AQRP project 14-030

Improving Modeled Biogenic Isoprene Emissions under Drought Conditions and Evaluating Their Impact on Ozone Formation

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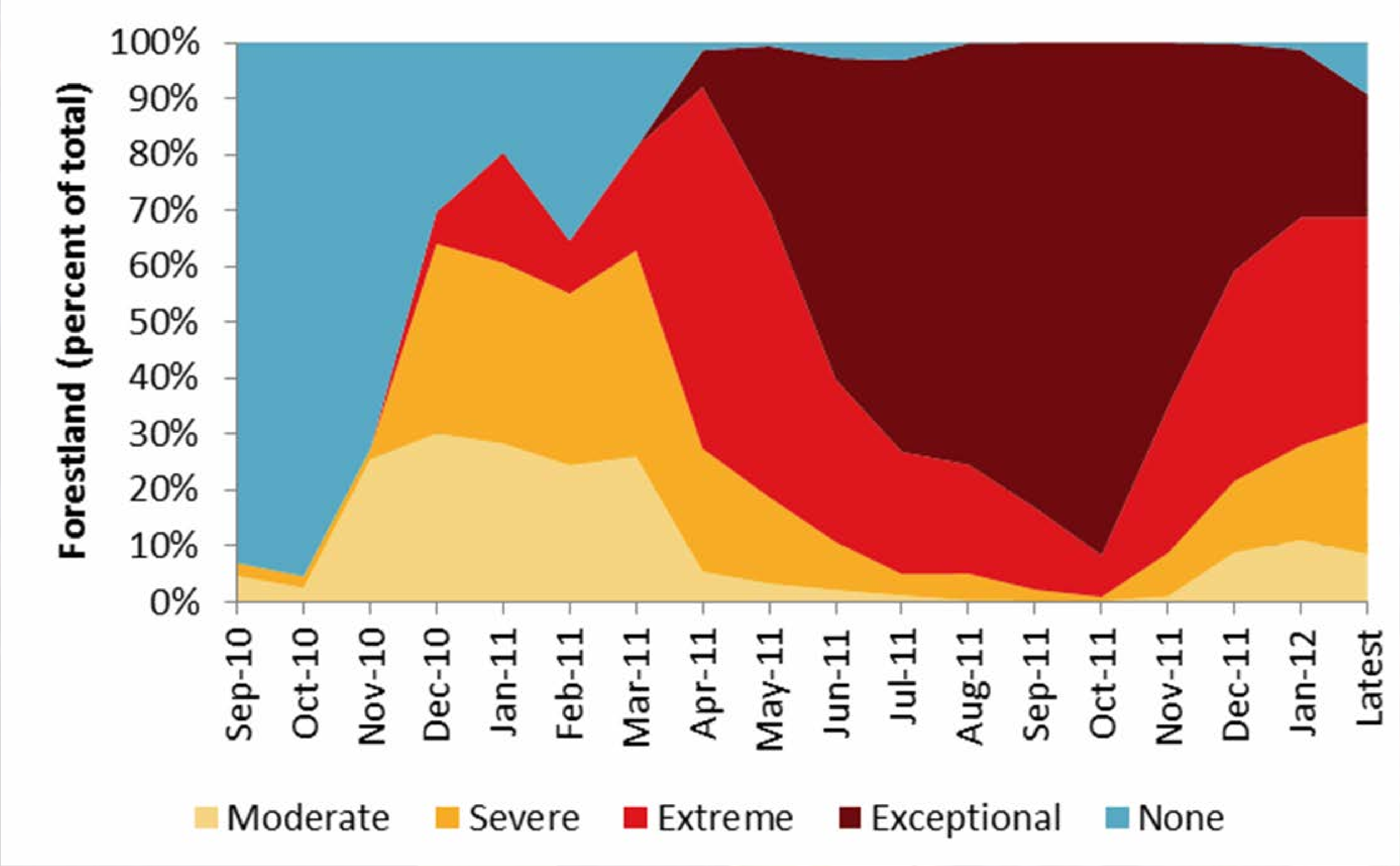
Motivation

- 2011 Texas drought had a major impact on vegetation in Texas
  - lower photosynthesis rates, early senescence
  - tree mortality of order 1-10% (300 million trees)
- high temperatures cause regionally high ozone
  - high emissions, fast chemistry
  - 2011 ozone values were only moderately high though
- drought reduced biogenic isoprene emissions
  - observed in leaf-level isoprene emissions field data, but
  - data base on drought response limited, and
  - model implementation not intensively tested

The 2011 Texas drought

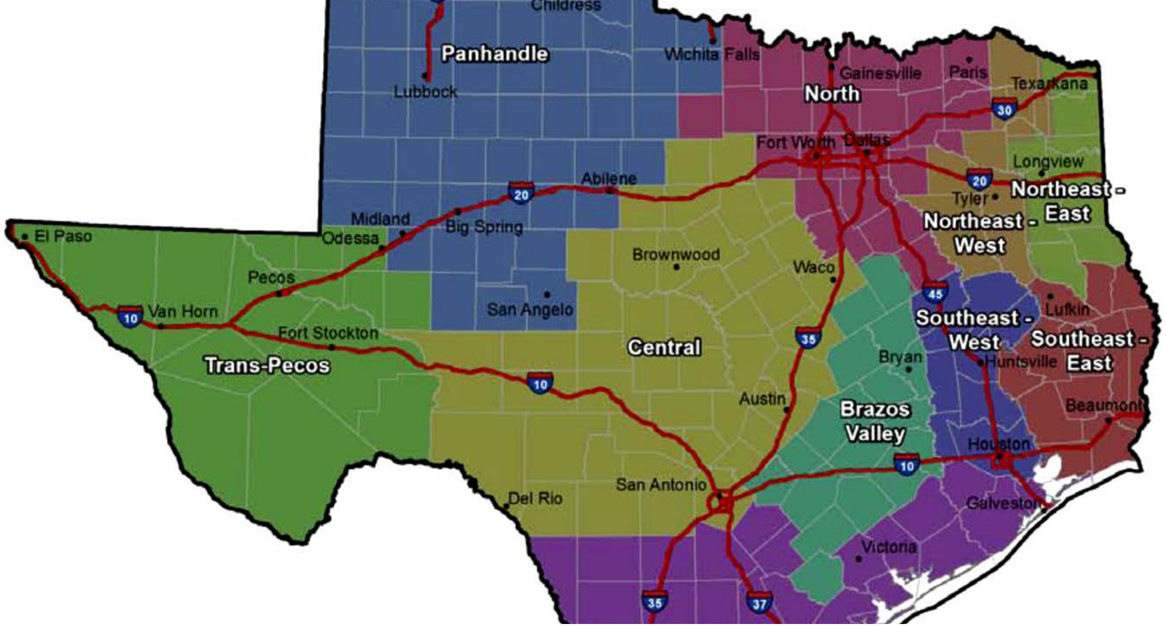


Chris Edgar, Texas Forest Service, 2012

Drought Impacts to Trees

- Fewer needles or leaves
- Early dormancy
- Reduced growth and loss of vigor
- Increased susceptibility to insects and disease
- Death

Chris Edgar, Texas Forest Service, 2012



East Texas:

4.2% of trees

8.6% of oak

4.1% of sweetgum

2.1% of pine

Region	Live trees prior to the drought (million trees)	Drought-related mortality (million trees)	Drought-related mortality (percentage)
Southeast - East	597.1	7.5	1.3
Southeast - West	289.7	18.8	6.5
Northeast - East	356.0	13.9	3.9
Northeast - West	309.4	25.3	8.2
North	370.5	30.9	8.3
Brazos Valley	256.4	24.9	9.7
South	431.2	31.7	7.4
Central	1,540.0	102.3	6.6
Panhandle	556.3	33.1	6.0
Trans-Pecos	163.4	12.2	7.5
Total	**4,869.9**	**300.6**	**6.2**

Chris Edgar, Texas Forest Service, 2012

Objectives

- evaluate BVOC emission models with focus on isoprene
  - default or updated drought parameterization scheme
  - recently collected data during 2011 drought
  - new laboratory / greenhouse data
- evaluate WRF model in predicting meteorological conditions for air quality simulations under drought conditions
- evaluate sensitivity of CMAQ ozone predictions in southeast Texas using drought parameterizations for isoprene emissions (2011 vs. 2007)

Project overview

- controlled drought experiments in a greenhouse on campus; basal isoprene emissions
  - focus on potted post oak (*Quercus stellata*) and water oak (*Quercus nigra*) in typical sandy loam soil

- extensive WRF-CMAQ simulations for (east) Texas
  - BVOC emissions model MEGAN v2.1, BEIS 3.14
  - anthro-emissions from SMOKE v3.5.1 and 2011 NEI v6
  - comparisons to met data and AQ monitoring data
    - in-situ isoprene at TCEQ (auto-GC) sites

Greenhouse setup, I

Greenhouse setup, II

- Regular measurements
  - daily during drought treatment
  - treatment vs. control groups
- environmental monitoring
  - PAR, T, rH
  - soil moisture in pot
    - in situ
    - weighing

Biogenic emissions processing (1): The drought parametrization

- modified MEGAN 2.1

$$F_{isop} = \varepsilon_{isop} \times \gamma_i, \quad \gamma_i = \gamma_{PAR} \times \gamma_T \times \gamma_{SM} \times \gamma_j$$

$\gamma_{SM,\, i}$: soil moisture activity factor for soil layer i

θ : volumetric soil moisture

θ_w : wilting point, **$\Delta\theta_1 = 0.04$ (for CMAQ modeling: 0.06)**

$\gamma_{SM} = 1$ for $\theta > \theta_w + \Delta\theta_1$

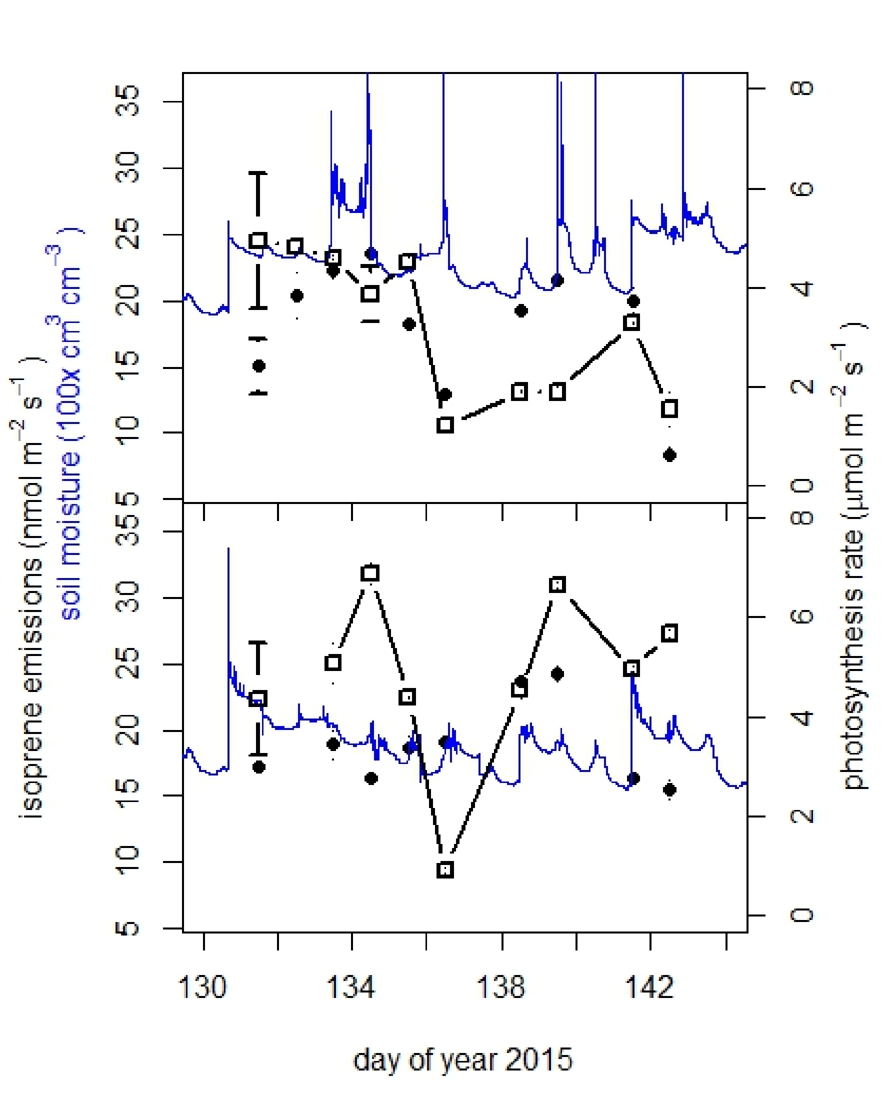
$\gamma_{SM} = (\theta - \theta_w) / \Delta\theta_1$ for $\theta_w < \theta < \theta_w + \Delta\theta_1$

$\gamma_{SM} = 0$ for $\theta \le \theta_w$

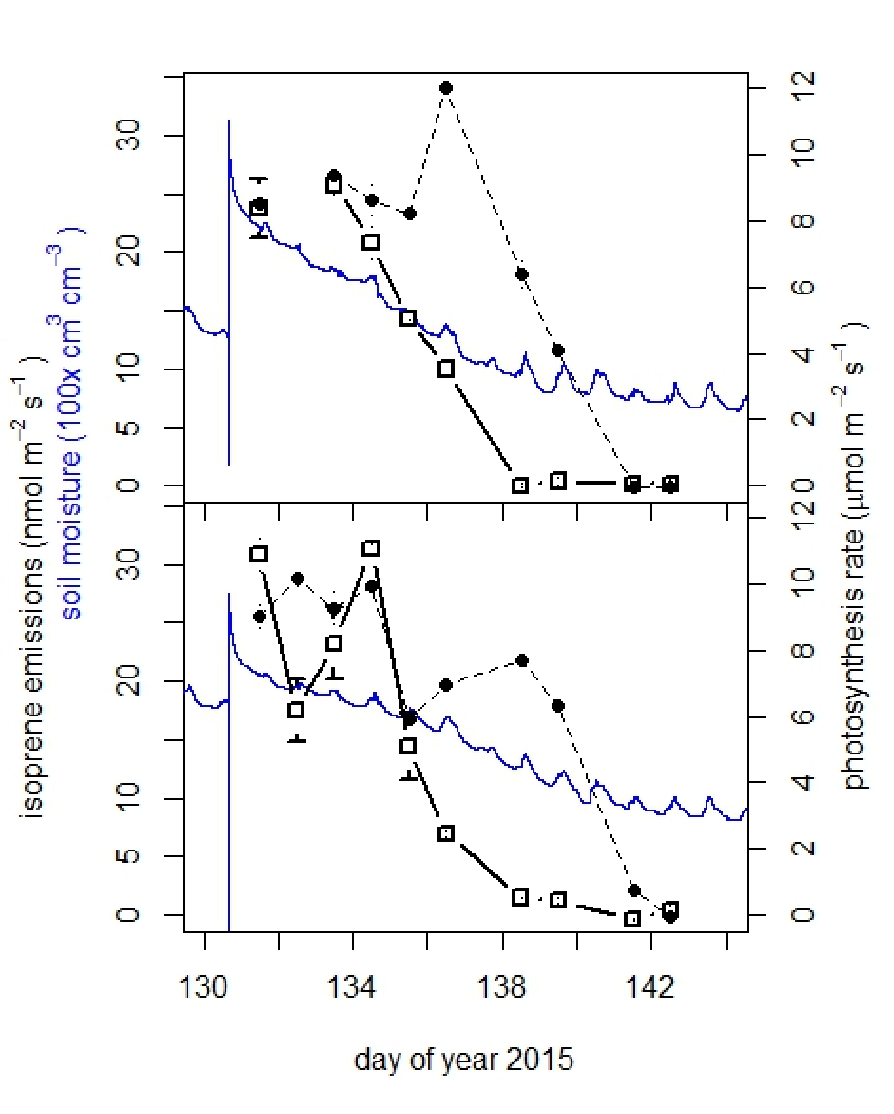
$$\gamma_{SM} = \sum_{k=1}^{N_{PFT}} \sum_{i=1}^{4} f_{PFT,k}\, \omega_{k,i}\, \gamma_{SM,i}$$

Potted water oak example

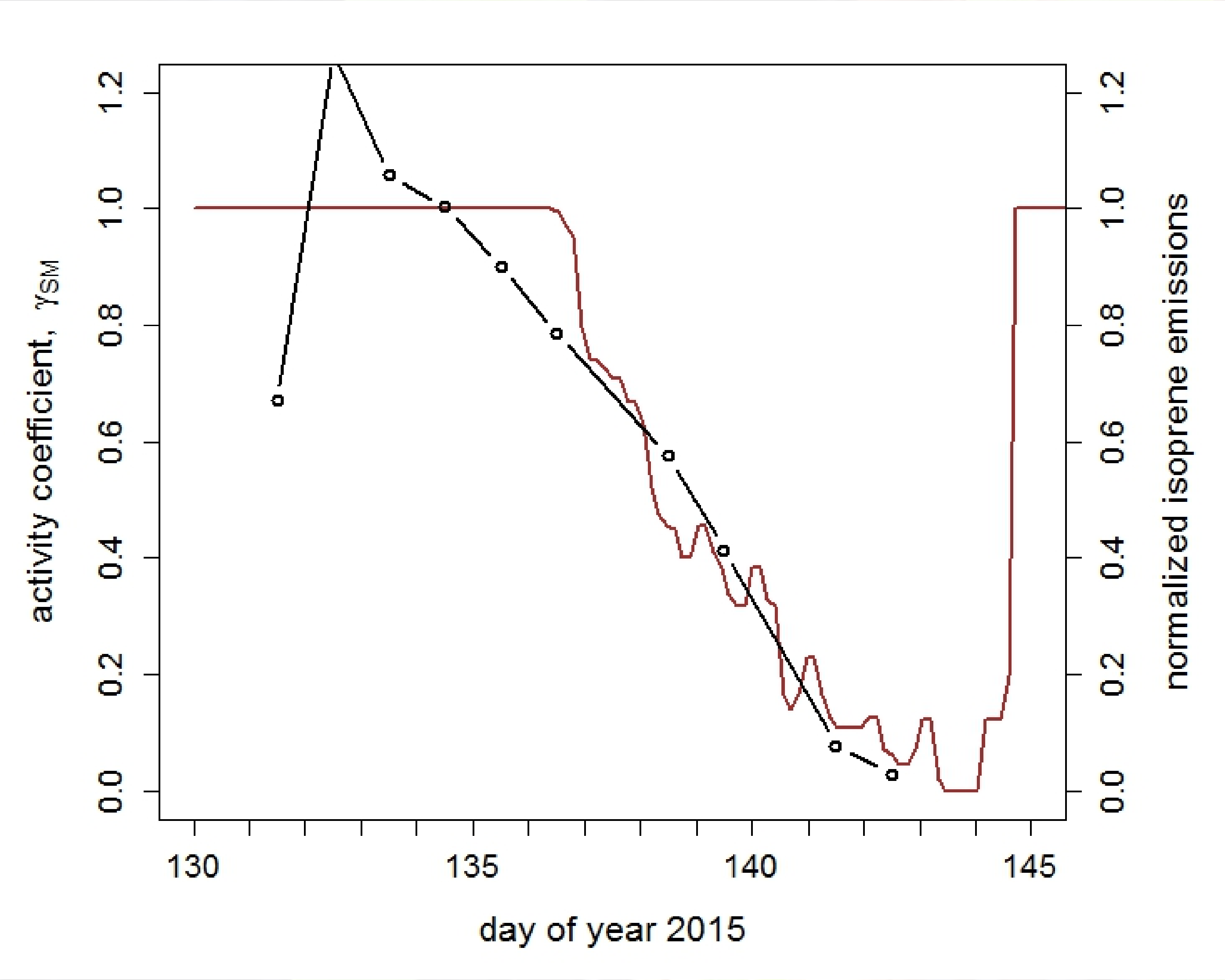
control



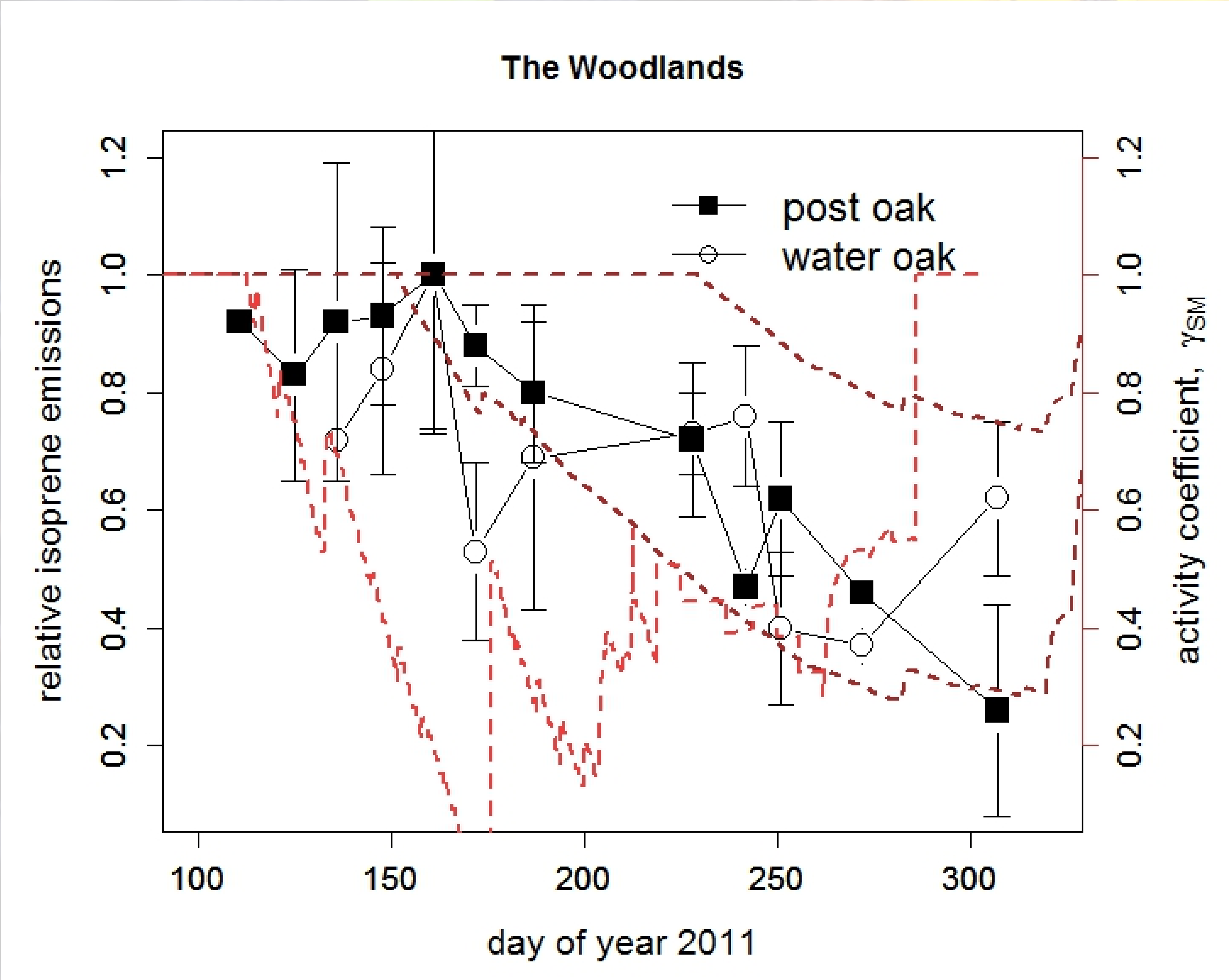
drought stressed



Potted post oak example

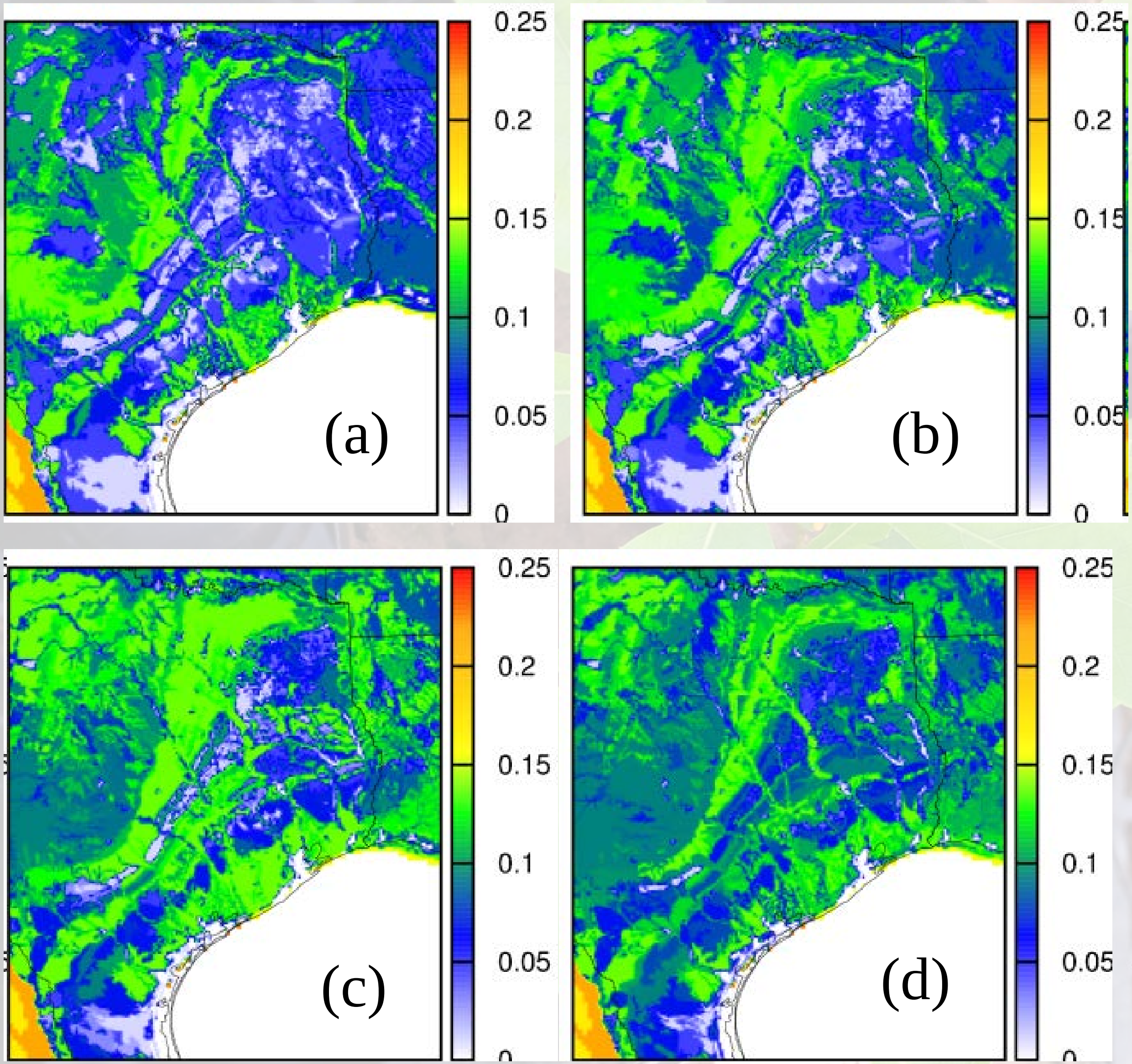


Normalized 2011 field data



simple soil model (Manfreda et al., 2014) vs. WRF/Noah average soil moisture 0-2 m depth

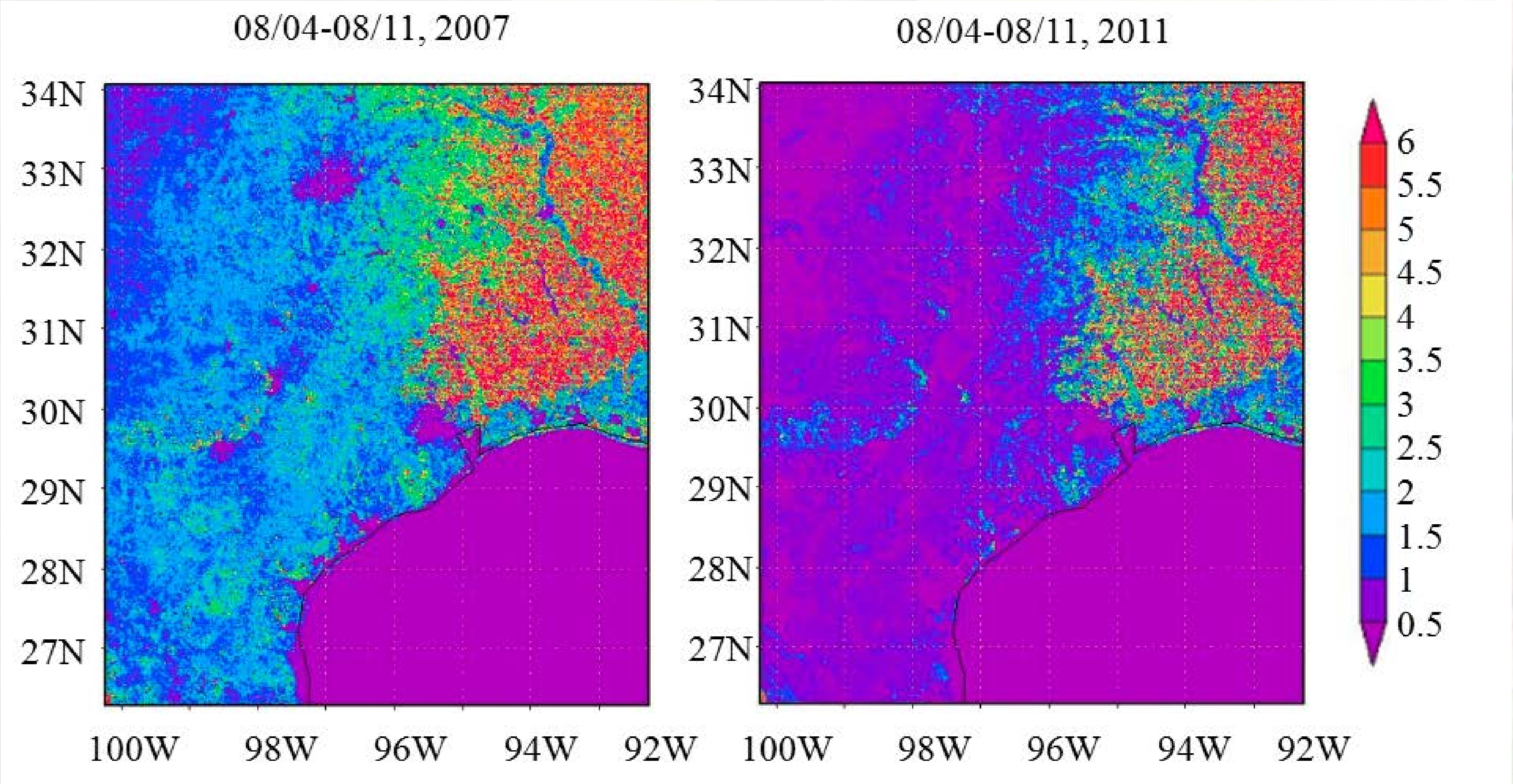
1-km wilting point fields (4-km domain)



(a): 0-0.1 m
(b): 0.1-0.4 m
(c): 0.4-1 m
(d): 1-2 m

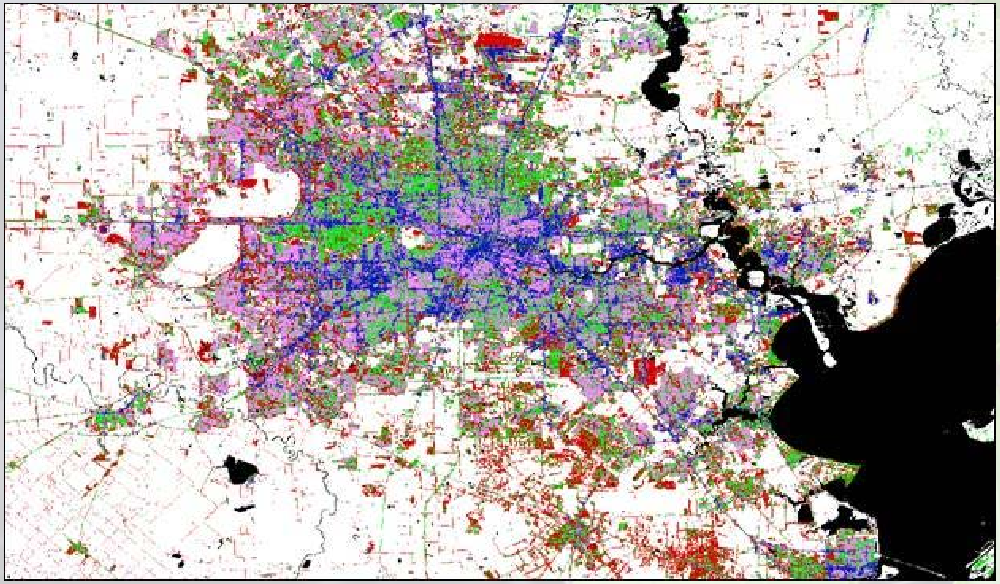
Biogenic emission processing (2)

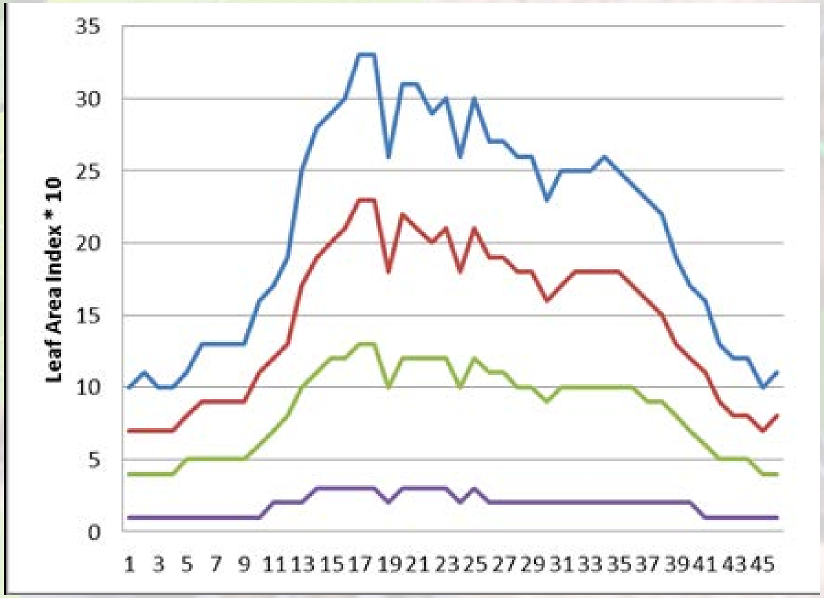
- Year specific MODIS LAI (MOD15A2)



Biogenic emission processing (3)

- Treatment of emissions from urban areas





TCEQ urban land use types for the Houston area. (Blue: developed high density; Green: developed low density; Purple: developed Medium density; Red: developed open areas.)

Developed open areas
Developed low density
Developed medium density
Developed high density

Soil moisture evaluation

July 2011 – All points in the TAMU North American Soil Database

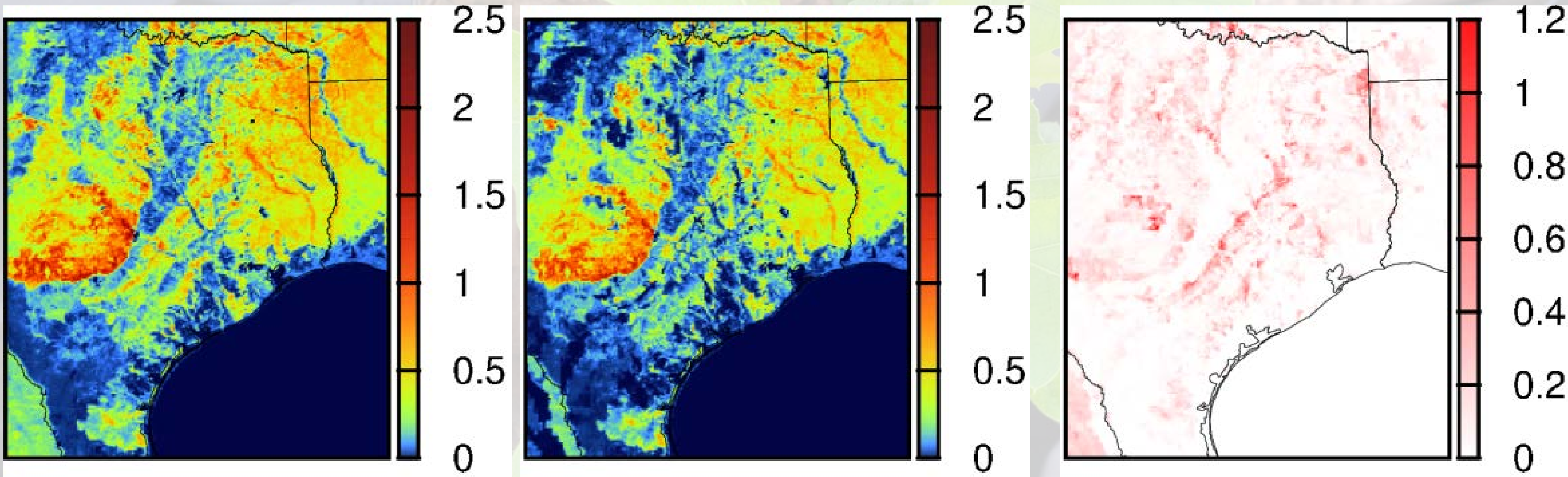
Depth	0.05m	0.1m	0.2m	0.25m	0.5m	0.6m	1m
avg_obs (m^3 m^{-3})	0.165	0.141	0.135	0.243	0.161	0.199	0.169
avg_pre (m^3 m^{-3})	0.131	0.109	0.129	0.158	0.119	0.141	0.116
MB	-0.03	-0.03	-0.01	-0.09	-0.04	-0.06	-0.05
RMSE (m^3 m^{-3})	0.05	0.07	0.06	0.09	0.05	0.06	0.10
GE (m^3 m^{-3})	0.04	0.06	0.06	0.09	0.05	0.06	0.09
MNB	-0.17	-0.02	0.24	-0.34	-0.21	-0.29	-0.08

(Performance of other months is similar)

Isoprene Emission
Effect of soil moisture

Monthly average emission July 2011 (mol s^{-1})

NSM SM Difference



NSM: Without considering soil moisture effect

SM: With soil moisture effect

Difference: NSM - SM

Isoprene concentrations – Auto GC sites

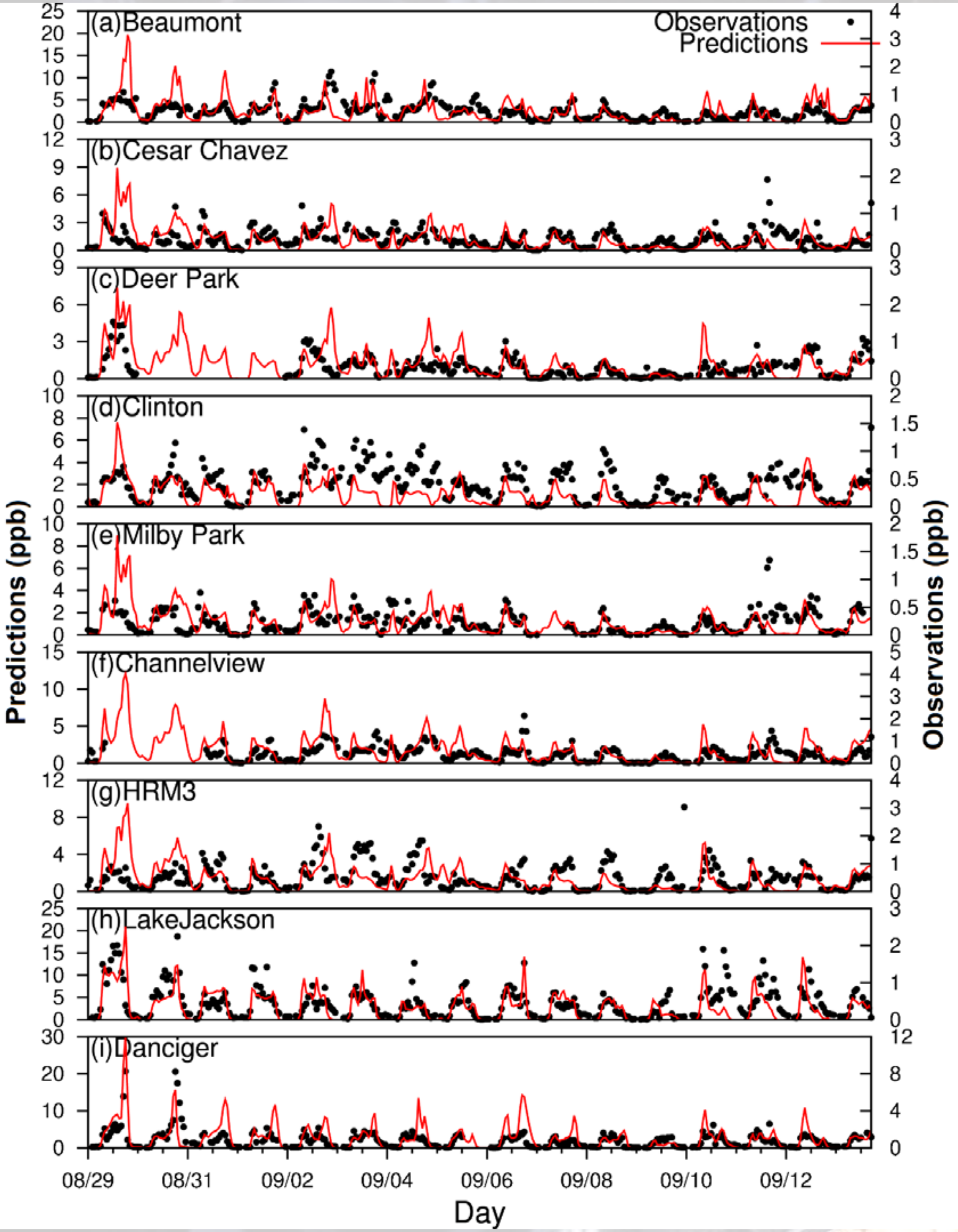
			SM		NSM	
sites	Name	Region	MNB	MNE	MNB	MNE
482010026	Channel View	Houston	2.54	2.71	3.25	3.41
482010069	Milby Park	Houston	1.20	1.91	1.66	2.30
482010617	Goodyear GC	Houston	7.22	7.33	10.72	10.81
482010803	HRM #3 Haden Rd	Houston	0.22	1.73	0.51	1.98
482011015	Lynchburg Ferry	Houston	2.47	3.35	3.18	4.02
482011035	Clinton	Houston	0.46	1.67	0.80	1.95
482011039	Houston Deer Park #2	Houston	3.62	3.77	4.43	4.56
482016000	Cesar Chavez	Houston	0.72	1.72	1.06	1.99
482450009	Beaumont Downtown	Houston	4.08	4.24	4.94	5.08
482451035	Nederland High School	Houston	3.23	3.43	4.00	4.17
481130069	Dallas Hinton	Dallas/Fort Worth	3.72	3.73	8.09	8.09
481211007	Lancester Cedardale	Dallas/Fort Worth	1.36	1.66	3.77	3.97
481211013	DISH Airfield	Dallas/Fort Worth	3.94	3.99	6.75	6.79
484390075	Eagle Mountain Lake	Dallas/Fort Worth	9.52	9.53	18.08	18.09
484391002	Fort Worth Northwest	Dallas/Fort Worth	5.19	5.20	8.72	8.72
484391009	Everman Johnson Park	Dallas/Fort Worth	1.87	1.92	2.35	2.39
484970088	Decatur Thompson	Dallas/Fort Worth	1.38	1.74	3.46	3.70
483550035	Oak Park	Corpus Christi	1.09	1.42	1.81	2.09
483550041	Solar Estates	Corpus Christi	1.81	2.01	2.47	2.63
483550083	Corpus Christi Palm	Corpus Christi	1.79	1.97	2.51	2.66

Isoprene concentrations
Non-Auto GC sites

Month	SM		NSM	
	MNB	MNE	MNB	MNE
April	2.12	2.30	2.61	2.73
May	2.13	2.22	2.51	2.59
June	2.43	2.52	3.28	3.33
July	2.76	2.84	3.38	3.44
August	2.13	2.23	3.52	3.60
September	3.67	3.79	4.88	4.93
October	1.09	1.44	1.84	2.11

a cut-off value of 0.1 ppb was applied

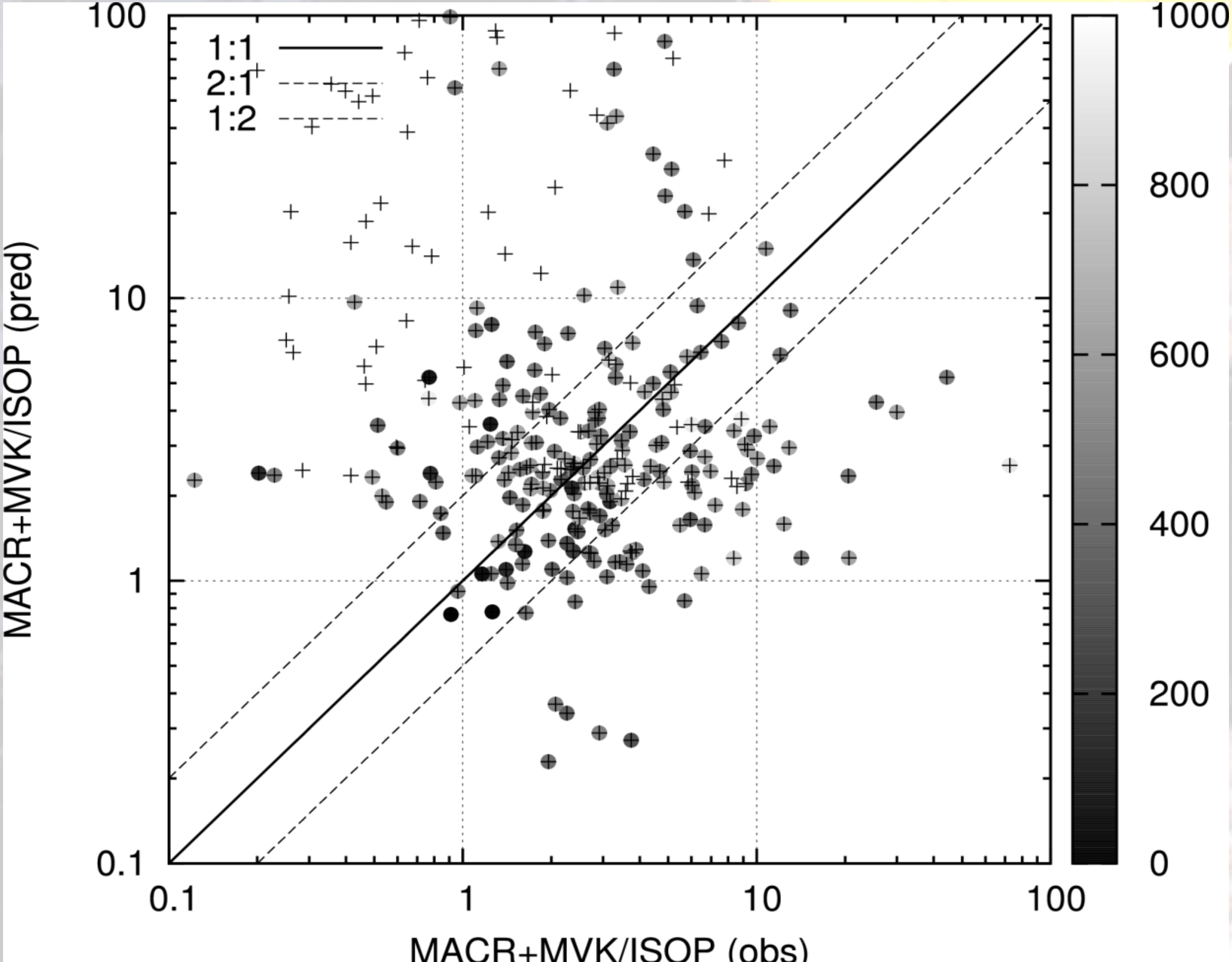
			SM		NSM	
SITE	NAME	TYPE	MNB	MNE	MNB	MNE
481671034	Galveston 99th Street	SUBURBAN	-0.29	0.41	-0.28	0.41
481670005	Texas City Ball Park	URBAN	0.25	0.87	1.83	1.88
482010057	Galena Park	URBAN	0.25	0.53	0.37	0.59
482010036	Jacinto Port	SUBURBAN	0.45	0.68	0.61	0.80
482010307	Manchester/Central	SUBURBAN	0.47	0.93	0.69	1.10
483550034	Dona Park	URBAN	0.60	0.64	0.61	0.64
484790017	Laredo Bridge	URBAN	0.78	1.08	0.91	0.99
482010058	Baytown	SUBURBAN	1.15	1.24	1.49	1.49
482010061	Shore Acres	SUBURBAN	1.45	1.50	1.64	1.68
482011049	Pasadena North	URBAN	1.52	1.58	1.94	2.00
482010024	Houston Aldine	SUBURBAN	1.53	1.54	2.07	2.08
482450011	Port Arthur West	URBAN	1.75	1.95	2.00	2.20
482570005	Kaufman	SUBURBAN	2.08	2.09	3.22	3.23
481390016	Midlothian OFW	SUBURBAN	2.17	2.17	7.68	7.68
484393009	Frisco 5th St	SUBURBAN	2.20	2.42	4.12	4.25
482450019	City Service Center / PA	SUBURBAN	2.62	2.78	2.72	2.87
482450018	Jefferson County Airport	SUBURBAN	2.67	2.67	2.81	2.81
482450017	Port Neches Avenue L	URBAN	2.71	2.74	2.90	2.94
481210034	Denton Airport South	RURAL	2.75	2.75	5.72	5.72
483390078	Conroe Relocated	SUBURBAN	2.85	2.85	3.86	3.86
482010055	Houston Bayland Park	SUBURBAN	2.98	3.24	3.72	3.98
482311006	Greenville	SUBURBAN	3.27	3.27	5.53	5.53
481830001	Longview	RURAL	3.34	3.34	4.17	4.17
481391044	Italy	RURAL	3.58	3.58	6.00	6.00
482030002	Karnack	RURAL	3.76	3.76	5.77	5.77
482450014	Groves	URBAN	3.87	3.97	4.24	4.34
482451050	Beaumont Mary	URBAN	4.29	4.29	4.66	4.66
480290677	Old Hwy 90	URBAN	5.33	5.33	9.08	9.08
482010029	Northwest Harris County	RURAL	5.60	5.60	7.66	7.66
480391003	Clute	SUBURBAN	11.83	11.85	12.25	12.25



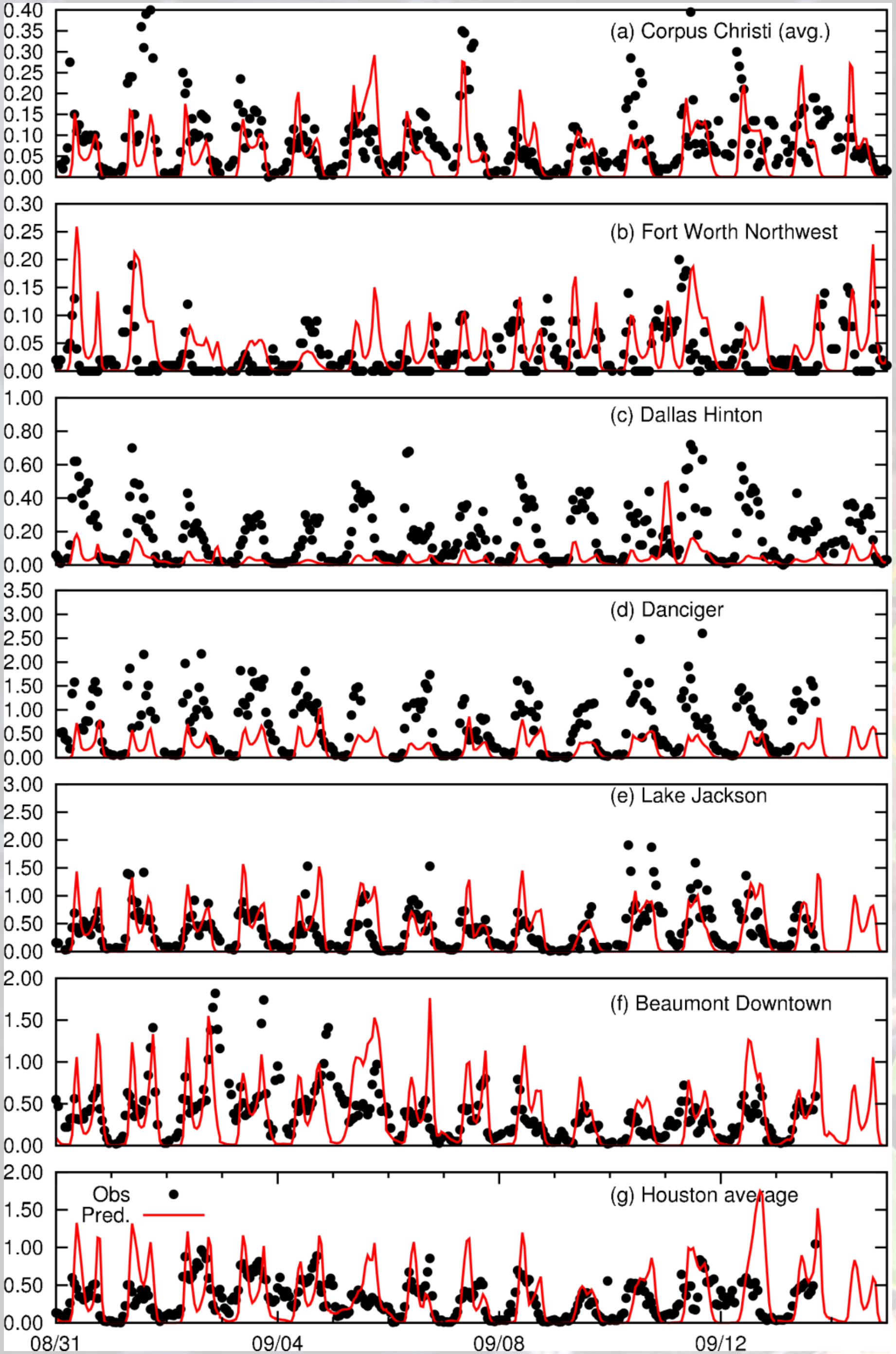
Isoprene over-prediction during TexAQS 2006

Site	MNB[*]	MNE	Biogenic (%)[#]
Beaumont	6.17 (7.74)[^]	6.28 (7.74)	74
Cesar Chavez	3.79 (4.67)	3.96 (4.69)	67
Deer Park	2.94 (3.65)	3.21 (3.72)	71
Clinton	1.87 (2.02)	2.19 (2.23)	85
Milby Park	3.31 (3.70)	3.48 (3.76)	75
Channelview	4.78 (5.50)	4.48 (5.51)	75
HRM3	2.77 (3.14)	2.99 (3.21)	80
LakeJackson	6.15 (6.27)	6.40 (6.51)	98
Danciger	2.78 (2.84)	3.01 (3.05)	98

Kota et al. , Atmospheric Environment, 110, 54-64, 2015



Kota et al. , Atmospheric Environment, 110, 54-64, 2015



BEIS 3.14 predicts reasonable isoprene concentrations during TexAQS 2006

Ying et al. (2015)
Env. Sci. and Tech., Accepted

Ozone Model Performance (SM case)

Month	MNB (±0.15)	MNE (<0.30)	Np[1]	APP	AAPP	AUP (±0.20)	AAUP	Np[2]
April	-0.13	0.14	2470	-0.14	0.15	-0.09	0.12	458
May	-0.10	0.13	1900	-0.12	0.14	-0.06	0.11	375
June	-0.08	0.17	2147	-0.17	0.21	0.01	0.13	439
July	-0.04	0.15	1422	-0.09	0.17	0.04	0.15	342
August	-0.06	0.16	4903	-0.08	0.17	0.03	0.17	718
September	-0.16	0.19	6293	-0.18	0.21	-0.11	0.17	989
October	-0.12	0.14	1981	-0.13	0.16	-0.08	0.13	444

$$\mathrm{APP} = \frac{C_{p,opeak} - C_{o,opeak}}{C_{o,opeak}}$$

Accuracy of paired peak

$$\mathrm{AUP} = \frac{C_{p,ppeak} - C_{o,opeak}}{C_{o,opeak}}$$

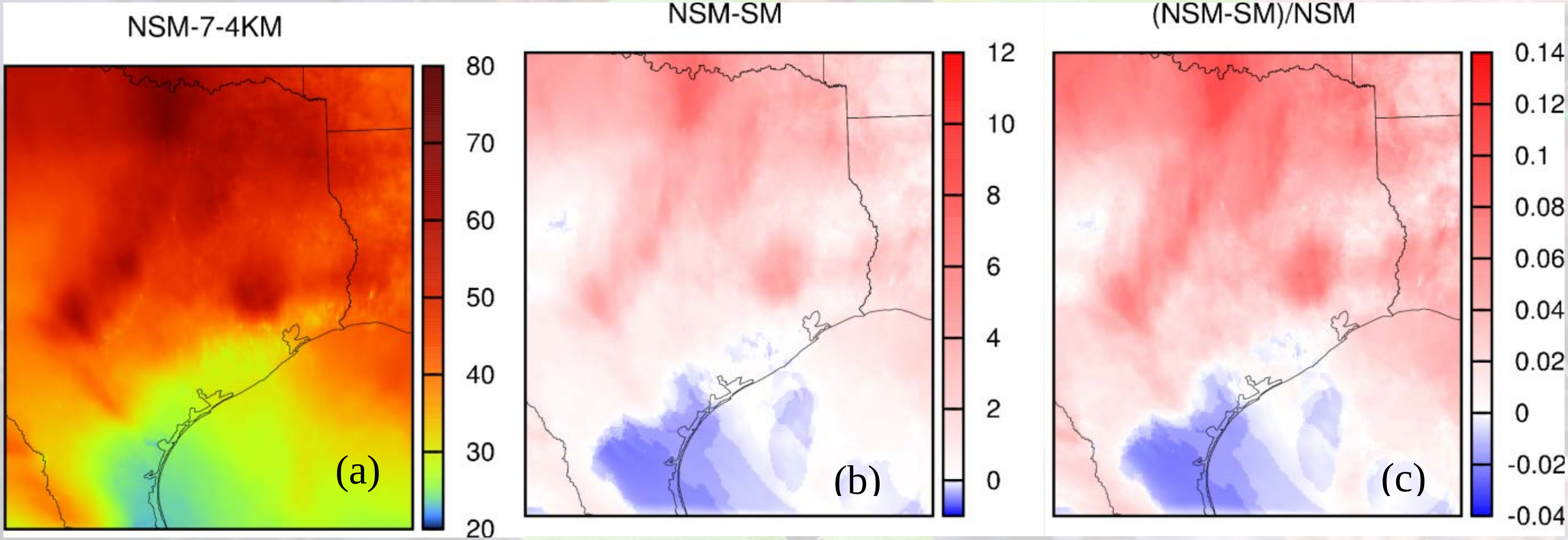
Accuracy of un-paired peak

$$\mathrm{MNB} = \frac{1}{N}\sum_{i=1}^{N}\frac{C_{m,i} - C_{o,i}}{C_{o,i}}$$

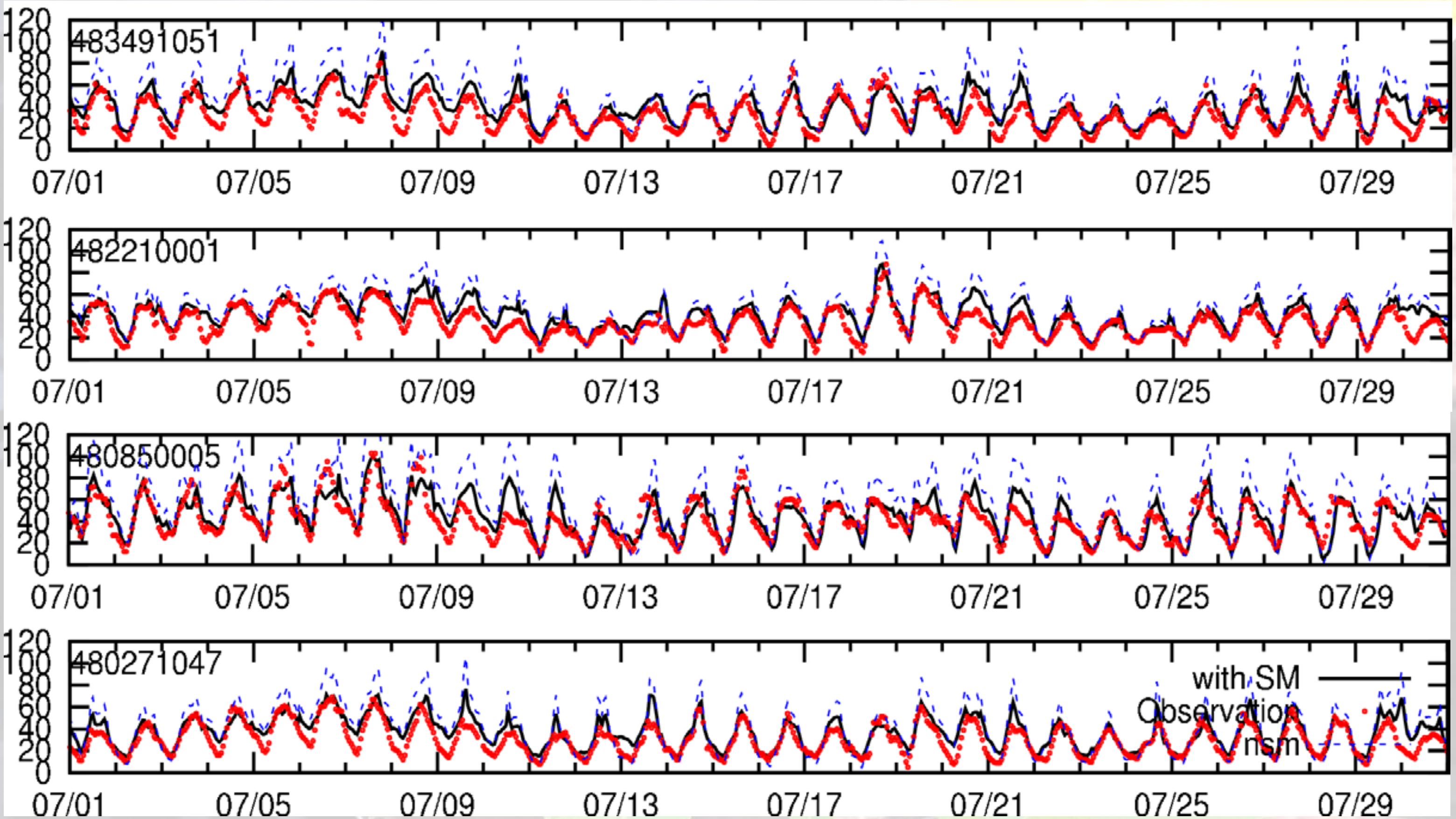
Mean Normalized Bias

Effect of soil moisture on 1-h peak ozone concentrations

- July 2011



Improves peak hour ozone performance



	July		August	
	SM	NSM	SM	NSM
APP	-0.09	0.05	-0.08	0.03
AAPP	0.17	0.17	0.17	0.18
AUP	0.04	0.14	0.03	0.15
AAUP	0.15	0.23	0.17	0.23

Conclusions

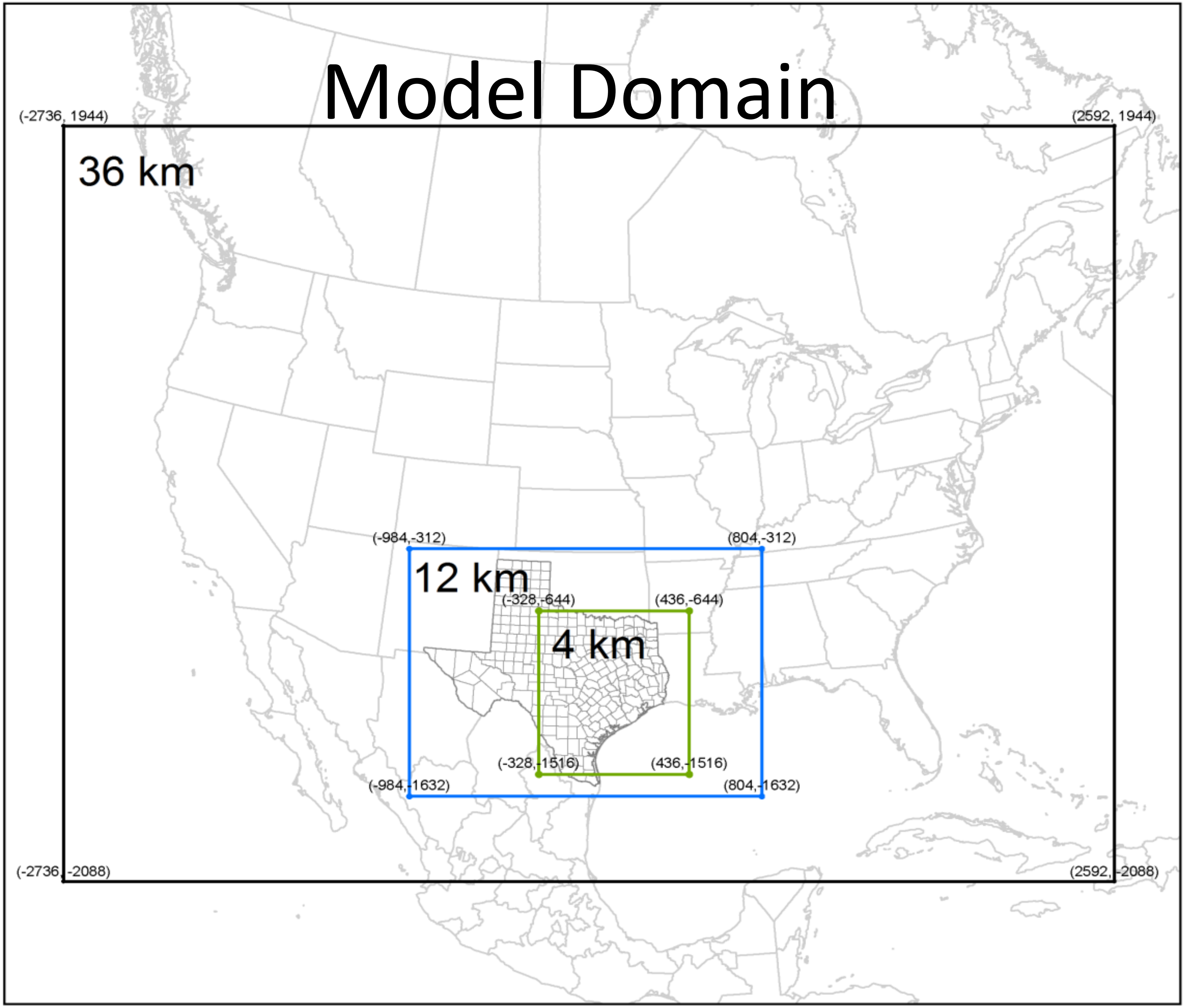
- current soil moisture parametrization is adequate
  - bigger issues with soil moisture itself, and rooting depth
  - soil moisture time series should be smoothed
- default parametrization reduced isoprene emissions during 2011 drought, but did not solve large over-prediction problem with MEGAN
- ozone performance was not significantly affected by isoprene over-prediction
  - but peak ozone performance improved with reduced isoprene emissions

Acknowledgements

PRA Monica Madronich
graduate student Peng Wang

extra slides

Model Domain



CMAQ Model Configuration

- Version 5.0.1
- Gas phase chemical mechanism: CB05 (cb05tucl)
- Aerosol mechanism: AERO6
- Offline biogenic emission using MEGAN v2.10
- Simulation periods: April – October 2007 and 2011. Only 2011 results are discussed here.

WRF simulation

- WRF version: 3.6
  - Land surface scheme: Noah
- 3-level nested domains (36, 12 and 4-km)
- Initialization:
  - Soil moisture: North American Land Data Assimilation System (NLDAS) – Noah Land surface model
  - Sea surface temperature: daily satellite-based observation
  - All other variables: 3-hr North American Regional Reanalysis (NARR) data (32-km resolution)
- Other data:
  - Leaf area index (LAI): 8-day MODIS product, MOD15A2
  - Land use/land cover classification: MOD12Q1
- Two sets of simulations
  - 1-day segments/3-hr spin-up
  - 8-day segments/1-day spin-up

WRF performance

July 2011

	TEMP (K)	**RAINS (mm/h)**	**WSPD (m/s)**	**WDIR (^{o})**	**RH (%)**
avg_obs	304.52	1.26	3.87	166.99	51.46
avg_pre	306.48	0.27	4.03	162.84	44.33
MB	2.05	-1	0.19	-2.97	-7.52
RMSE	3.63	1.77	1.91	64.58	16.28
GE	2.76	1.18	1.5	47.26	12.01

$$\mathrm{MB} = \frac{1}{N}\sum_{i=1}^{N}(C_{m,i} - C_{o,i}) \qquad \mathrm{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(C_{m,i} - C_{o,i})^2} \qquad \mathrm{GE} = \frac{1}{N}\sum_{i=1}^{N}|C_{m,i} - C_{o,i}|$$

Anthropogenic emission processing

- SMOKE v3.5.1
- 2011 NEI v6
  - 4 on-road source sectors: on-network, on-road; on-network, refueling; off-network, fuel-vapor venting; off-network, non-venting
  - 6 point source sectors: EGU peaking units; EGU non-peaking units; off-shore Class 3 CMV and drilling platforms; oil-and-gas extraction; wildfire and prescribed burning; other point sources
  - 7 other non-road and non-point sources