# Updates for AQM V5.1 for $O_3$ and PM2.5 48 hour predictions

Verification Stats:
http://www.emc.ncep.noaa.gov/mmb/aq/fvs/web/html/regular.html

Spatial Maps:
http://www.emc.ncep.noaa.gov/mmb/aq/cmaqparabc/web/html/index.html

04/19/2018

G    **Schedule**

## Project Information & Highlights

**Leads:** Jeff McQueen/Jianping Huang (EMC), Steven Earle(NCO)

**Scope:** Upgrade area source oil and gas emissions; Add ozone bias correction and update unified PM bias correction;  Transition to vlab; transition latest unified emission preprocessor.

**Expected benefits:**  AQM is improved and unified through improved emissions and post-processing.

 **Dependencies:** Transition code, emissions from ARL and ESRL/PSD; BlueSky smoke outputs from Hysplit.

| Milestones & Deliverables | Date | Status |
|---|---|---|
| ARL Code Delivery and evaluations presented | 10/15/17 | Completed |
| Freeze system code /  (EE meeting  Jan 23, 2018) | 2/16/18 | Completed |
| Complete full retrospective/real time runs/evaluation/CCB | 4/19/18 | On Track |
| Conduct OD Brief and deliver code to NCO | 4/24/18 | On Track |
| Issue Technical Information Notice | TBD | On track |
| Complete IT testing | TBD | TBD |
| Operational Implementation | **9/23/18** | TBD |

G    **Issues/Risks**

**Issue:**   Increased run time for premaq/cmaq extension to 72 h may exceed delivery time deadline; codes not delivered  by deadline
**Mitigation:**  Descoped, ARL to run a parallel this summer.

**Issue:** Updates to NEI mobile emissions delivered too late  and evaluations were incomplete; **Mitigation**: Descoped,  ARL to run a parallel this summer for AQ forecasters.

G    **Resources**

**Staff**: 0.7 Fed (J. McQueen) + 2.2 contract (1.0 J. Huang + 0.9 H-C Huang  + 0.3 P. Shafran), incl. dev

**Funding Source**: STI/NAQFC

**Compute: Dev**: 120 nodes;**Para:** 40 nodes ;

**Ops:** *CONUS: 24 nodes/cycle for 35 mins;*  AK: 4 nodes/cycle for 25  mins ; HI: 1 node/cycle for 7 mins

**Archive:  Ops:** 450 gb/day (+1 gb)

| | | |
|---|---|---|
| **R** | **Management Attention Required** | |
| **Y** | **Potential Management Attention Needed** | |
| **G** | **On Target** | 2 |

# Team

- Jianping Huang, EMC : code design/transition
- Ho-Chun Huang, EMC: wild fire smoke emission development
- Jeff McQueen, EMC: system evaluation, graphics web page support

- Pius Lee, ARL: team leader, oil/gas emissions development
- Youhua Tang & Daniel Tang, ARL: Emissions development

- Jim Wilczak, Irina, Djalalova, Dave Allerud, ESRL/PSD: bias correction development

- Li Pan, ARL/EMC:  research system development and testing
- Sarah Lu, SUNY/Albany: Global model LBCs
- Perry Shafran, EMC: O3/PM grid2obs verification
- Boi Voung, EMC: WMO Header generation for new products

- Ivanka Stajner, Sikchya Udaphayay, Jose Tirado-Delgado, NWS/STI:  AQ program management

# Summary of Upgrades

- Updates to anthropogenic emissions (NOAA/ARL)
  - *Oil & gas sector emission update to 2017 from NEI 2011*
  - *Species ratio adjustment for Colorado winter VOC emissions*

- Updates to Kalman Filter ANalog (KFAN) Bias Correction (ESRL/PSD)
  - *Included ozone bias correction*
  - *Added processing for rare events (V8)*
  - *Increased number of sites to over 900 sites*
  - *Consistent CMAQ V5 predictions training data*
  - *Add the use of downward SW radiation for analog selection*

- *Update Alaska/Hawaii system to same CONUS V5.0.2*
  - *Moved to Cray (same as CONUS)*
  - *Small impact, was to be delivered in FY17 upgrade*

# Emission Upgrades
# NOAA/ARL

➢ **Point source** Static for outside the border:

     - Canada 2011 Environment Canada Emission
       Inventory (ECEI);
     - Mexico inventory (MI) 2012 version 2.2

➡ **Upgrade** based on 2016 Continuous Emission Monitoring (CEM ) & scaled by the Energy Outlook released by DoE in Jan 2018

➢ **Area source: Upgrade for Oil and Gas Sector by including:**

➡     Activity data from 2016 production inventories
➡     - Contributions from fracking
     - Latest Formaldehyde to total-VOC ratios

# Point Source Upgrade

– Annual upgrade
– *Expect small impact*

## Difference plots (upgraded minus prod) for 4/4/2018

**Maximum 8 h ave O$_3$ (ppbv)**          **24 h ave PM$_{2.5}$ (µg m$^{-3}$)**
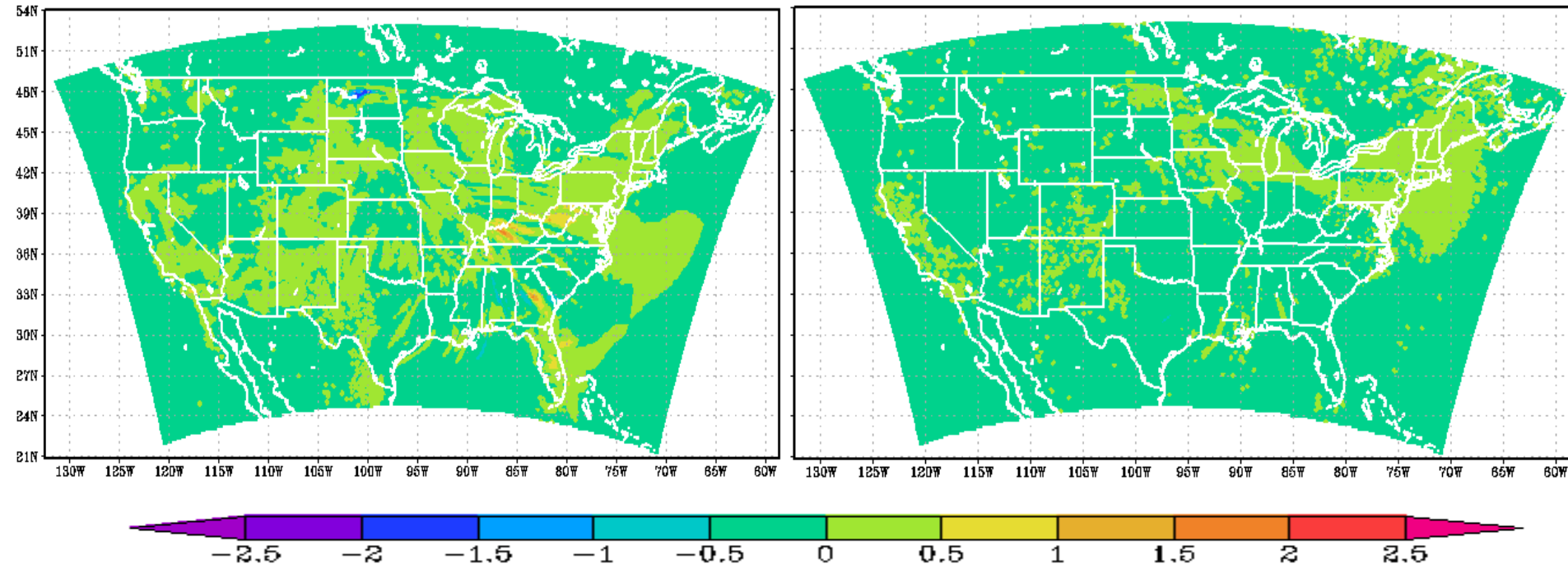
# Source: Oil and gas activity upgrade
## – *expect significant local impact*

## O$_3$ (ppb) distribution valid at 18Z July 18 2017

**Prod**　　　　　　　　　　　➡ **Upgraded**
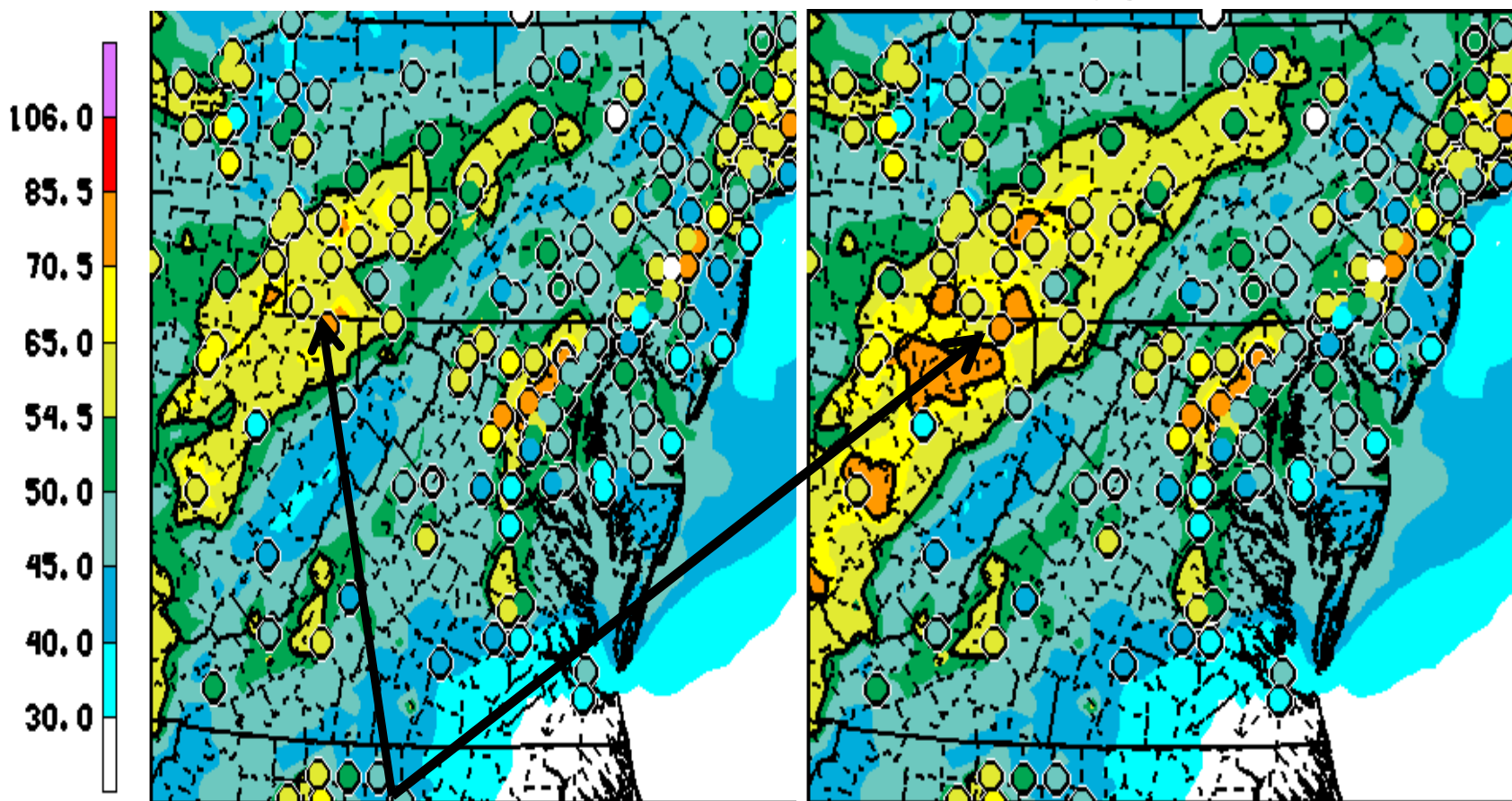


**Morgan Town, WV**

# Source: Oil and gas speciation upgrade
## – *expect significant local impact*

## O$_3$ (ppb) distribution valid at 13Z Feb 23 2018



Prod

➡ Upgraded

Denver, CO
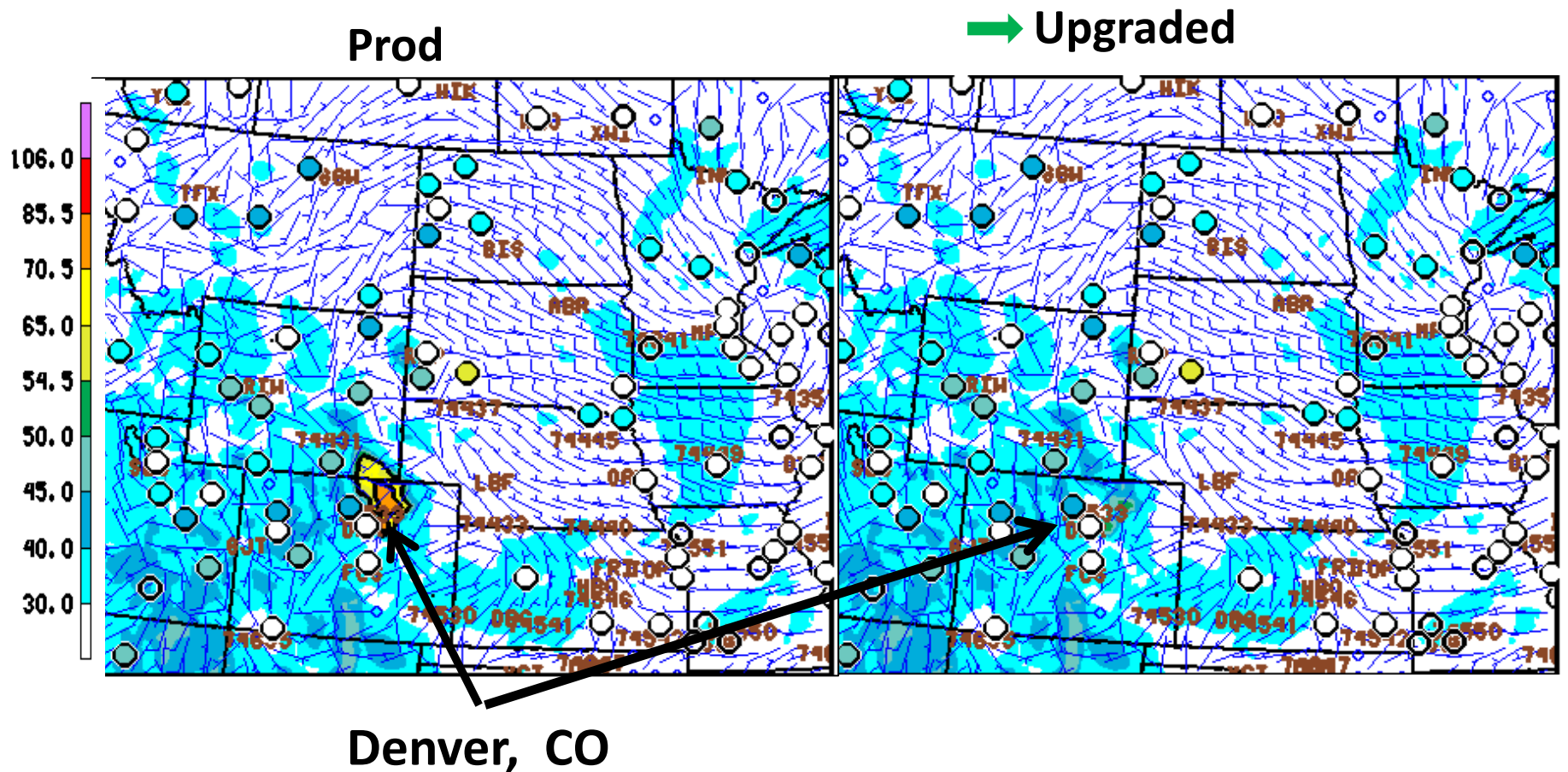
# ESRL Bias Correction
# Jim Wilczak, ESRL/PSD

- Analog post-processing schemes require the ability to find good analogs from past forecasts in the post-processing training data.  Short training data sets are less likely to have extreme (rare) events.

- Forest fires are extremely episodic, and can create extreme values of PM2.5 and other AQ variables including ozone.

- CMAQ has some skill at forecasting forest fire effects because of the inclusion of satellite-derived data assimilation of fire position, size and intensity. Therefore when an extreme high PM2.5 concentration is forecast, it is likely to be true.

- A standard analog post-processing technique will mistakenly reduce the forecast high PM if the best historical analogs it can find are from non-fire days.

- New algorithm:  if algorithm is unable to find good analogs, compute the difference between the current forecast and its analogs, and add this difference to the standard KFAN forecast.
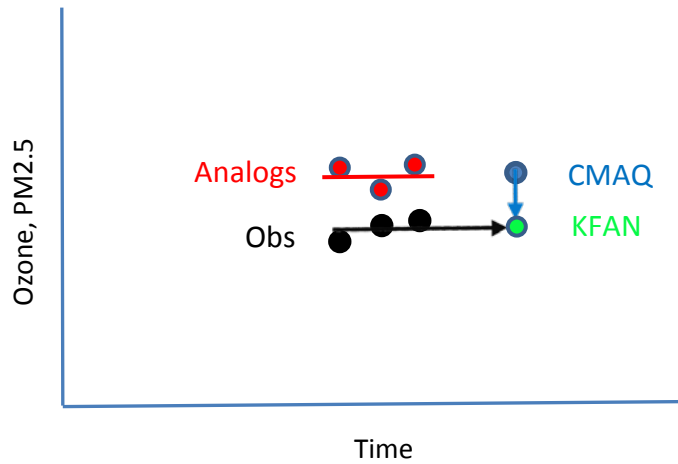
Standard KFAN bias correction with good analogs
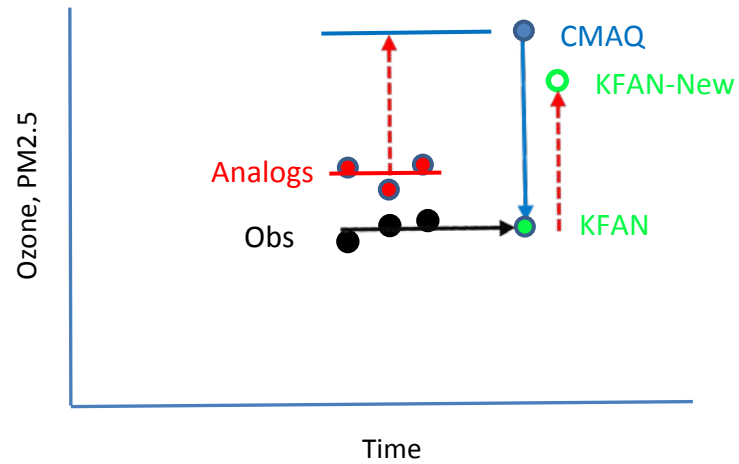
New KFAN bias correction with very poor analogs

# Bias correction configuration

| | Ozone | PM2.5 |
|---|---|---|
| Variables used to determine analogs | 1) Ozone concentration<br>2) Wind direction, 10 meters<br>3) Wind speed, 10 meters<br>4) Temperature, 2 meters<br>5) Solar radiation reaching surface<br>*6) PBL height (ACM2 based Richardson number)*<br>*7) NOx concentration*<br>*8) NOy concentration* | 1) PM2.5 concentration<br>2) Wind direction, 10 meters<br>3) Wind speed, 10 meters<br>4) Temperature, 2 meters<br>5) Solar radiation reaching surface |
| Number of analogs used | 10 | 10 |
| Training period | Rolling 12 months | Rolling 12 months (skip July 4 and July 5) |
| Training model configuration | CMAQ 5.0.2 | CMAQ 5.0.2 |

# AQM V5.1 Cray Testing

- **<u>Emissions tests</u>**
  - Retrospectives: July-August 2017
  - Near Real-time: December-Present

- **<u>KFAN Bias Correction tests for ozone and PM2.5</u>**
  - Retrospectives: July 2017-Jan. 2018
  - Near Real-Time (w/ emissions): Feb-Present

# Prod, EXP and *EXP bias corrected* $O_3$
# Diurnal time-series
## **July 2017**



1-h Avg OZON obs (PPB) avged by fcst hrs
20170701 to 20170731
West–US

**WEST U.S.**

- Observed–Mean
- OPERATIONAL Forecast–Mean
- EXPERIMENTAL Forecast–Mean
- Unif–Bias–corrected–V8 Forecast–Mean

FORECAST HOUR 12 UTC CYCLE

1-h Avg OZON obs (PPB) avged by fcst hrs
20170701 to 20170731
East–US

**EAST U.S.**

- Observed–Mean
- OPERATIONAL Forecast–Mean
- EXPERIMENTAL Forecast–Mean
- Unif–Bias–corrected–V8 Forecast–Mean

FORECAST HOUR 12 UTC CYCLE
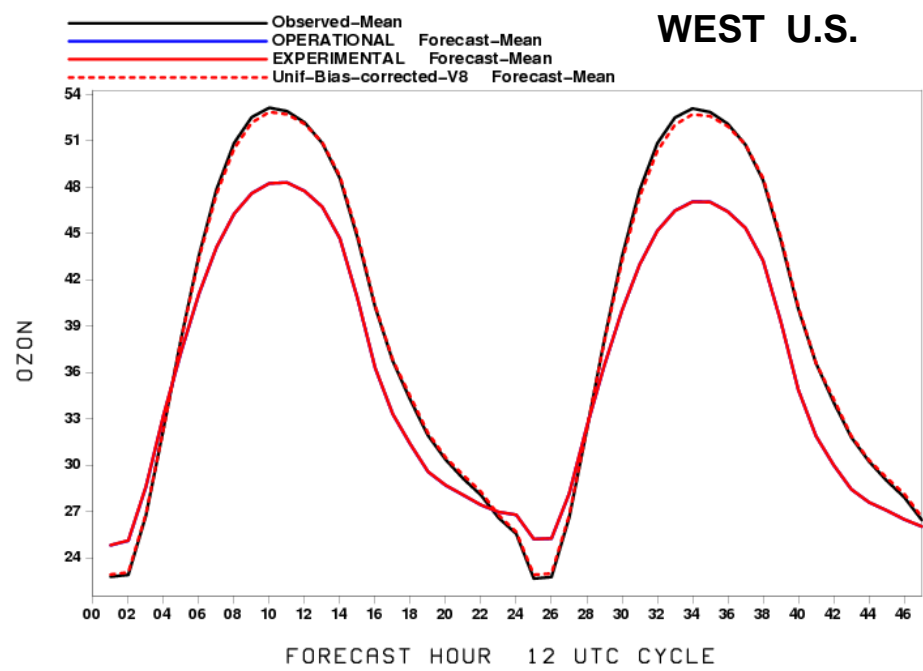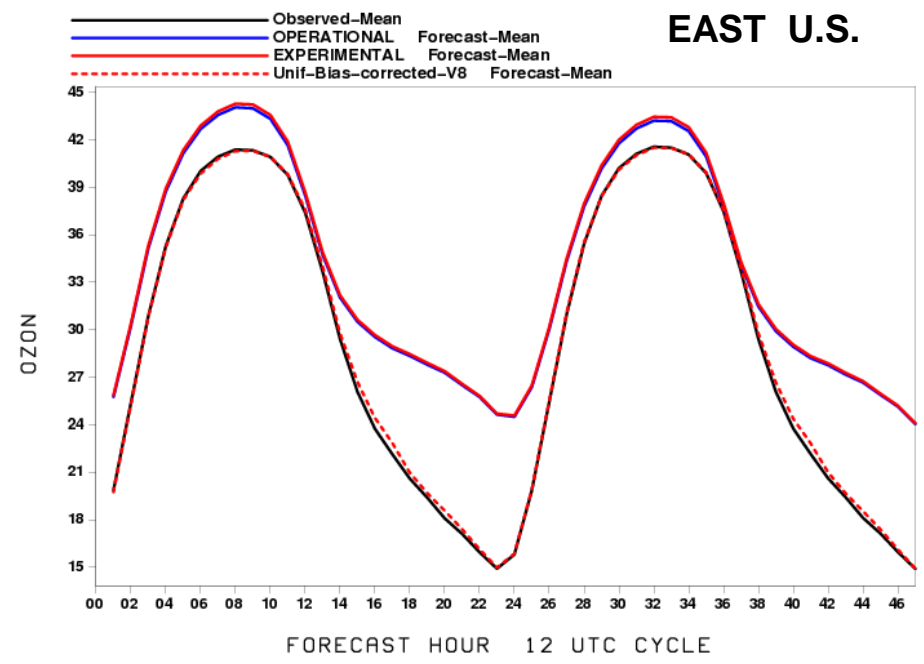
*Exp Unified Bias Correction* near perfect
Prod & V5.1: - typical over-prediction East
            - under-prediction West

13

# Day 2  8 hr daily max O$_3$
## Valid July 19, 2017
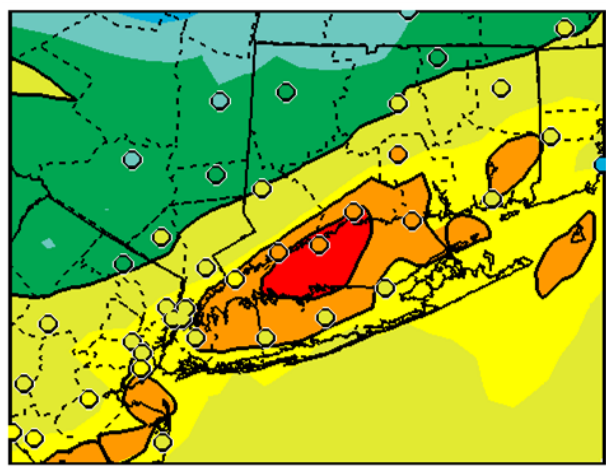


Production
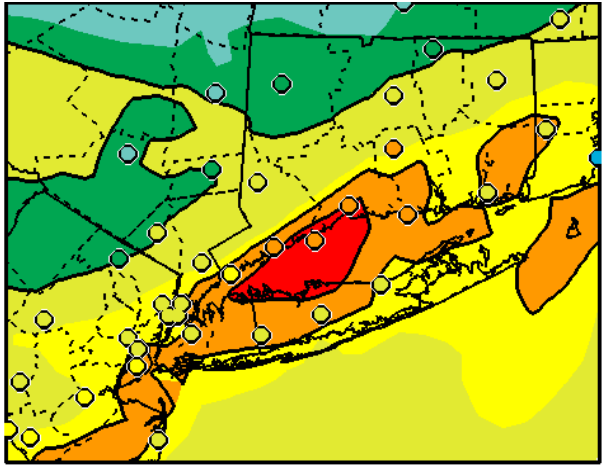
Experimental
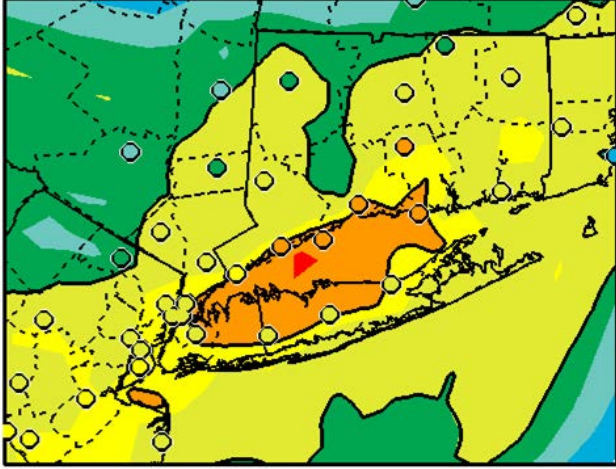
Exp. Bias Corrected

PARA5 4X-DAY  DAY2 OZMX08 (PPB) 20170718 12Z CYC

Bias Correction with rare event update:
- No longer overcorrects daily  max O3 over LIS

# Day 2  8hr daily max O₃
## Valid July 19,2017



PARA BIAS COR V8  DAY2 OZMXO8 (PPB) 20170718 12Z CYC

PROD  DAY2 OZMXO8 (PPB) 20170718 12Z CYC

OBS:      77 ppb
Prod:     67
Exp BC:  61

EXP - OPER BC aqm DAY2 O8 hr avg OZMX from 20170718 12 UTC Run
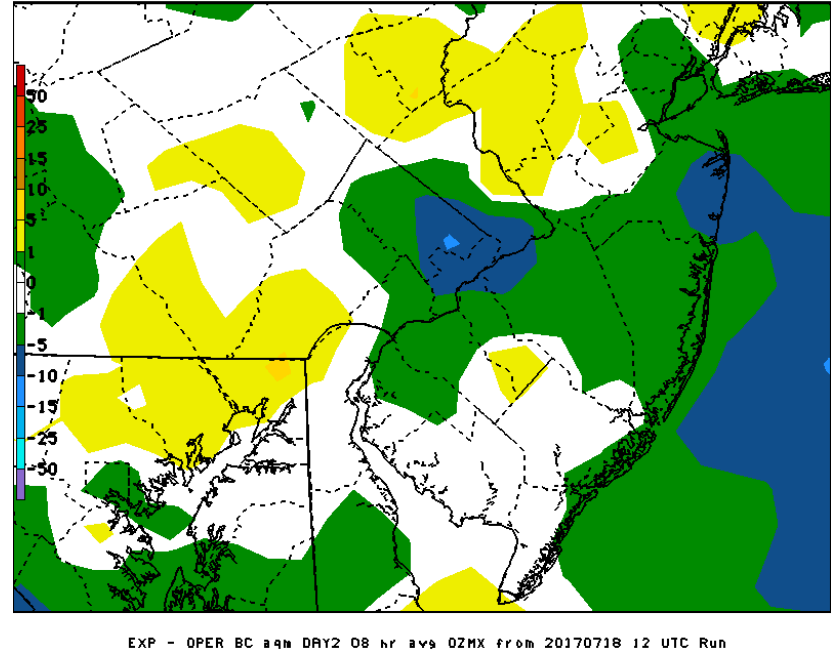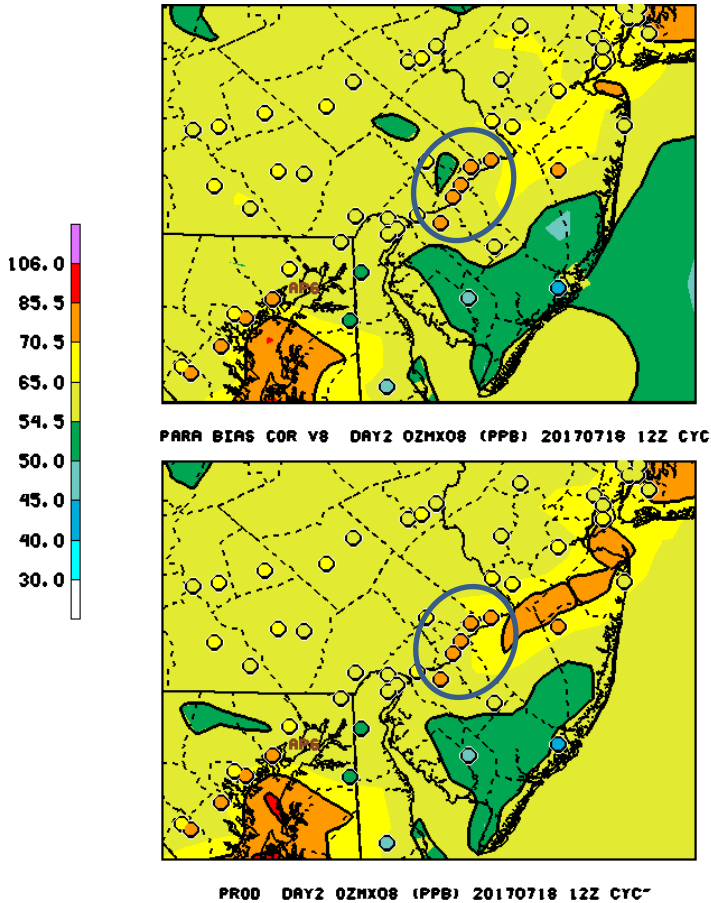
EXP BC - Production

Philadelphia experimental bias-corrected
O₃ predictions  degraded from Raw production
predictions by 5-10 ppb

DAY 2  −8 Avg OZON  BIAS  (PPB) 1500 −> 1200 UTC
West−US

OPERATIONAL    27 −> 48 hrs BIAS
EXPERIMENTAL    27 −> 48 hrs BIAS
Unif−Bias−corrected−V8    27 −> 48 hrs BIAS

WEST  U.S.

DAY 2  −8 Avg OZON  BIAS  (PPB) 1500 −> 1200 UTC
East−US

OPERATIONAL    27 −> 48 hrs BIAS
EXPERIMENTAL    27 −> 48 hrs BIAS
Unif−Bias−corrected−V8    27 −> 48 hrs BIAS
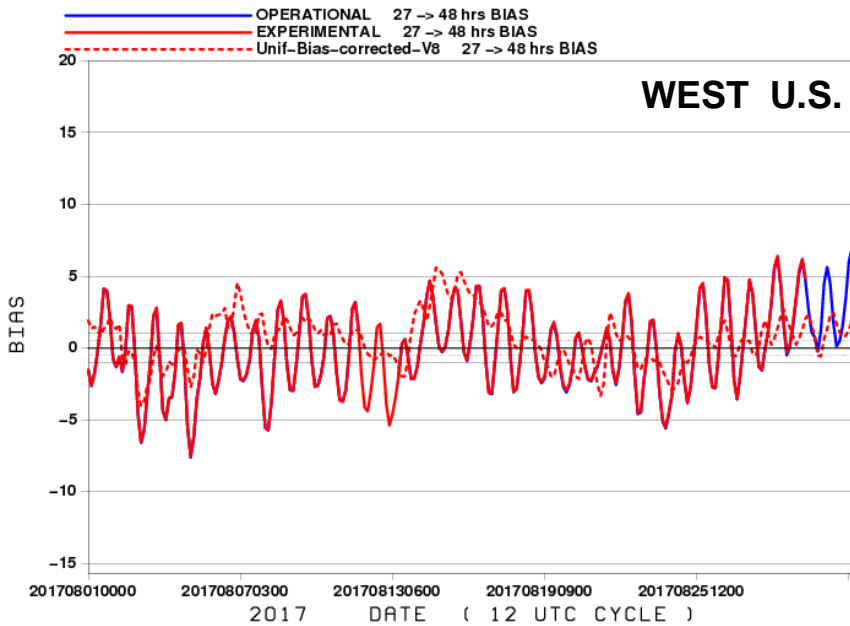
EAST  U.S.
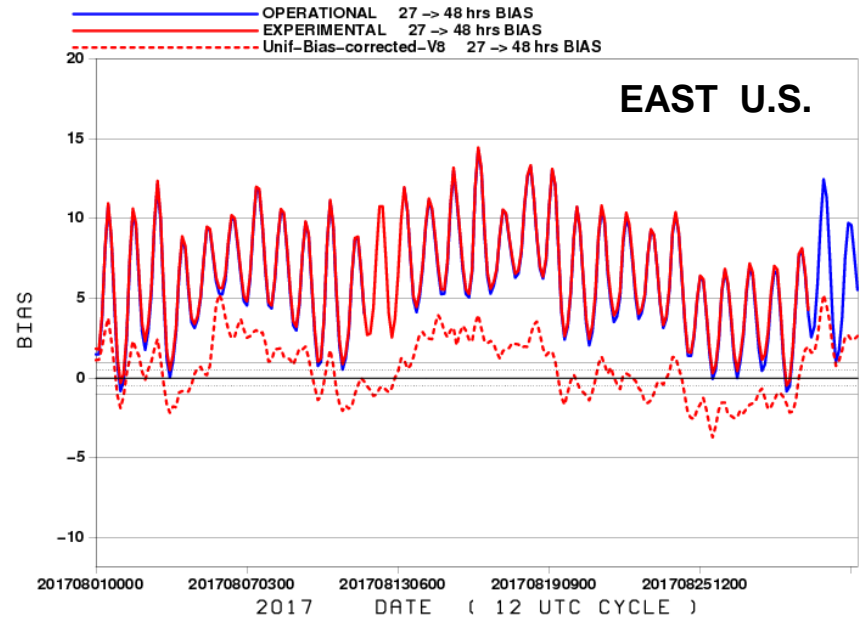
*Exp Bias Correction* reduces large overpredictions esp. over East

16

# Day 2  8 hr daily max O₃



Valid Aug 28, 2017
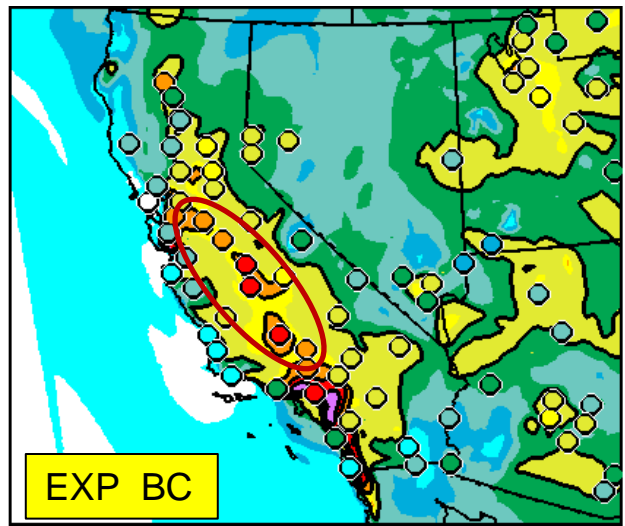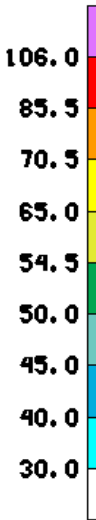
EXP BC

PARA BIAS COR V8    DAY2 OZMXO8 (PPB)    TUE 170829/12(
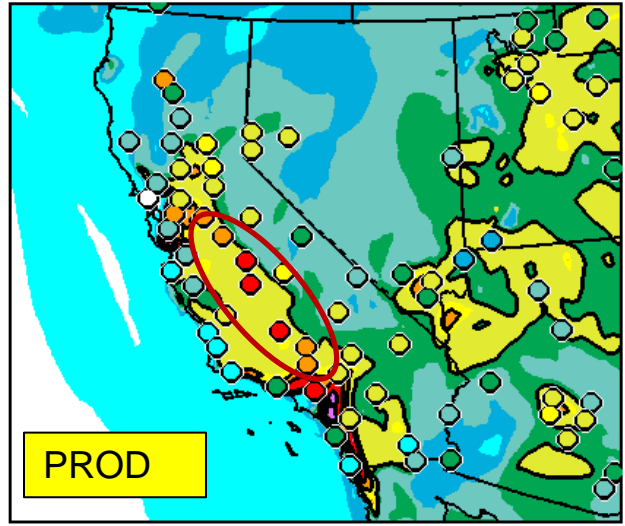
PROD

PROD    DAY2 OZMXO8 (PPB)    TUE 170829/1200V048
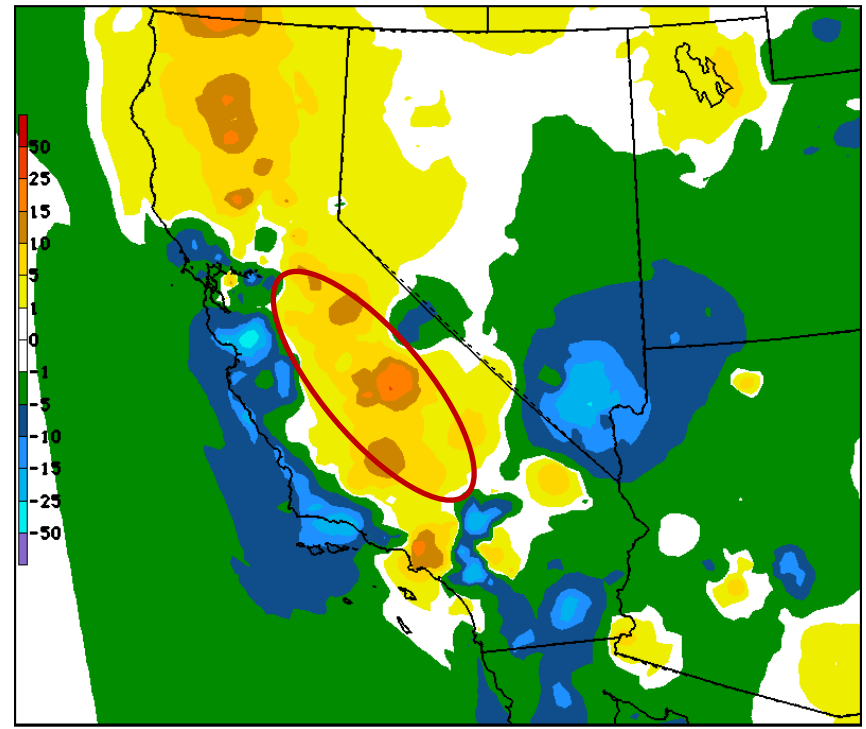
EXP - OPER BC aqm DAY2 O8 hr avg OZMX from 20170827 12 UTC Run

**EXP BC - Production**

BC:    Helps correct underprediction over California valleys
       from fire influenced O₃ production

# Day 1 8hr daily max O₃
## Valid Sept. 2,2017
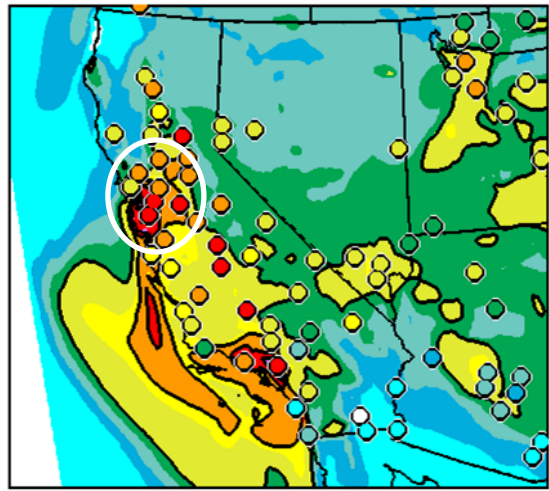


PARA5 4X-DAY DAY1 OZMXO8 20170902 12Z CYC

**EXP Raw**
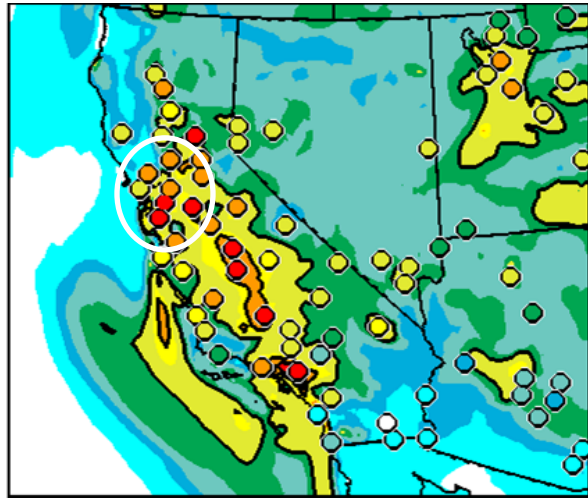
PARA PARABC BIAS COR DAY1 OZMXO8 20170902 12Z

**Old EXP BC**
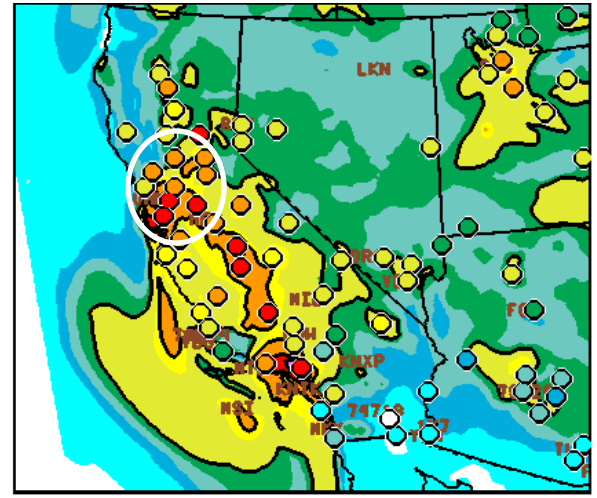
PARA BIAS COR V8 DAY1 OZMXO8 (PPB) 20170902 12Z

**V8 EXP BC**

- BC: helps correct under-prediction over California valleys
- New ozone BC w/ calibration for rare events captures enhanced ozone from fires East of San Francisco better than old EXP BC

# **Raw PM Production** vs
# *PM Production Bias correction* vs
# *Experimental Bias Correction (V8)*
# Predictions

1-h Avg PM25 obs (ug-m3) avged by fcst hrs
20170701 to 20170731
West-US

1-h Avg PM25 obs (ug-m3) avged by fcst hrs
20170701 to 20170731
East-US
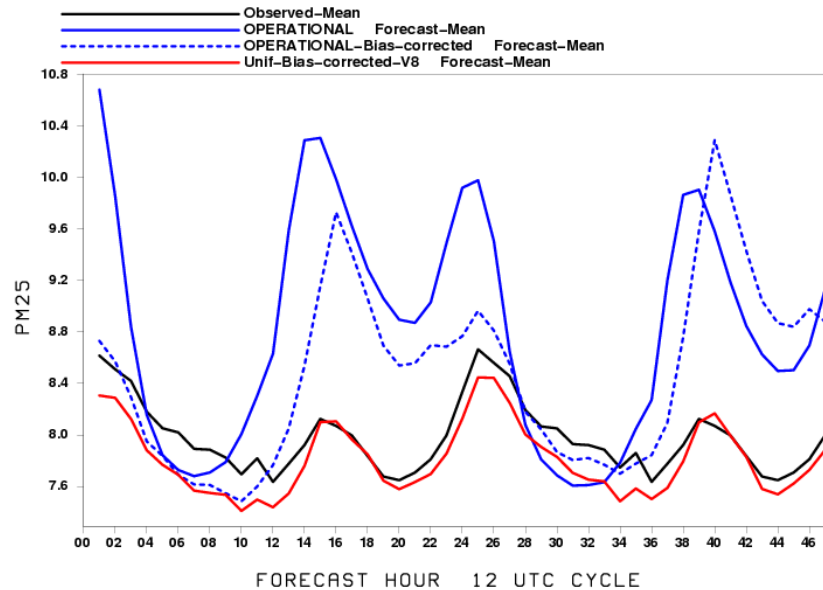
- Large improvement with Exp. Bias correction esp. over East
- *Note: Operational bias correction still using old V4 training predictions*

# Prod, *Prod BC*, Exp BC PM2.5
## Diurnal Time Series
### **August, 2017**



1–h Avg PM25 obs (ug–m3) avged by fcst hrs
20170801 to 20170831
West–US
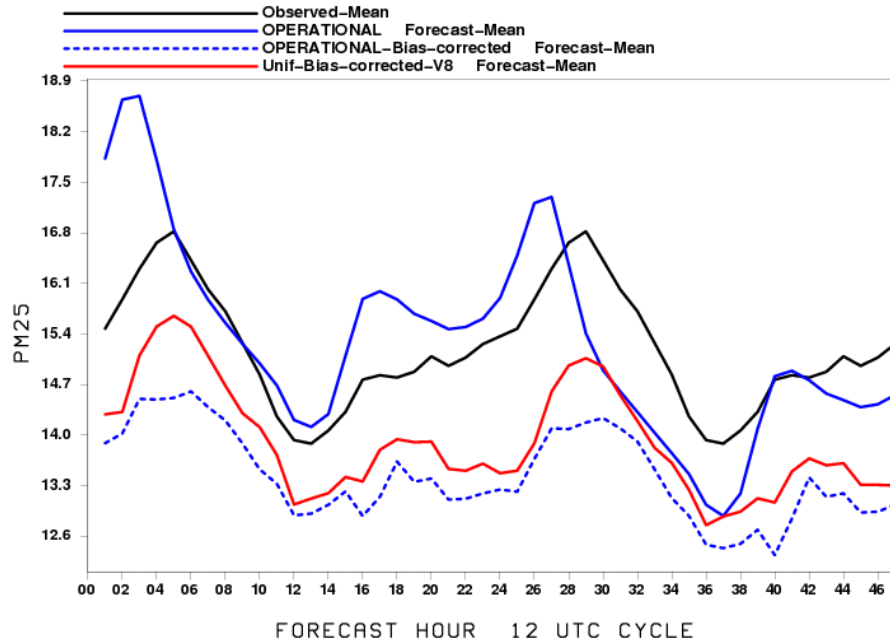
1–h Avg PM25 obs (ug–m3) avged by fcst hrs
20170801 to 20170831
East–US
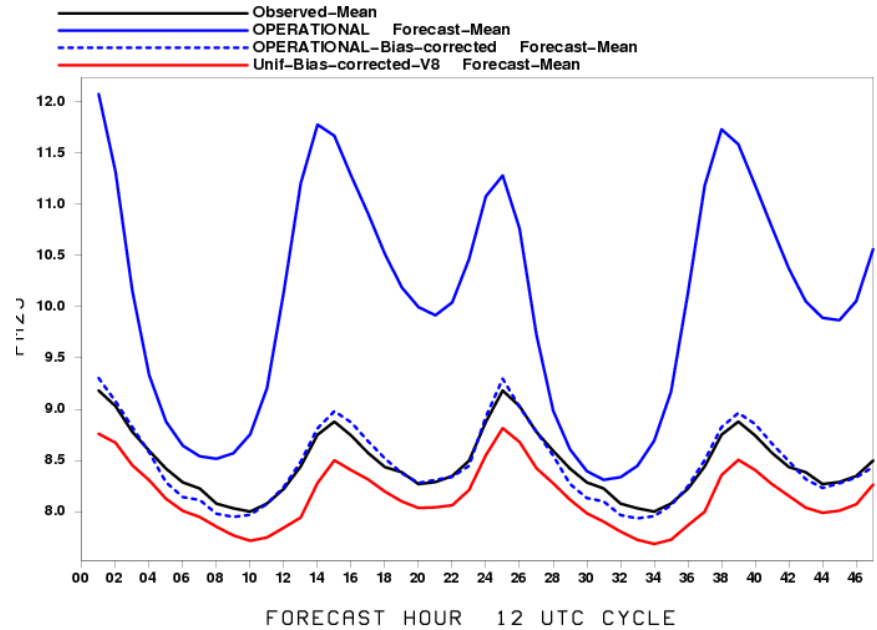
- Improvement with Exp. Bias correction over West compared to Prod BC
- All BC results are degraded compared to raw predictions over West
    - Extensive fires over NW US
- *Note: Operational bias correction still using old V4 training prediction*

# Prod, *Prod BC*, Exp BC PM2.5
## Daily Time Series
## **August, 2017**



DAY 1  −1 Avg PM25  obs (ug-m3) 1500 -> 1200 UTC
West-US                                                            WEST

DAY 1  −1 Avg PM25  obs (ug-m3) 1500 -> 1200 UTC
East-US                                                            EAST
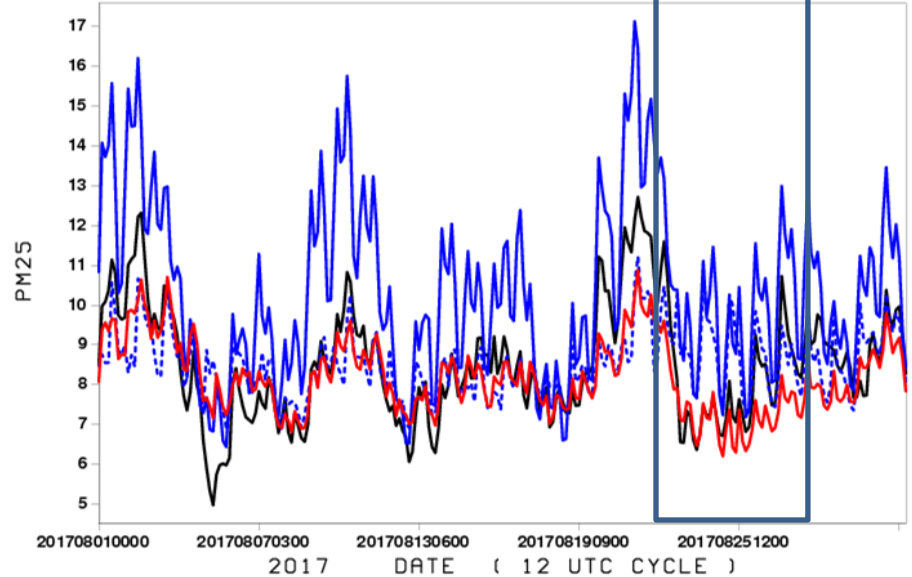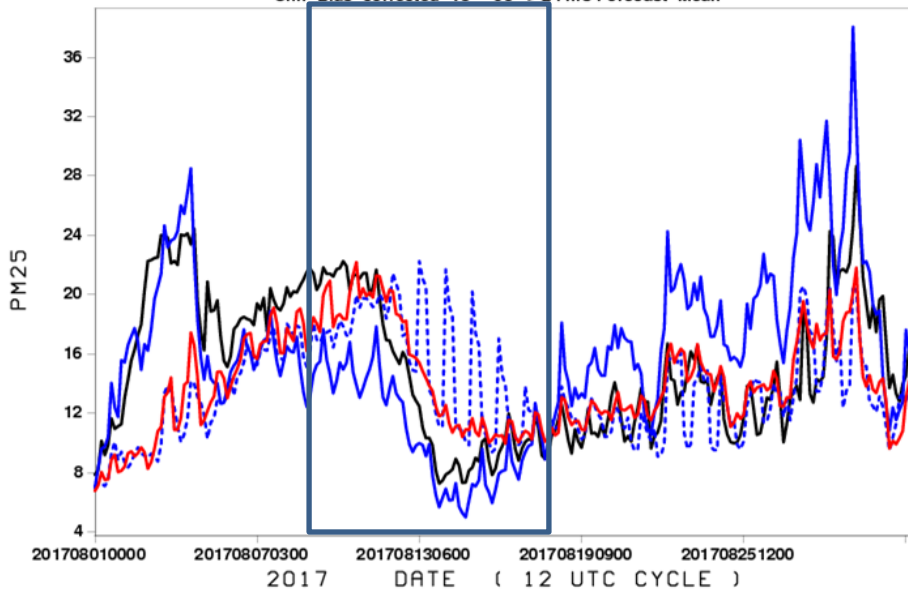
**Exp Bias correction**
- West: - Removes post wild-fire event noise
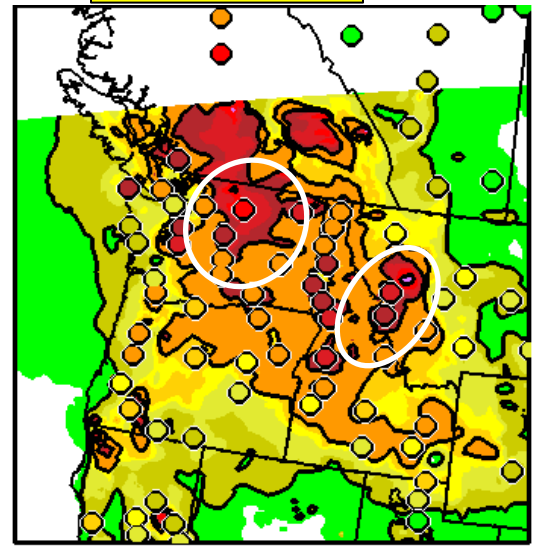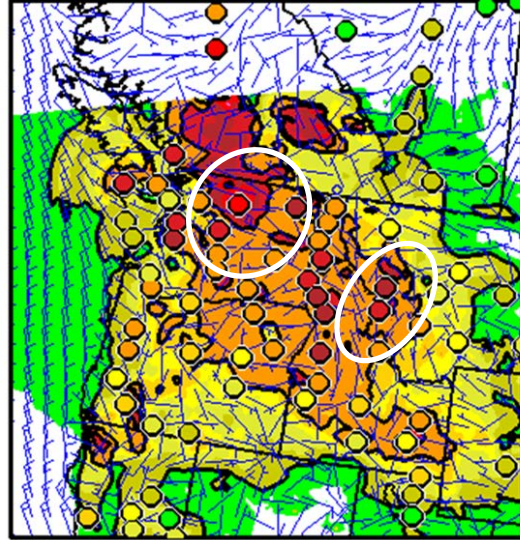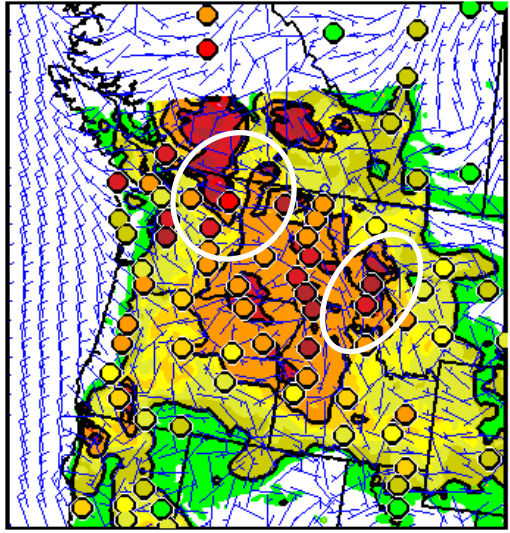          - Overcorrects some fire events esp. early Aug
- East: Similar to prod BC, some improvement around 8/25/17

22

# Day 2  1hr daily max PM2.5
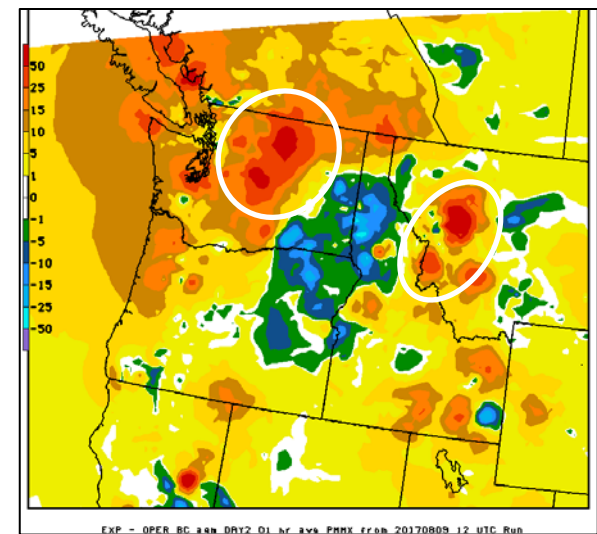## Valid August 9,2017



PROD

PROD  BC

EXP V8  BC
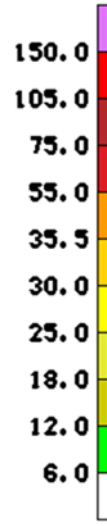
Fire case: some improvement over Washington and Western Montana w/ EXP bias correction
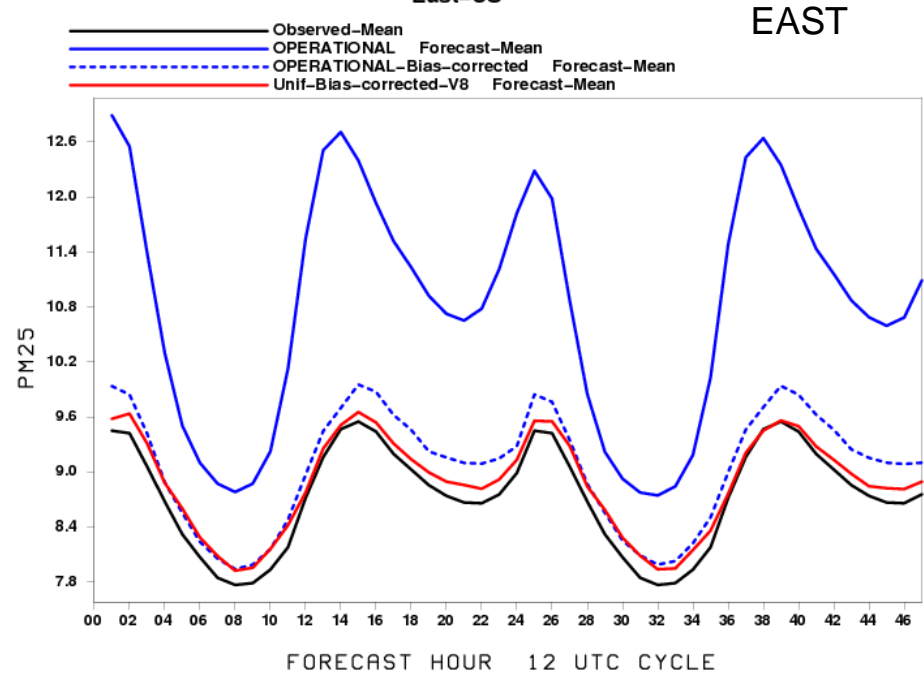
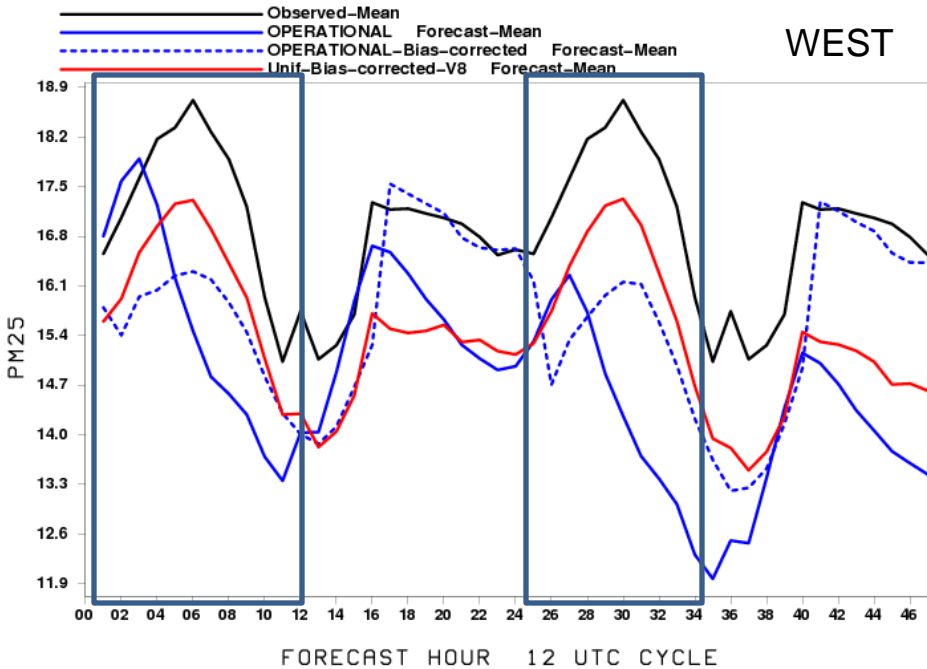# Prod, *Prod BC*, Exp BC PM2.5
## Diurnal Time Series
## **September 2017**



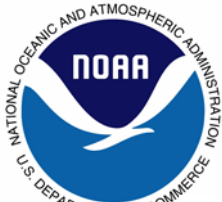1-h Avg PM25 obs (ug-m3) avged by fcst hrs
20170901 to 20170930
West-US

WEST

1-h Avg PM25 obs (ug-m3) avged by fcst hrs
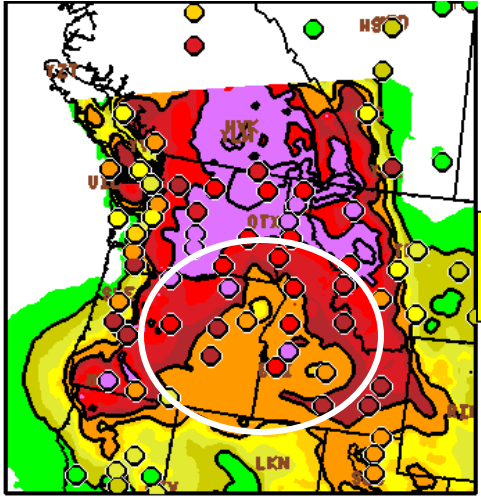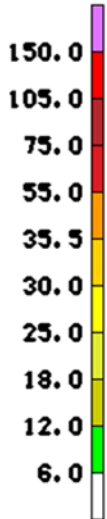20170901 to 20170930
East-US

EAST

- Improvement with Exp. Bias correction over West during the daytime compared to prod BC
- Best improvement over East with bias correction
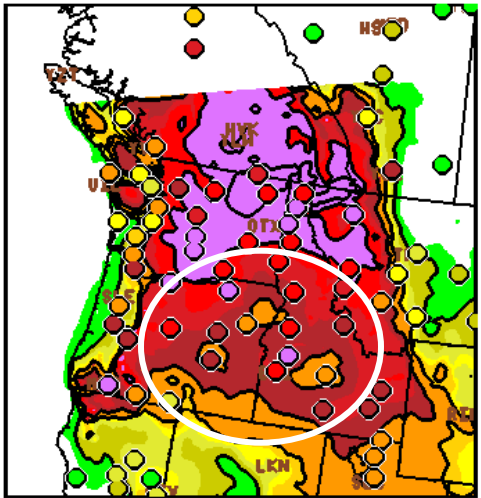- *Note: Operational bias correction using old V4 training prediction*

# Day 2  24hr daily AVE PM2.5
## Valid Sept. 6,2017
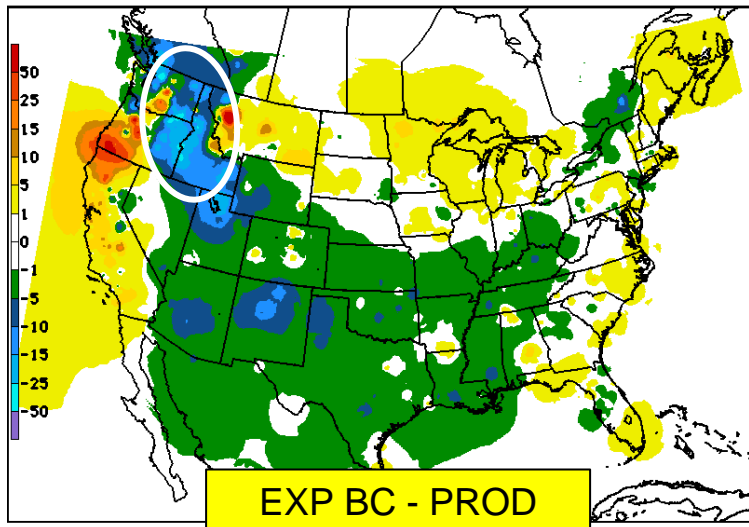


EXP
BC V8

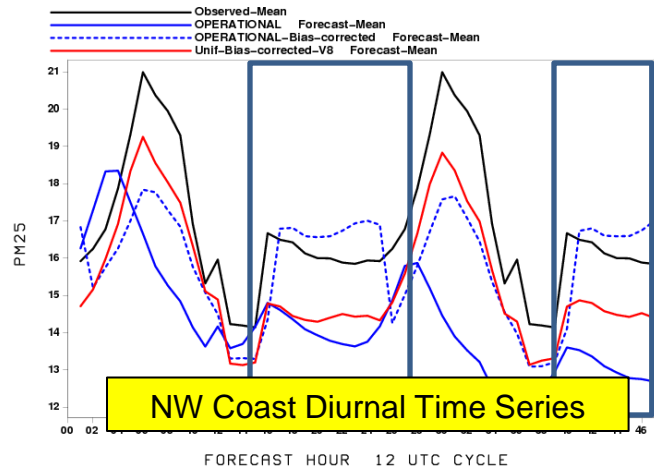PARA BIAS COR V8   DAY2 PMAV24 (UG/M3) 20170905 12Z

PROD
"raw"

PROD   DAY2 PMAV24 (UG/M3) 20170905 12Z CYC

EXP BC - PROD

EXP - OPER BC aqm DAY2 24 hr avg PMAV from 20170905 12 UTC Run

1-h Avg PM25 obs (ug-m3) avged by fcst hrs
20170901 to 20170930
NWEST-Coast

Observed-Mean
OPERATIONAL   Forecast-Mean
OPERATIONAL-Bias-corrected   Forecast-Mean
Unif-Bias-corrected-V8   Forecast-Mean

PM25

NW Coast Diurnal Time Series

FORECAST HOUR   12 UTC CYCLE

EXP PM bias correction overcorrects raw forecasts over East OR/West ID
(due to night-time overcorrection ?)

# Prod, *Prod BC*, Exp BC PM2.5
# Diurnal Time Series
## January 2018



**1–h Avg PM25 obs (ug–m3) avged by fcst hrs**
**20180101 to 20180131**
**West–US**

- Observed–Mean
- OPERATIONAL     Forecast–Mean
- OPERATIONAL–Bias-corrected     Forecast–Mean
- EXPERIMENTAL     Forecast–Mean
- Unif–Bias–corrected–V8     Forecast–Mean

WEST

FORECAST HOUR   12 UTC CYCLE

**1–h Avg PM25 obs (ug–m3) avged by fcst hrs**
**20180101 to 20180131**
**East–US**

- Observed–Mean
- OPERATIONAL     Forecast–Mean
- OPERATIONAL–Bias-corrected     Forecast–Mean
- EXPERIMENTAL     Forecast–Mean
- Unif–Bias–corrected–V8     Forecast–Mean
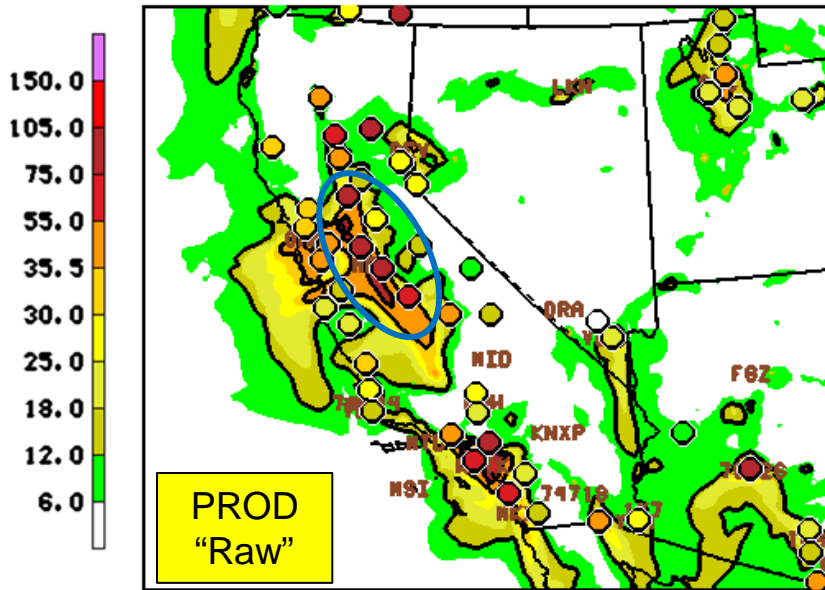
EAST

FORECAST HOUR   12 UTC CYCLE
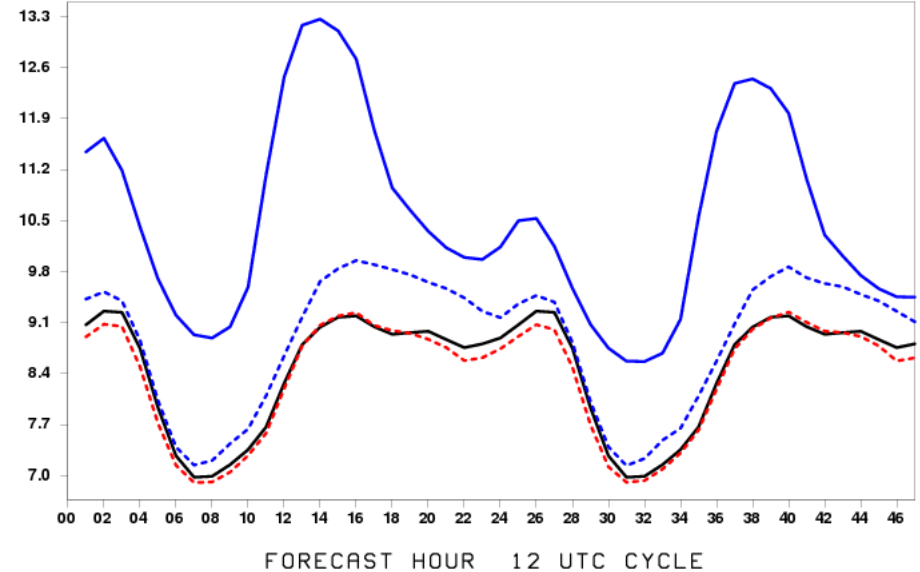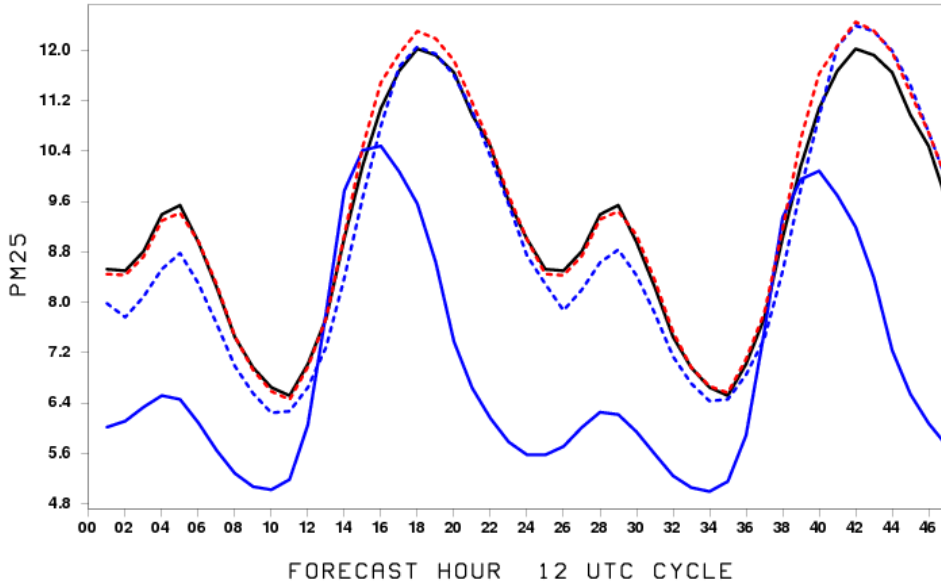
- Less PM (improved) over East with experimental bias correction processing
*Note: Operational bias correction now using correct V5 training predictions*
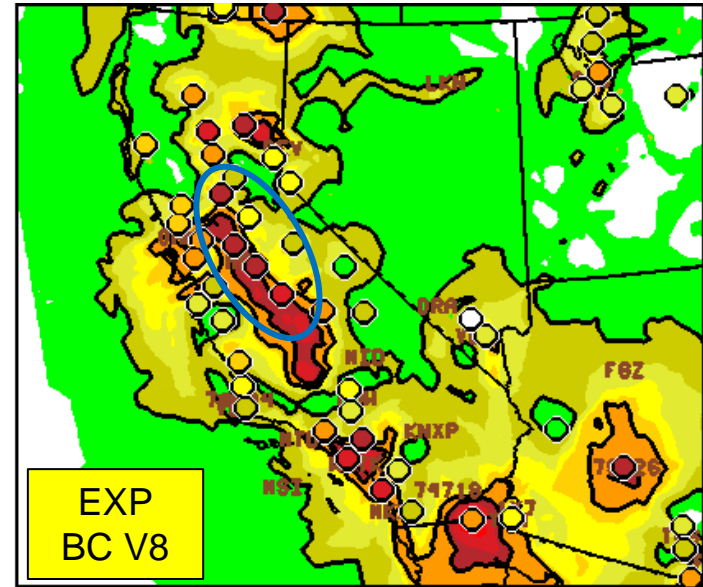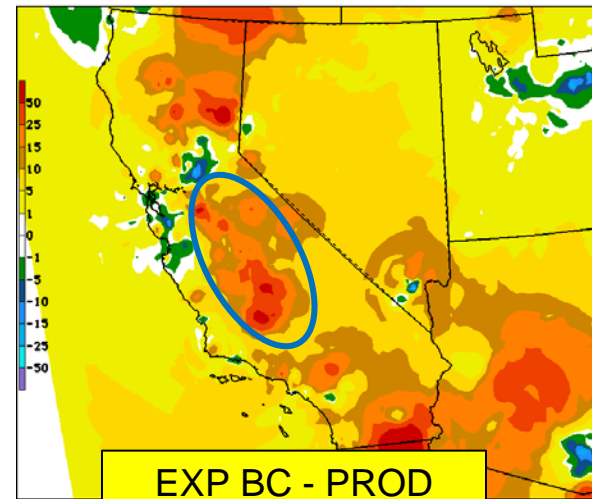
# Day 2 daily 1hr Max PM2.5
## Valid Jan.2, 2018



PROD "Raw"

150.0
105.0
75.0
55.0
35.5
30.0
25.0
18.0
12.0
6.0

PROD DAY2 PMMX01 (UG/M3) 20180101 12Z CYC

EXP BC V8

BIAS COR V8 DAY2 PMMX01 (UG/M3) 20180101 12Z

Bias correction better captures stagnation episode in Central Valley

EXP BC - PROD

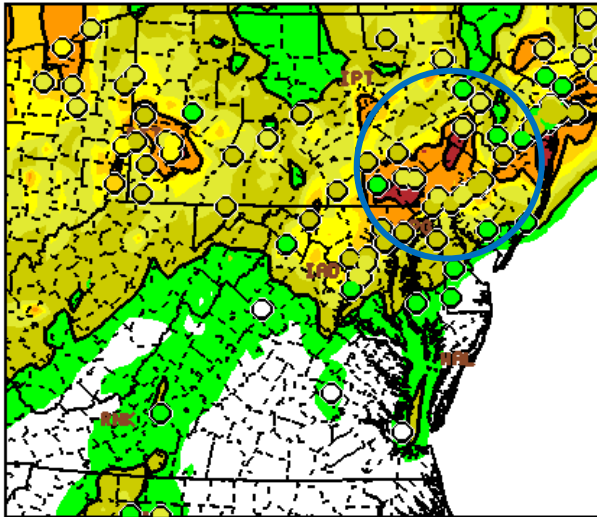EXP - OPER BC aqm DAY2 O1 hr avs PMMX from 20180101 12 UTC Run

# Day 2  daily 1hr Max PM2.5
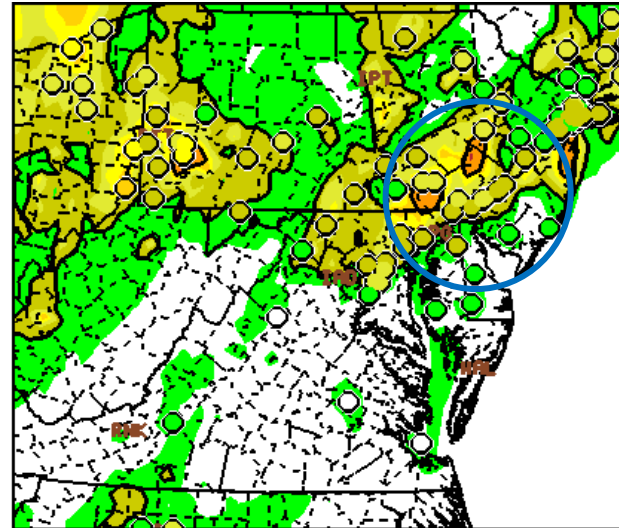## Valid Jan.28, 2018



PROD "Raw"

EXP BC V8
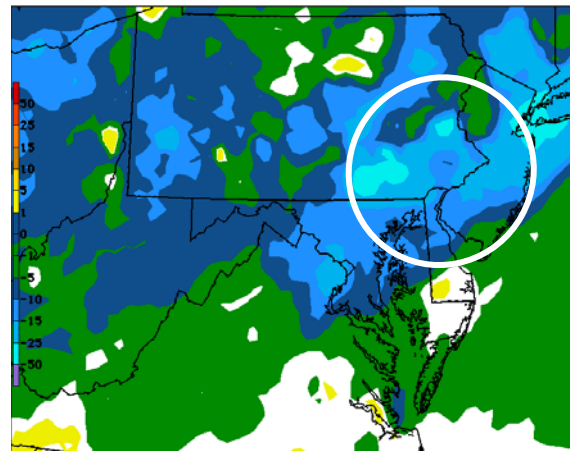
PROD  DAY2 PMMX01 (UG/M3) 20180127 12Z CYC

PARA BIAS COR V8  DAY2 PMMX01 (UG/M3) 20180127 12Z

Significant improvement with Bias correction

EXP BC - PROD

EXP - OPER BC 24h DAY2 01 hr avg PMMX from 20180127 12 UTC Run

# EMC Case Analysis

- **EXP Ozone Bias Correction**: Large improvement without degrading most exceedance cases in Summer
  - *Philadelphia exceptions noted*

- **Summer PM Bias Correction** :
  - Overall improvement statistically correcting raw model over-predictions  (still too much PM near fires at night)
  - Still some overcorrection during fire events but improvements after high PM events

- **Winter PM Bias Correction**:
  - Improved over West  and North East with bias correction especially during strong stagnation episodes
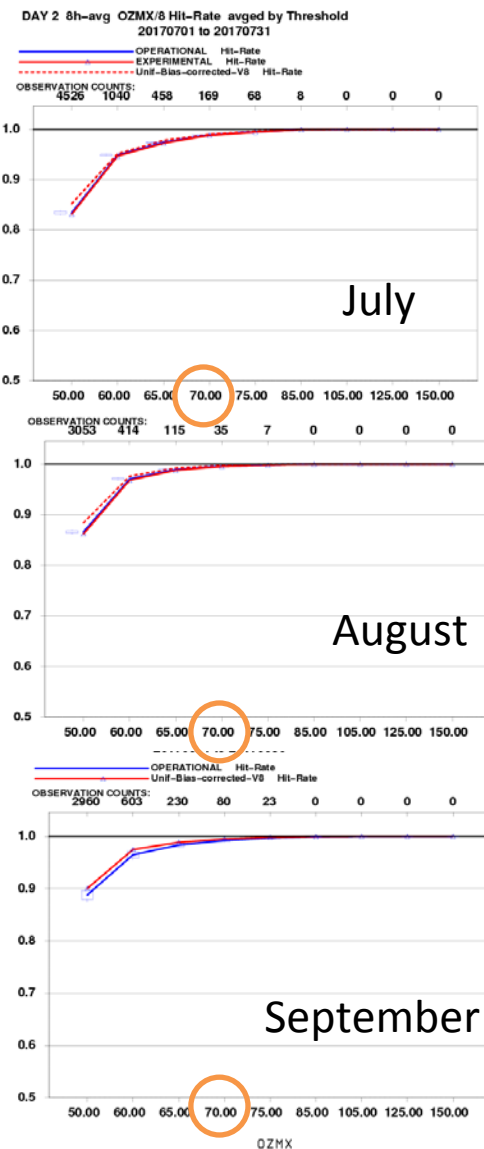
# Statistical performance of ozone prediction
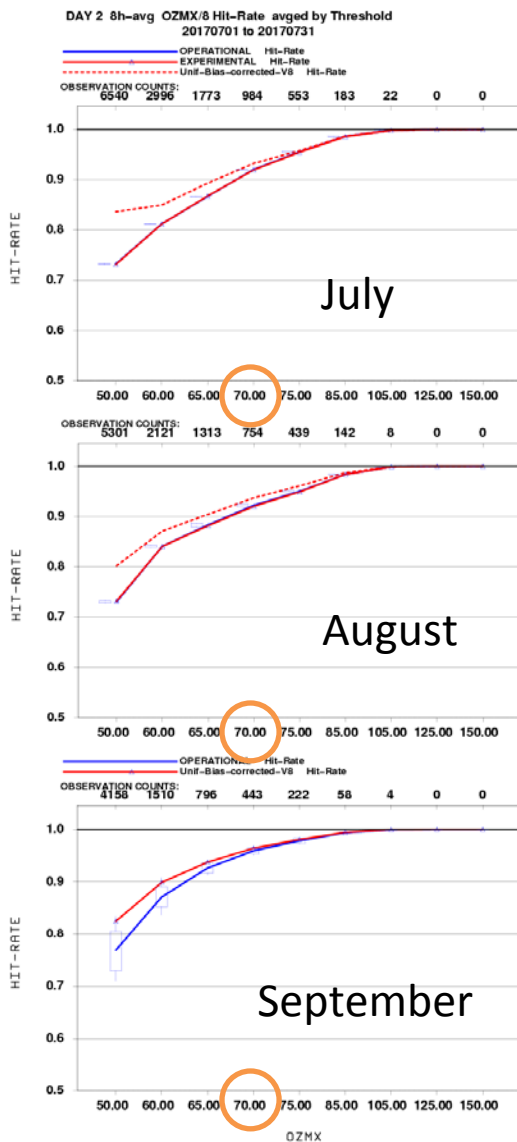## *NWS/STI*

**Fraction correct for 8h ozone maximum (day 2)**



Western US

Eastern US

| BC compared to Raw | Exper. ozone 8h max BC | |
|---|---|---|
| Day 2 | West | East |
| July | ++ | + |
| August | ++ | + |
| September | ++ | + |

- Experimental bias correction for ozone is better than raw model, especially in the Western US

**Fraction correct for 24-hour average PM2.5 (day 2)**

| BC compared to Raw | Operational PM2.5 24h avg BC --- | | Exper. PM2.5 24h avg BC | |
|---|---|---|---|---|
| Day 2 | West | East | West | East |
| July | + | + | ++ | ++ |
| August | -- | + | +/- | ++ |

### Western US
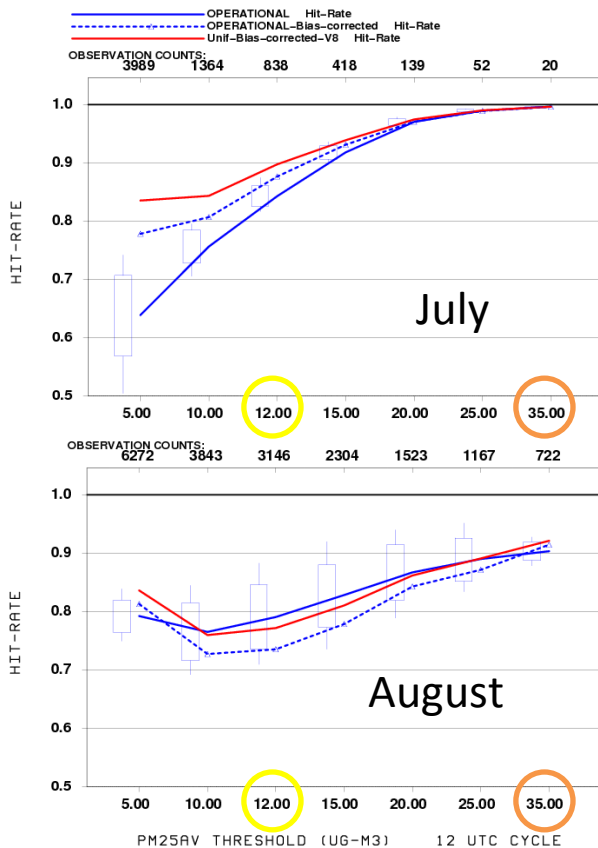


### Eastern US



- Experimental bias correction is better than operational one

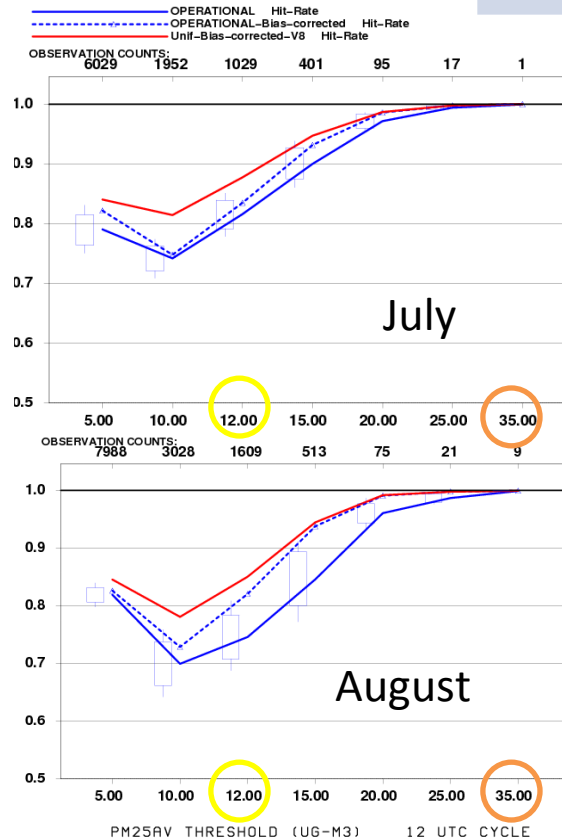- Experimental bias correction is much better than raw model in July and in for Eastern US in August

**Fraction correct for 24-hour average PM2.5 (day 2)**

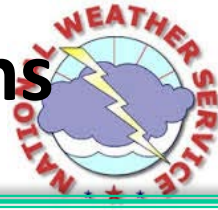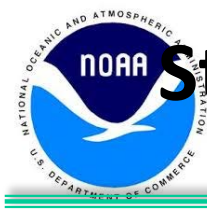| BC compared to Raw | Operational PM2.5 24h avg BC --- | | Exper. PM2.5 24h avg BC | |
|---|---|---|---|---|
| Day 2 | West | East | West | East |
| September | -/+ | + | + | ++ |
| January | + | + | ++ | ++ |

### Western US



### Eastern US



- Experimental bias correction is better than operational one

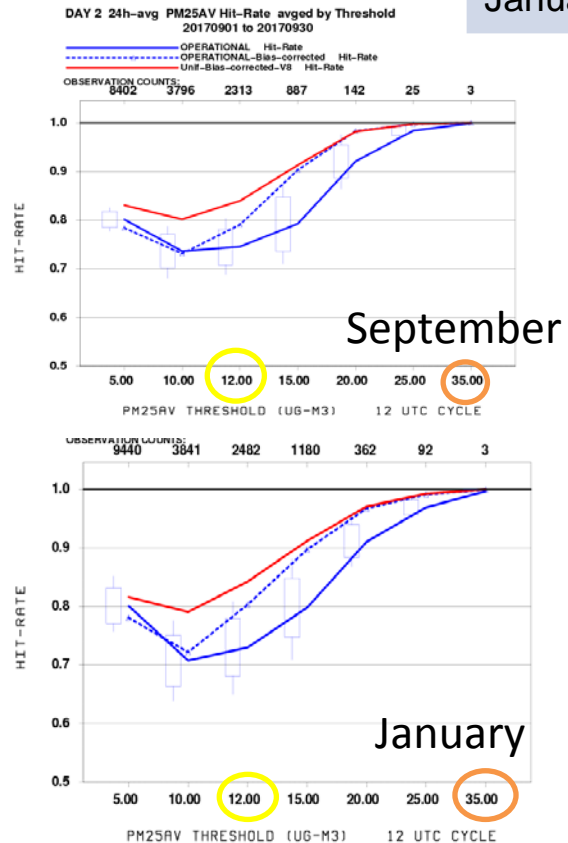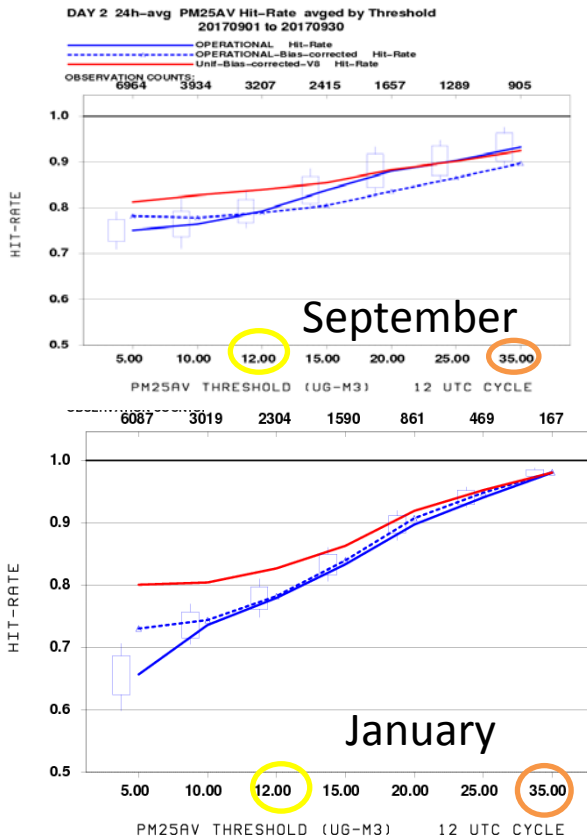- Experimental bias correction is much better than raw model in January and in for Eastern US in September

# Summary evaluation of bias corrected predictions

| BC compared to Raw | Operational PM2.5 24h avg BC | | Exper. PM2.5 24h avg BC | | Exper. ozone 8h max BC | |
|---|---|---|---|---|---|---|
| Day 2 | West | East | West | East | West | East |
| July | + | + | ++ | ++ | ++ | + |
| August | -- | + | +/- | ++ | ++ | + |
| September | -/+ | + | + | ++ | ++ | + |
| January | + | + | ++ | ++ | | |

Fraction Correct for day 2 predictions indicates:

- New ozone bias corrected prediction is better than raw model prediction
- Updated PM2.5 bias correction is better than both raw model predictions and operational bias corrected predictions

# Testing with Forecaster Feedback
## NWS/STI

- Forecasters' feedback was collected after the evaluation period of March 8, 2018 through April 6, 2018.

- Frozen model version predictions were provided by EMC retrospectively for July - September 2017 and January 2018 and in real time since March 2018.

- EMC provides parallel prediction maps and predicted values at monitor sites in text form to air quality forecasters.

# Summary of Forecaster Feedback

Received recommendation to <u>implement as proposed</u> from AQ forecasters in

- California

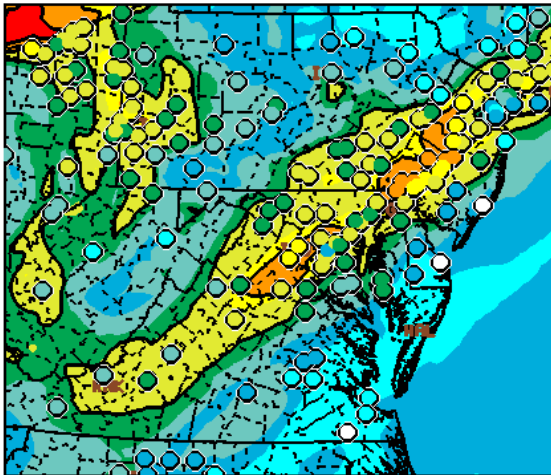- Maryland

- Virginia

- Connecticut

- Alabama

Additional feedback was received from forecasters in Maine, Minnesota, and North Carolina without a recommendation.

Pennsylvania forecaster recommended further testing.

# Ozone Feedback: Maryland/DC
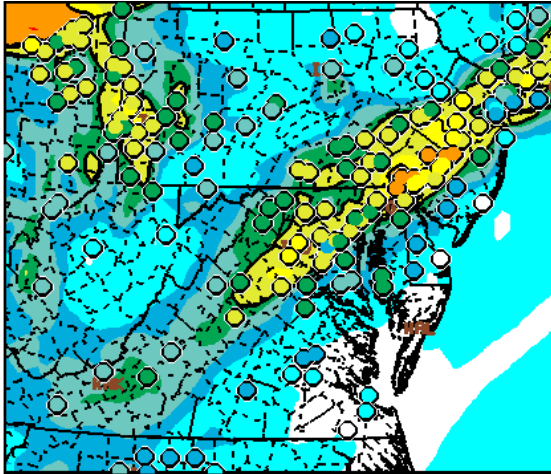


PARA BIAS COR V8  DAY2 OZMXO8 (PPB) 20170924 12Z CYC

PROD  DAY2 OZMXO8 (PPB) 20170924 12Z CYC

**During Exeedance Event on Sept 25, 2017, Bias correction was significantly better**

- Significant improvement in Bias correction forecast, particularly around DC.

- Bias correction correctly nailed the single exceeding monitor (FairHill) on this day.

- Caveat – the Bias correction appears to over correct west of DC
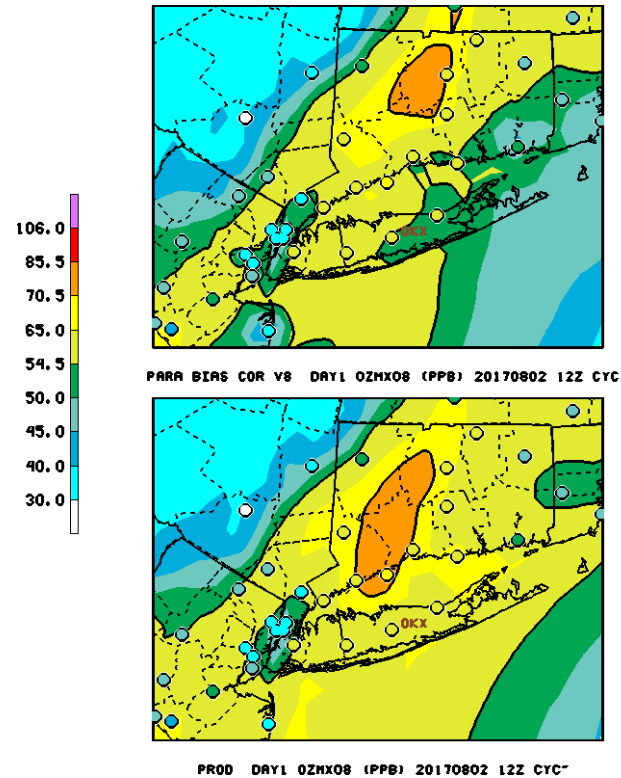
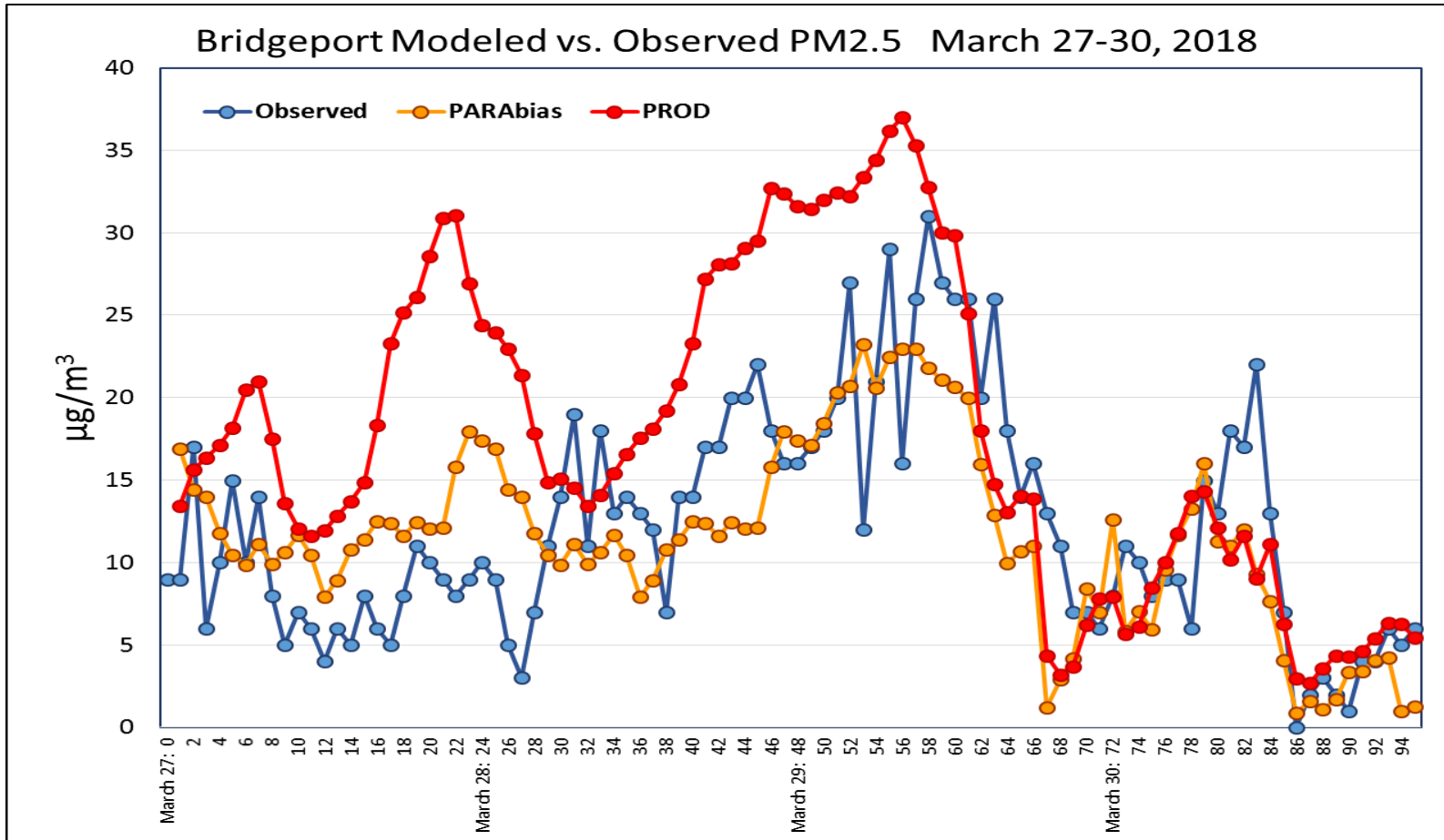# Ozone Feedback: Connecticut

**August 2, 2017 12z**

Day 2
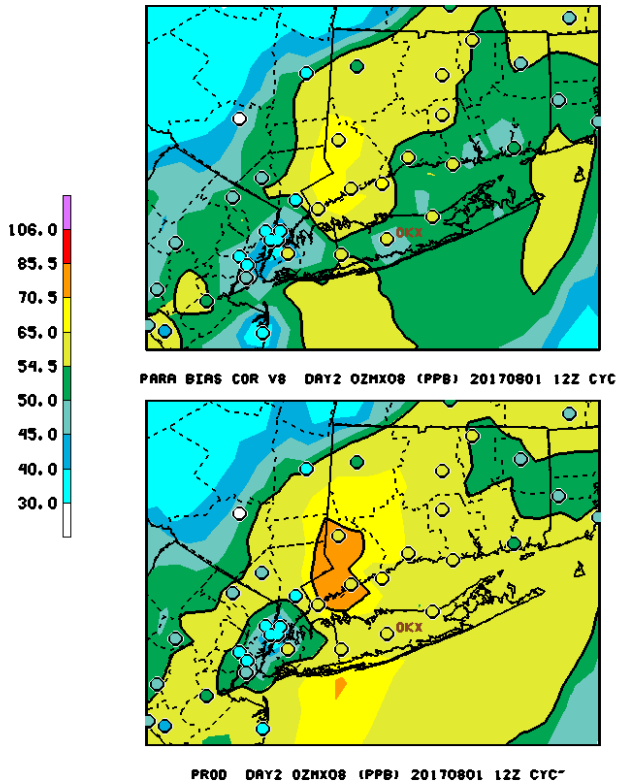
Day 1



- The BIAS tended to be more accurate with higher ozone levels;
- But on some days, e.g. July 2,3,11ᵗʰ, both models performed poorly;
- BIAS= 18  WINNER!
- PROD= 12

# PM2.5 Feedback: Connecticut



Bridgeport Modeled vs. Observed PM2.5   March 27-30, 2018

The PARA bias (and PROD bias) correction are almost always a better predictor for PM2.5 levels than the PROD run

# BACKUPS

# FY19 Goals

- Extend forecast to 72 hours
- Update anthropogenic emissions to NEI 2014V2
- Implement diurnal wild-fire smoke emission profiles

- CMAQ V5.2.1 update:
  - Extended speciation (marine chemistry)
  - Aerosol impacts on photolysis

- Begin transition to FV3-Chem
  - Offline coupling at first ?
  - FV3GFS vs FV3REG met driver
  - BlueSky vs topdown VIIRS/MODIS active fire data
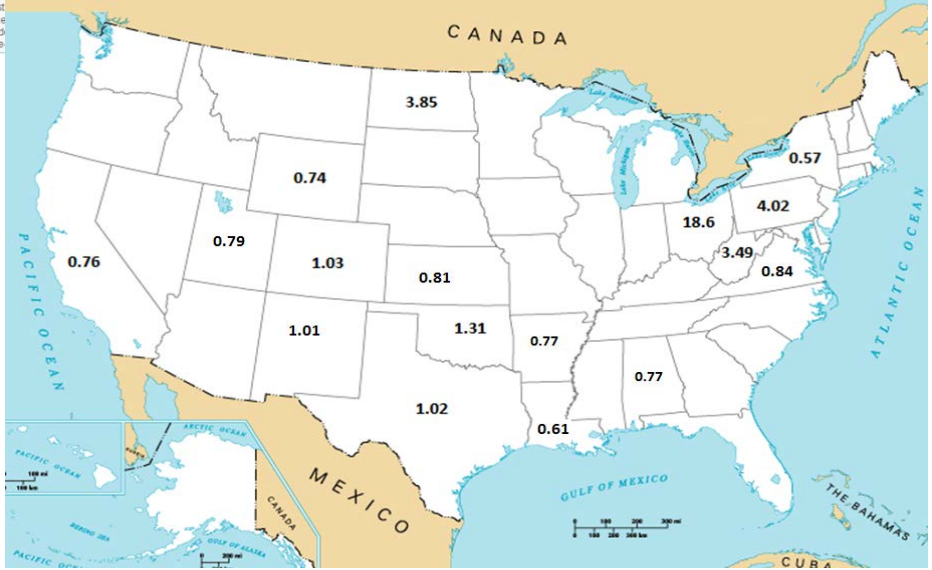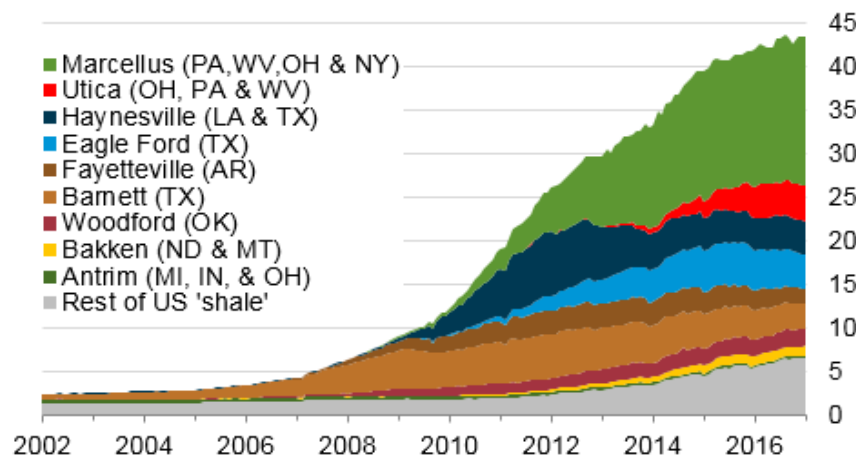  - Update bias correction for new model behaviors

# Emissions updates: oil and gas sector



**2014 Energy Information Administration on Shale Plays**

Testing of State-specific scaling for Oil_n_Gas area source
- July 11-21 sensitivity run confirmed that Marcellus area O3 increased
- Under-prediction in O3 in the Marcellus area was reduced
- However the over-prediction in O3 elsewhere was exacerbated



Monthly dry shale gas production
billion cubic feet per day

- Marcellus (PA,WV,OH & NY)
- Utica (OH, PA & WV)
- Haynesville (LA & TX)
- Eagle Ford (TX)
- Fayetteville (AR)
- Barnett (TX)
- Woodford (OK)
- Bakken (ND & MT)
- Antrim (MI, IN, & OH)
- Rest of US 'shale'

Sources: EIA derived from state administrative data collected by DrillingInfo Inc. Data are through January 2017 and represent EIA's official shale gas estimates, but are not survey data. State abbreviations indicate primary state(s).
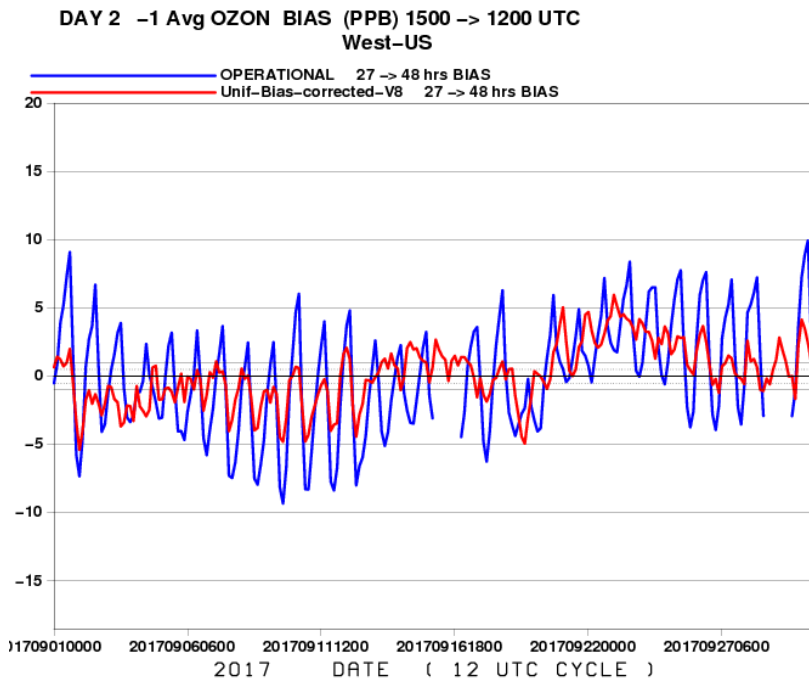


**Adjustment factor applied to NEI2011 oil and gas area source sector**

# 1h avg O₃ Day 2 Daily Time Series BIAS
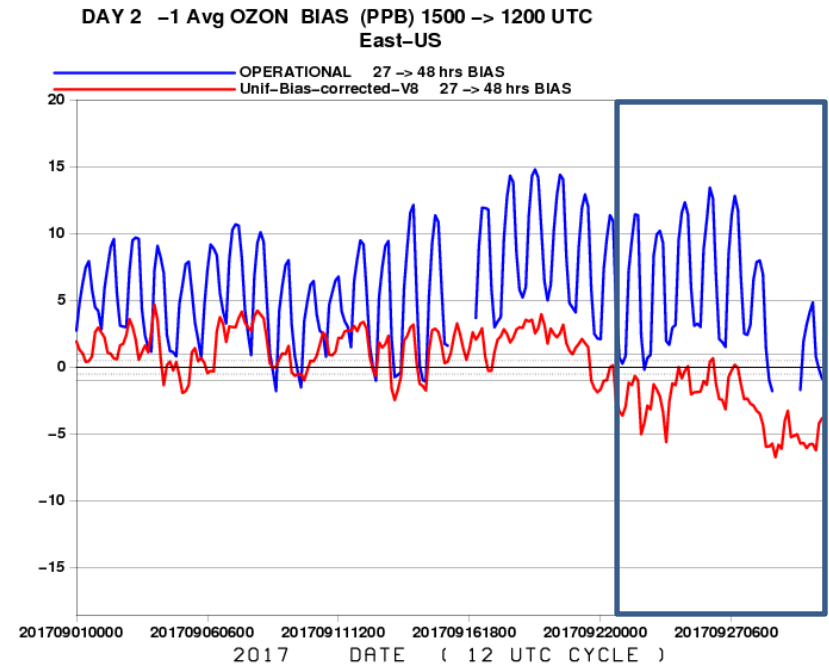## Prod and EXP bias corrected
### September 2017



**WEST**

**EAST**

O3 Bias Correction - Improved, similar trend to raw except underprediction over East later in month

43