Developmental Activities of Emissions Inputs and Air Quality Modeling Tools for the NOAA National Ozone Forecast Guidance

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ARL Accomplishments in FY2010: Part I

- Yearly emission updates for operational CBIV and Parallel CB05
  - 2008 CEM
  - 2010 projection for EGU point sources
- Improvements of inputs for the Hawaii and Alaksa domains
  - Hawaii domain –Land use/Land cover
  - Alaska domain –Land use/Land cover, OCEAN,
- Emissions Quality Control
  - Mechanism: CBIV and CB05
  - Sources: Area, mobile, and biogenic
  - Domains: CONUS, HI, and AK
  - Other changes: No fire, small fire, CMAQ 4.7
- Weekly discussion of ozone and PM forecasts
  - Evaluation graphics (spatial tile plot, scatter, time series)
  - Identification of good and bad forecast areas

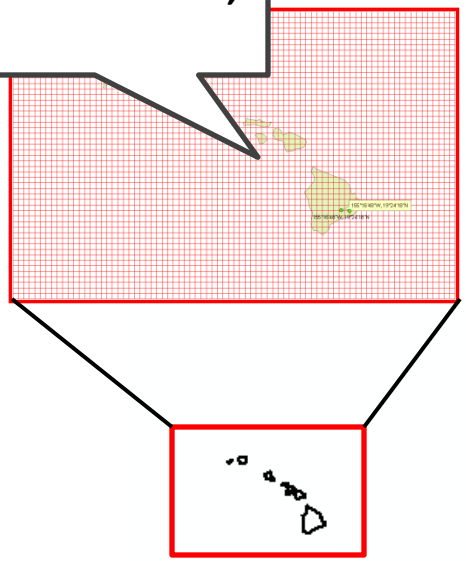
AQFC Emission Updates

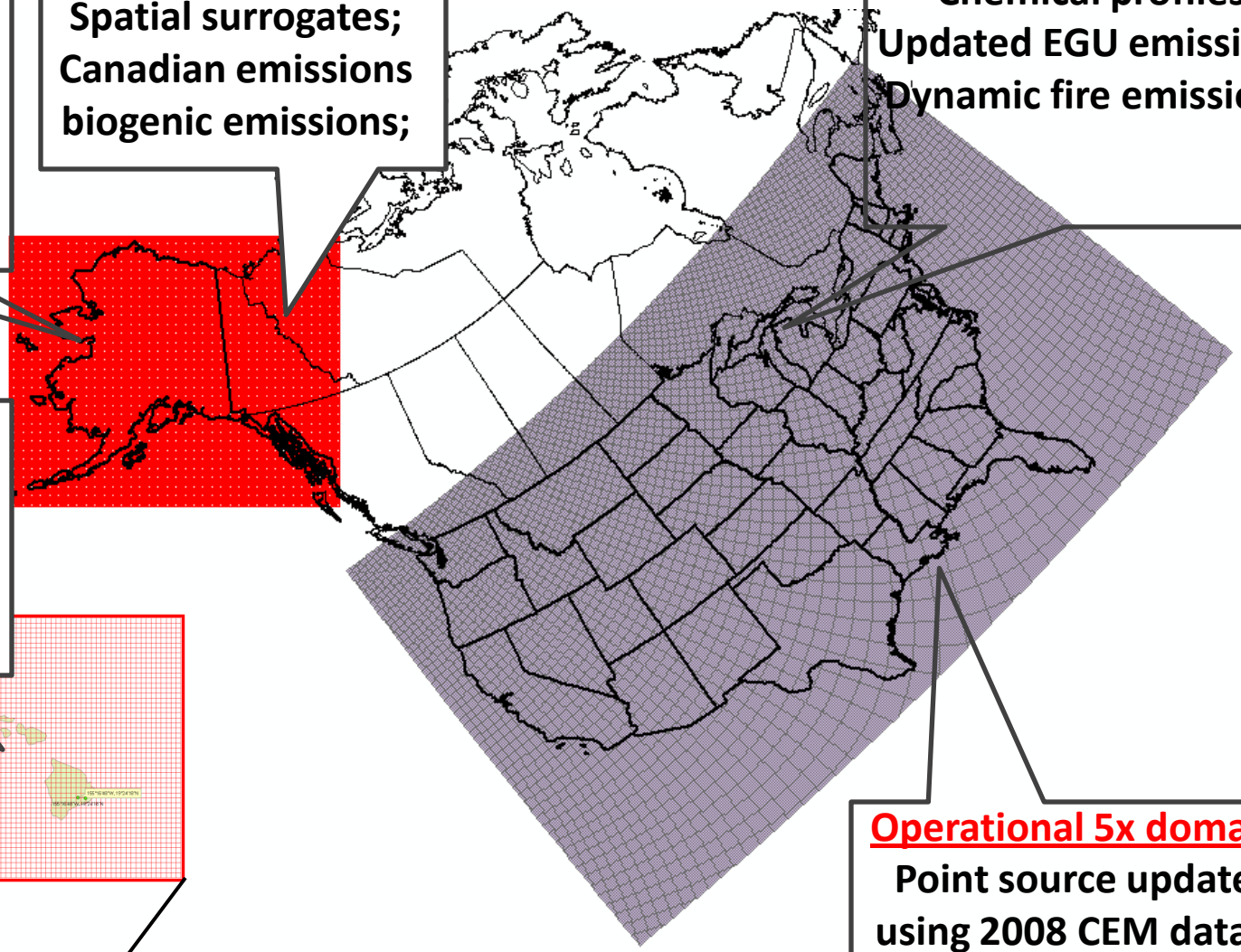
Alaska domain:
BELD dataset;
biogenic emissions;
Sea-salt emissions;
EGU updates;

Spatial surrogates;
Canadian emissions
biogenic emissions;

Experimental 5x :
SMOKE updated to v2.6;
Chemical profiles;
Updated EGU emissions;
Dynamic fire emissions;

Hawaii domain:
BELD dataset;
biogenic emissions;
Sea-salt emissions;





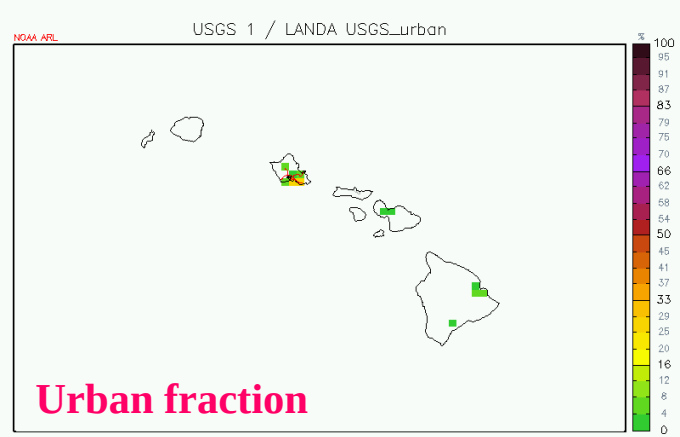
Operational 5x domain:
Point source updates
using 2008 CEM data &
2010 EGU projection

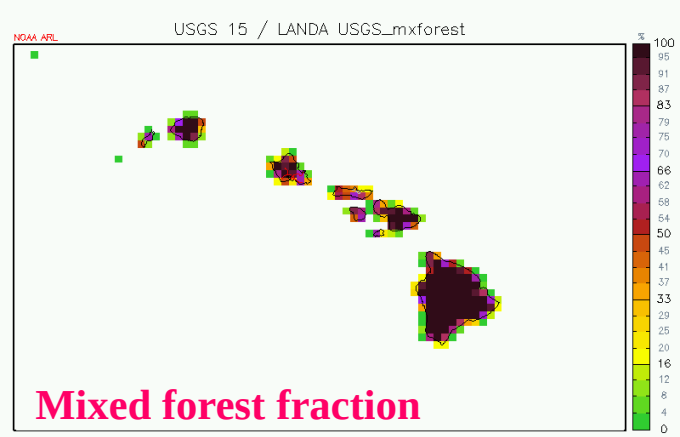
Land Use Land Cover (LULC) in HI domain

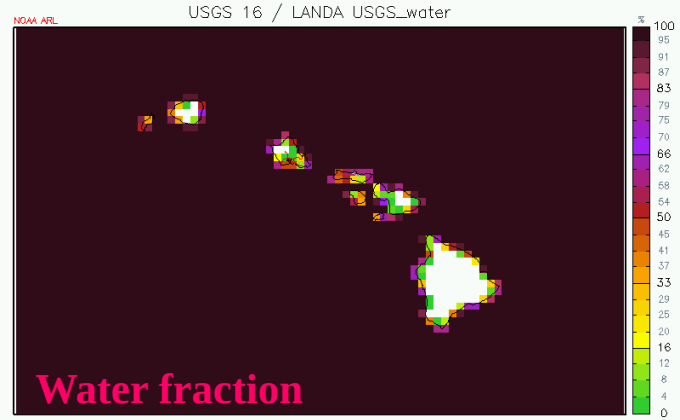
- USGS 30s vegetation type data is used to process LULC in HI
- 3 dominant LULC in Hawaii are water, mixed forest, and urban
- LAND* files are used to generate land sea mask and biogenic emission

Mapping from USGS to LAND* files

	A	B	C	D	E	F	G	H	I
1		USGS			LANDA file			LAND_TOTAL file	
2	1	urban		1	USGS_urban				
3	2	dryland cropland and pasture		2	USGS_drycrop		6	AGRICULTURE	
4	3	irrigated cropland and pasture		3	USGS_irrcrop				
5	4	mixed dry/irrigated cropland and pasture							
6	5	cropland/grassland		4	USGS_cropgrass				
7	6	cropland/woodland		5	USGS_cropwdlnd				
8	7	grassland		6	USGS_grassland				
9	8	shrubland		7	USGS_shrubland				
10	9	mixed shrubland/grassland		8	USGS_shrubgrass				
11	10	savanna		9	USGS_savanna				
12	11	deciduous braodleaf forest		10	USGS_decidforest		5	FOREST	
13	12	deciduous needleleaf forest							
14	13	evergreen broadleaf		11	USGS_evbrdleaf				
15	14	evergreen needleleaf		12	USGS_coniferfor				
16	15	mixed forest		13	USGS_mxforest				
17	16	water bodies		14	USGS_water				
18	17	herbaceous wetland							
19	18	wooden wetland		15	USGS_wetwoods				
20	19	barren or sparsely vegetated		16	USGS_sprsbarren				
21	20	herbaceous tundra							
22	21	wooded tundra		17	USGS_woodtundr				
23	22	mixed tundra		18	USGS_mxtundra				
24	23	bare ground tundra							
25	24	snow or ice		19	USGS_snowice				
26									



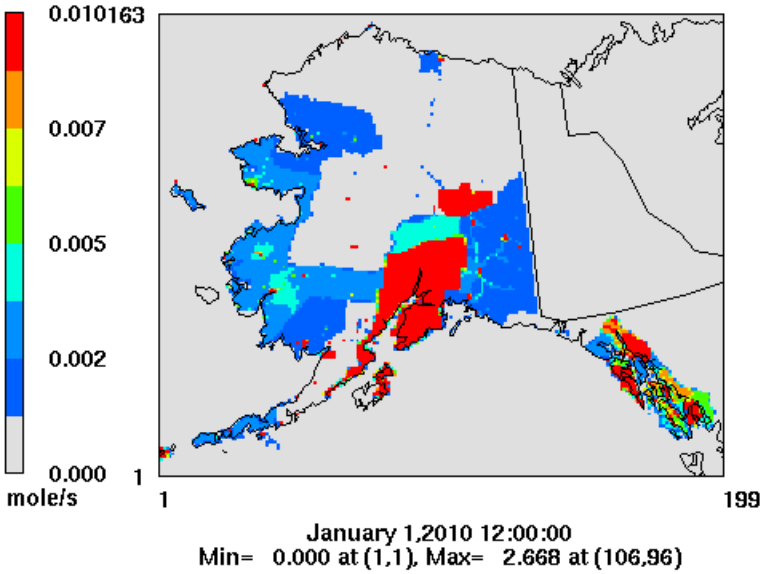


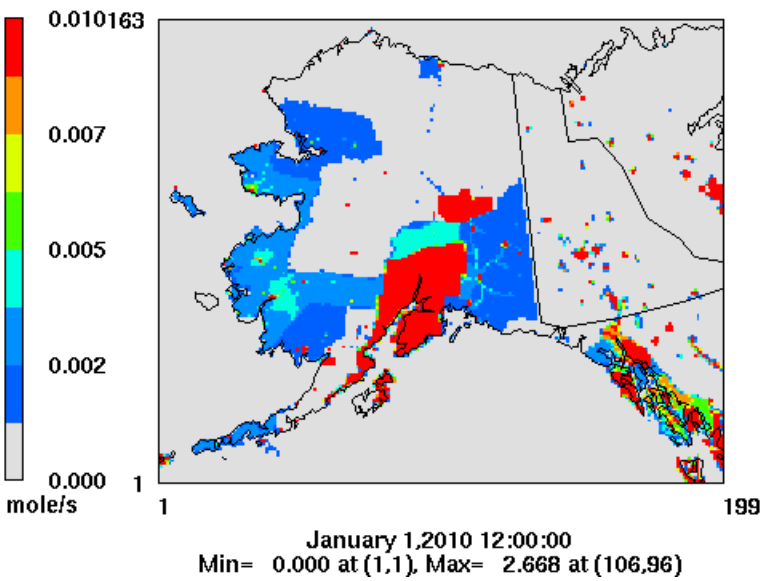


Updated Biogenic and Canadian Anthropogenic Emissions for the Alaska domain

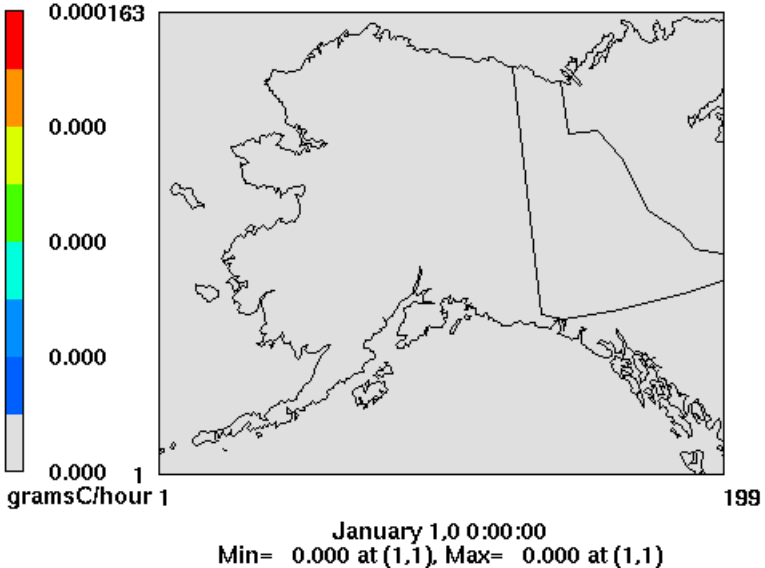
Prototype | **Updated**

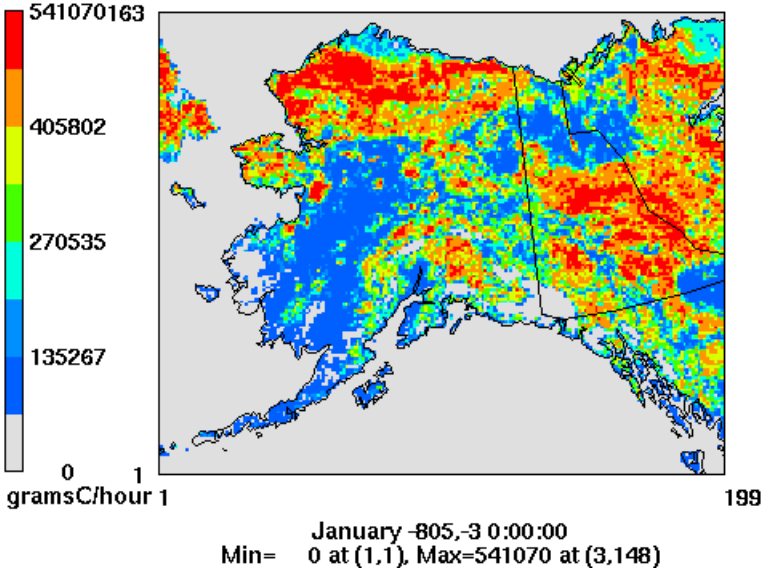
Area





Biogenic

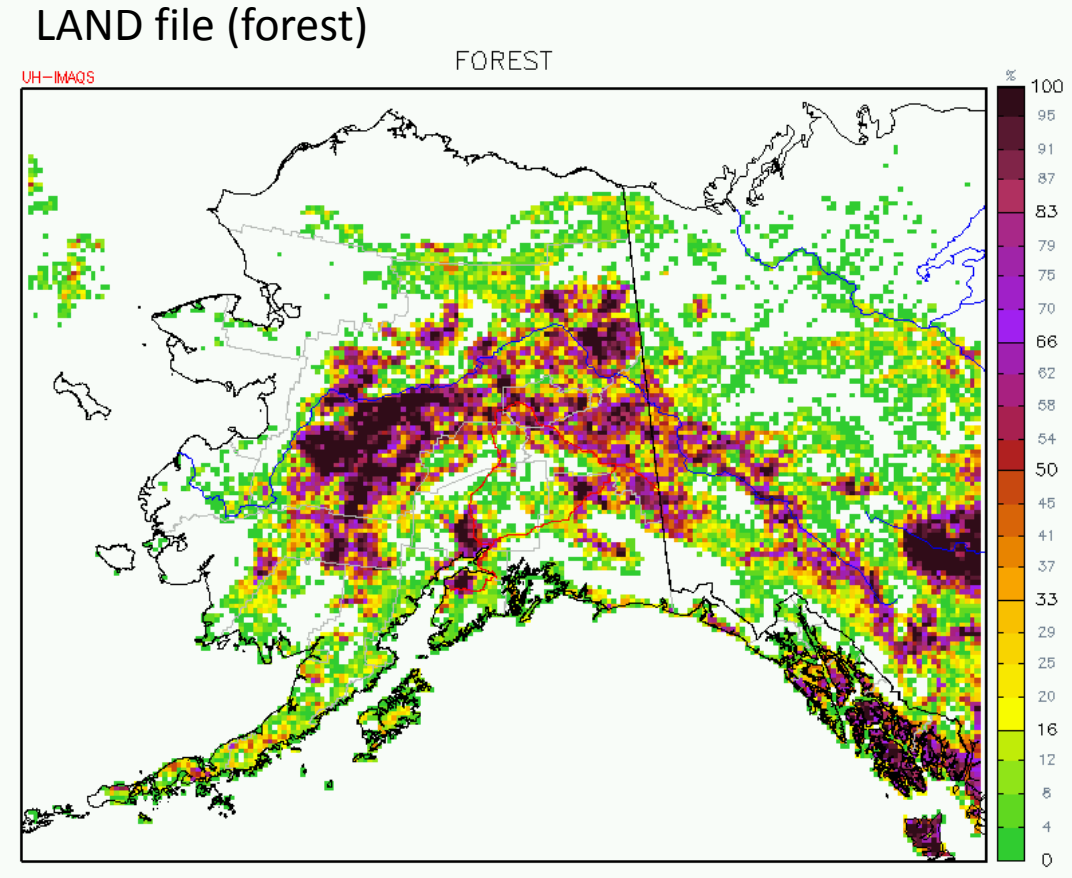




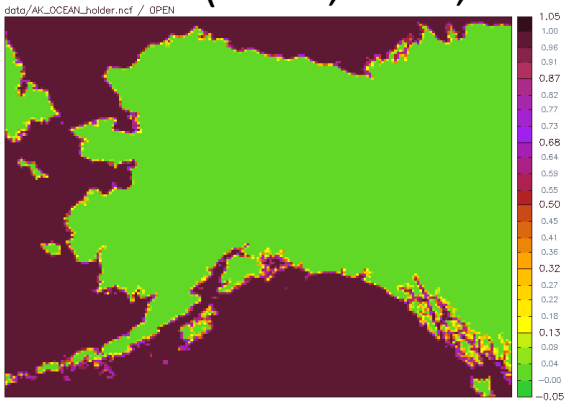
Alaska (AK) domain

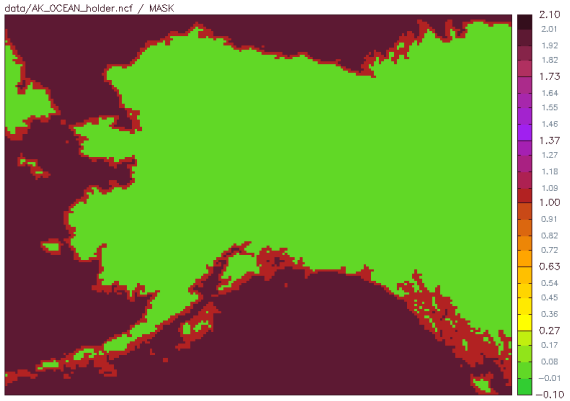
LAND* files and OCEAN files were updated with USGS LULC (global 1km resolution)

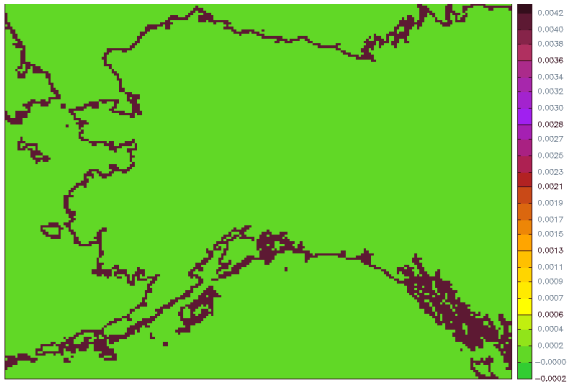
LAND file (forest)



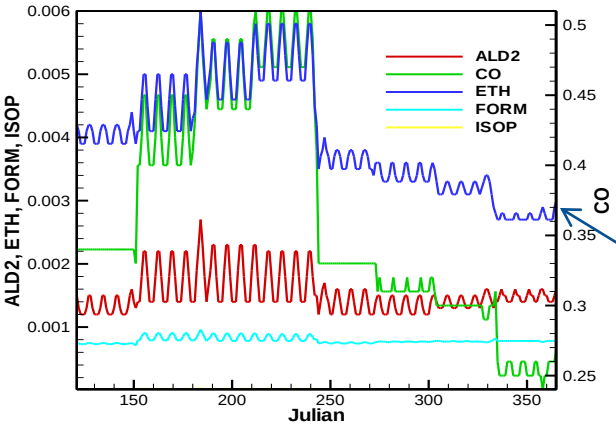
Ocean file (OPEN,MASK,SURF)

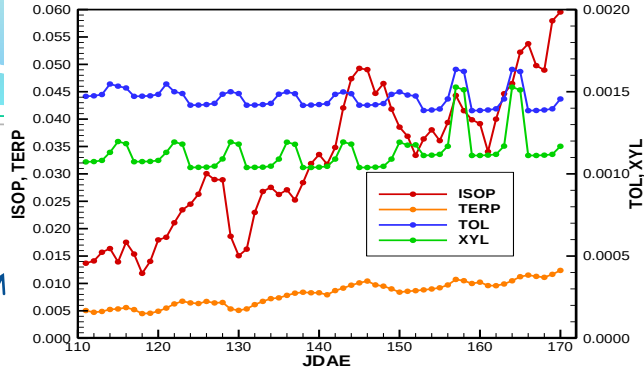






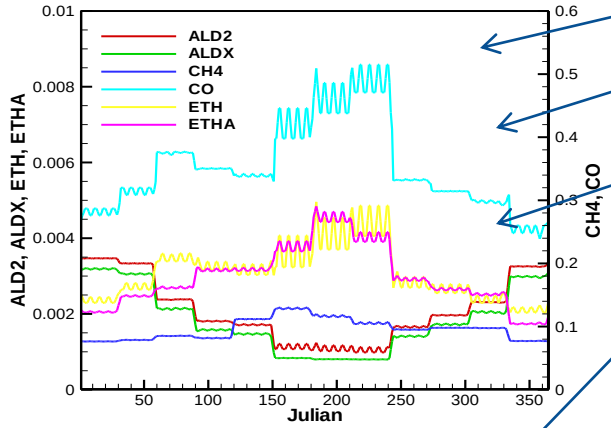
Quality Control of Emissions Data



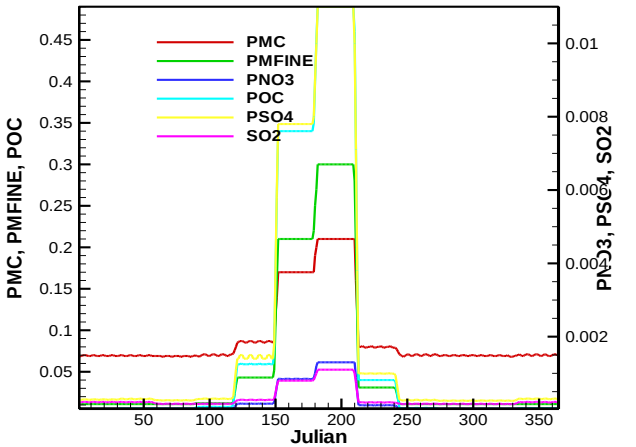


- Mechanism:
  CBIV and CB05
- Sources:
  Area, mobile, and biogenic
- Regions:
  CONUS, HI, and AK
- Others:
  No fire, small fire, CMAQ 4.7

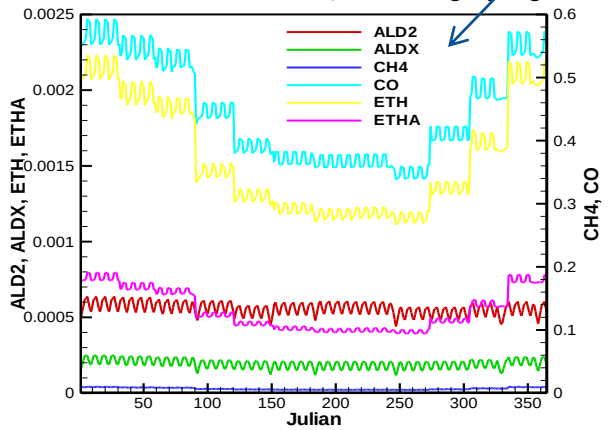
2010 CB05 area emission, mole/s or g/s per grid cell



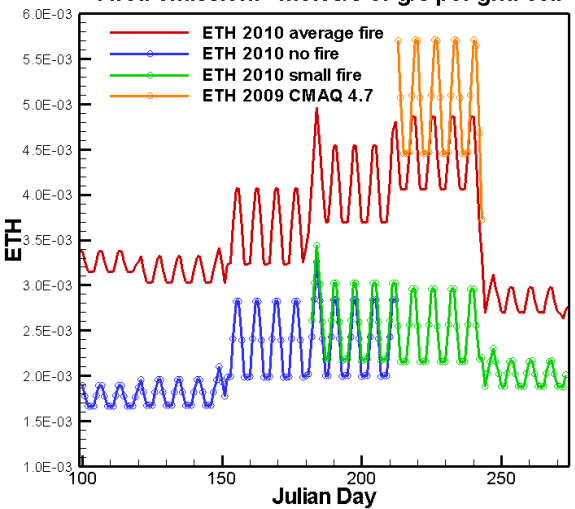
2010 CB05 area emission, mole/s or g/s per grid cell



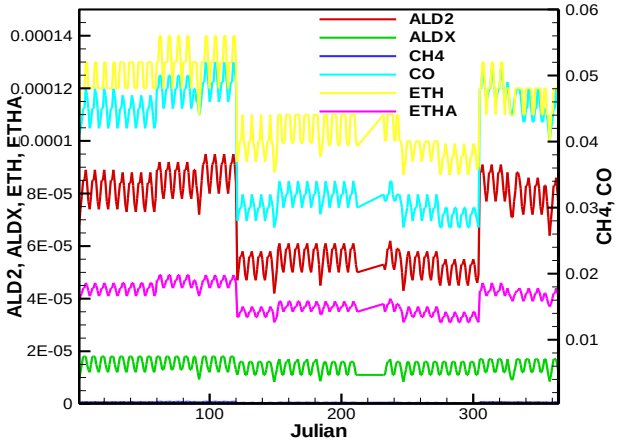
2010 CB05 mobile emission, mole/s or g/s per grid cell



Area emission: moles/s or g/s per grid cell

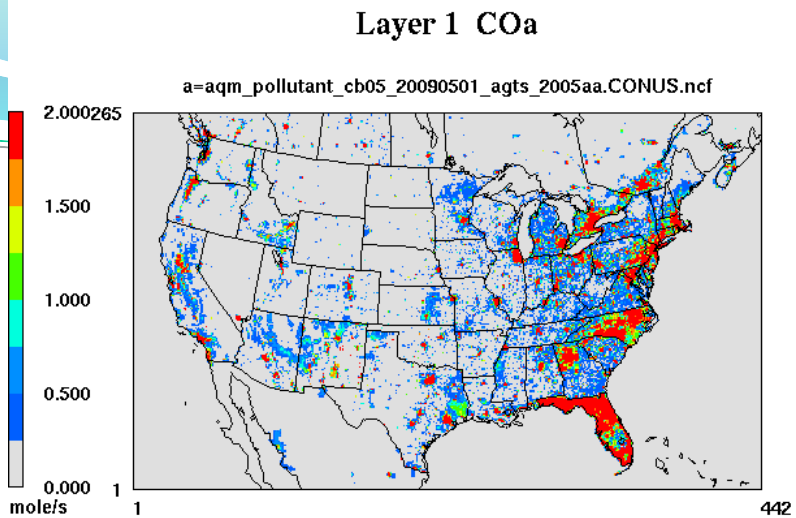


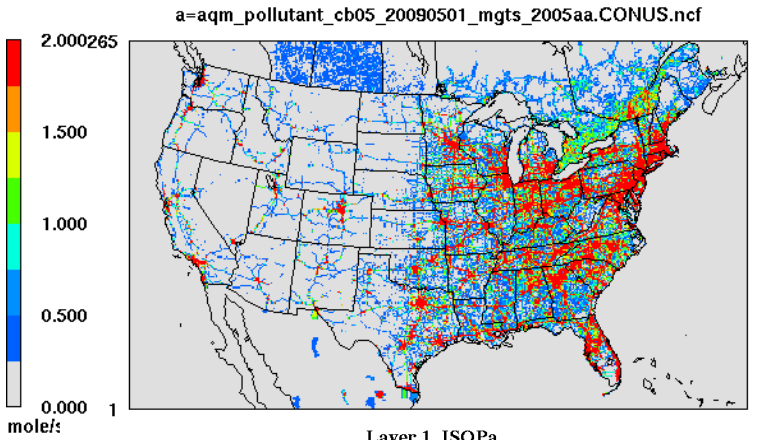
2010 HI CB05 mobile emission, mole/s or g/s per grid cell

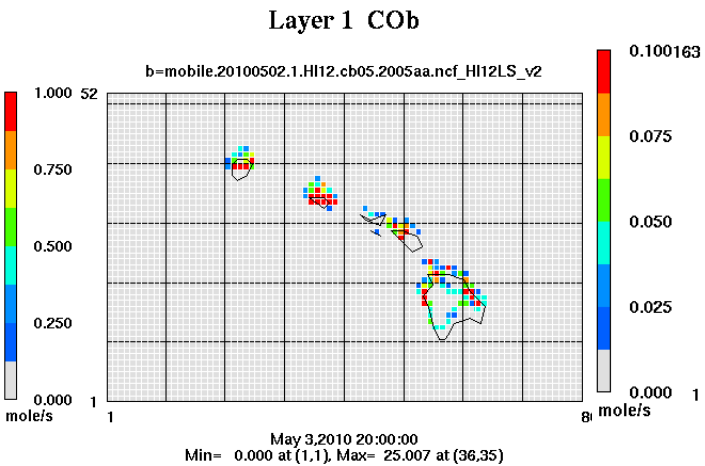


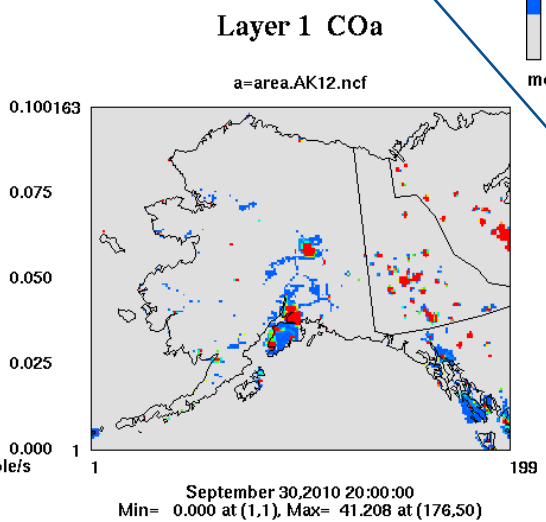
Emissions & Quality Controls

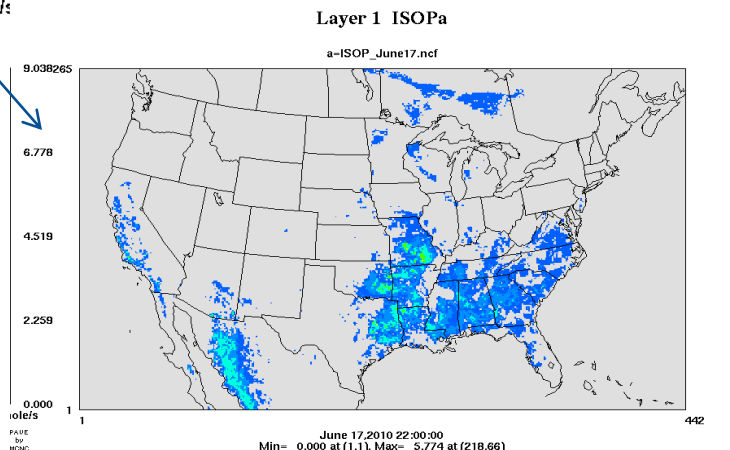
- **Mechanism:**
  CBIV and CB05
- **Sources:**
  Area, mobile, and biogenic
- **Regions:**
  CONUS, HI, and AK
- **Others:**
  No fire, small fire, CMAQ 4.7



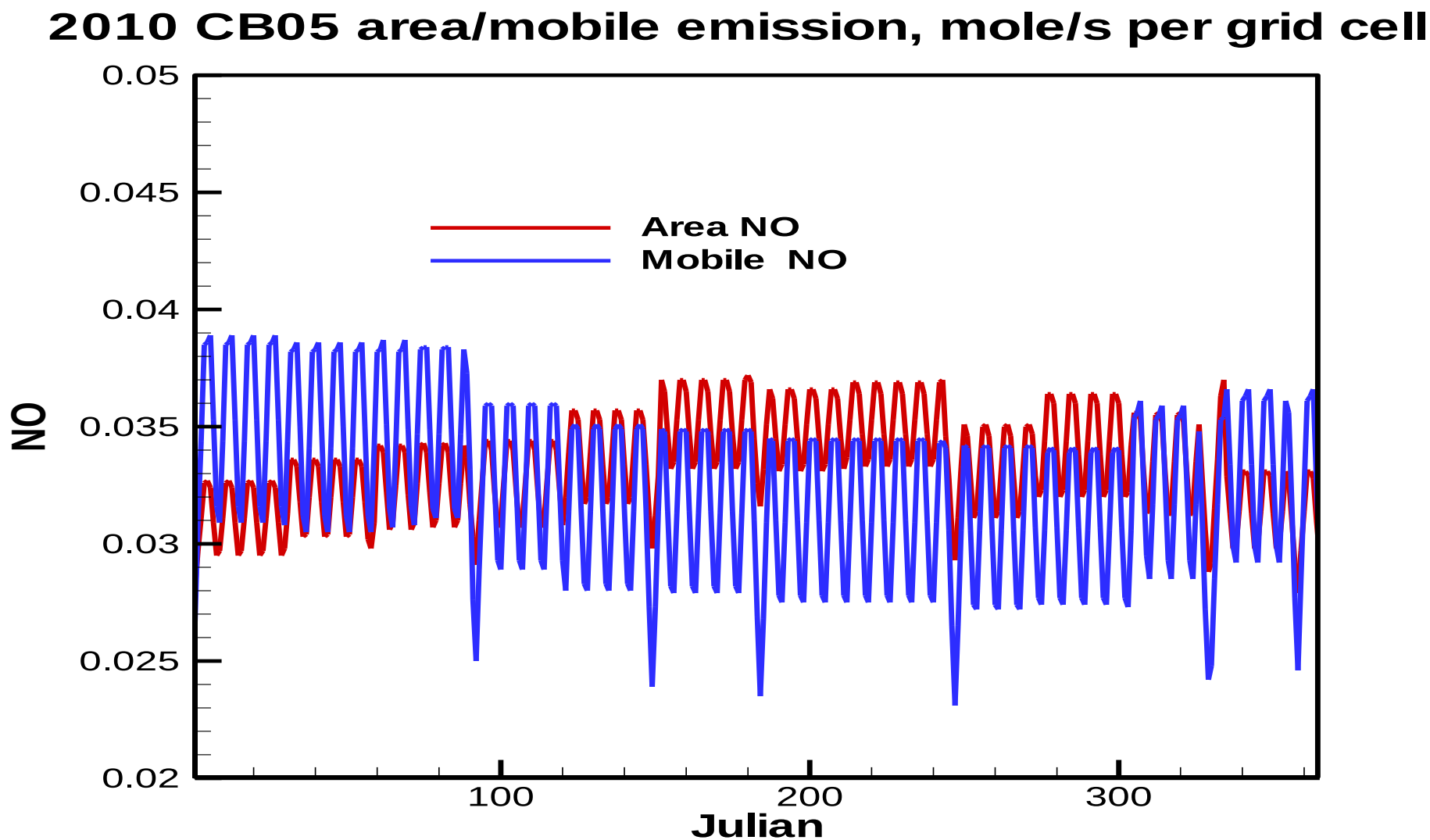




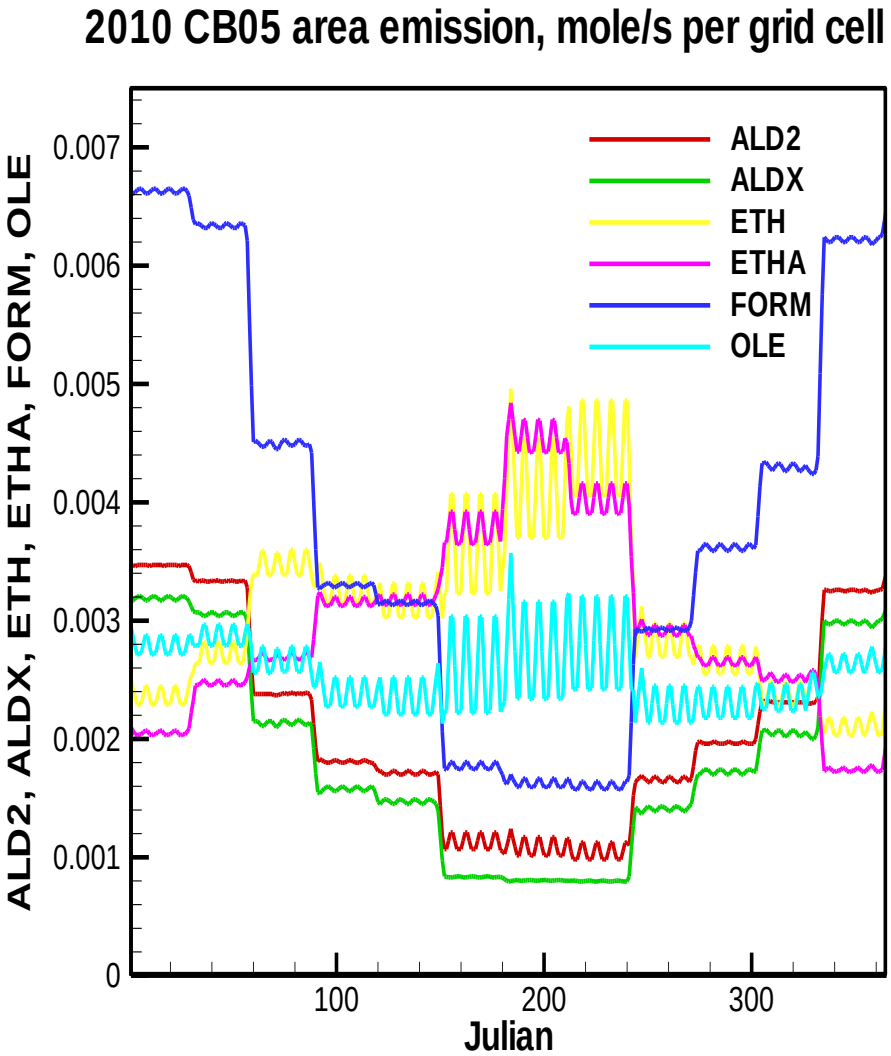


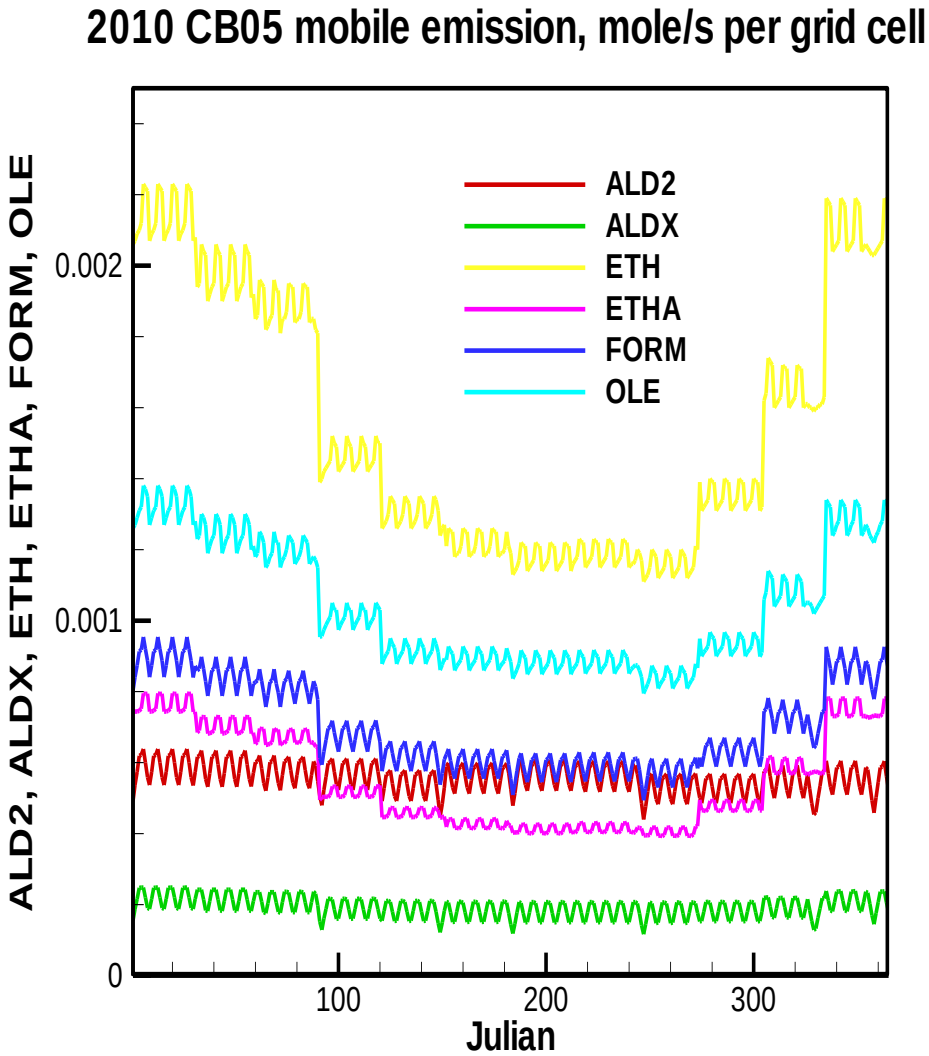


CONUS NO Emissions from Area and mobile sources, NO= 9 × NO_2

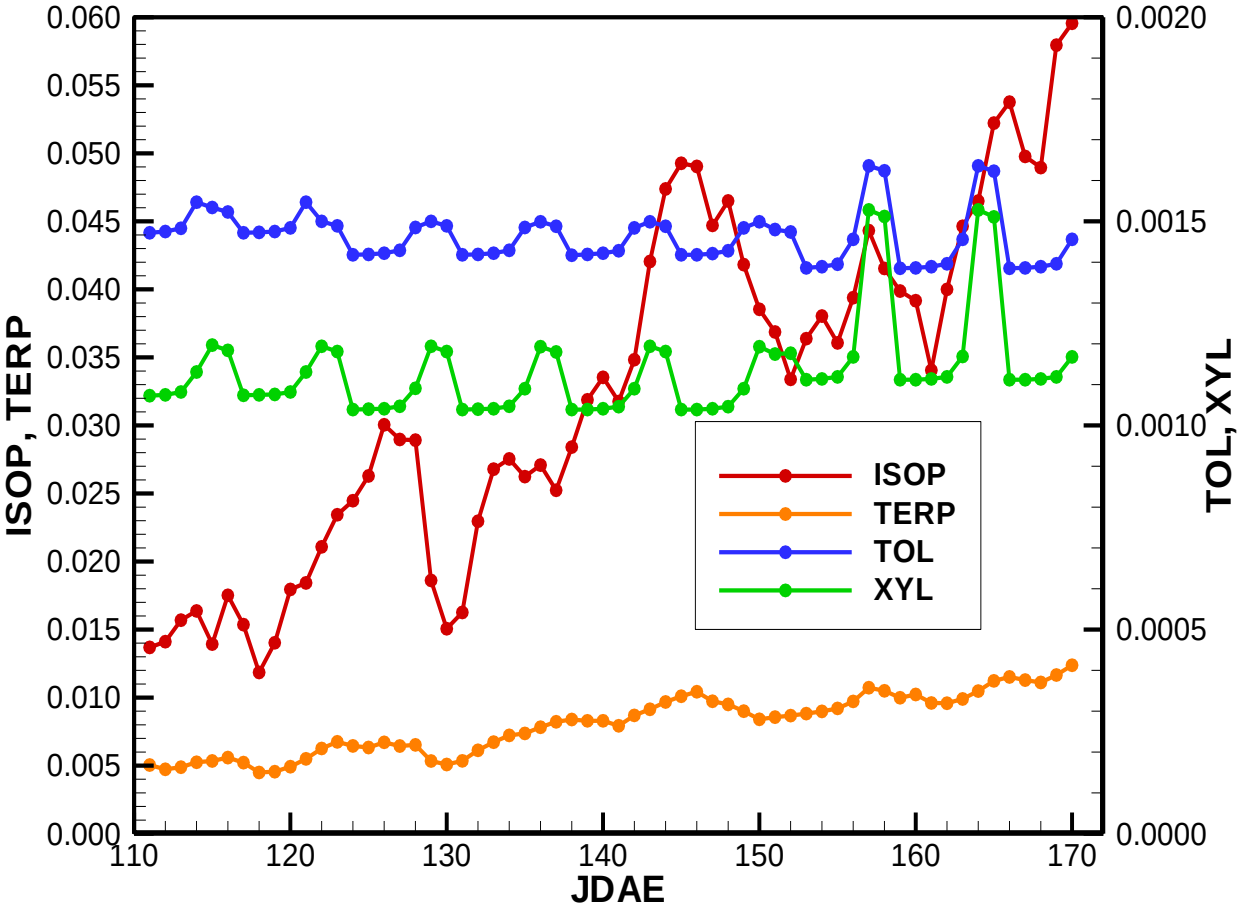


CONUS VOCs from area & mobile sources

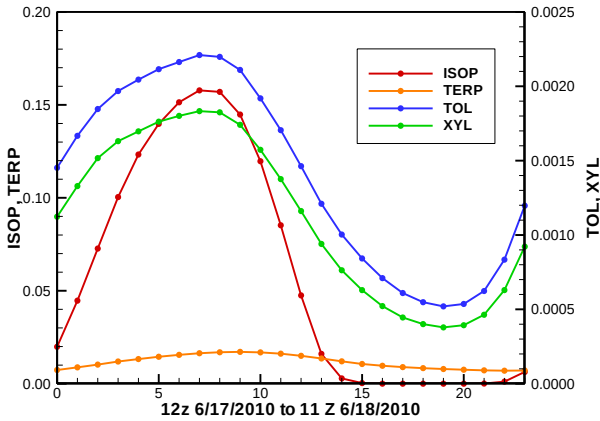




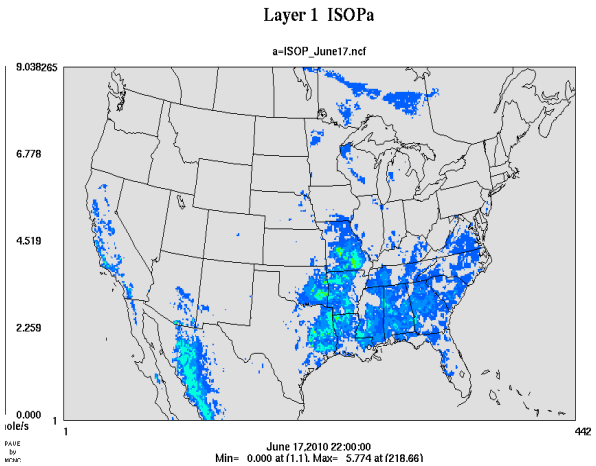
Biogenic Emissions



Daily variations of biogenic emissions from 4/20/2010 to 6/18/2010.



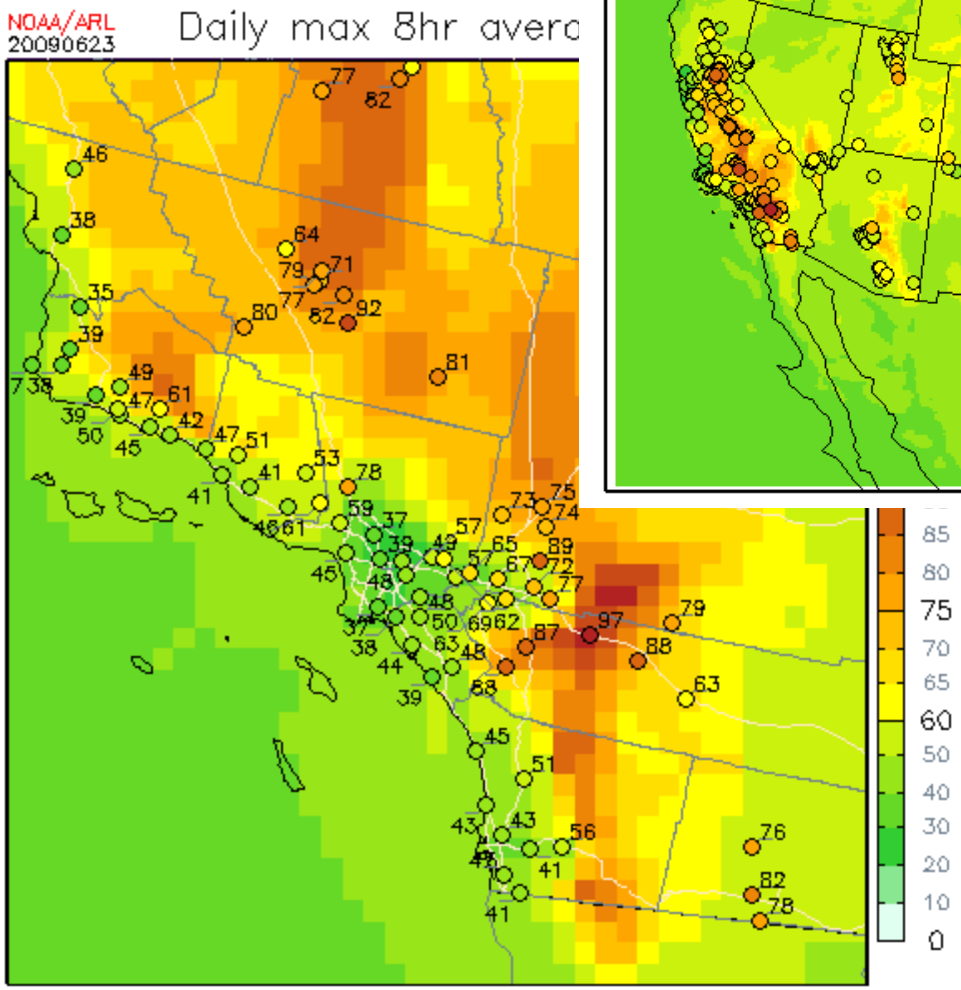
Diurnal variations of biogenic emissions on 6/17/2010

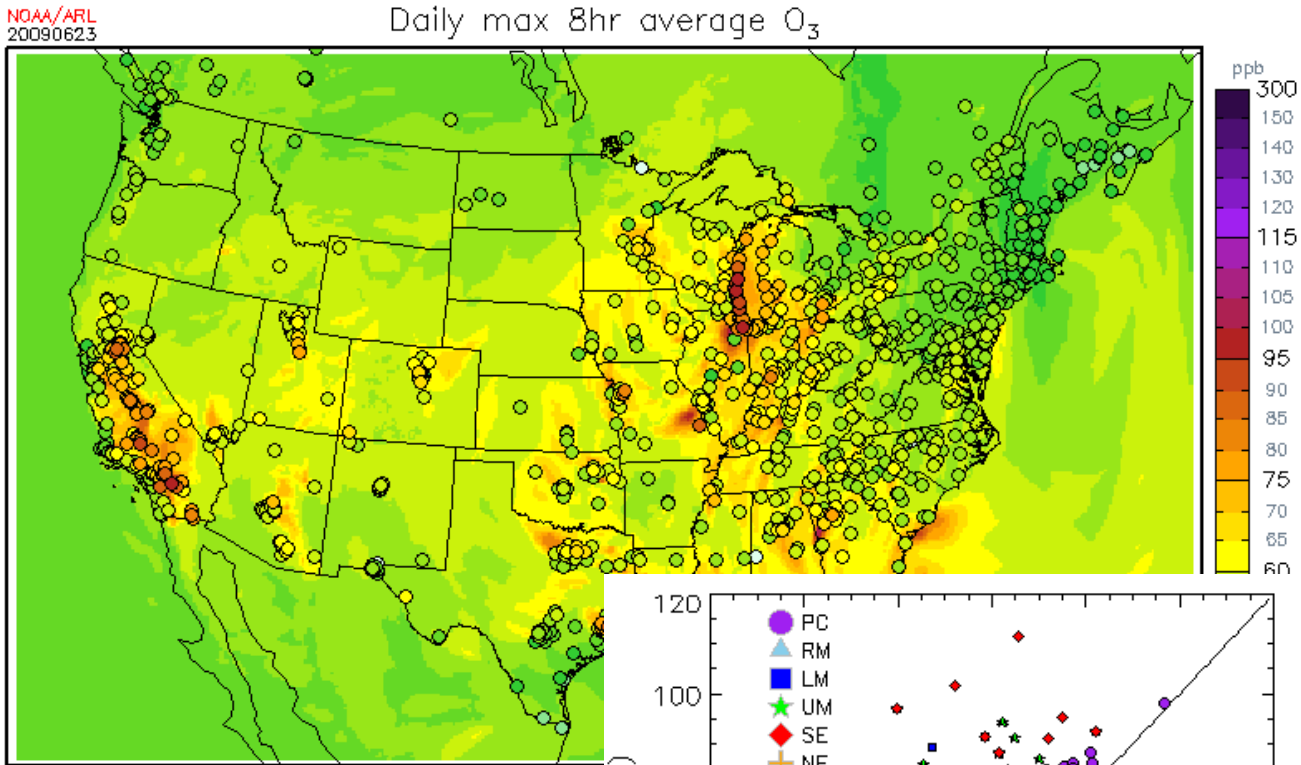


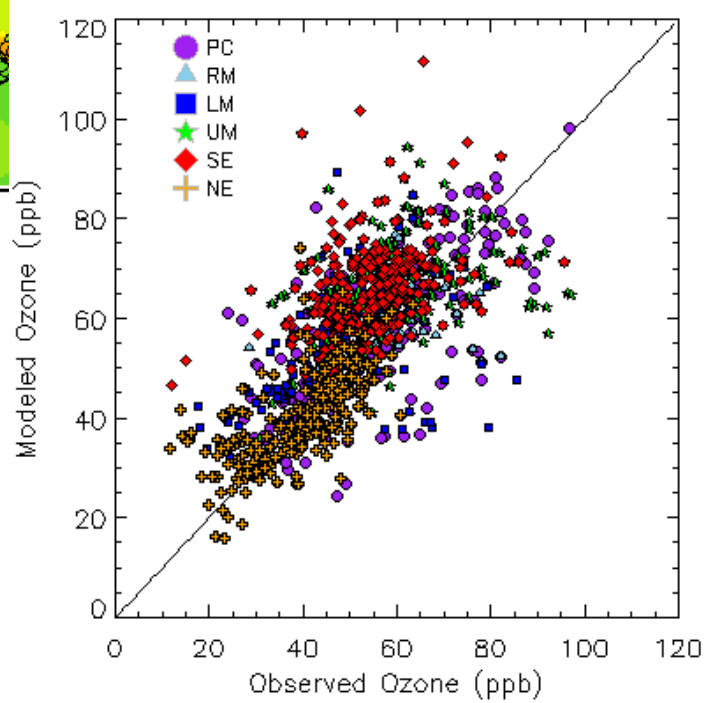
Spatial variations of biogenic emissions of ISOP at 22Z on 6/17/2010.

National Air Quality Forecast & Evaluation

Regional AQ (LA)







ARL Accomplishments in FY2010-Part 2

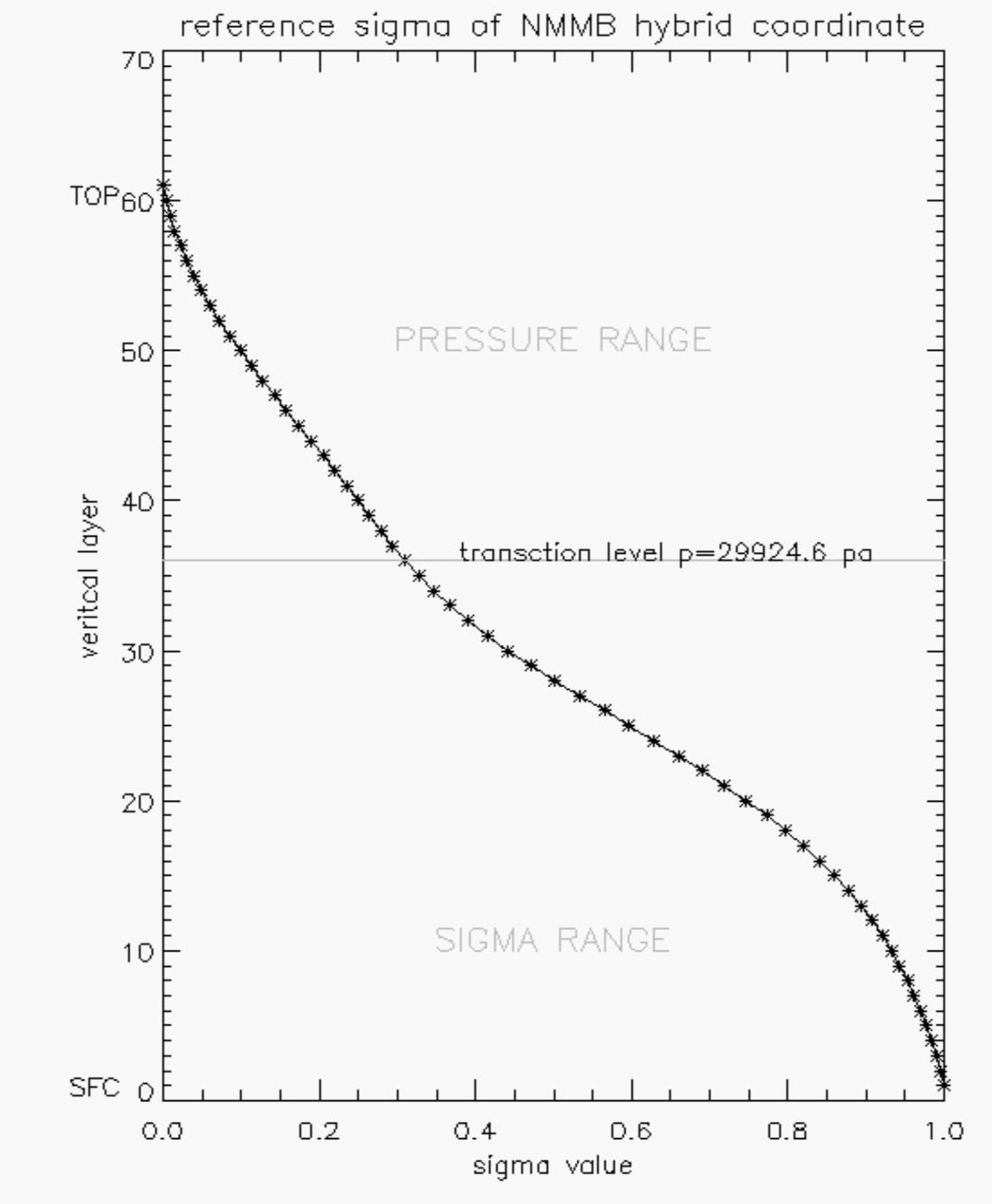
- Adapting CMAQ to NMM-B formulations (PREMAQ/CMAQ)
  - terrain following sigma pressure coordinate – lower part
  - pressure coordinate – upper part
  - Blending of two coordinates utilizing spline curve
  - Generation of Jacobian and contravariant velocity components
- Horizontal mapping
  - Lambert Conformal for production run & experimental run
  - Rotated latitude longitude (RLL) for developmental run (TBD)
  - Development of SMOKE-B (RLL)
- CMAQ versions
  - CMAQ4.6/CB05/AERO4 LCC
  - CMAQ4.7/CB05/AERO5 LCC

Although the vertical structures are similar, the hybrid coordinate system changed from a pure pressure-σ system to a "blended" system

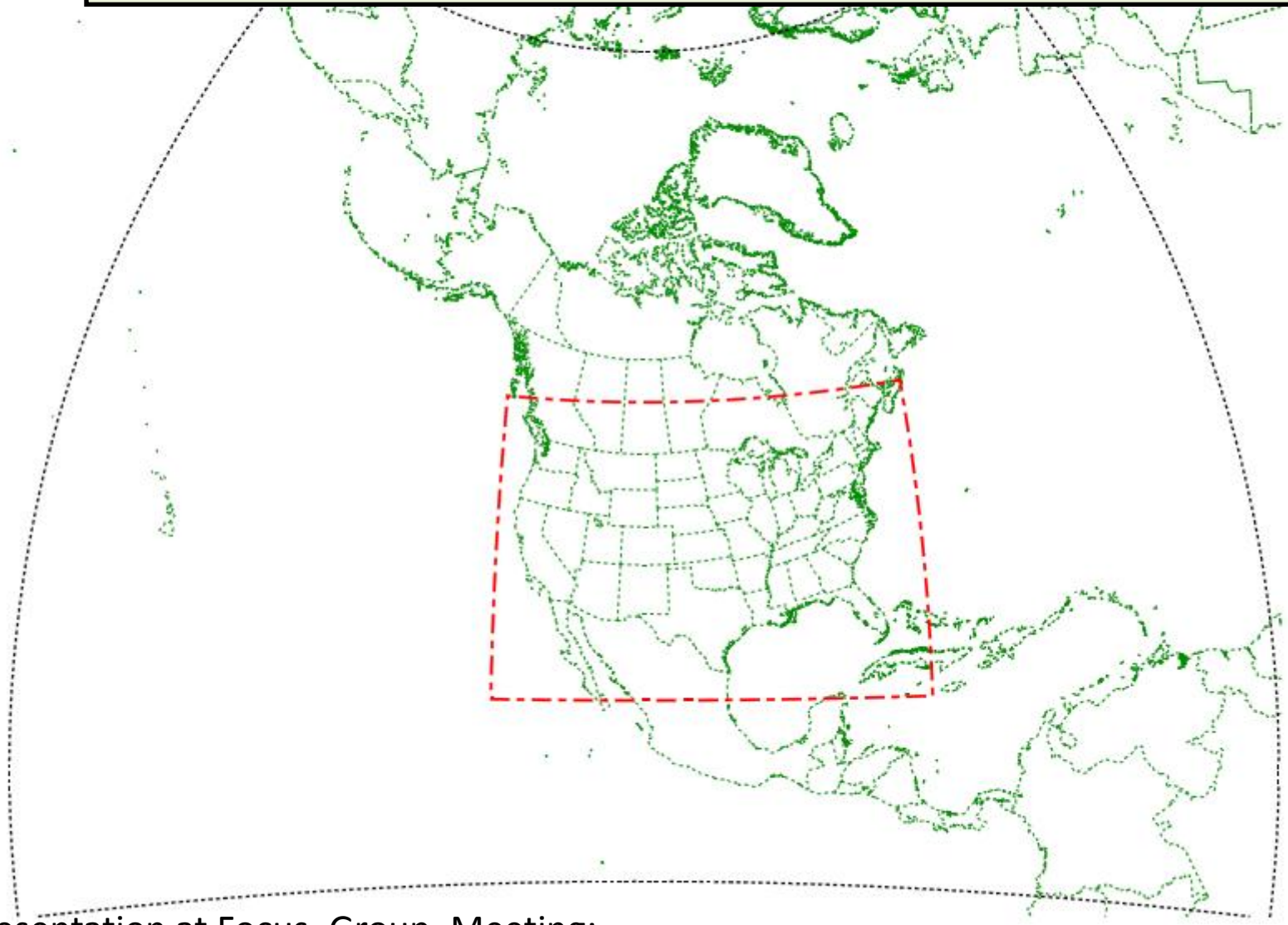
Formulations	WRF-NMM	NMMB
Pressure level	$p_{hydro}(x,y,\sigma\,\vert\,t)=\eta_1(\sigma)\cdot PD_{Top}+\eta_2(\sigma)\cdot PD(x,y\,\vert\,t)+P_T$	
Thickness of upper pressure stratum	$PD_{TOP}=P_{ref}(k_c)-P_T$	
Terrain following stratum *	$PD(x,y\vert t)=P_{sfc}(x,y\vert t)-P_{ref}$	$PD(x,y\vert t)=P_{sfc}(x,y\vert t)-P_T$
Interface between strata $P_{ref}(k_c)$	420 hPa	299 hPa
Model top P_T	2 hPa	
Characteristics of $\eta_1(\sigma)$ and $\eta_2(\sigma)$	Between (0,1), and monotonic increasing	Between (0,2) and not monotonic increasing

New “mixed” hybrid vertical grid structure

In contrary to ops wrf-nmm, the top portion is no longer a sole function of pressure



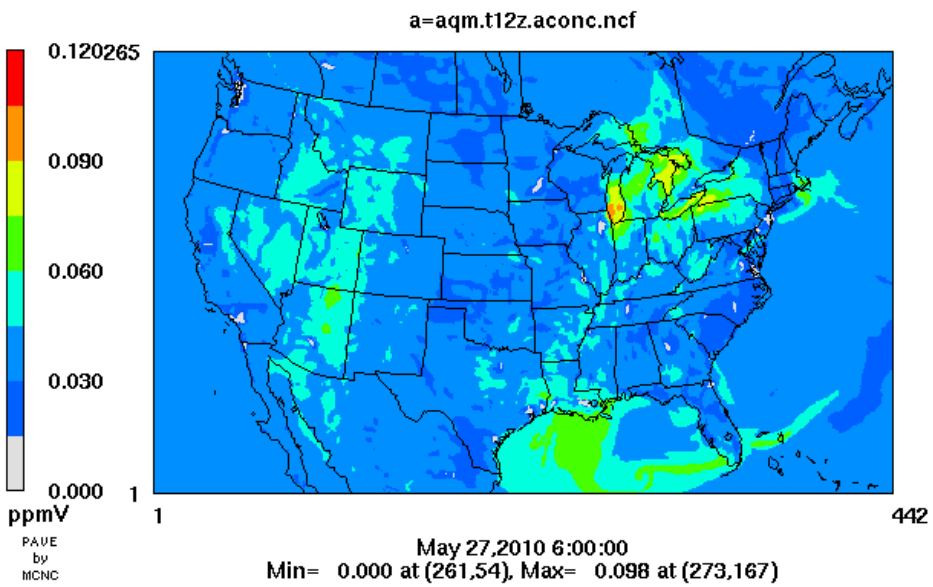
NAQFC CONUS (red) domain within the new NMMB North American Domain (black-dotted)



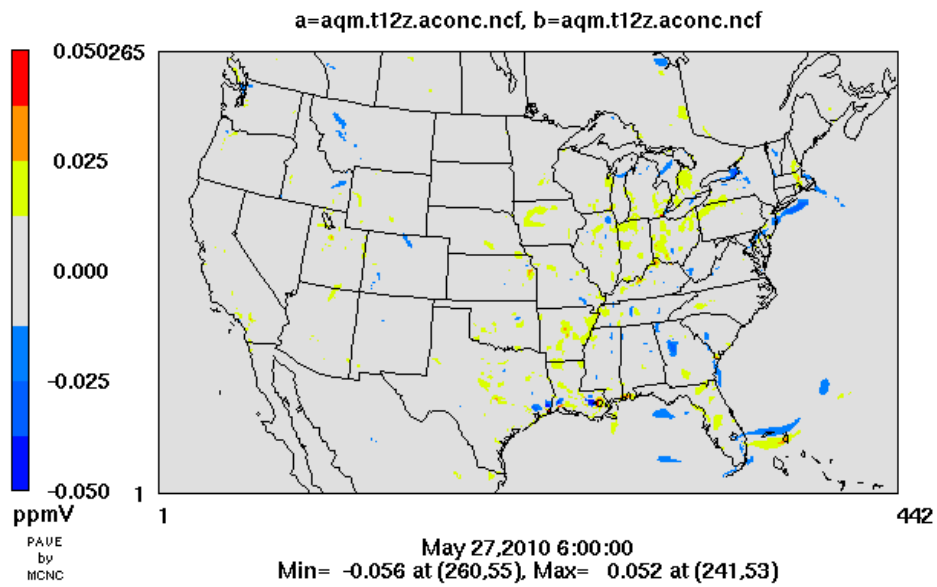
ARL presentation at Focus_Group_Meeting:
September 15, 2010

NMMB Expr-5x run (a) versus Expr run (b) after 42 hr, initialized 12Z May 25th

(a)

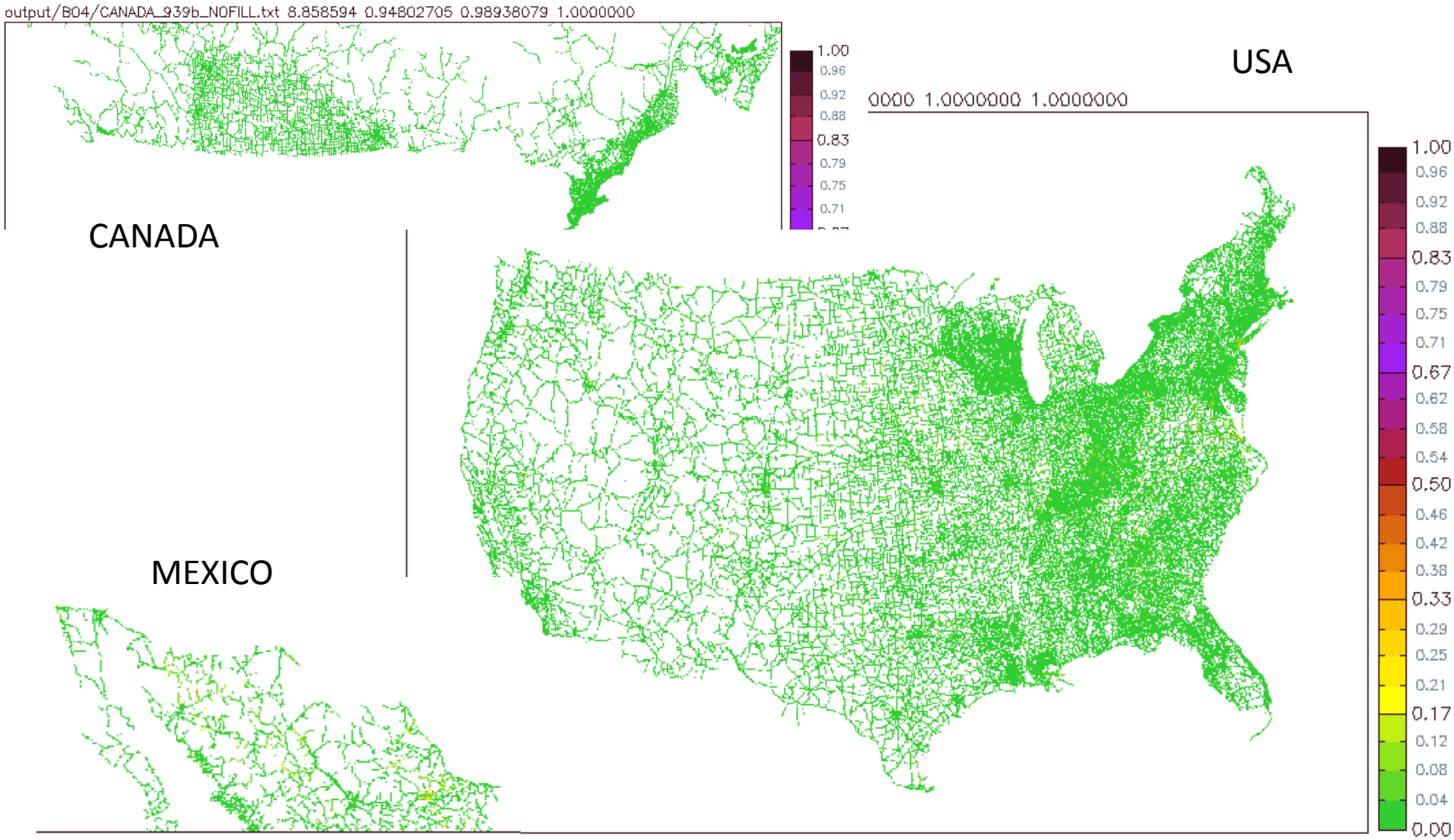


(a - b)



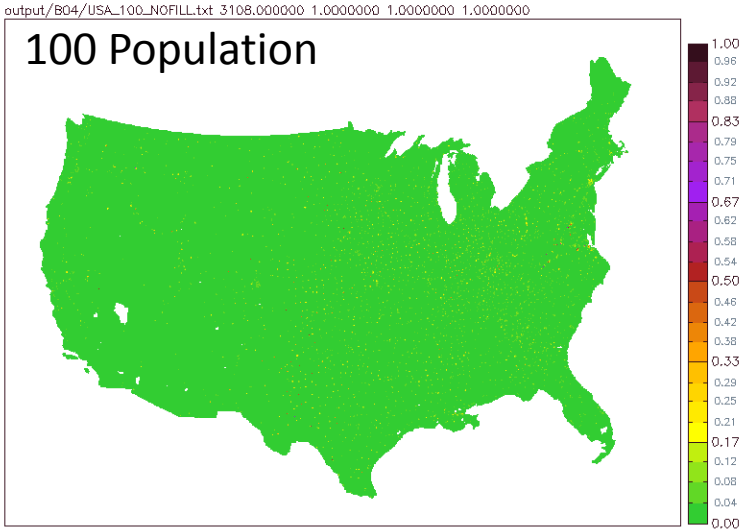
FY11 AQFC Emission Updates

- ✓ Update experimental CB05 run to CMAQ4.7;
- ✓ Update EGU emissions based on CEM 2009 data and DOE 2011 Projection;
- ✓ Remove climatological wildfires and prescribed burning emissions from the currently NEI, and replace them with dynamic fires;
- ✓ Bring online wind-blown dust emissions;
- ✓ Revised anthropogenic dust emissions (paved and unpaved road, construction, agricultural dust, mining and quarrying);
- ✓ Forecast near real-time volcanic emissions for Hawaii;
- ✓ Development of SMOKE-B for rotated lat/lon projectioni;


output/B04/CANADA_939b_NOFILL.txt 8.858594 0.94802705 0.98938079 1.0000000
1.00
0.96
0.92
0.88
0.83
0.79
0.75
0.71
CANADA
USA
0000 1.0000000 1.0000000
1.00
0.96
0.92
0.88
0.83
0.79
0.75
0.71
0.67
0.62
0.58
0.54
0.50
0.46
0.42
0.38
0.33
0.29
0.25
0.21
0.17
0.12
0.08
0.04
0.00
MEXICO

RLL 4km surrogates (examples)

output/B04/USA_100_NOFILL.txt 3108.000000 1.0000000 1.0000000 1.0000000



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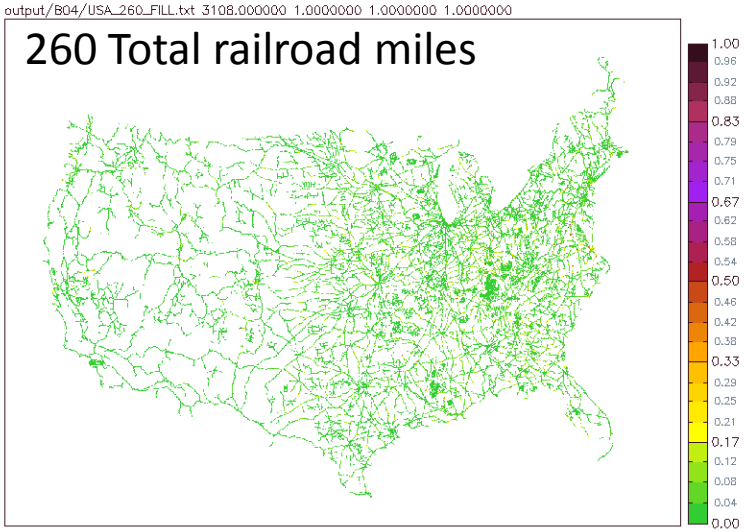

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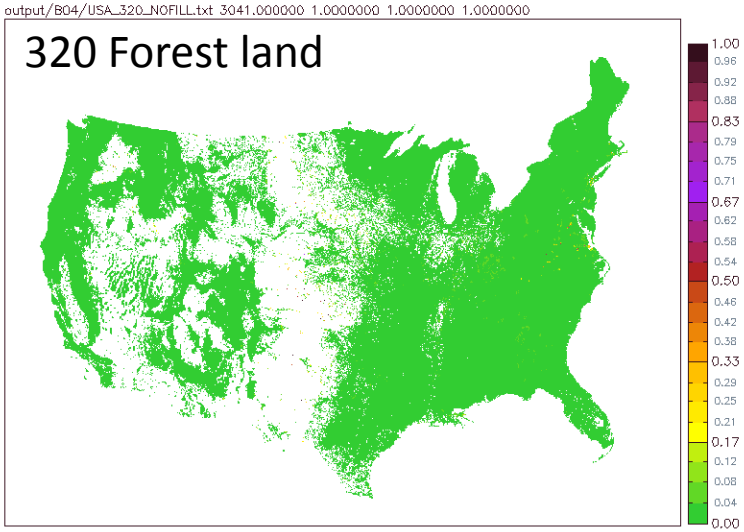

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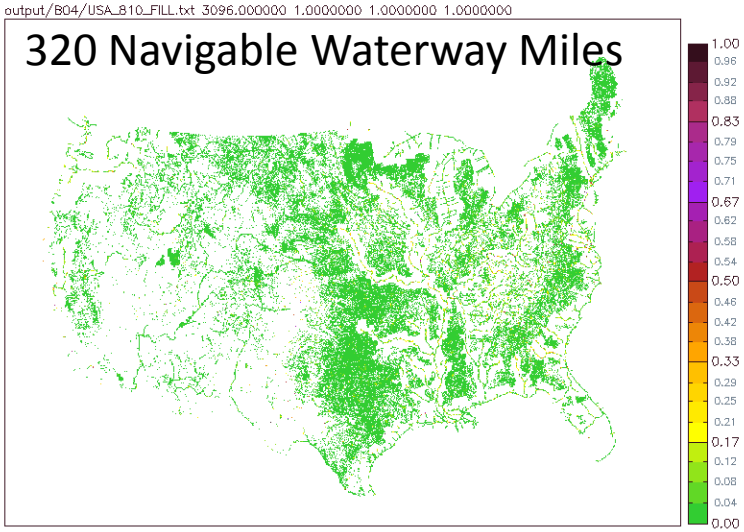
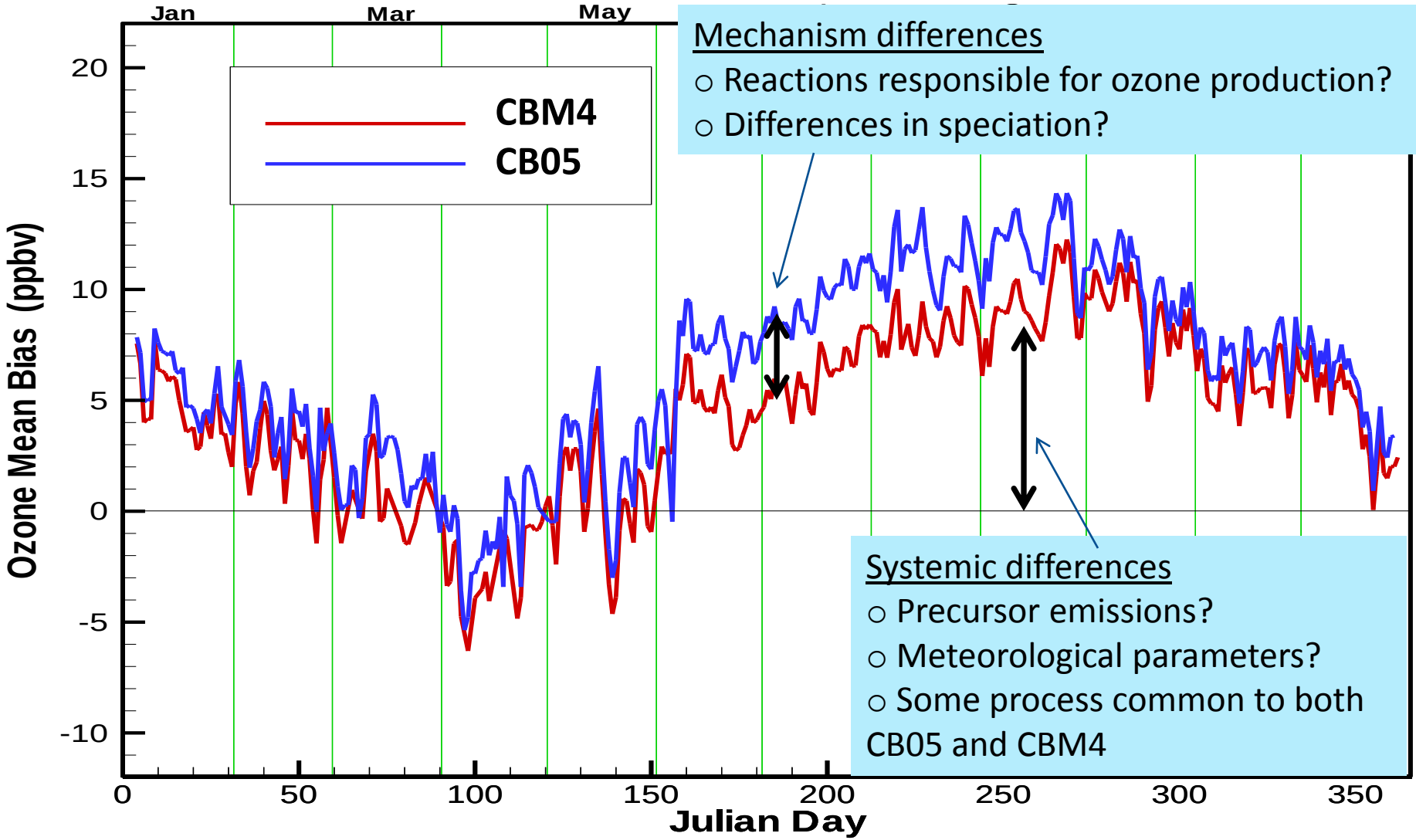


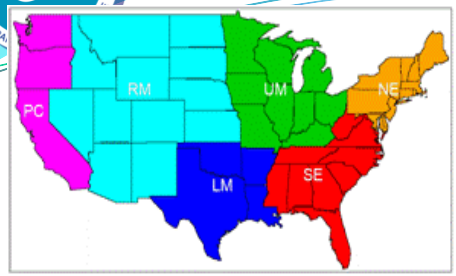
Evaluation of NAQFC: CB05 Ozone > CBM4 Ozone



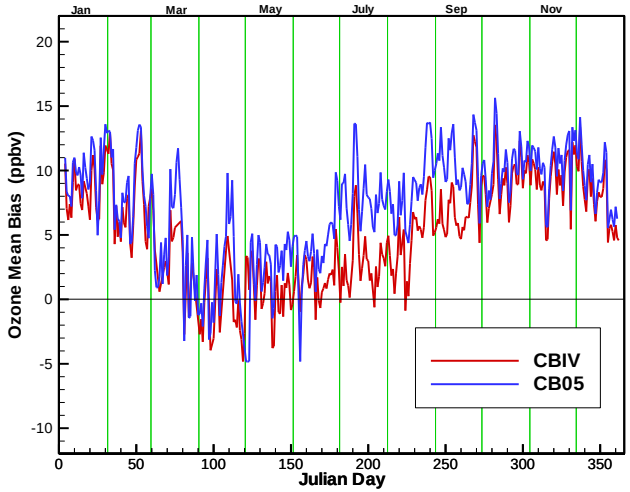
Mechanism differences
- Reactions responsible for ozone production?
- Differences in speciation?

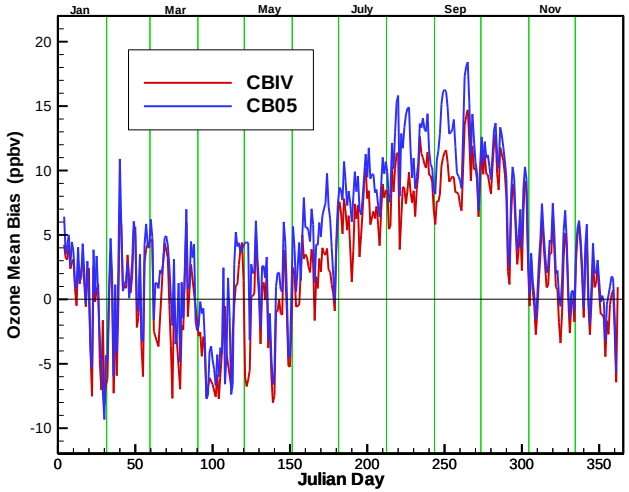
Systemic differences
- Precursor emissions?
- Meteorological parameters?
- Some process common to both CB05 and CBM4

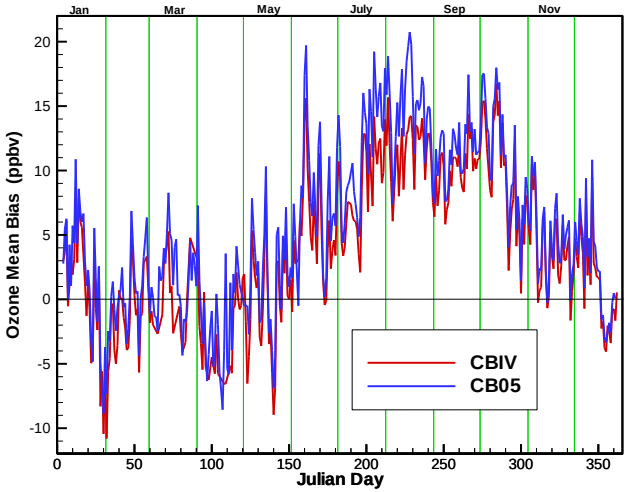
2009 CBIV & CB05 comparison-**Ozone Bias** in 6 Regions

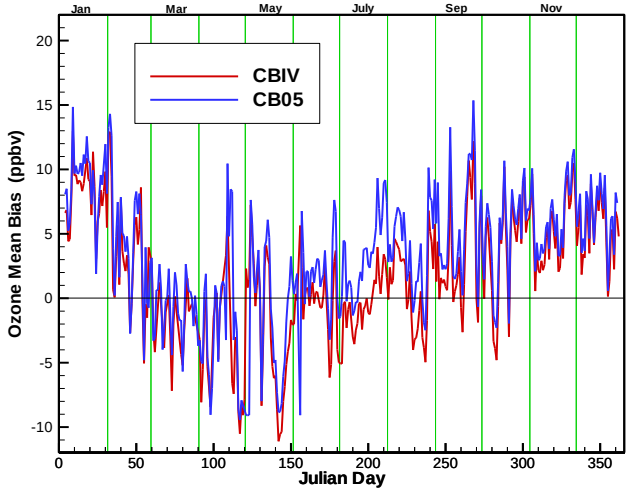


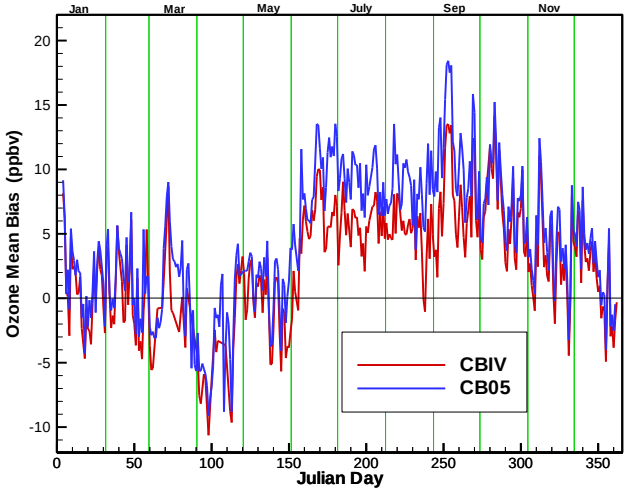
Rocky Mountain Region	Upper Midwest	Northeast US
Pacific Coast Region	Lower Midwest	Southeast US

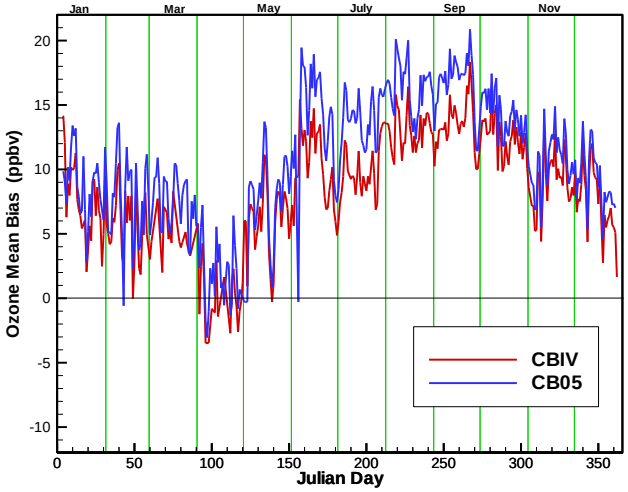












How to reduce model ozone high biases?

- A two-prong approach – On the one hand, adopt a set of short-term operational modifications; on the other, focus on the longer-term basic science research

1) Operational modifications: Perform model sensitivity study
   - aerodynamic resistance
   - canopy height as deposition surface in the forest area
   - BC & minimum PBL height

2) Science investigation: Research model algorithms
   - Main causes of higher P(O3) in CB05 (current)
   - Effects of dynamic consistency (TBD)
   - Emissions uncertainty (TBD)

09Base – Aerodynamic resistance estimated with Monin-Obukhov equation

2009 August Monthly Average difference

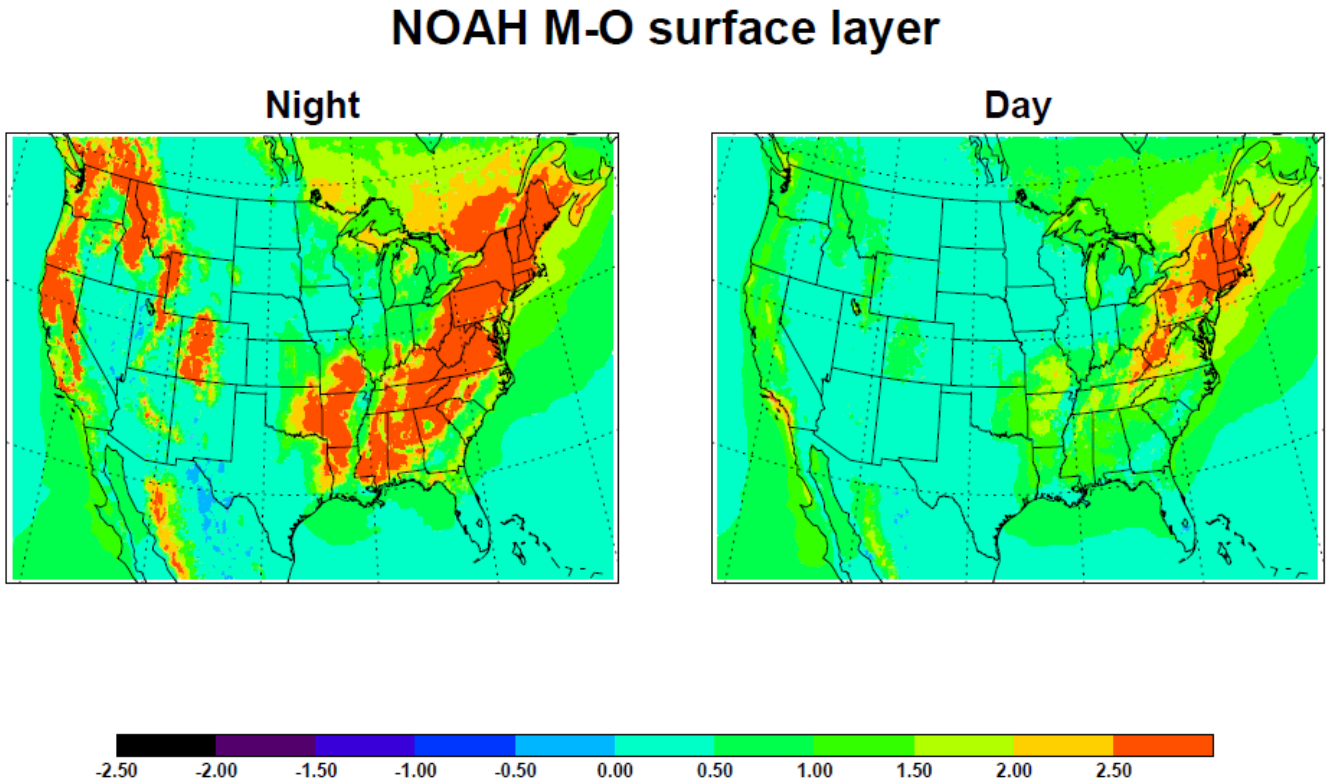


Figure 1. The surface O3 difference between two model simulations (standard simulation - sensitivity test to estimate the aerodynamic resistance using the M-O equation with NOAH LSM inputs (instead of using surface exchange coefficient at default) during the nighttime (6PM-6AM local time) and daytime (6AM-6PM local time) over the US for August 2009

09Base – Aerodynamic resistance considering canopy height ~ 10 m

August Monthly Average difference

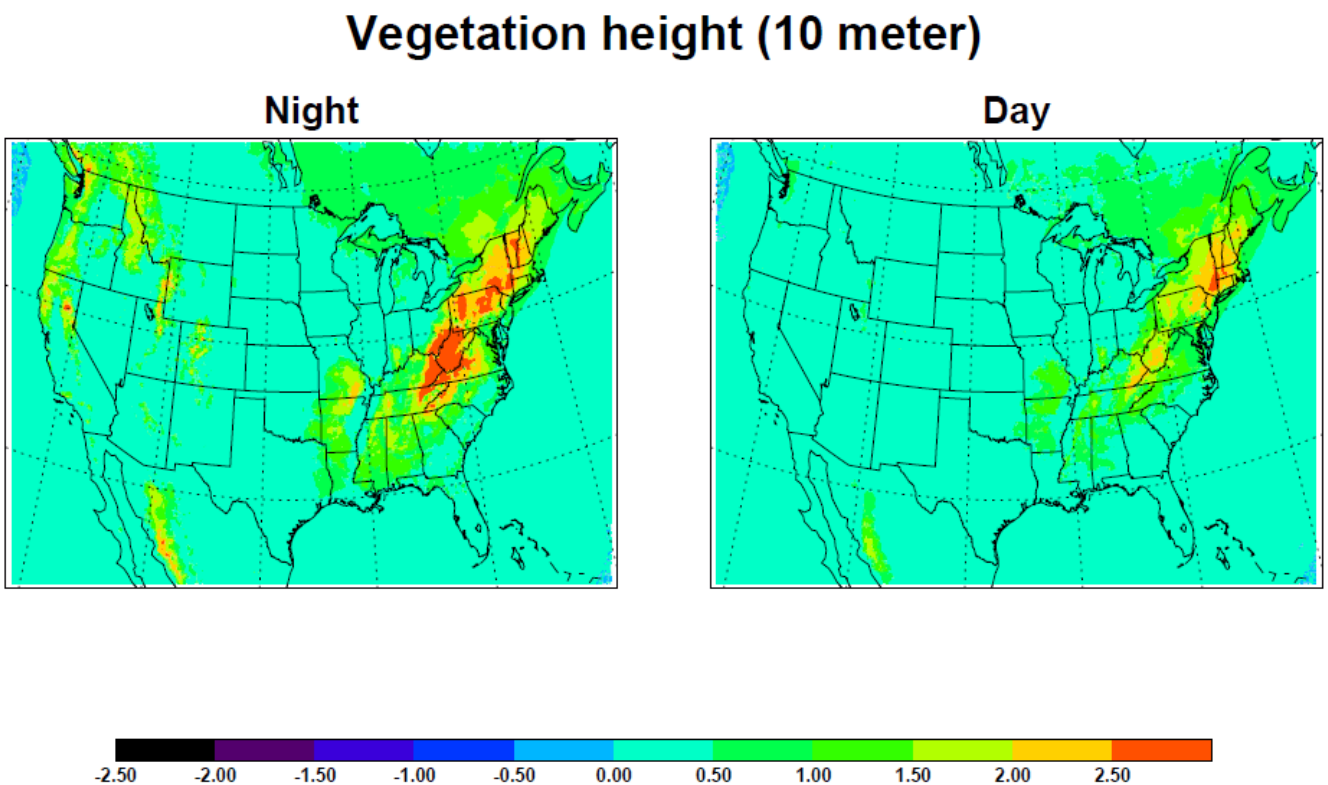


Figure 2. The surface O3 difference between two model simulations (standard simulation - sensitivity test to estimate the aerodynamic resistance by considering the canopy height (10M) during the nighttime (6PM-6AM local time) and daytime (6AM-6PM local time) over the US for August 2009

09Base – with ozone BC change & min. PBL height (50m)

August Monthly Average difference

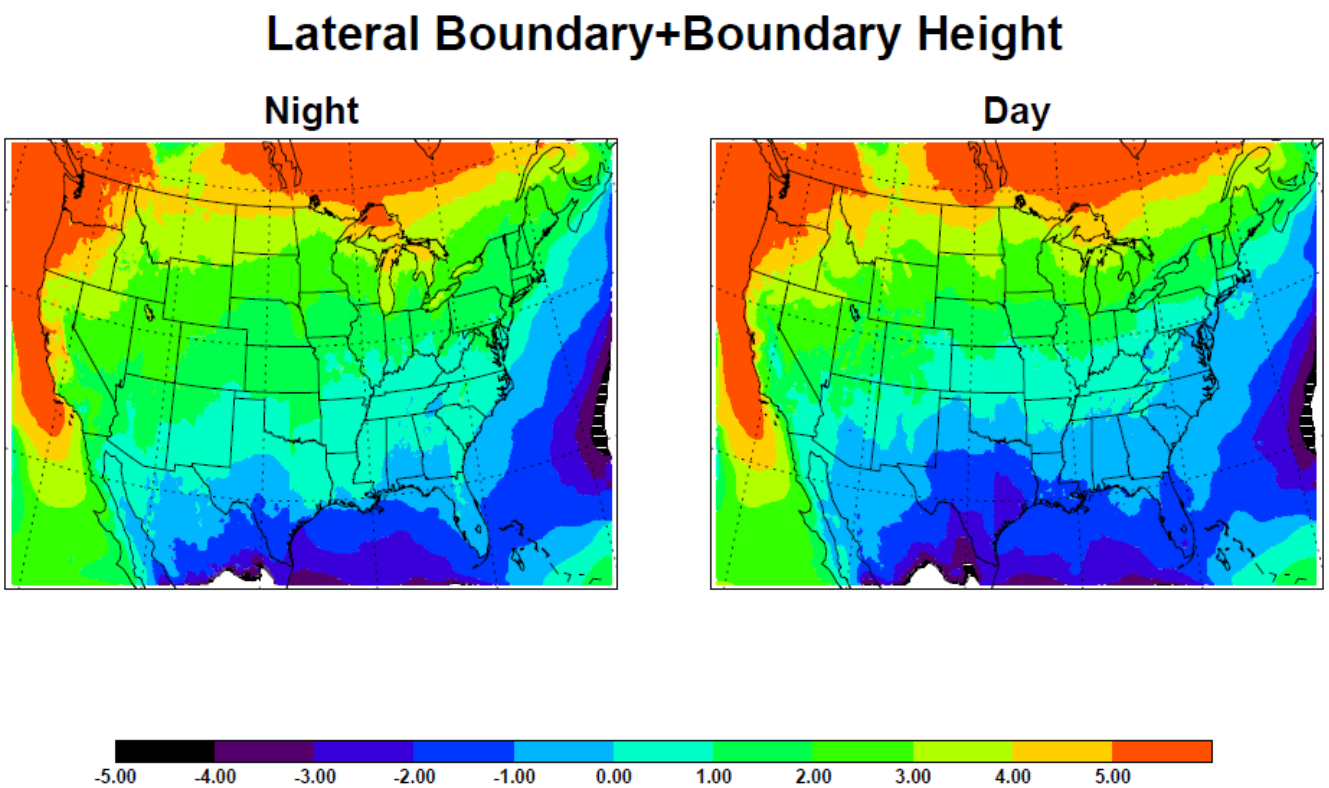


Figure 3. The surface O3 difference between two model simulations (standard simulation - sensitivity test including GEOS-Chem lateral boundary condition and constraining the minimum boundary layer height (50 meter) during the nighttime (6PM-6AM local time) and daytime (6AM-6PM local time) over the US for August 2009

09Base – combo (all three changes)

09August Monthly Average difference

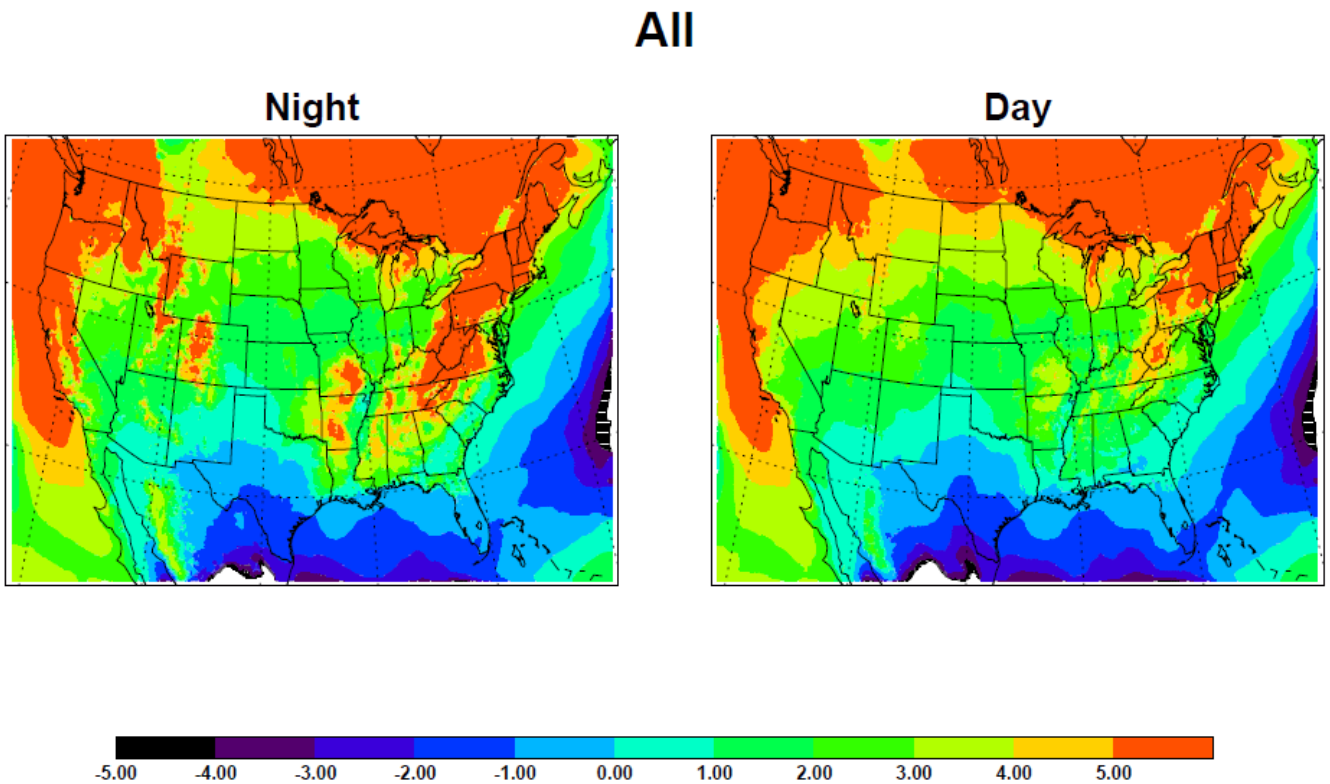


Figure 4. The surface O3 difference between two model simulations (standard simulation - sensitivity test including GEOS-Chem lateral boundary condition, constraining the minimum boundary layer height (50 meter), using M-O equation and canopy height for Ra estimate during the nighttime (6PM-6AM local time) and daytime (6AM-6PM local time) over the US for August 2009

CMAQ (base) – EPA AIRS Observation

August Monthly Average difference

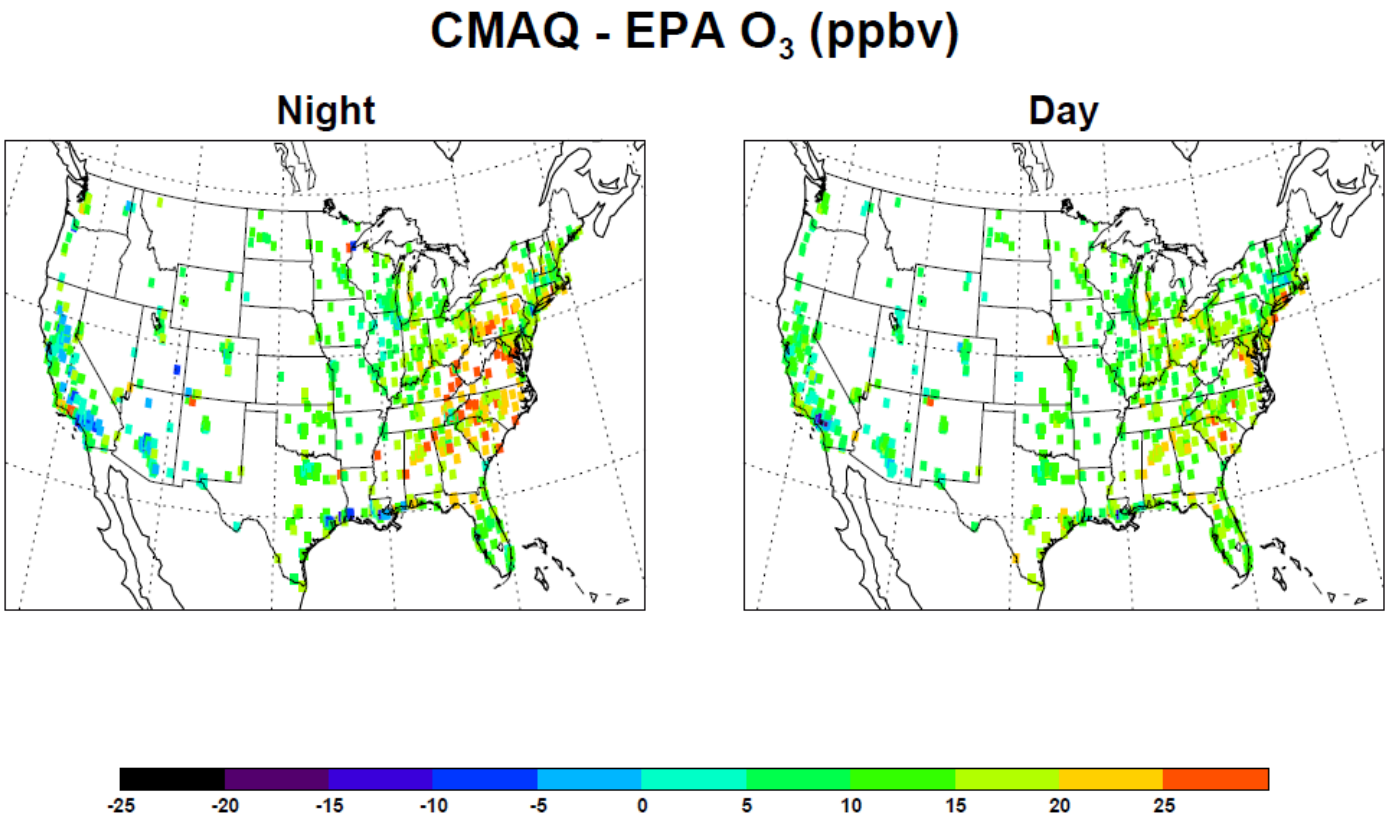


Figure 5. The surface O3 difference between AQS observation and CMAQ (base) for the nighttime (6PM-6AM local time) and daytime (6AM-6PM local time) over the US for August 2009.

CMAQ (all) – EPA AIRS Observation

August Monthly Average difference

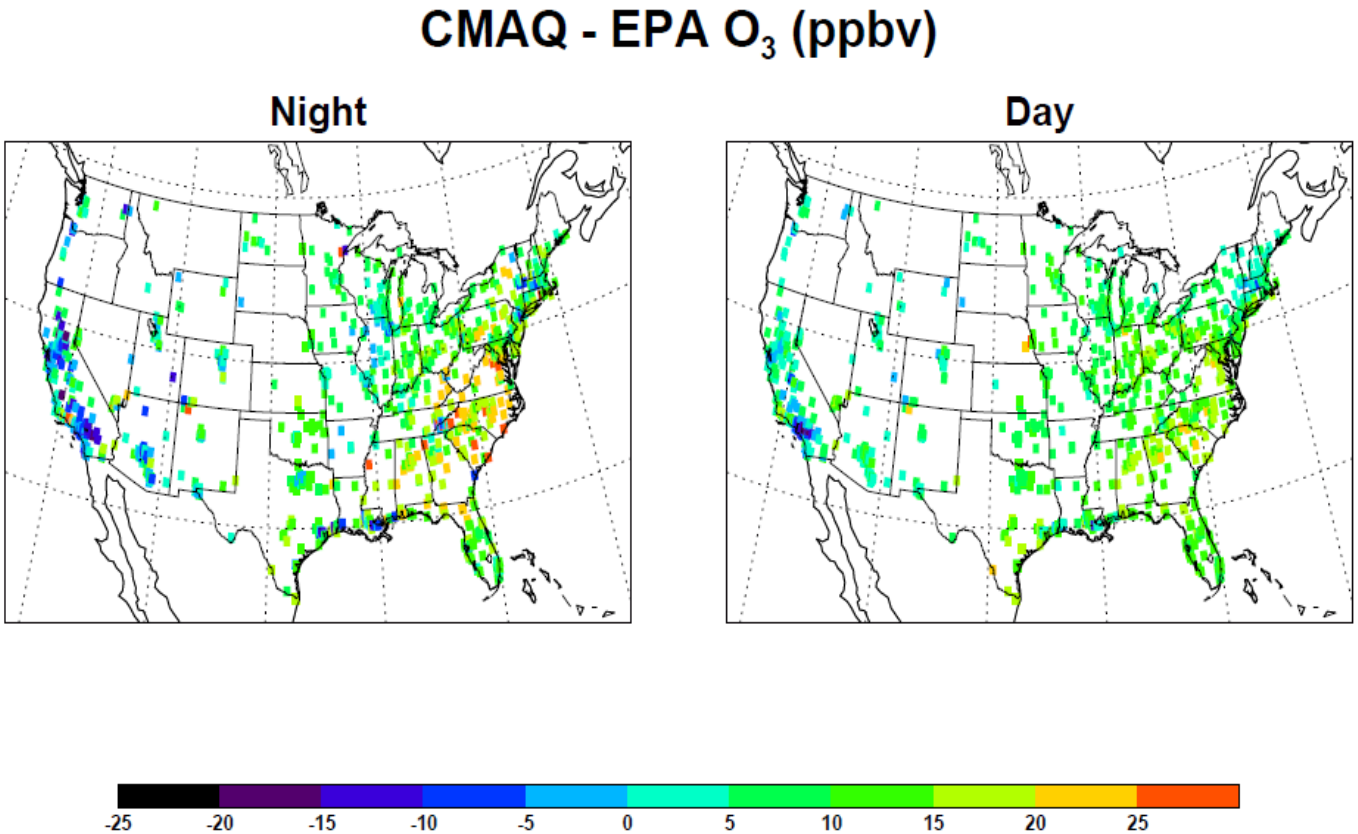
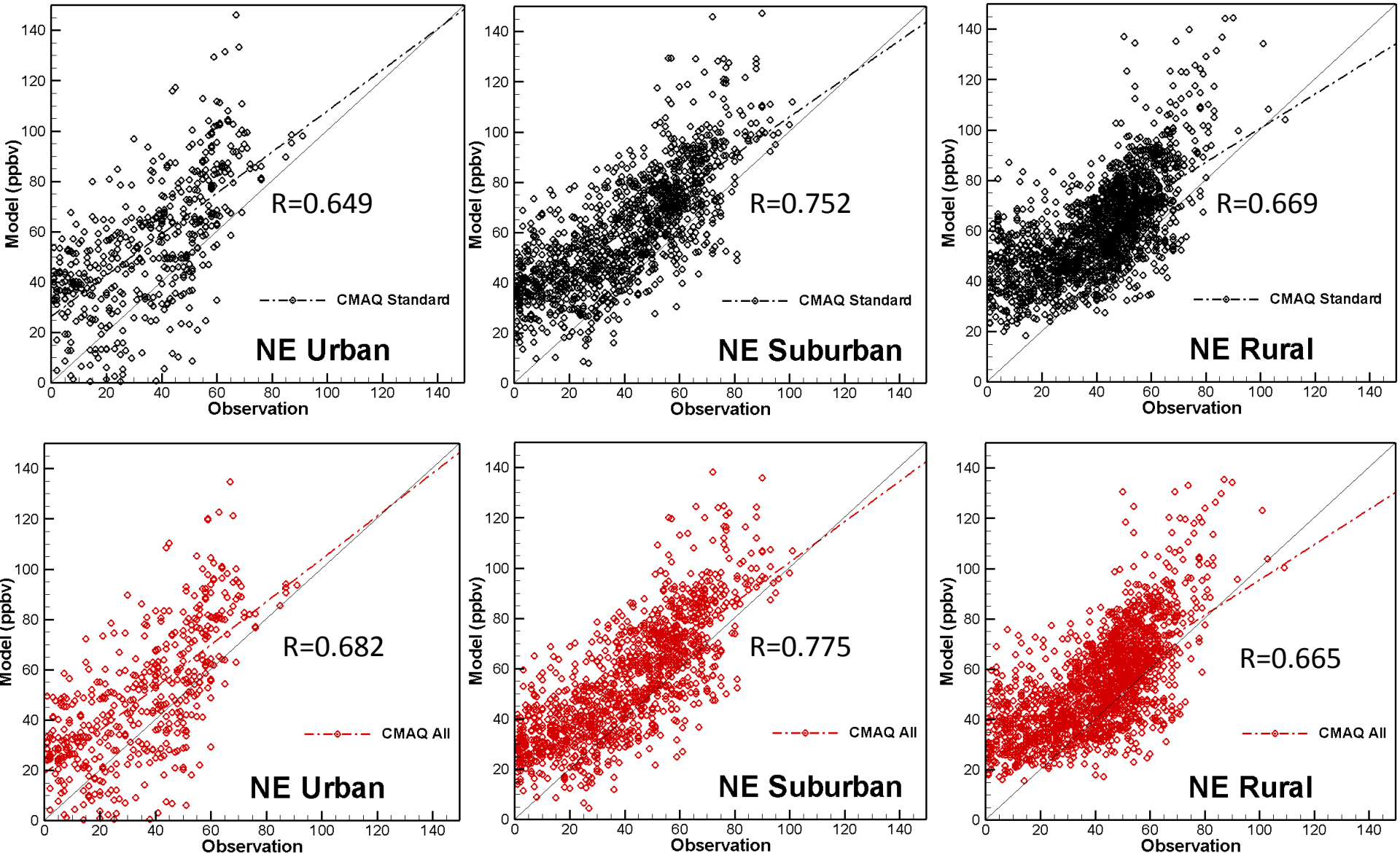


Figure 5. The surface O3 difference between AQS observation and CMAQ “all” simulation for the nighttime (6PM-6AM local time) and daytime (6AM-6PM local time) over the US for August 2009.

Improved results after RA2 and BCs changes

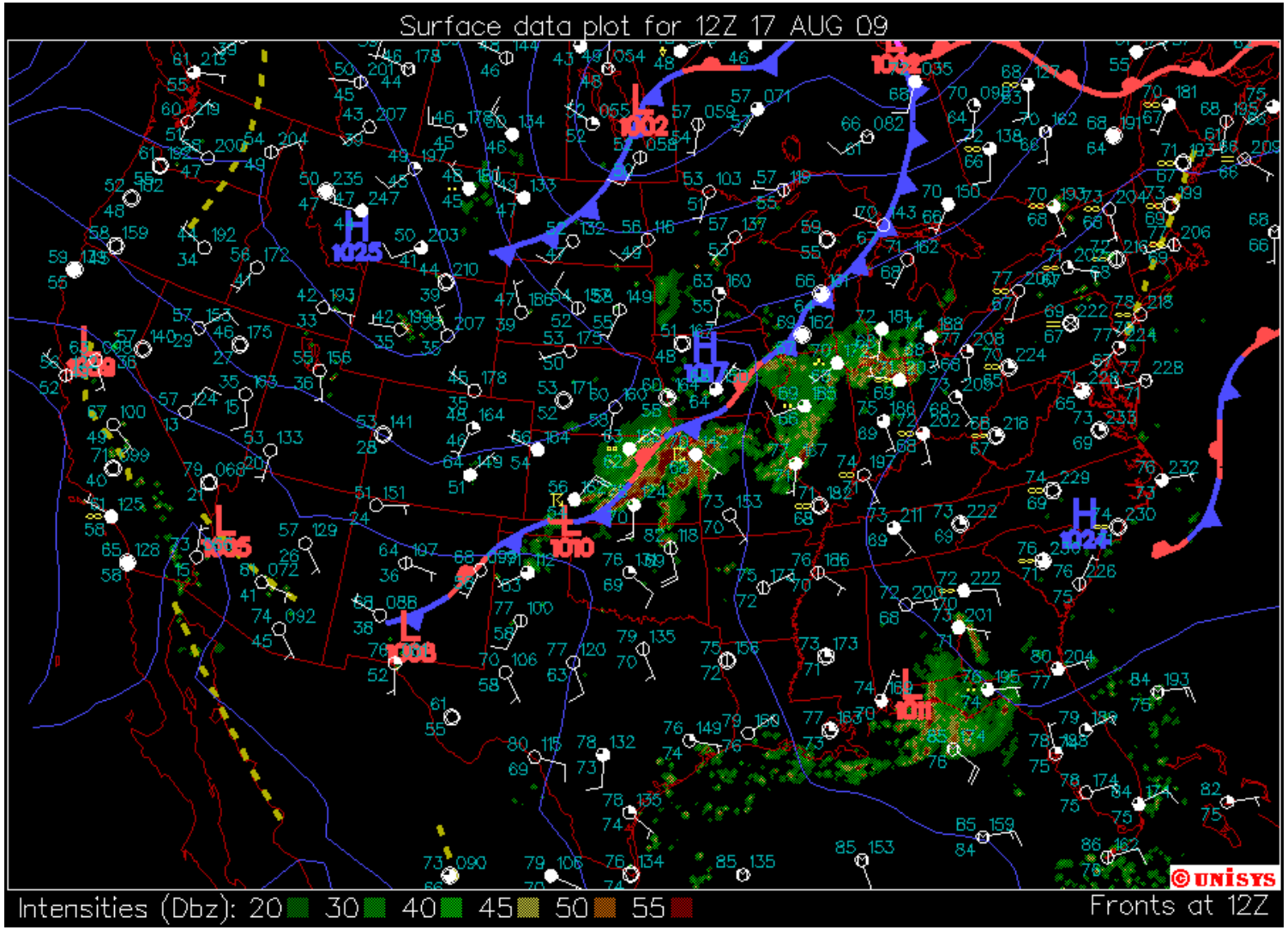
(evaluated at Urban/Suburban/Rural AIRNow sites in Northeast US, on Aug 17, 2009)



After reviewing daily Weather Charts for August 2009

- Frequent frontal passages have significant impact on air quality simulation accuracy
- Importance of location of warm sectors in the UM and NE regions which affect model biases
- Accurate simulations of clean-up and recovery cycles are key for the success of air quality prediction

Weather Chart of August 17, 2009



Impact of Claudette Tropical Storm - August 17 2009

Issues of using August 17, 2009 as the day to "judge" performance of air quality system

- How accurately was the TS Claudette simulated?
- How well did we simulate precipitations associated with thunderstorm events?
- What are the impacts of these convective storms on the realistic simulation of wind flows?
- How well did we simulate the stationary front and PBL evolution in the Northeastern coastal areas?

By Dr. Rick Saylor

Science Algorithm Study: Updates to the Carbon Bond Chemical Mechanism: CB05

G. Yarwood, S. Rao, M. Yocke, and G. Whitten, *Updates to the Carbon Bond Chemical Mechanism: CB05*, Final Report to U.S. EPA, December 8, 2005.

1. Incorporates current (as of 2005) kinetic and photolysis data.
2. Extends the CB mechanism to better support PM modeling needs such as SOA formation.
3. Adds extra species and reactions to treat additional VOCs for air toxics study.
4. Includes effect of reactive chlorine emissions in VOC degradation and oxidant chemistry.

- Explicit methylperoxy radical, methyl hydroperoxide and formic acid.
- Lumped higher organic peroxides, organic acids and peracids.
- Higher aldehyde species ALDX making ALD2 explicitly acetaldehyde.
- Recycling of NO_y from organic nitrates.
- Additional NO_x recycling from HNO_3, N_2O_5 and HO_2NO_2.
- Higher peroxyacyl nitrate species from ALDX called PANX.
- Explicit terpene gas phase chemistry.

Box Model Equations

$$\frac{dC_i}{dt} = \frac{q_i}{H(t)} + R_i - \frac{v_{d,i}}{H(t)} C_i + k_v (C_i^b - C_i) \qquad \frac{dH}{dt} \le 0$$

$$\frac{dC_i}{dt} = \frac{q_i}{H(t)} + R_i - \frac{v_{d,i}}{H(t)} C_i + k_v (C_i^b - C_i) + \frac{C_i^a - C_i}{H(t)} \frac{dH}{dt} \qquad \frac{dH}{dt} > 0$$

C_i = concentration of species *i* in the box (μg/m³)

$H(t)$ = time dependent mixed layer height (m)

q_i = emission of species *i* into the box (μg/m²-s)

R_i = chemical production rate of species *i* within the box (μg/m³-s)

$v_{d,i}$ = dry deposition velocity of species *i* (m/s)

C_i^b = background concentration of species *i* (μg/m³)

C_i^a = concentration of species *i* above the mixed layer (μg/m³)

k_v = mixing rate of background air (s^{-1})

Simulation Conditions

$$\frac{dC_i}{dt} = \frac{q_i}{H} + R_i$$

- Fixed mixing layer height = 1000 m, $\frac{dH}{dt} = 0$
- No dry deposition, $v_{d,i} = 0$
- No mixing with background air, $k_v = 0$
- Fixed initial conditions:

T	= 298 K
p	= 1 atm
RH	= 50%
O_3	= 10 ppbv
CO	= 100 ppbv
CH_4	= 1600 ppbv

NO_x = all VOCs = 0

Zaveri and Peters (1999) **JGR**, **104**, *30387-30415*.

Simulation Suite

Scenario	NO_x (µmol m^{-2} h^{-1})	ISOP (µmol m^{-2} h^{-1})	R_{NMHC} (mol NMHC/mol NO_x)	CO (µmol m^{-2} h^{-1})
u001	5	0	10	800
u002	20	0	10	800
u003	40	0	10	800
u004	5	0	1	800
u005	20	0	1	800
u006	40	0	1	800
u007	5	0	100	800
u008	20	0	100	800
u009	40	0	100	800
r001	1	50	1	80
r002	5	50	1	80
r003	10	50	1	80
r004	1	50	0.1	80
r005	5	50	0.1	80
r006	10	50	0.1	80
r007	1	50	10	80
r008	5	50	10	80
r009	10	50	10	80

Hourly emission = E_0 * cos(zenith angle)

Sensitivity Tests

Name	Description (changes made to CB05 from base mechanism)
xNTRrecycle	NTR recycling reactions removed
xiNOxrecycle	inorganic NOx recycling reactions removed
xallNOxrecycle	both NTR and inorganic NOx recycling reactions
xPANX	all PANX reactions removed (no ALDX emissions)
xPANXrecycle	PANX recycling reactions removed
xPANrecycle	PAN recycling reactions removed
PANcbm4	PAN chemistry as in CBM4 (xPANX + CBM4 PAN rate constants)
PANjpl06	PAN and PANX rate constants from JPL 2006
xNTR-PANcbm4	xNTRrecycle + PANcbm4 (no NTR recycle and CBM4 PAN chem.)
xNTR-PANcbm4-xPANX	xNTRrecycle + PANcbm4 + xPANX (no NTR recycle, CBM4 PAN chemistry, and no PANX chemistry)
xPANX-xNTR	xPANX + xNTRrecycle (no PANX chem. and no NTR recycle)
noALDXemis	no ALDX emissions and ALD2 emissions as in base CBM4

Organic Nitrate (NTR) Chemistry in CB05

Production –

R115.	ROR + NO_2	→	NTR
R129.	TO2 + NO	→	… + 0.1 NTR + …
R133.	CRO + NO_2	→	NTR
R144.	ISOP + NO_3	→	… + 0.8 NTR + …
R55.	XO2N + NO	→	NTR
R147.	ISPD + NO_3	→	… + 0.85 NTR + …
R156.	ISOP + NO_2	→	… + 0.8 NTR + …
R152.	TERP + NO_3	→	… + 0.53 NTR + …

Destruction –

R61.	NTR + OH	→	HNO_3 + …	**xNTRrecycle**
R62.	NTR + hv	→	NO_2 + HO_2 + …	

Reactive N is recycled back into the gas phase via R61 & R62. NTR is an irreversible N sink in CBM4, but is a reversible temporary reservoir of N in CB05.

Inorganic NO_x Recycling Reactions in CB05

R51. $HO_2NO_2 + h\nu \rightarrow 0.61\ HO_2 + 0.61\ NO_2 + 0.39\ OH + 0.39\ NO_3$

R52. $HNO_3 + h\nu \rightarrow OH + NO_2$

R53. $N_2O_5 + h\nu \rightarrow NO_2 + NO_3$

xiNOxrecycle

CBM4 does not include these recycling pathways for NO_x.

NOTE: Removing these in the box model sensitivity test will likely overestimate the effect it will have on ozone in the full 3-D model because some HO_2NO_2, HNO_3 and N_2O_5 will be removed via other model processes (e.g., deposition and heterogeneous reactions).

NTR and Inorganic NO_x Recycling Reactions in CB05

R51. $HO_2NO_2 + h\nu \rightarrow 0.61\ HO_2 + 0.61\ NO_2 + 0.39\ OH + 0.39\ NO_3$

R52. $HNO_3 + h\nu \rightarrow OH + NO_2$

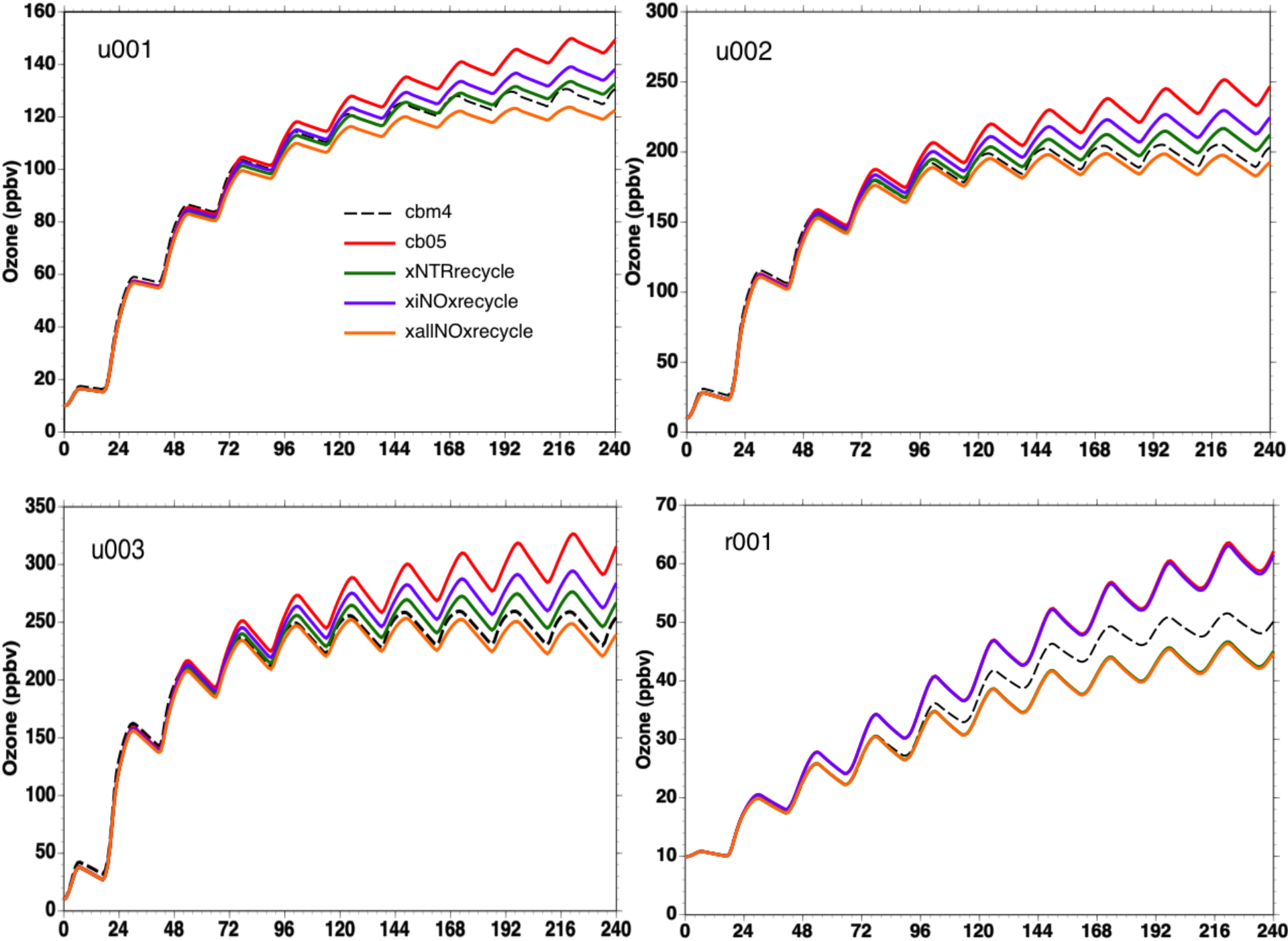
R53. $N_2O_5 + h\nu \rightarrow NO_2 + NO_3$

R61. $NTR + OH \rightarrow HNO_3 + \ldots$

R62. $NTR + h\nu \rightarrow NO_2 + HO_2 + \ldots$

xallNOxrecycle

All NO_x recycling reactions that are included in CB05 but absent in CBM4.


u001
u002
u003
r001
Ozone (ppbv)
cbm4
cb05
xNTRrecycle
xiNOxrecycle
xallNOxrecycle
0
24
48
72
96
120
144
168
192
216
240

Preliminary Conclusions and Next Steps

Box model sensitivity tests indicate that the primary causes of higher ozone biases from CB05 simulations are the additional NO_x recycling pathways that were added to better represent the fate of NO_x over multi-day timescales. This has resulted in a larger "effective" NO_x level in the model (even with the same NO_x emissions), resulting in more O_3 produced.

- Full-model sensitivity tests are underway to confirm the results of the box model simulations.

- Future work will investigate individual chemical formation pathways of organic nitrates, compare predicted organic nitrate concentrations with available measurements, review all reactive N deposition parameters, and systematically re-evaluate NO_x emission sources.

$PM_{2.5}$ Tendency = δ =

(Day 2 24-hr-avg) – (Day 1 24-hr-avg)

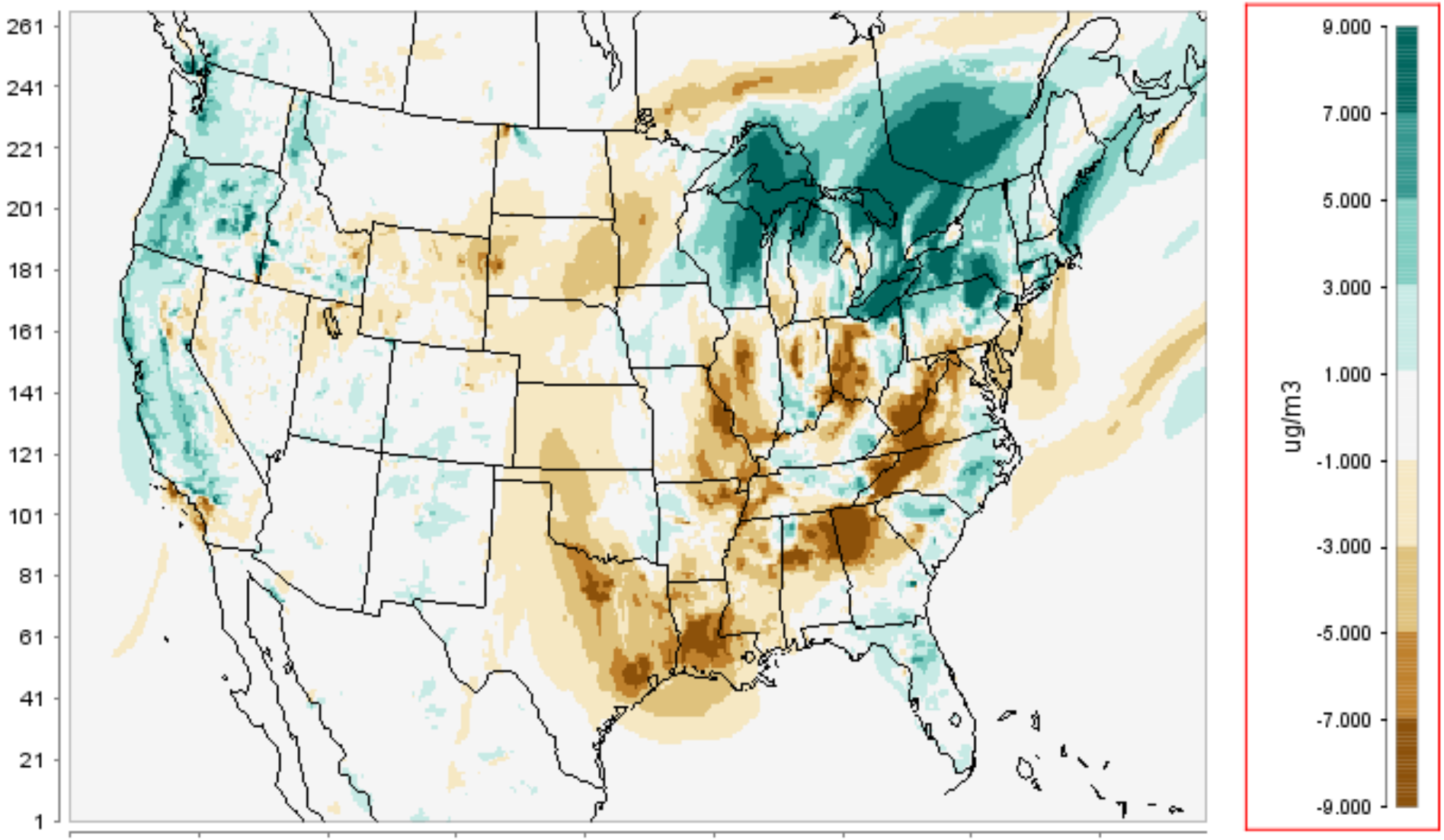
Questions:

- How well does the model perform in predicting this quantity in comparison with observations?

- Would it be a useful product for local AQ forecasters?

Example for August 15-August 14, 2009

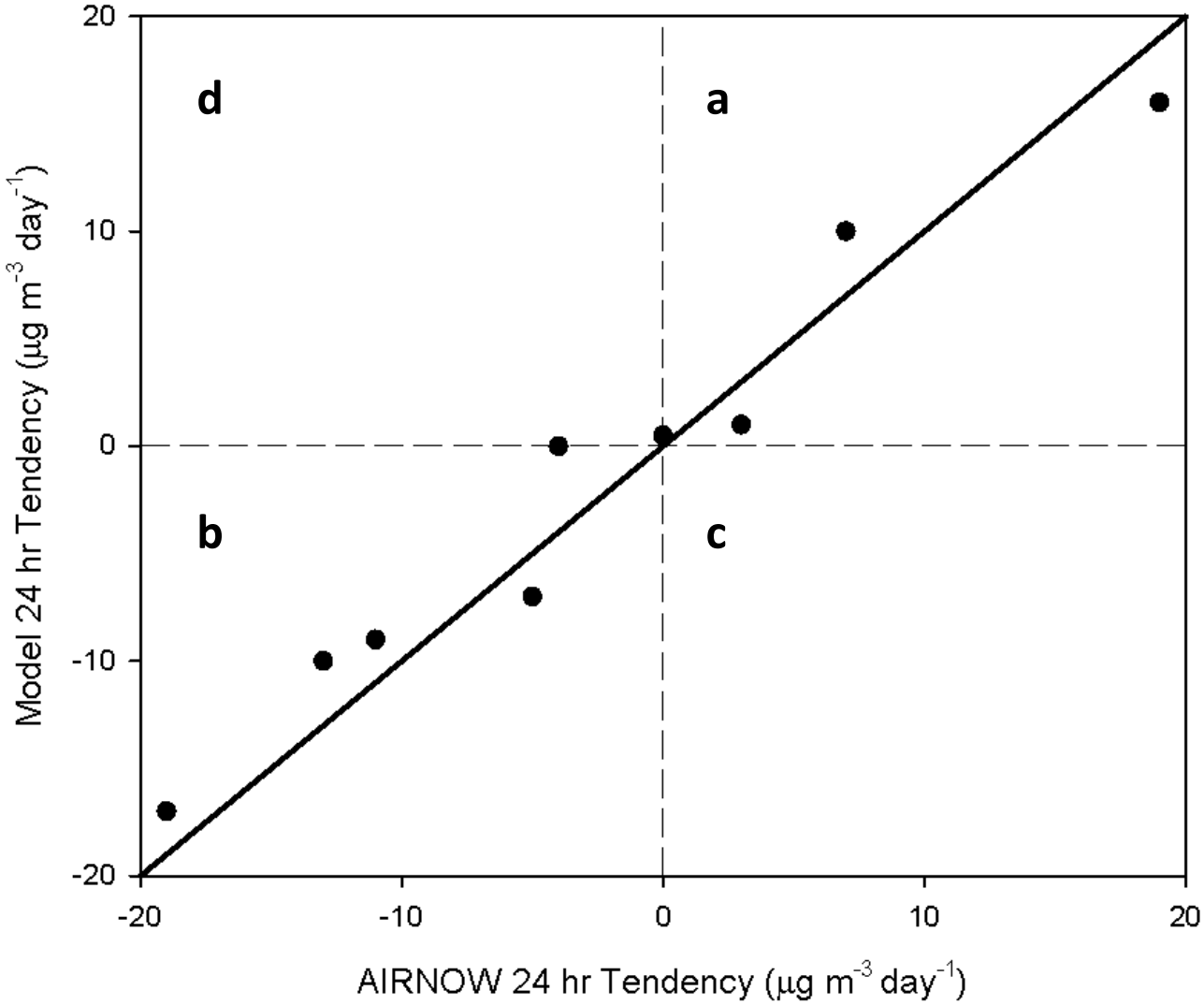
PM2.5 24 hr Tendency Day 1 to Day 2



August 14, 2009 12:00:00 UTC

Min (329, 119) = -1.491E1, Max (71, 199) = 27.75

Example Only!

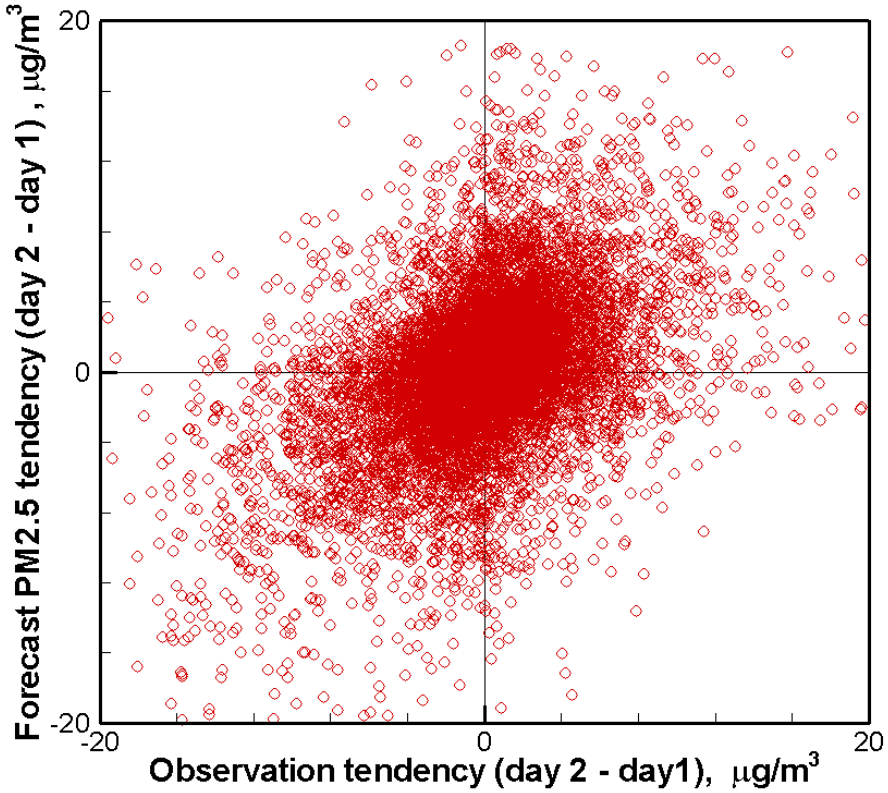


Fraction Sign Correct = f_{sc} = (a+b)/(a+b+c+d)

Example Model Skill for $PM_{2.5}$ Tendency

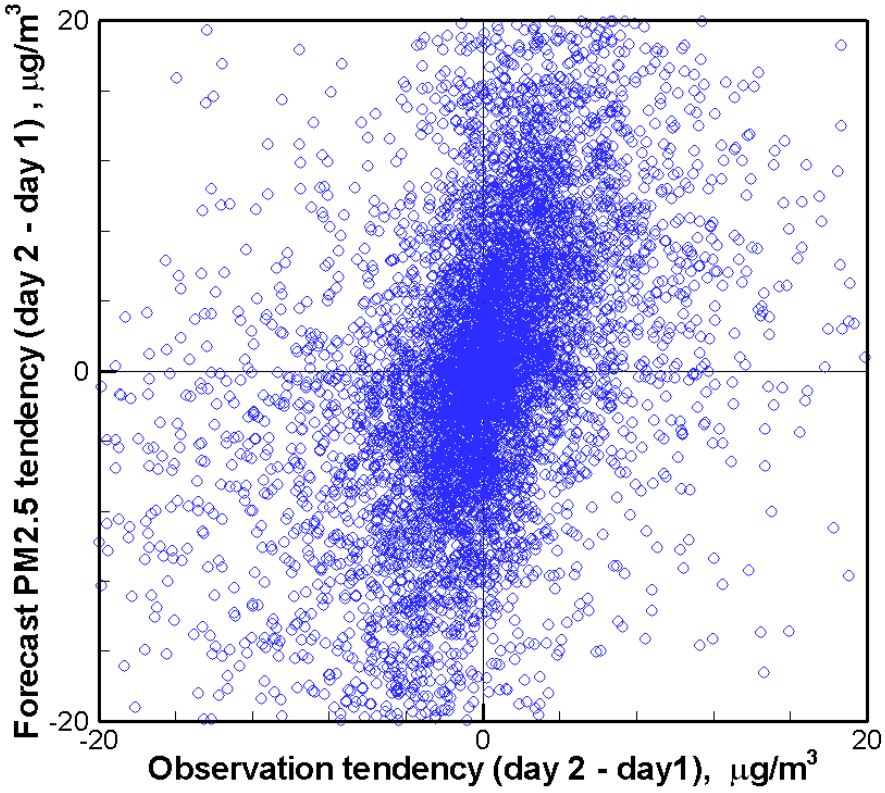
Aug 10-30, 2009

$r = 0.412$ $f_{sc} = 0.64$



Dec 10-26, 2009

$r = 0.434$ $f_{sc} = 0.69$



Observation tendency calculated from AIRNow data

Omit data where both $|\delta_{model}|$ and $|\delta_{obs}| < 5\ \mu g/m^3/d$, i.e., only δ's above a "trigger" threshold are included

August

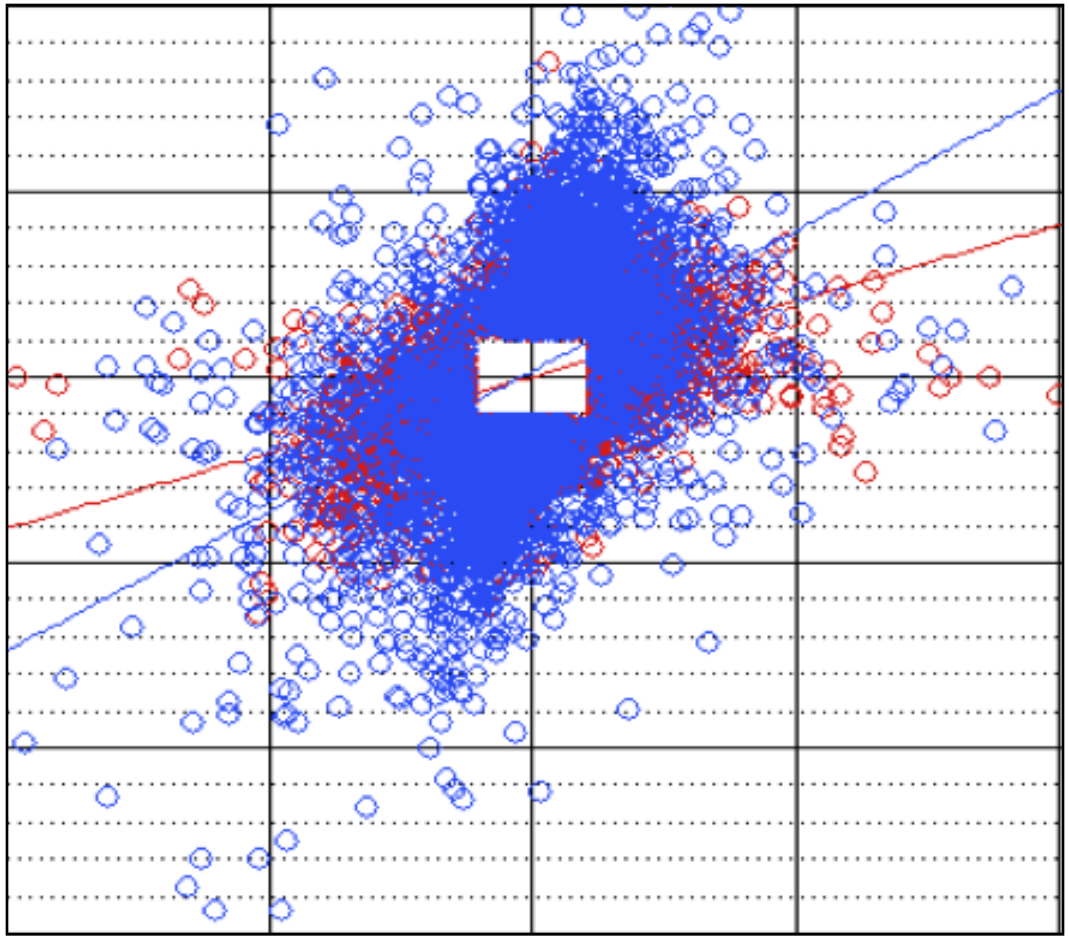
$f_{sc} = 0.75$

$r = 0.437$

December

$f_{sc} = 0.77$

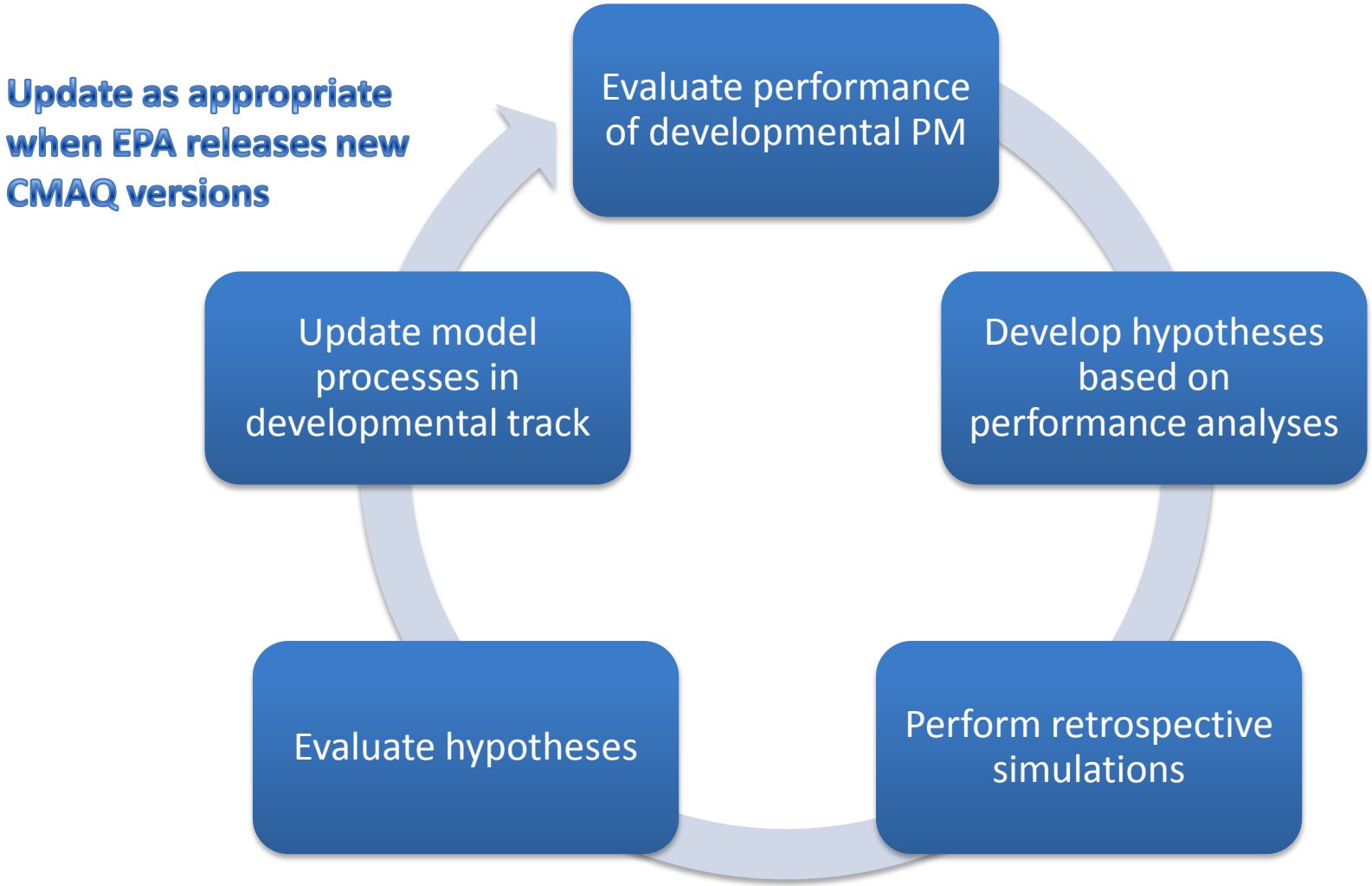
$r = 0.444$



Future Research Topics for Improving $PM_{2.5}$ Prediction

- Evaluation of AERO5 PM module
  - additional SOA precursors and nonvolatile SOA
  - corrected SOA heat of vaporization
  - updated heterogeneous chemical processes
  - updated aerosol thermodynamics

- Improvements in biogenic emissions
  - update algorithms
  - better linkage to ambient meteorology
  - seasonally appropriate surface and vegetation parameters (e.g., LAI, snowcover)

- Investigate apparent linkage between ozone overpredictions and $PM_{2.5}$ underpredictions

Continuous Evaluation-Test-Update Cycle for $PM_{2.5}$