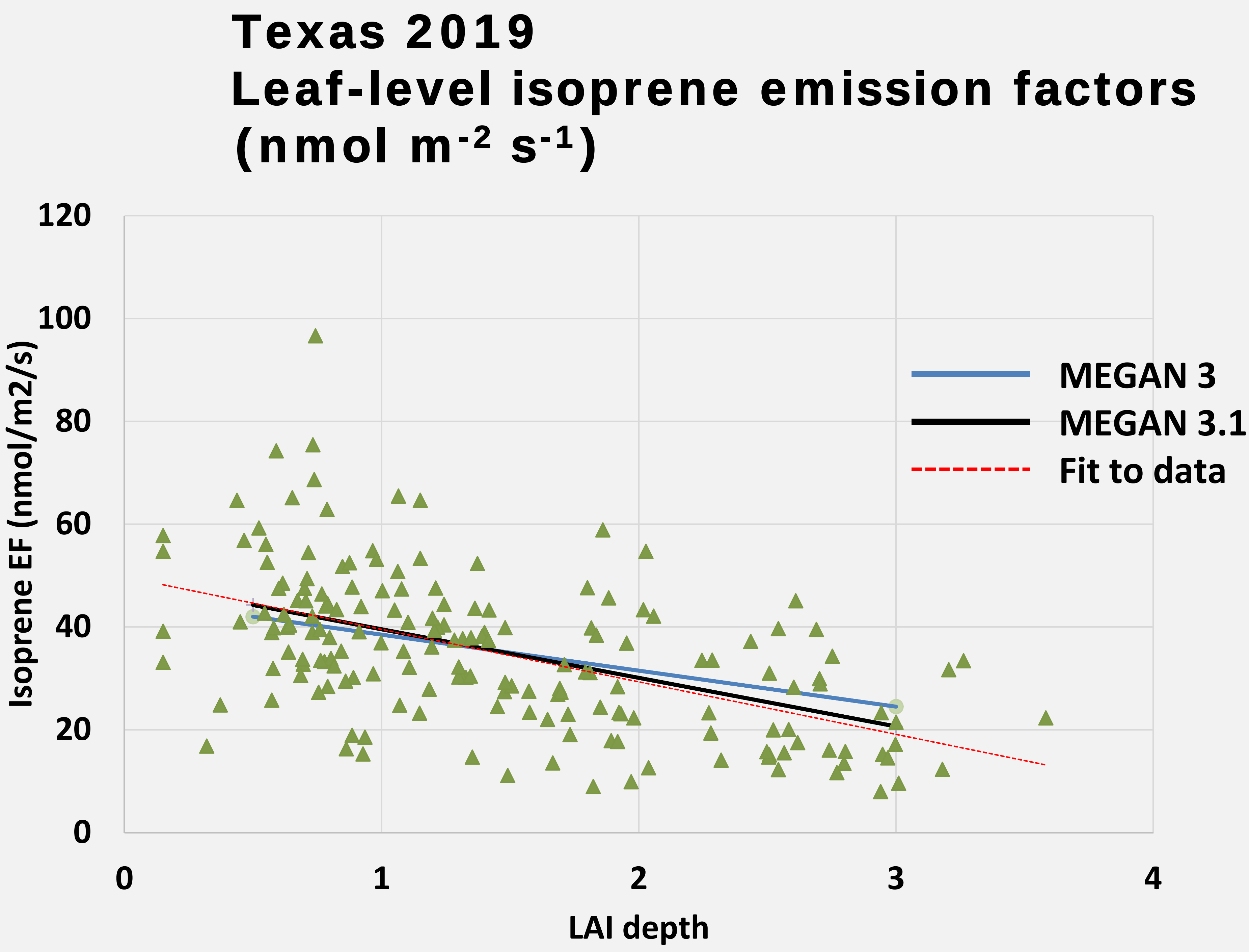
Species	nmol m^{-2} s^{-1}	µg g^{-1} h^{-1}
Post Oak	24±13 (n=18)	53
Shumard Oak	27±15 (n=8)	89
Sweetgum	30±12 (n=8)	84
Southern Live Oak	33±13 (n=91)	55
Swamp Chestnut Oak	35±6 (n=10)	81
Water Oak	45±17 (n=43)	86
BEIS	24	79

Literature values of isoprene EF (nmol m^{-2} s^{-1})

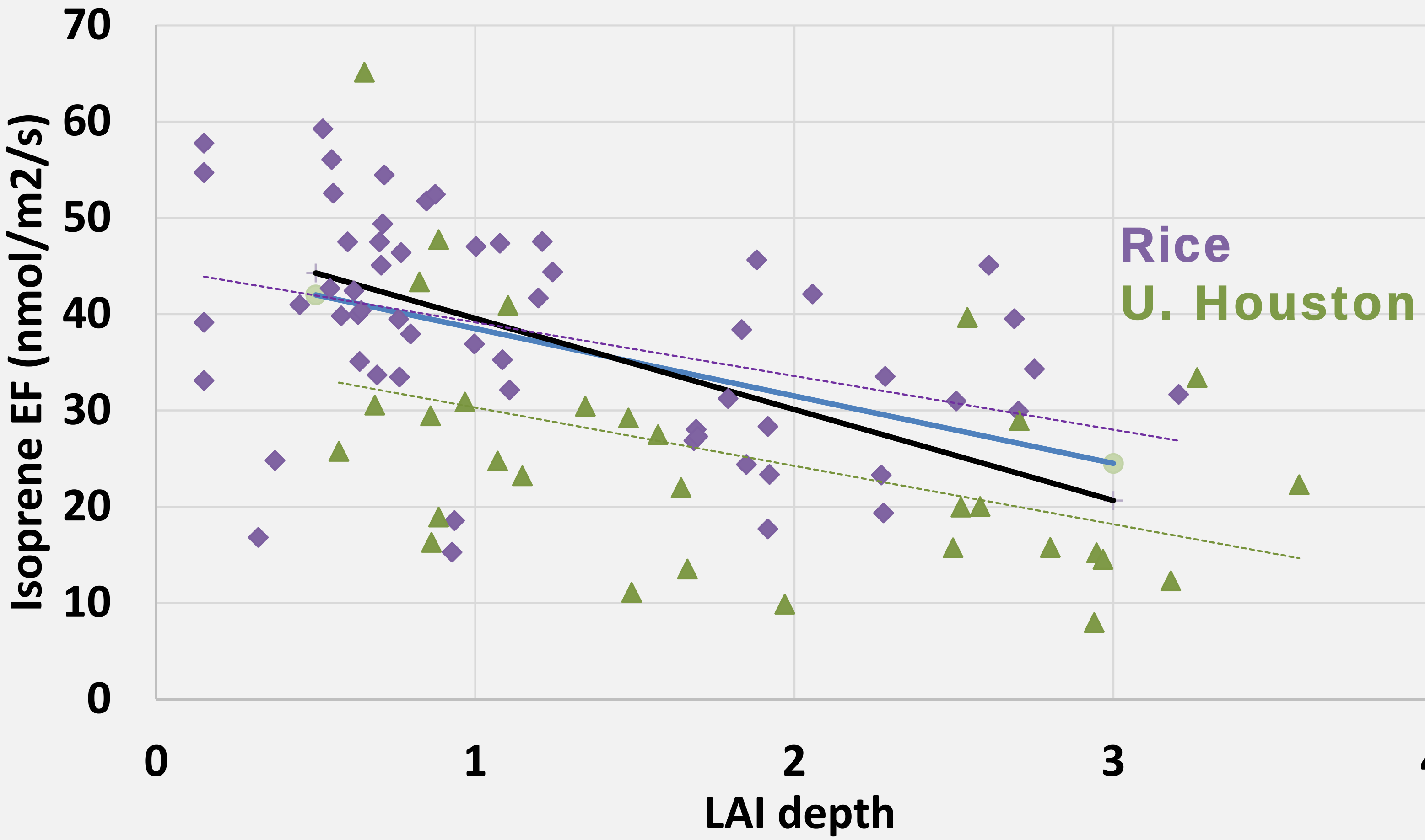
	Low quality (j=0)	High Quality (j=4)
Post Oak	21 to 39	29 to 50
Sweetgum	5 to 22	25 to 44
Southern Live Oak		40
Water Oak		46

Texas 2019
Leaf-level isoprene emission factors
(nmol m^{-2} s^{-1})

	All	Sun	Shade	LAI = 1.5
Post Oak	24	28	17	27
Shumard Oak	27	39	15	28
Sweetgum	30	35	23	28
S. Live Oak	33	38	20	37
Swamp Ch. Oak	35	35	---	30
Water Oak	45	48	25	43


Texas 2019
Leaf-level isoprene emission factors
(nmol m-2 s-1)
Isoprene EF (nmol/m2/s)
120
100
80
60
40
20
0
0
1
2
3
4
LAI depth
MEGAN 3
MEGAN 3.1
Fit to data

Texas 2019 isoprene emission factors



For the 3 species with measurements on both campuses: Isoprene EFs were 10 to 30% higher at Rice

Possible reasons:

- **LAI depth does not accurately represent light environment**
- **Weekly weather**
- **Location**
- **Genetics**

Speciated terpenoid emission factors

2 Custom inert gas exchange systems with off-site GCTOFMS analysis near Austin in June 2019

>50 terpenoids emitted by 20 tree species

Conifers (6)
Ash Juniper
Redcedar
Baldcypress
Shortleaf pine
Longleaf pine
Loblolly pine

Urban Broadleaf (5)
Camphor
Crepe myrtle
Magnolia
Chinese Tallow
Pecan

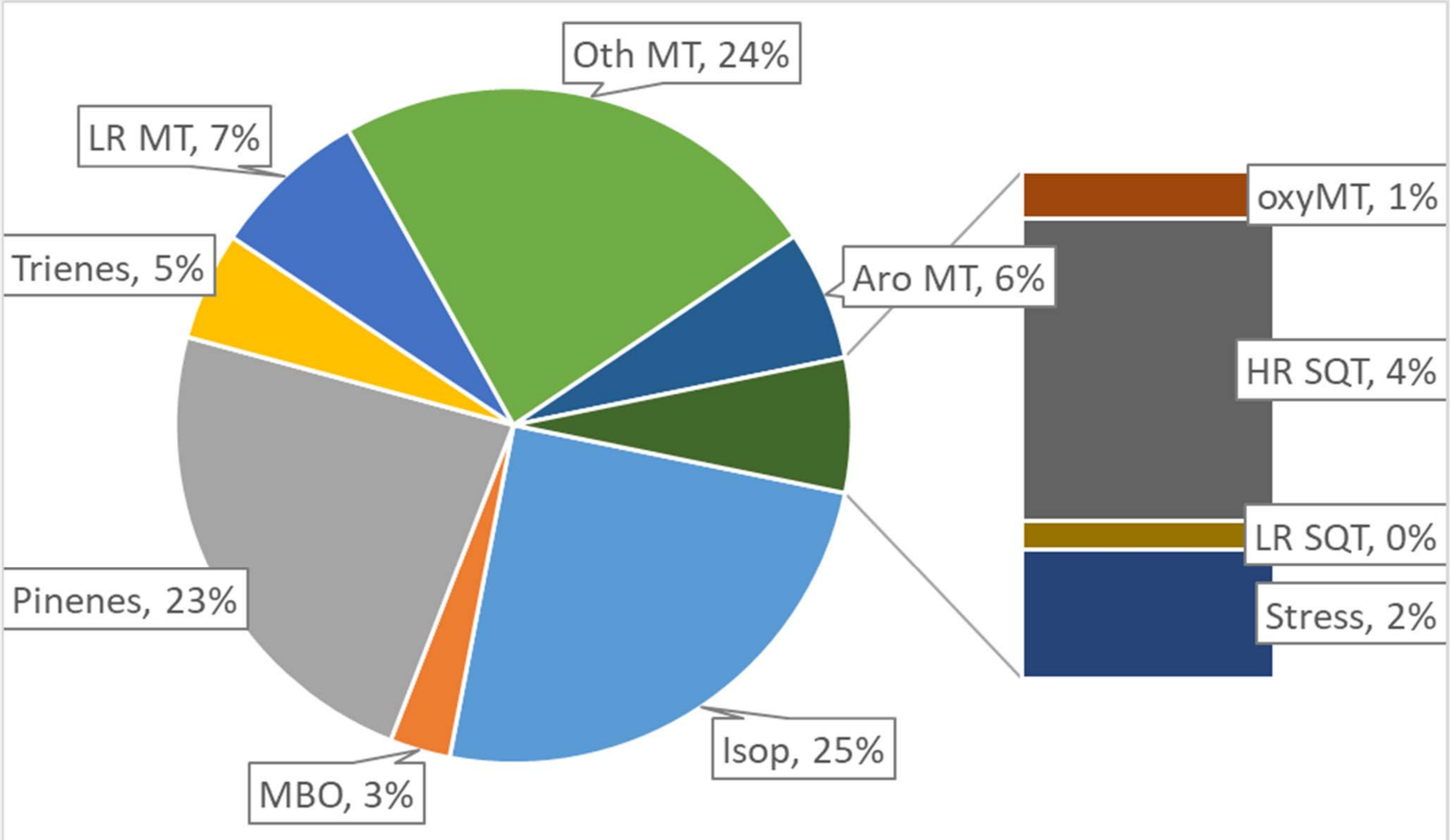
Rural Broadleaf (9)
Hackberry
Sweetgum
Honey mesquite
Plateau live oak
Southern live oak
Water oak
Willow oak
Post oak
Cedar elm

>50 terpenoids emitted by 20 tree species

<u>**Distributed across 11 of the 20 MEGAN3 compound categories**</u>

Class 1 (1): Isoprene
Class 2 (1): Methyl butenol
Class 3 (2): pinenes (a-pinene, b-pinene)
Class 4 (4): triene MT (myrcene, c-b-ocimene, t-b-ocimene, allo-ocimene)
Class 5 (7): less reactive MT (cyclo-fenchene, a-fenchene, 2-bornene, tricyclene, camphene, 3-carene, 4-careen)
Class 6 (10): other MT (limonene, a-thujene, thujadiene, sabinene, a-phellandrene, b-phellandrene, a-terpinene, g-terpinene, terpinolene, MT1509)
Class 7 (3): C10 aromatics (m-cymene, o-cymene, p-cymenene)
Class 8 (8): oxygenated MT (Carveol, Eucalpytol, camphor, thujanol, a-terpineole, bornyl acetate, anisol, terpineol acetate)
Class 9 (9): Highly reactive sesquiterpenes (b-bourbonene, b-caryophyllene, a-humulene, g-Muurolene, a-muurolene, d-cadinene, g-cadinene, SQT1628, SQT 1837)
Class 10 (7): less reactive sesquiterpenes (Ylangene, a-cubebene, b-cubebene, longifolene, a-copaene, b-copanee, cubebol)
Class 17 (3): stress compounds isoprene products and homoterpenes (methyl vinyl ketone, methacrolein, DMNT)

Speciated terpenoid emission factors



Average contribution of each MEGAN terpenoid class for the 20 tree species

Sum of non-isoprene terpenoid emission factors (nmol m^{-2} s^{-1})

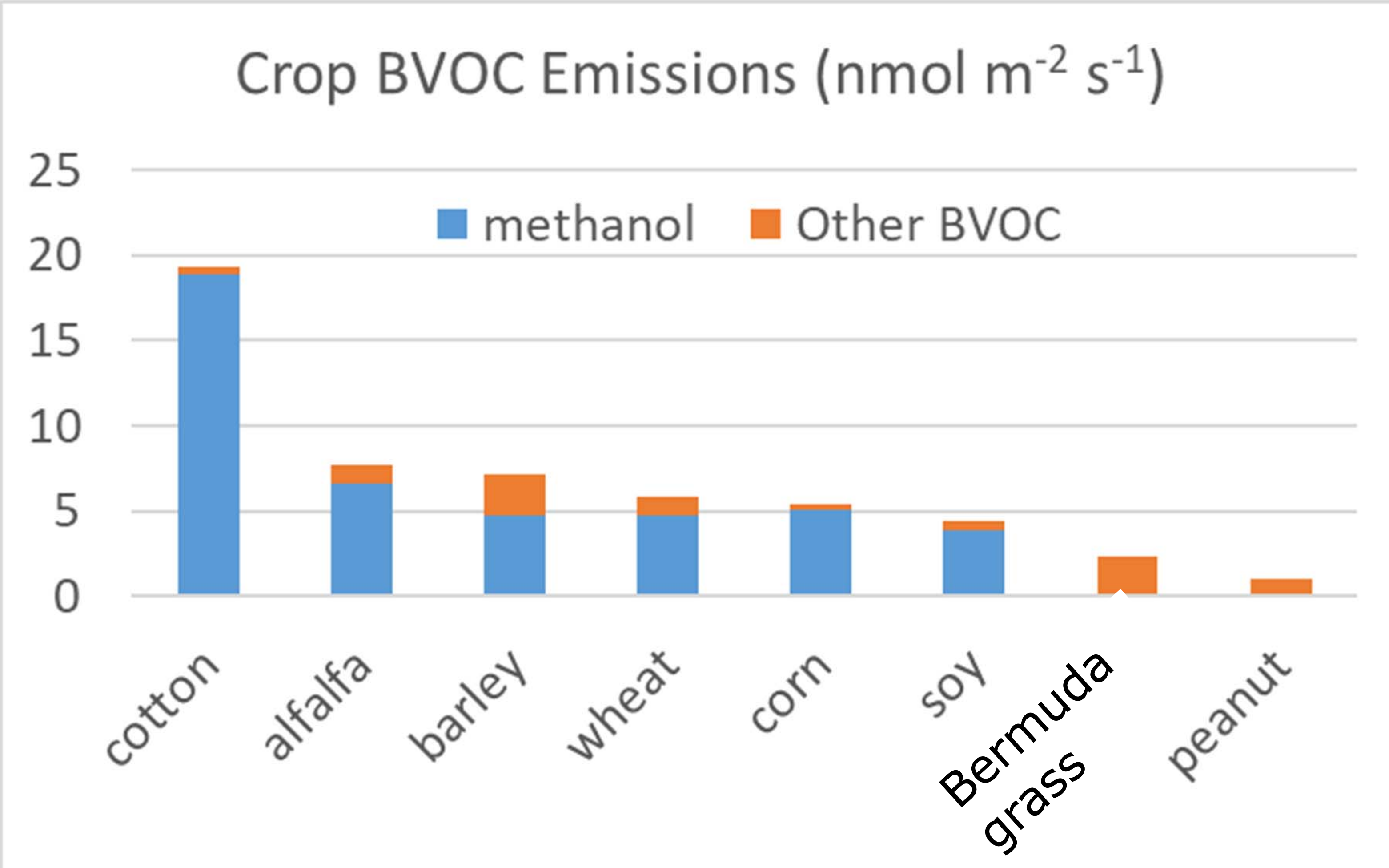
Magnolia:	1.21	**59%** a-pinene, sabinene, b-pinene, o-cymene, camphene
Loblolly pine:	0.93	**74%** a-pinene, b-pinene, b-phellandrene
Post oak:	0.70	**68%** MVK, methacrolein, DMNT, b-bourbonene
Chinese Tallow:	0.11	**61%** methancrolein

26% to 41% of the terpenoid emission is associated with small peaks and/or compounds that are not typically reported

Crop BVOC emission factors

Custom inert gas exchange systems with in-situ PTRFOTMS analysis on UCI campus in June 2019

Crop BVOC emission factors



Other BVOC are primarily sesquiterpenes, acetaldehyde, acetone, acetic acid, and DMS

Ratio of observed to predicted (MEGAN2.1) crop BVOC emissions

~1000: Benzene

~100: Toluene, sesquiterpenes, DMS

10 to 30: acetic acid, isoprene, MVK and methacrolein

5: Monoterpenes

3: Methanol

~1: acetone and acetaldehyde

MEGAN3 predicts substantial isoprene emissions for several crop species based on older j=0 data. The observed isoprene is much lower but is non-zero.

Task 2. MEGAN model Improvements (MEGAN3.1)

<u>Deliverables</u>

- CODE: MEGAN 3.1 FORTRAN Emission Preprocessor and Emission Calculator. MEGAN3.1 Emission Factor Processor python code.
- INPUT files: Preprocessors, EFP.
- User Guides

Task 2. MEGAN model Improvements (MEGAN3.1)

1. Replaced soil NO code (Yienger and Levy approach) used by MEGAN (and BEIS) with state-of-the-art BDSNP approach. This model was already available to the community in GEOS-chem and WRF-CMAQ but required on-line AQ model. Also this allows MEGAN users to use a single model.
2. Added input files and preprocessor code for BDSNP
3. Updated BVOC EF vs LAI depth parameterization
4. Updated MEGAN EFP python code
5. Updated MEGAN EFP input files to integrate emission factors from Task 1 and other data.

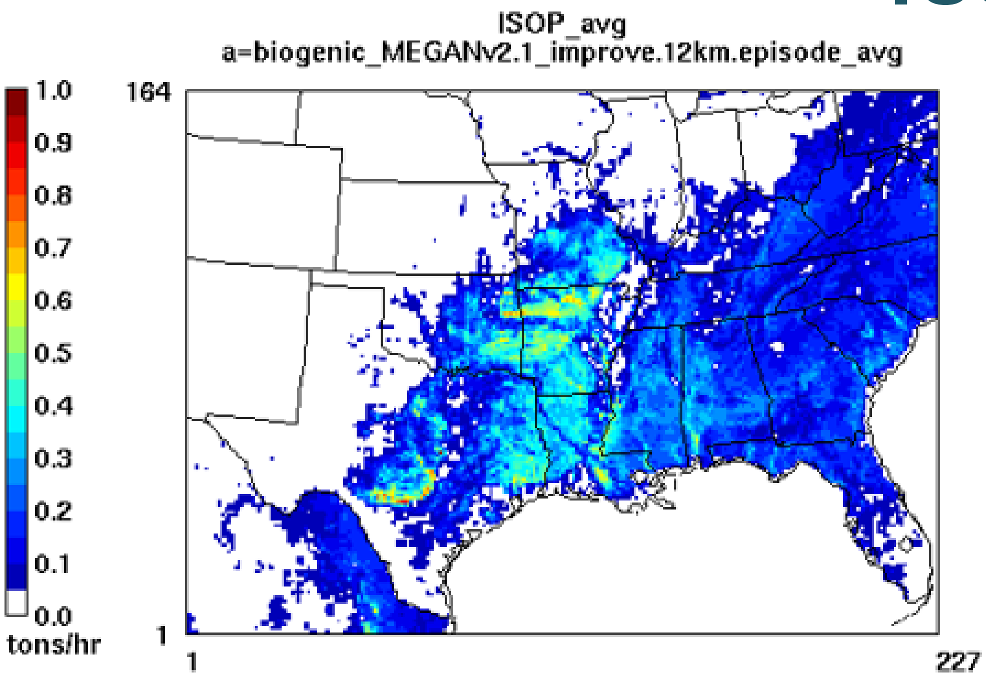
Task 3. MEGAN3.1 sensitivity study

Deliverables

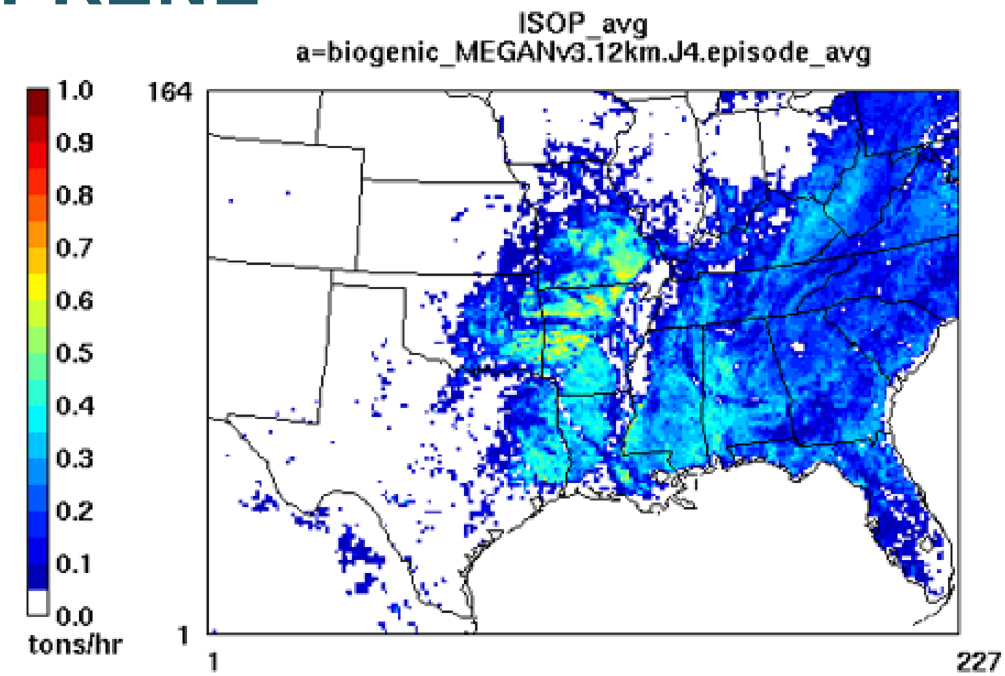
- Biogenic (VOC and NO) emissions inputs and outputs files for:
  - MEGANv3.1
  - MEGAN3
  - MEGANv2.1
  - BEIS3

ISOPRENE

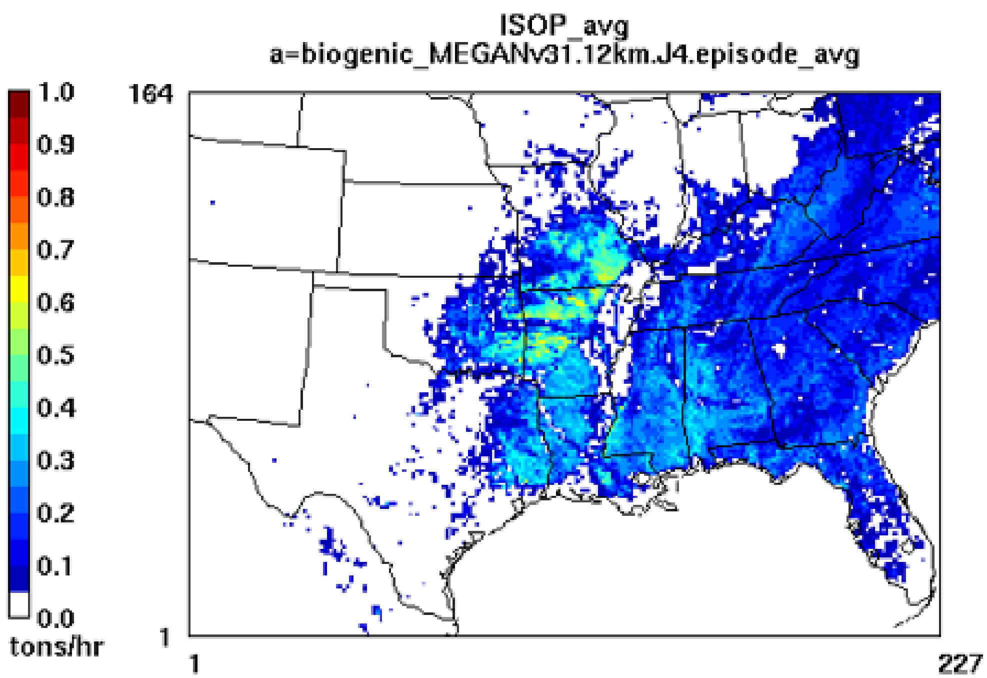
MEGANv2.1_improve



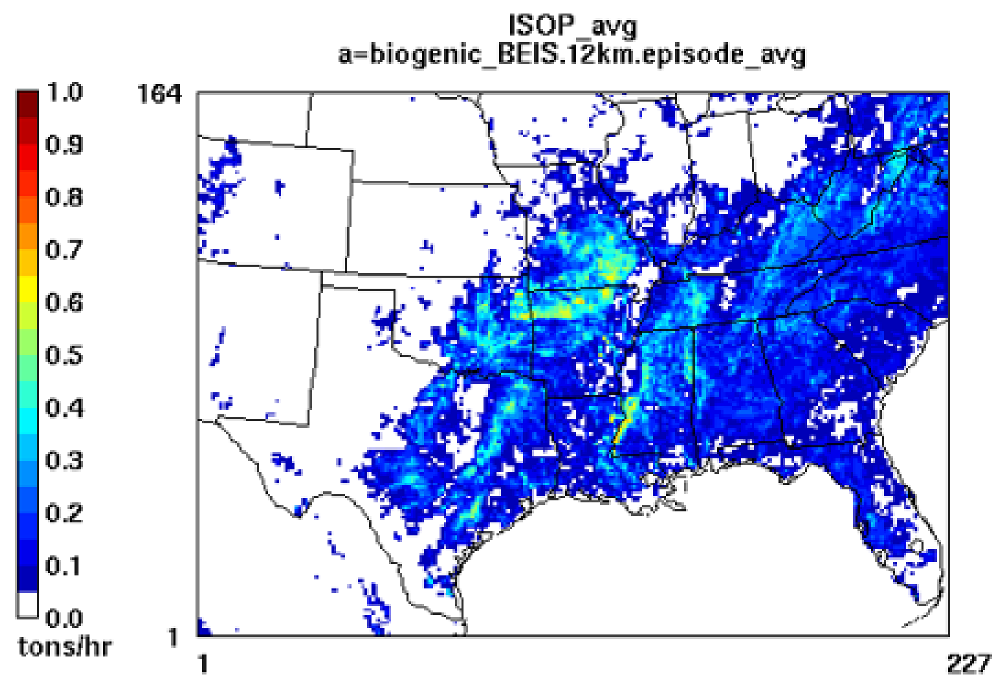
MEGANv3(J4)



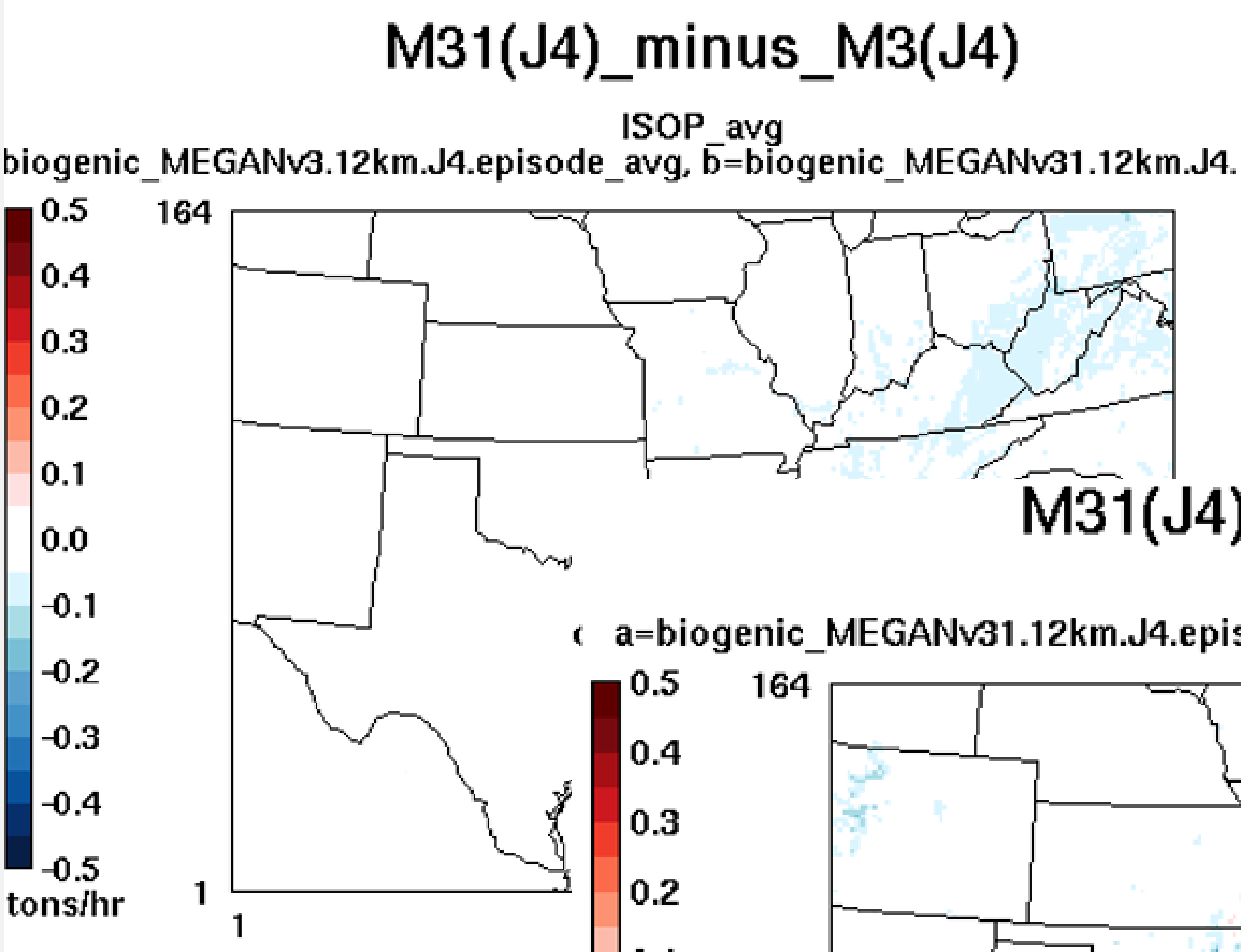
MEGANv31(J4)



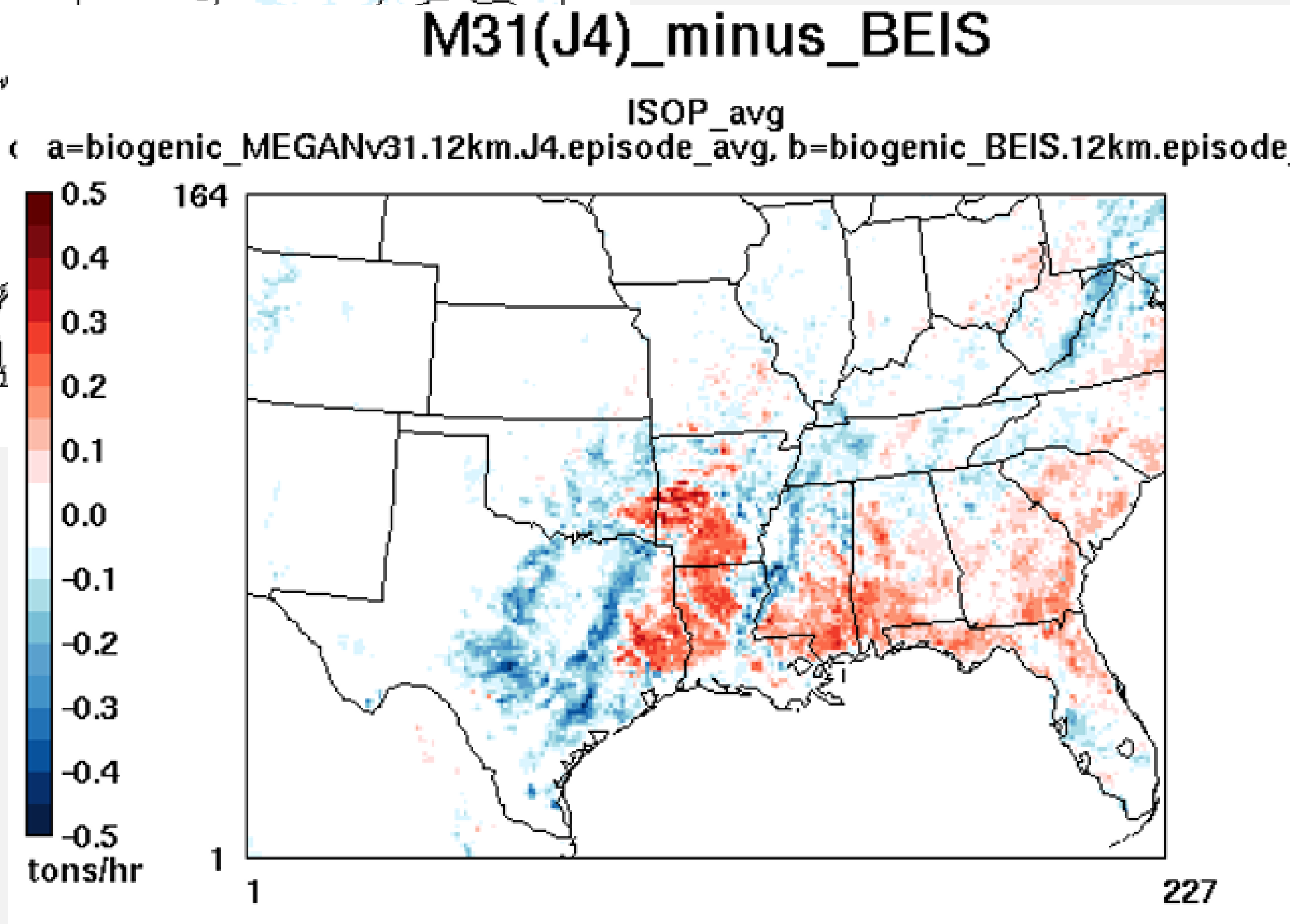
BEIS



ISOPRENE



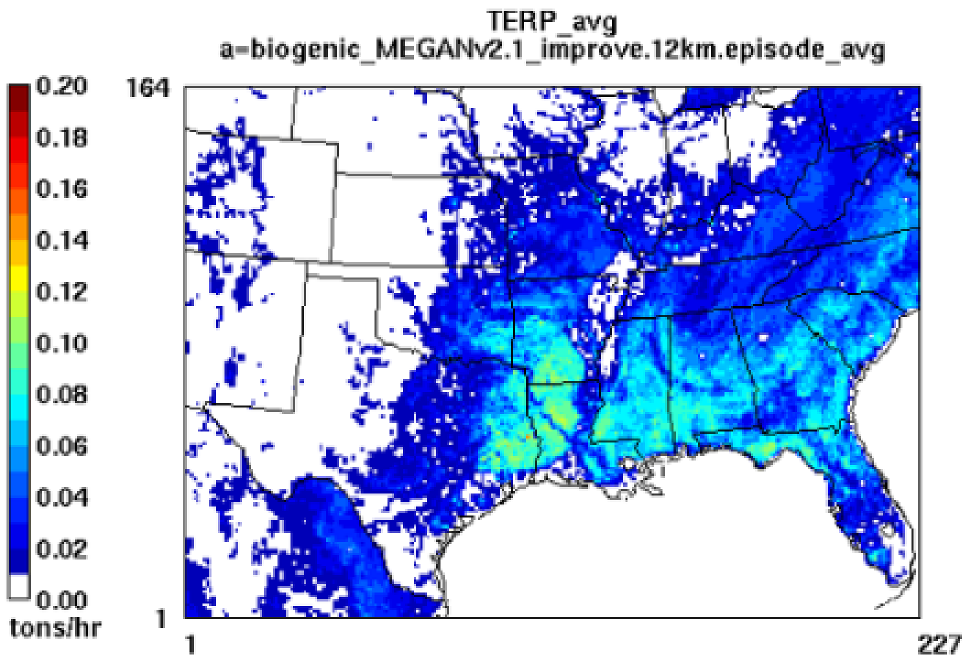
M31(J4)_minus_M3(J4)
ISOP_avg
biogenic_MEGANv3.12km.J4.episode_avg, b=biogenic_MEGANv31.12km.J4.
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
-0.4
-0.5
tons/hr
164
1
1



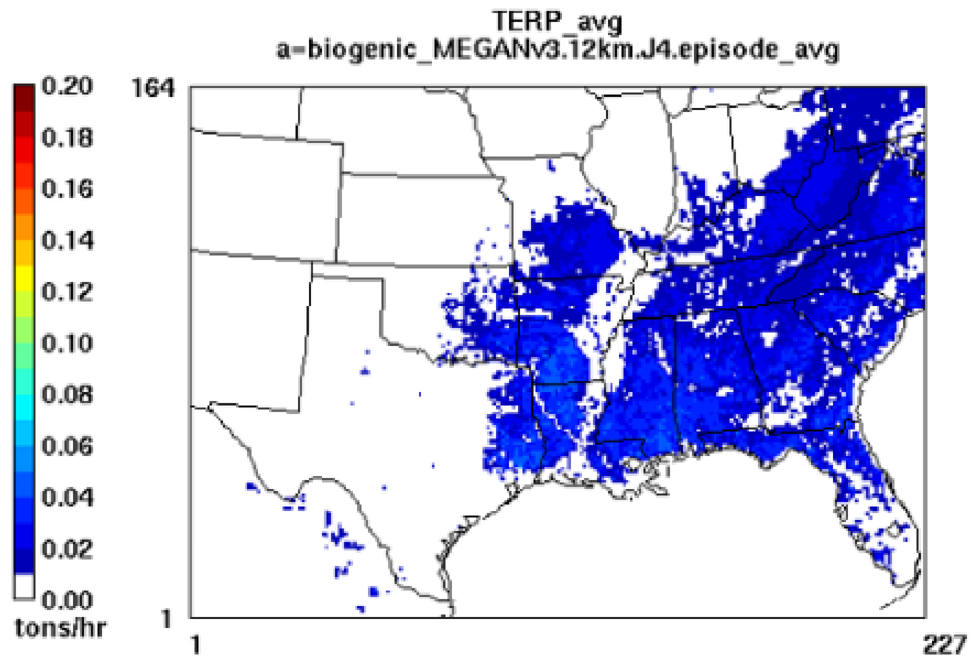
M31(J4)_minus_BEIS
ISOP_avg
a=biogenic_MEGANv31.12km.J4.episode_avg, b=biogenic_BEIS.12km.episode_
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
-0.2
-0.3
-0.4
-0.5
tons/hr
164
1
1
227

MONOTERPENE

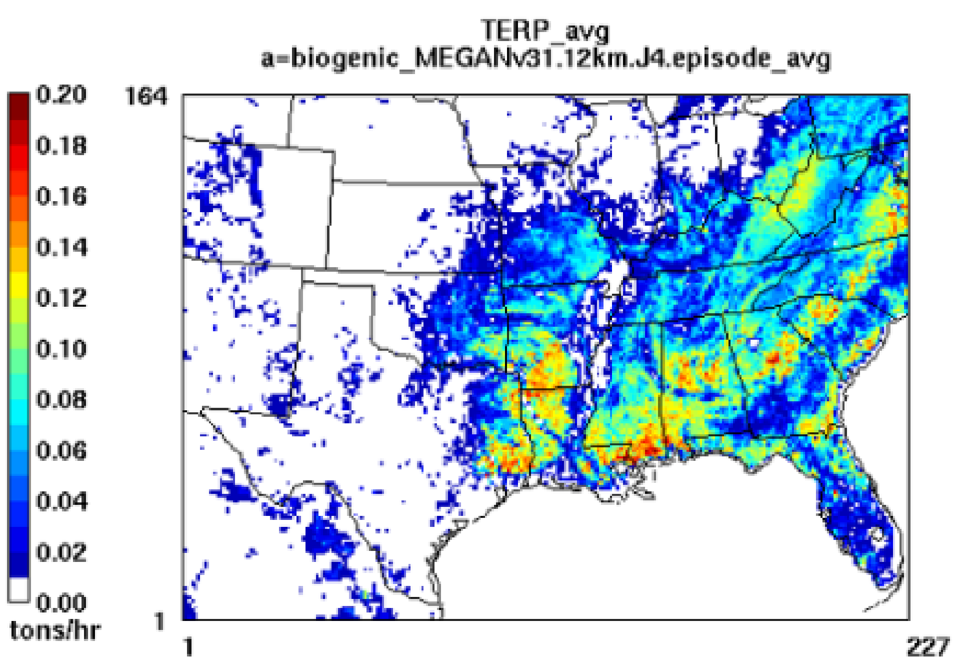
MEGANv2.1_improve



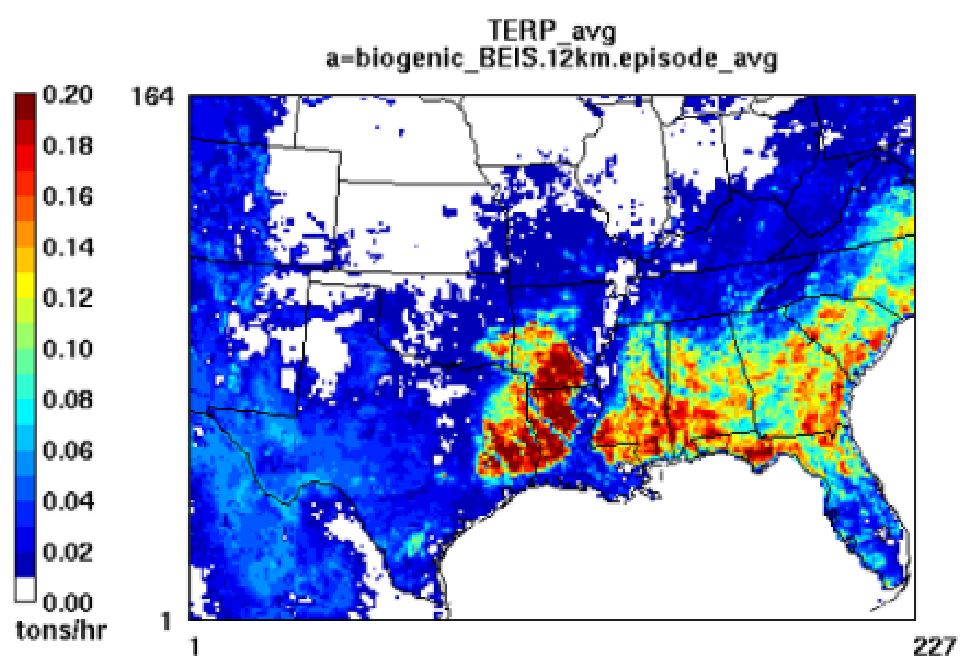
MEGANv3(J4)



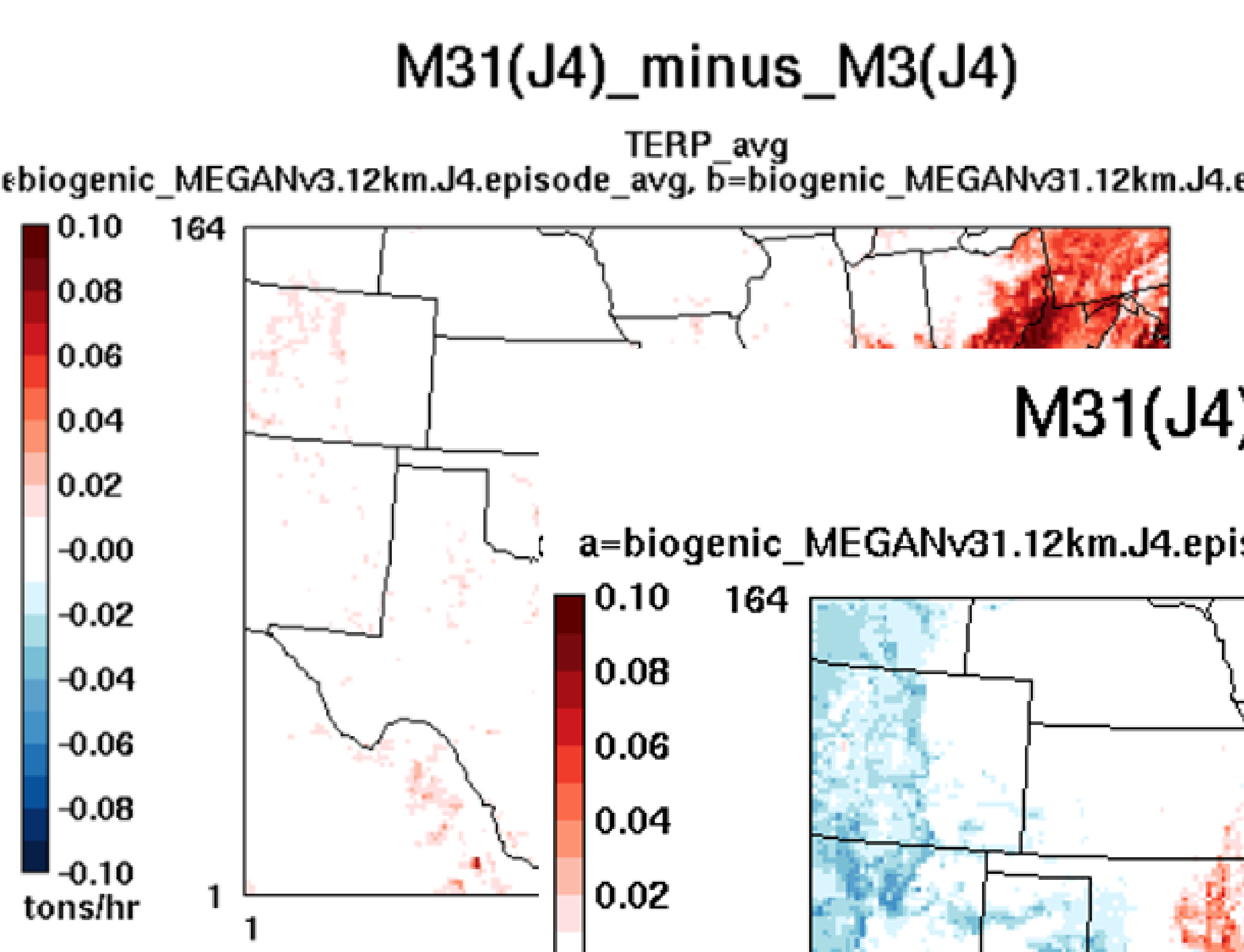
MEGANv31(J4)

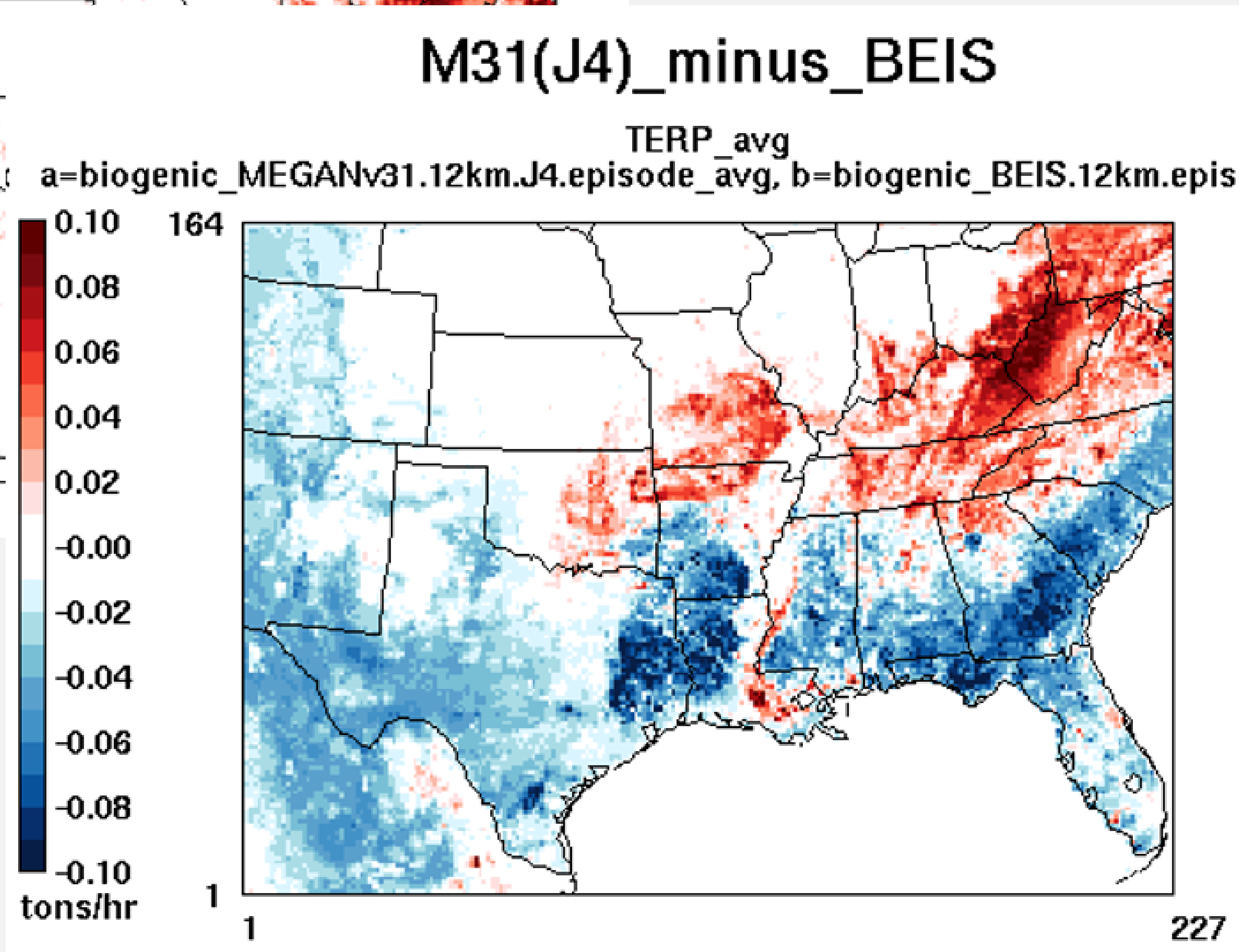


BEIS

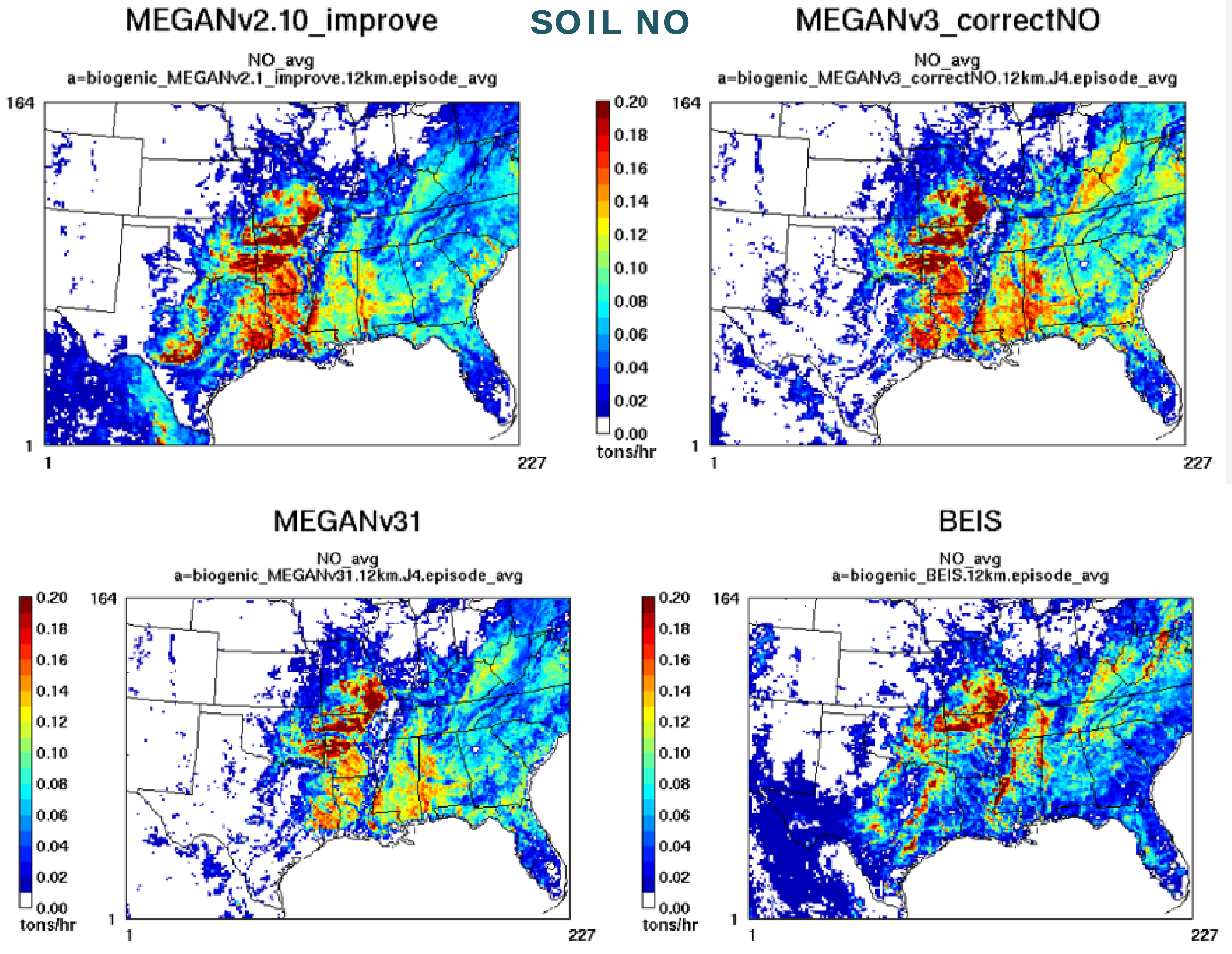


MONOTERPENE



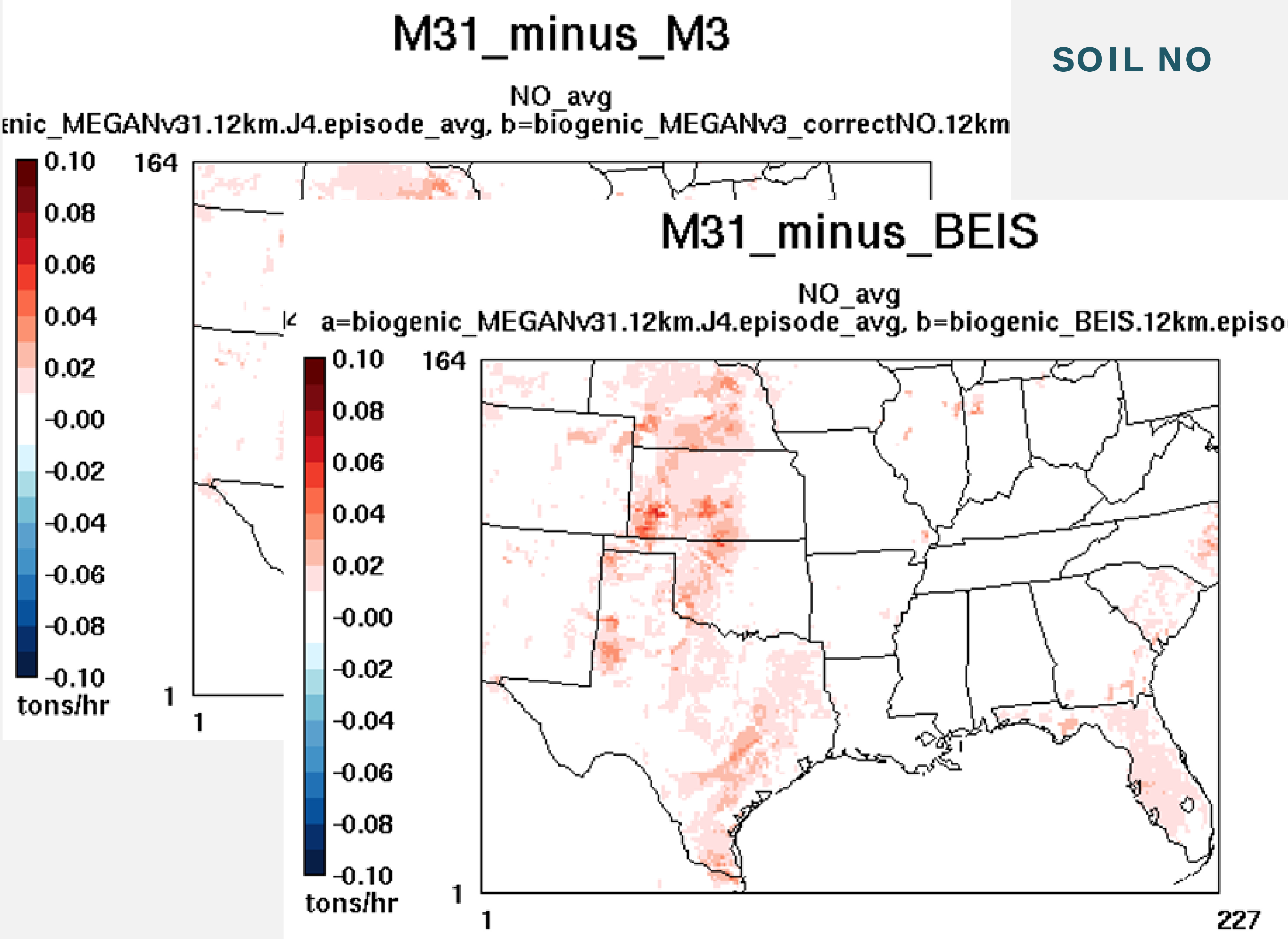


SOIL NO



MEGANv2.10_improve
NO_avg
a=biogenic_MEGANv2.1_improve.12km.episode_avg
MEGANv3_correctNO
NO_avg
a=biogenic_MEGANv3_correctNO.12km.J4.episode_avg
MEGANv31
NO_avg
a=biogenic_MEGANv31.12km.J4.episode_avg
BEIS
NO_avg
a=biogenic_BEIS.12km.episode_avg
0.20
0.18
0.16
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
tons/hr
164
1
227

SOIL NO


M31_minus_M3
NO_avg
enic_MEGANv31.12km.J4.episode_avg, b=biogenic_MEGANv3_correctNO.12km
0.10
0.08
0.06
0.04
0.02
-0.00
-0.02
-0.04
-0.06
-0.08
-0.10
tons/hr
164
1
1
M31_minus_BEIS
NO_avg
a=biogenic_MEGANv31.12km.J4.episode_avg, b=biogenic_BEIS.12km.episo
0.10
0.08
0.06
0.04
0.02
-0.00
-0.02
-0.04
-0.06
-0.08
-0.10
tons/hr
164
1
1
227

Key Points

- Southern live oak and Water oak isoprene EF is ~40 nmol/m2/s while others are 30 nmol/2/s (BEIS is 24 nmol/m2/s).
- EF variability requires investigating multiple trees/leaves and quantifying light environment (LAI depth).
- >50 terpenoids (non-isoprene total 0.04 to 2 nmol/m2/s) dominated by well known terpenes but about a third is associated with many small peaks and compounds that are typically not reported.
- Isoprene and pinenes tend to comprise about half of the EF with the rest spread over a wide range of MEGAN emission categories.
- EFs of previously unstudied Texas native trees (Ashe juniper, Plateau live oak, Shumard oak, Swamp chestnut oak, Cedar elm) emit at rates similar to other members of their genera.
- Texas broadleaf trees range from very low (crepe myrtle, camphor, Chinese tallow tree) to high (Post oak, Magnolia, Pecan) terpenes.
- Texas crops have low isoprene (in contrast to some past reports) but significant sesquiterpenes, acetaldehyde, acetone, acetic acid, and DMS.

Recommendations for future work

- **Investigate heat stress (>35C) induced terpenoid emissions from dominant Texas trees with field enclosure and ambient measurements to evaluate and improve MEGAN3.1 predictions.**
- **Improve Texas landcover (species composition and cover) data for BVOC model simulations using existing data and field surveys, especially in urban areas and shrublands.**
- **Evaluate model predictions with light, temperature and EF measurements throughout tree canopies, especially in open and heterogeneous canopies, and compare results for different locations and environments.**
- **Identify and quantify the processes controlling location-dependent isoprene EF variability.**
- **MEGAN3.1 should be used for estimating emissions of NO and biogenic VOC emissions in Texas while continuing to improve MEGAN landcover and other inputs.**