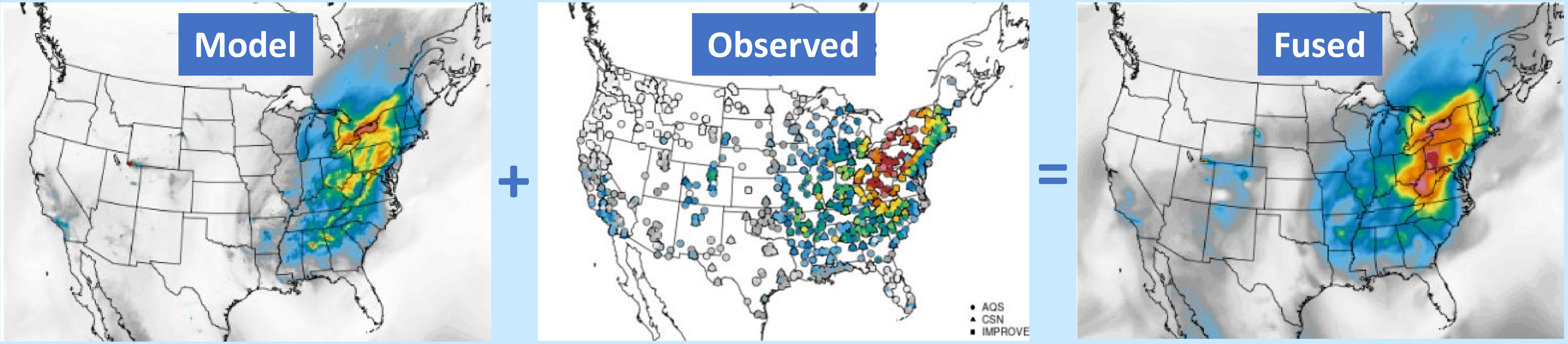
Improved air quality estimates using EQUATES CMAQ and data fusion with Downscaler: A cross-validation study using 18 years of $PM_{2.5}$ and ozone modeling

Kristen Foley, Adam Reff, Jeanette Reyes, Sharon Philips, Barron Henderson, Christian Hogrefe (US EPA)

Acknowledgments: Veronica Berrocal (University of California, Irvine)



EQUATES: EPA's Air Quality Time Series Project

A collaboration across different parts of EPA to develop modeled meteorology, emissions, air quality and pollutant deposition for 2002 - 2019. Modeling datasets were publicly released in 2021 and have been widely distributed and used by researchers in and outside of EPA.
In this talk "EQUATES" = output from CMAQv5.3.2 simulations using consistent emissions and meteorology.

Downscaler: Fused Air Quality Surfaces using Downscaling (FAQSD or **DS**)

Bayesian statistical model developed by researchers from UC Urvine, Duke, BYU, and EPA to create fused daily average ozone and $PM_{2.5}$ estimates for the contiguous US based on air quality modeling and observations. In this talk "EQUATES DS" = EQUATES CMAQ + observations fused using DS.

CDC DS: DS ozone and $PM_{2.5}$ fused estimates to inform the CDC's National Environmental Public Health Tracking Network

The 2002-2020 CDC DS data were developed by EPA over the last 15 years based on the best air quality modeling data available at the time. Fused ozone and $PM_{2.5}$ data are publicly available through EPA's RSIG, including comprehensive technical support documents (Annual Reports) for each year.

Background and Motivation

Environmental Research
Volume 196, May 2021, 110432

Examining $PM_{2.5}$ concentrations and exposure using multiple models

James T. Kelly[a], Carey Jang[a], Brian Timin[a], Qian Di[b], Joel Schwartz[c], Yang Liu[d], Aaron van Donkelaar[e f], Randall V. Martin[e f g], Veronica Berrocal[h], Michelle L. Bell[i]

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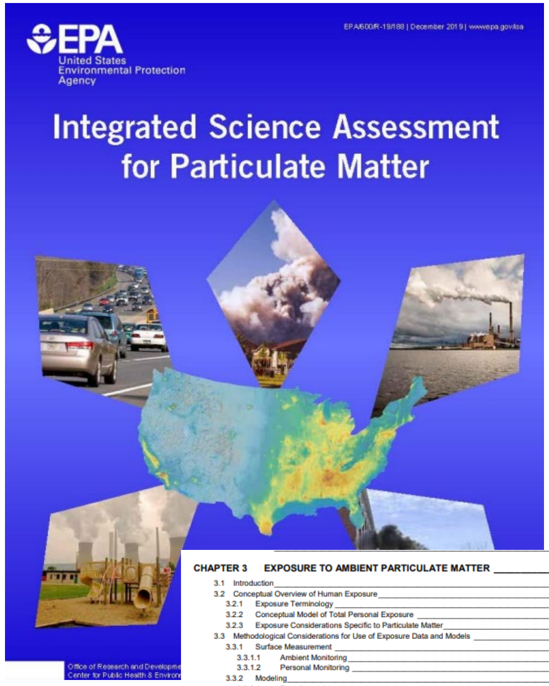
Many data fusion methods in the literature have been applied and evaluated by EPA.

Many EPA data products rely on fused estimates including BenMap, EJScreen, CEJST, and the NetAssess2025 Tool.



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Data fusion applications in the Air Quality Modeling Group

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July 2023, Durham, NC

Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the U.S. Environmental Protection Agency.

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Estimating US Background Ozone Using Data Fusion

T. Nash Skipper, Yongtao Hu, M. Talat Odman, Barron H. Henderson, Christian Hogrefe, Rohit Mathur, and Armistead G. Russell*

Cite This: Environ. Sci. Technol. 2021, 55, 4504–4512 Read Online

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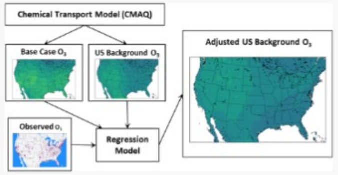
ABSTRACT: US background (US-B) ozone (O_3) is the O_3 that would be present in the absence of US anthropogenic (US-A) emissions. US-B O_3 varies by location and season and can make up a large, sometimes dominant, portion of total O_3. Typically, US-B O_3 is quantified using a chemical transport model (CTM) though results are uncertain due to potential errors in model process descriptions and inputs, and there are significant differences in various model estimates of US-B O_3. We develop and apply a method to fuse observed O_3 with US-B O_3 simulated by a regional CTM (CMAQ). We apportion the model bias as a function of space and time to US-B and US-A O_3. Trends in O_3 bias are explored across different simulation years and varying model scales. We found that the CTM US-B O_3 estimate was typically biased low in spring and high in fall across years (2016–2017) and model scales. US-A O_3 was biased high on average, with bias increasing for coarser resolution simulations. With the application of our data fusion bias adjustment method, we estimate a 28% improvement in the agreement of adjusted US-B O_3. Across the four estimates, we found annual mean CTM-simulated US-B O_3 ranging from 30 to 37 ppb with the spring mean ranging from 32 to 39 ppb. After applying the bias adjustment, we found annual mean US-B O_3 ranging from 32 to 33 ppb with the spring mean ranging from 37 to 39 ppb.



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Environmental Research
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Examining $PM_{2.5}$ concentrations and exposure using multiple models

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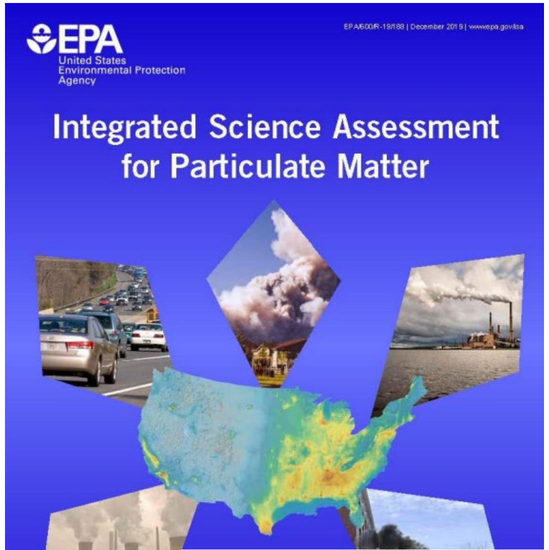
Data fusion provides a method to decrease model bias and increase correlation between model output and measurement data, providing a more complete and accurate picture of air pollutant concentrations.



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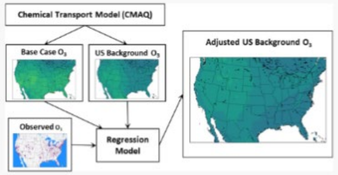

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EQUATES Downscaler Objectives

- Create EQUATES daily average $PM_{2.5}$ and Maximum daily 8-hr Ozone (MDA8 O_3) fused estimates for 2002-2019 for the contiguous US.

  → EQUATES DS fused estimates provide a consistent timeseries of bias-adjusted model estimates for epidemiological studies and other applications.

- Use cross validation to evaluate $PM_{2.5}$ and MDA8 O_3 estimates from
  - EQUATES DS vs EQUATES CMAQ output (fused vs raw)
  - EQUATES DS vs CDC DS (fused vs fused)

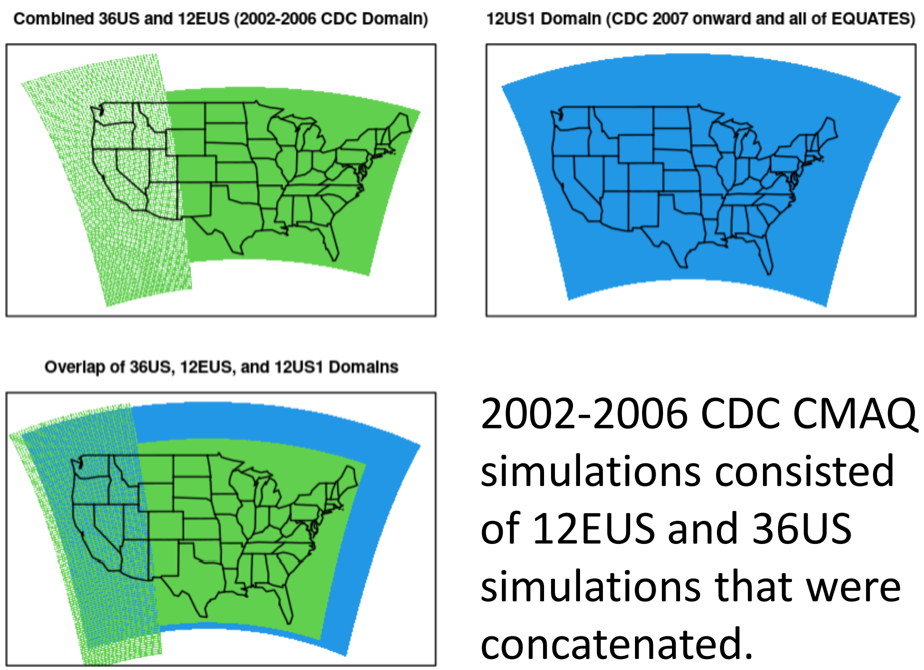
  → What is the impact of using improved CMAQ modeling datasets on the final fused surfaces?

A sample of this evaluations is included in this presentation.

How different are the model data used in the CDC and EQUATES DS estimates?

CMAQ Version for CDC and EQUATES Fused Surfaces

	CDC	EQUATES
2002	CMAQv4.6 (12km + 36km)	CMAQv5.3.2
2003	CMAQv4.7 (12km + 36km)	CMAQv5.3.2
2004	CMAQv4.7 (12km + 36km)	CMAQv5.3.2
2005	CMAQv4.7 (12km + 36km)	CMAQv5.3.2
2006	CMAQv4.7 (12km + 36km)	CMAQv5.3.2
2007	CMAQv4.7.1	CMAQv5.3.2
2008	CMAQv4.7.1	CMAQv5.3.2
2009	CMAQv4.7.1	CMAQv5.3.2
2010	CMAQv4.7.1	CMAQv5.3.2
2011	CMAQv5.0.2	CMAQv5.3.2
2012	CMAQv5.0.2	CMAQv5.3.2
2013	CMAQv5.1	CMAQv5.3.2
2014	CMAQv5.2	CMAQv5.3.2
2015	CMAQv5.2.1	CMAQv5.3.2
2016	CMAQv5.3	CMAQv5.3.2
2017	CMAQv5.3.1	CMAQv5.3.2
2018	CMAQv5.3.2	CMAQv5.3.2
2019	CMAQv5.3.2	CMAQv5.3.2



2002-2006 CDC CMAQ simulations consisted of 12EUS and 36US simulations that were concatenated.

CDC and EQUATES model inputs (e.g., emissions, meteorology) and configurations differ for every year, even 2018 and 2019 which used the same CMAQ version.

Fused Air Quality Surfaces using Downscaling

Biometrics JOURNAL OF THE INTERNATIONAL BIOMETRIC SOCIETY

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Full Access

BIOMETRICS 68, 837–848
September 2012

Space-Time Data fusion Under Error in Computer Model Output: An Application to Modeling Air Quality

Veronica J. Berrocal,[1,*] Alan E. Gelfand,[2,**] and David M. Holland[3,***]

[1]Department of Biostatistics, University of Michigan, Ann Arbor, Michigan 48109, U.S.A.
[2]Department of Statistical Science, Duke University, Durham, North Carolina 27708, U.S.A.
[3]U.S. Environmental Protection Agency, National Exposure Research Laboratory, Research Triangle Park, North Carolina 27711, U.S.A.

User's Manual for Downscaler Fusion Software

Thomas Leininger[1] David Holland[2] Matthew Heaton[3]

August 24, 2013

[1]Duke University, Durham, NC 27708.
[2]U.S. Environmental Protection Agency, National Exposure Research Laboratory, RTP, NC 27711.
[3]Department of Statistics, Brigham Young University, Provo, UT 84602.

Formulation of the Downscaler Bayesian statistical model

Presents three spatial formulations of the Downscaler

1. Univariate Downscaler
2. Gaussian Markov Random field (GMRF) smoothed downscaler
3. Smoothed downscaler using spatially varying random weights

Matlab code to implement the Downscaler approach

Implements formulation 3. with some modifications.

Smoothed Downscaler using spatially varying random weights

$$Y(\mathbf{s}) = \tilde{\beta}_0(\mathbf{s}) + \beta_1 \tilde{x}(\mathbf{s}) + \epsilon(\mathbf{s}) \qquad \epsilon(\mathbf{s}) \sim N(0, \tau^2) \qquad (7)$$

$$\tilde{x}(\mathbf{s}) = \sum_{k=1}^{g} \boxed{w_k(\mathbf{s})} x(B_k). \qquad (8)$$

$$x(B) = \mu + \boxed{V(B)} + \eta(B) \qquad \eta(B) \overset{ind}{\sim} N(0, \sigma^2) \qquad (4)$$

Parameterized random spatial processes; Bayesian estimation of parameters is used to determine poster *distribution* of $\tilde{x}(s)$.

Berrocal et al., 2012

* Ozone transformation = square root
PM2.5 transformation = natural log

- $Y(s)$ = Transformed* observed daily value at site **s**
- $\tilde{\beta}_0(\boldsymbol{s})$ = spatially varying additive bias correction (mean-zero GP with exponential covariance)
- $\tilde{\beta}_1$ = global multiplicative bias correction
- $\tilde{x}(s)$ = weighted average of smoothed CMAQ estimates
- $\varepsilon(s)$ = white noise processes
- $w_k(s)$ = random spatially varying weights that can have directionality to allow for spatial misalignment of modeled and observed processes (e.g., plumes in the wrong place)
- $x(B_k)$ = smoothed version of transformed* CMAQ estimate at grid cell B_k; allows grid cells surrounding **s** to inform estimate $\hat{Y}(\mathbf{s})$.
- μ = global mean (applied to all grid cells)
- $V(B)$ = a mean-zero Gaussian Markov random field with a conditionally autoregressive structure
- $\eta(s)$ = white noise processes

Smoothed Downscaler using spatially varying random weights

$$Y(\mathbf{s}) = \tilde{\beta}_0(\mathbf{s}) + \beta_1 \tilde{x}(\mathbf{s}) + \epsilon(\mathbf{s}) \qquad \epsilon(\mathbf{s}) \sim N(0, \tau^2) \qquad (7)$$

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Berrocal et al., 2012

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Spatially Varying Random Weights

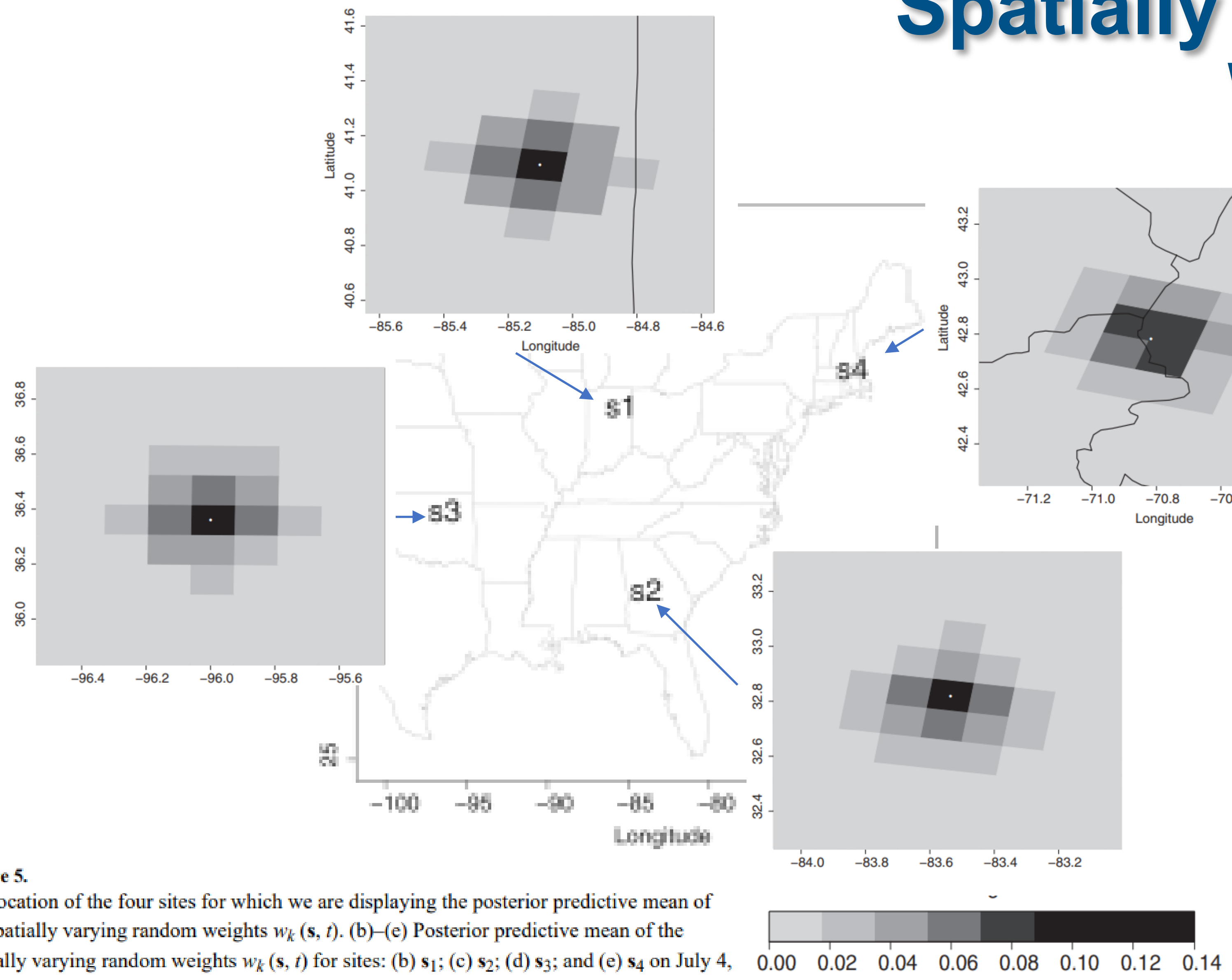
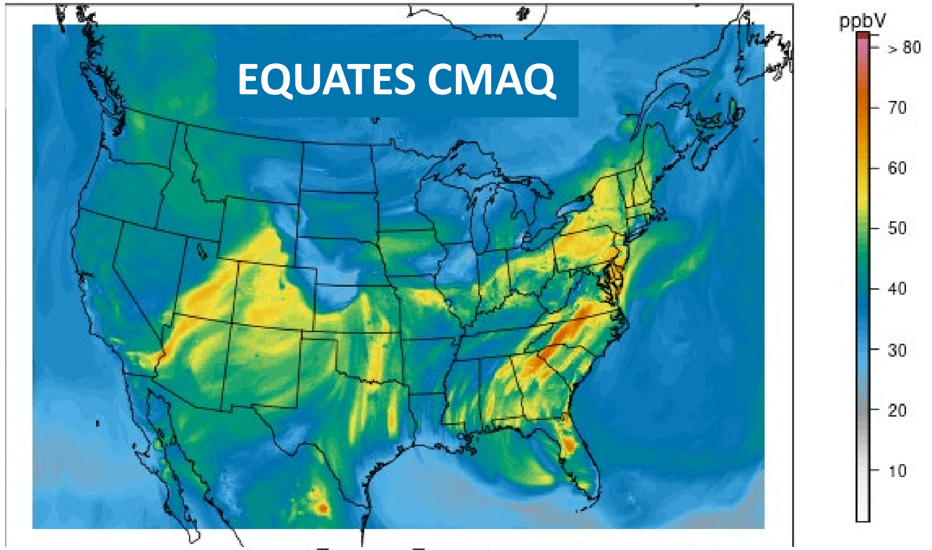
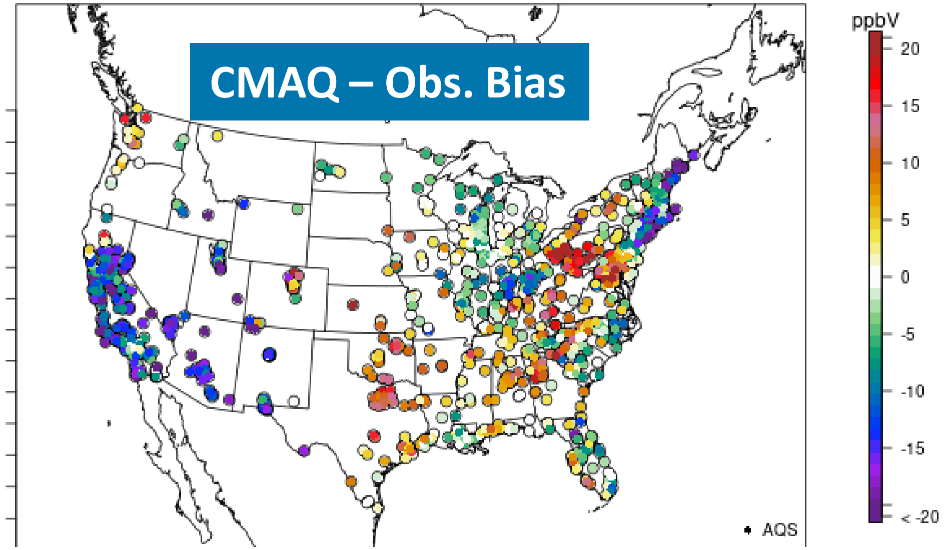


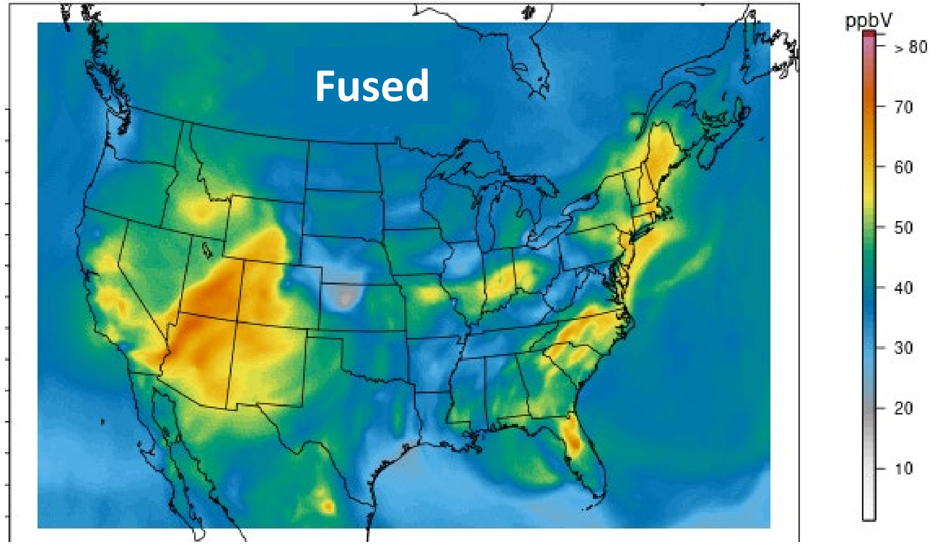
Figure 5.
(a) Location of the four sites for which we are displaying the posterior predictive mean of the spatially varying random weights $w_k(\mathbf{s}, t)$. (b)–(e) Posterior predictive mean of the spatially varying random weights $w_k(\mathbf{s}, t)$ for sites: (b) $\mathbf{s}_1$; (c) $\mathbf{s}_2$; (d) $\mathbf{s}_3$; and (e) $\mathbf{s}_4$ on July 4, 2001. Berrocal et al., 2012

- Posterior predictive mean of the spatially varying weights $w_k(s)$ at four locations.
- Weights are *not* a circular contour around the prediction site but have directionality (analogous to anisotropy in spatial variogram fitting).
- Directionality can be different depending on the site due emissions sources, land use and topography, wind flow patterns, etc.
- Weights are parameterized such that only the **window of 6 x 6 grid cells** surrounding, and including, grid cell B_k are assigned a weight.

Example Downscaler Fused Ozone Field







Aug 10, 2002 Example Maximum Daily 8-hr Ozone (MDA8 O_3)

- CMAQ is biased low in the west and biased high in much of the eastern US. DS adjusts the model output accordingly.
- Fused surface is smoother than the CMAQ output, muting peak values and spatial gradients.
- Spatial gradients (e.g., flow patterns) from the model are still retained, leading to a surface that is more spatially heterogeneous than a spatial field of purely interpolated observations, particularly in areas with fewer monitors.

Development of Cross Validation Approach

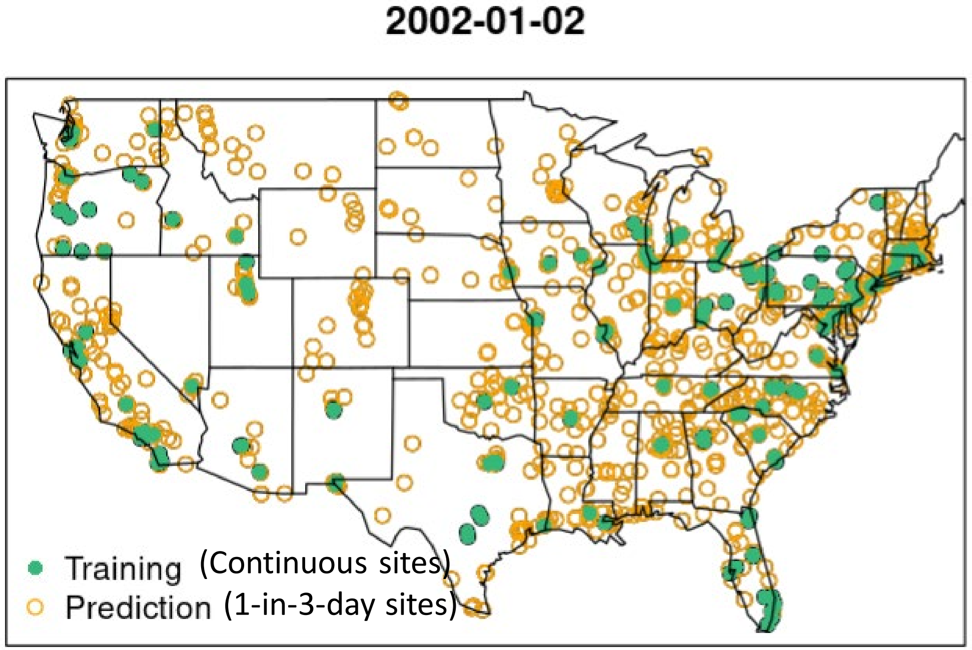
To evaluate the fused surfaces, we implemented two types of cross validation.

<u>10-fold CV</u> - used for MDA O_3 and $PM_{2.5}$

DS model is fit using 90% of sites (training) to estimate remaining 10% (prediction).

<u>1-in-3-day CV</u> - used for $PM_{2.5}$

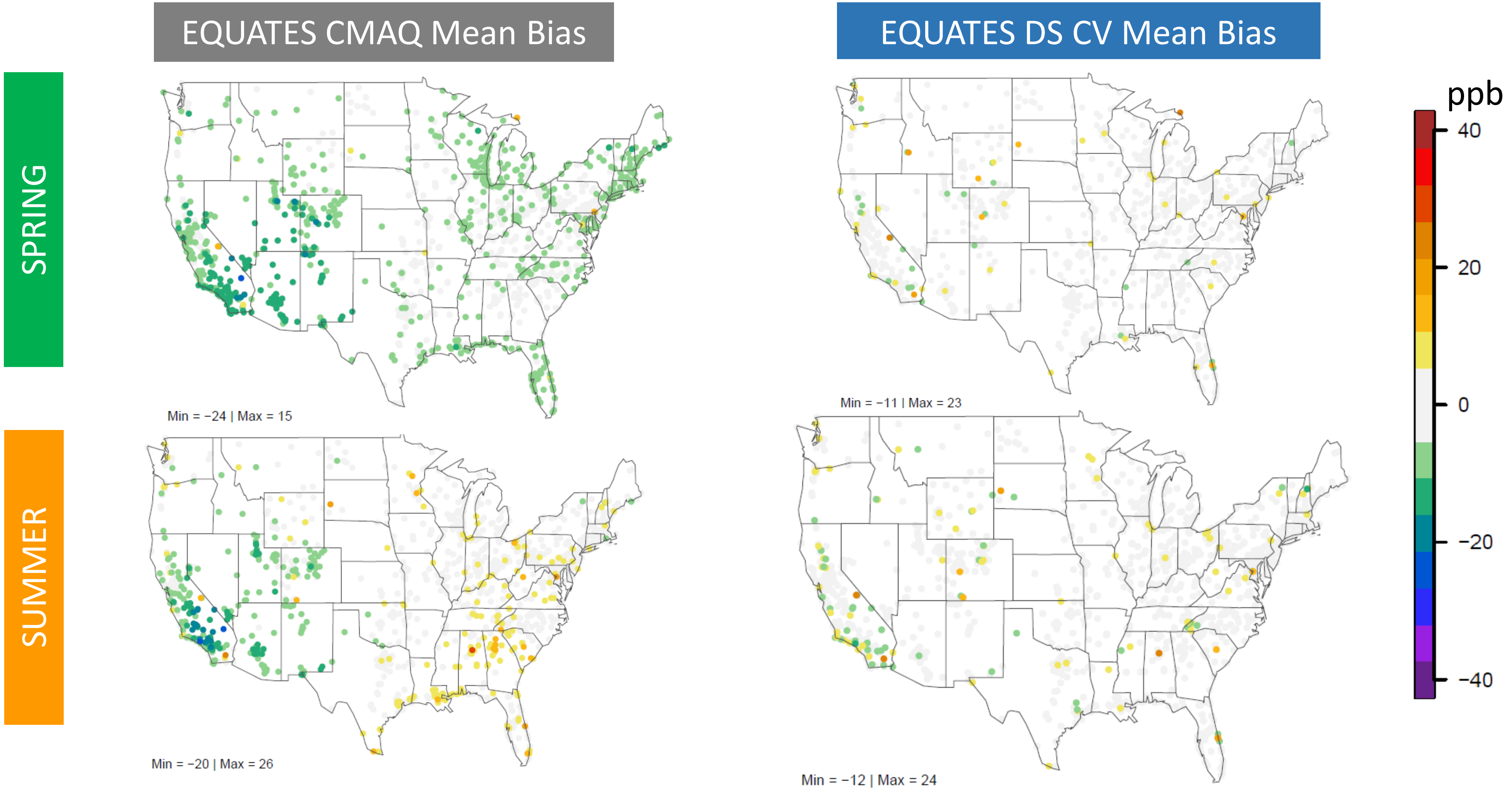
Daily average $PM_{2.5}$ from continuous FEM and daily filter sites are used as the **training sites** and 1-in-3-day and 1-in-6-day filter sites are used as the **prediction sites**.



MDA8 Ozone Results Summary

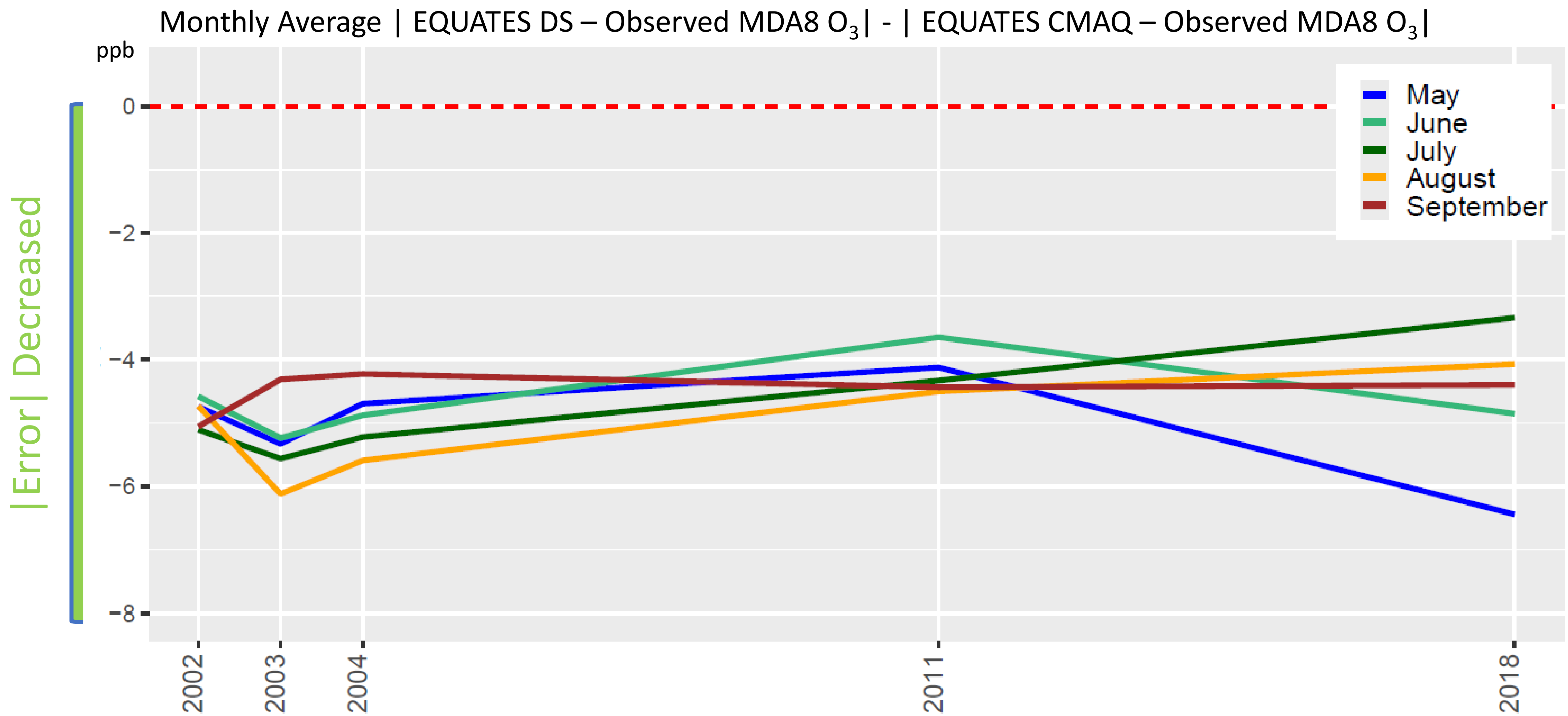
Decreased Bias using DS

2018 Spring/Summer Model – Obs. MDA8 O_3 Mean Bias



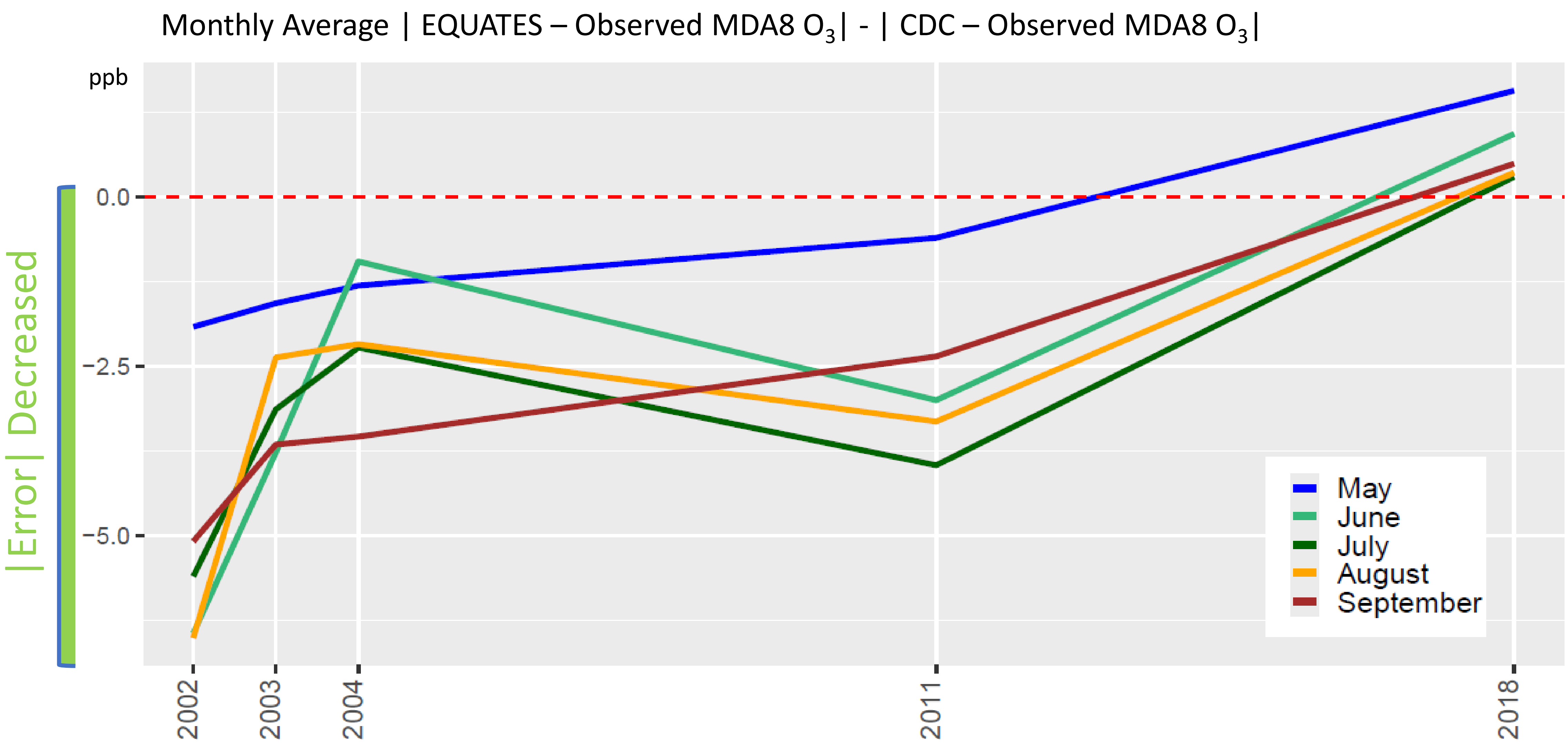
Not a surprise – fused estimates decrease model bias!

How different are the Fused and CMAQ MDA8 O_3 CV errors?



3 to 6 ppb average decrease in absolute estimation error using DS compared to 'raw' CMAQ output.

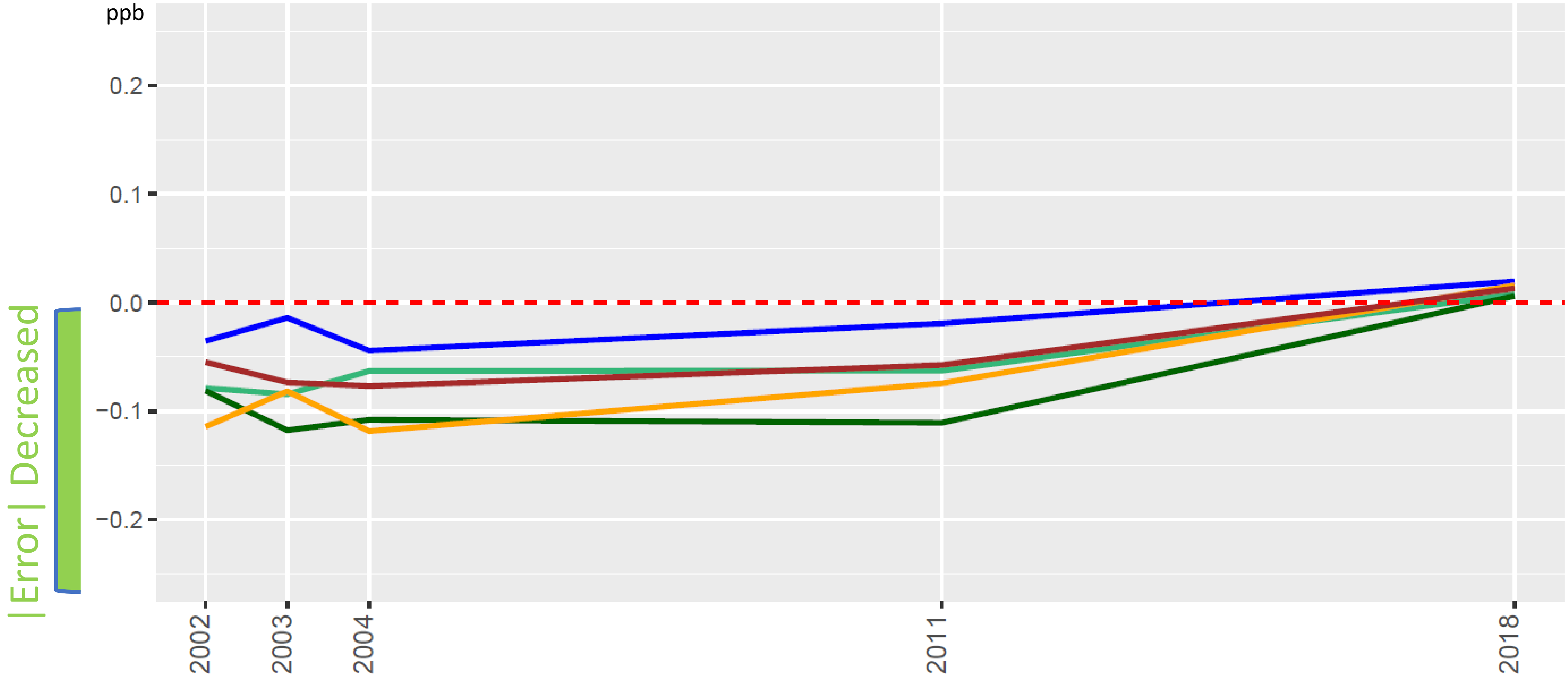
How different are the EQUATES and CDC CMAQ MDA8 O_3 CV errors?



EQUATES 'raw' CMAQ output has lower error than CDC CMAQ simulations in 2002-2004, 2011.

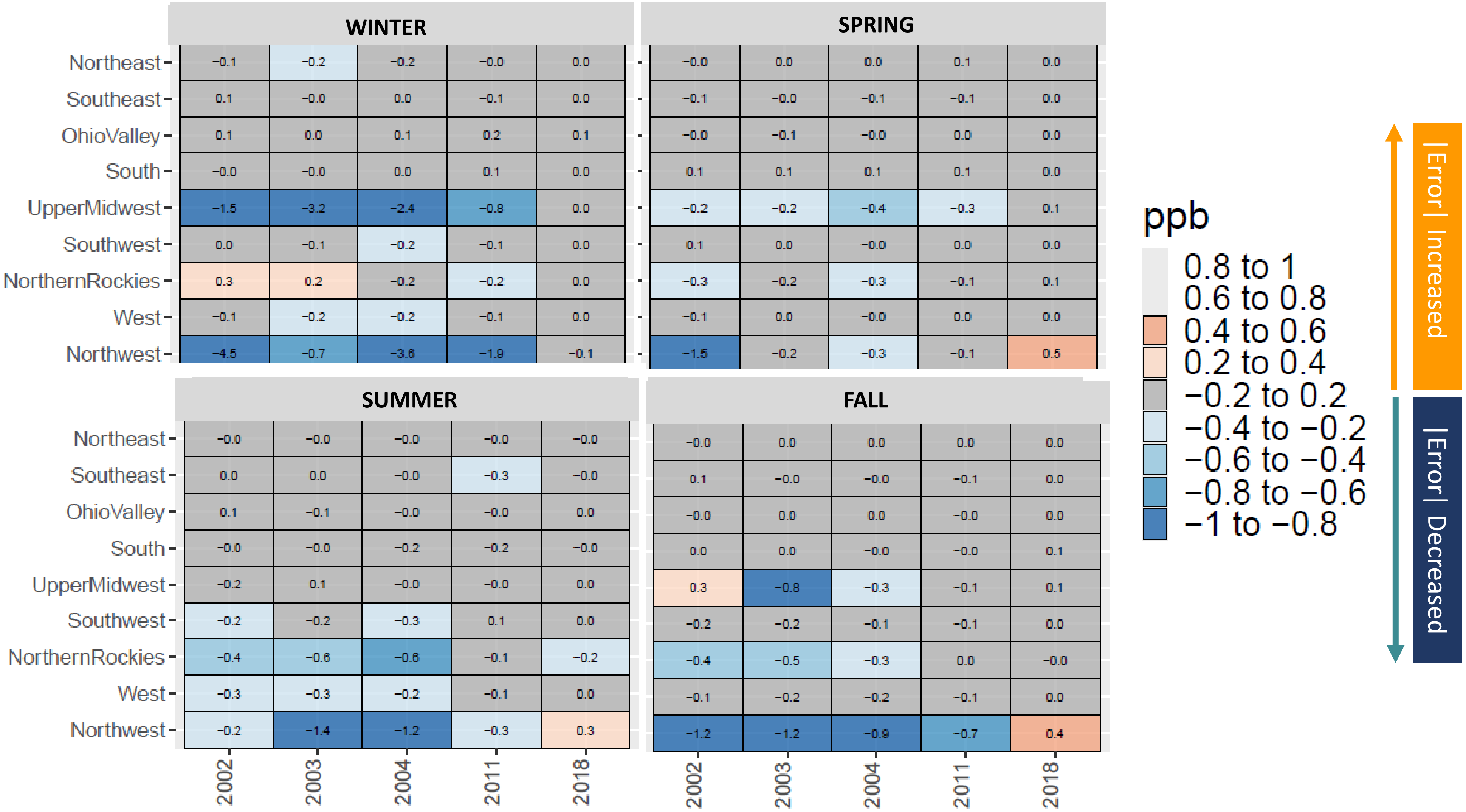
How different are the EQUATES and CDC Fused MDA8 O_3 errors?

Monthly Average | EQUATES DS – Observed MDA8 O_3| - | CDC DS – Observed MDA8 O_3|



EQUATES DS estimates have slightly lower average error (<0.13 ppb) than CDC DS in 2002-2004, 2011.

Seasonal/Regional Average of
|EQUATES DS – Observed MDA8 O_3| - |CDC DS – Observed MDA8 O_3|

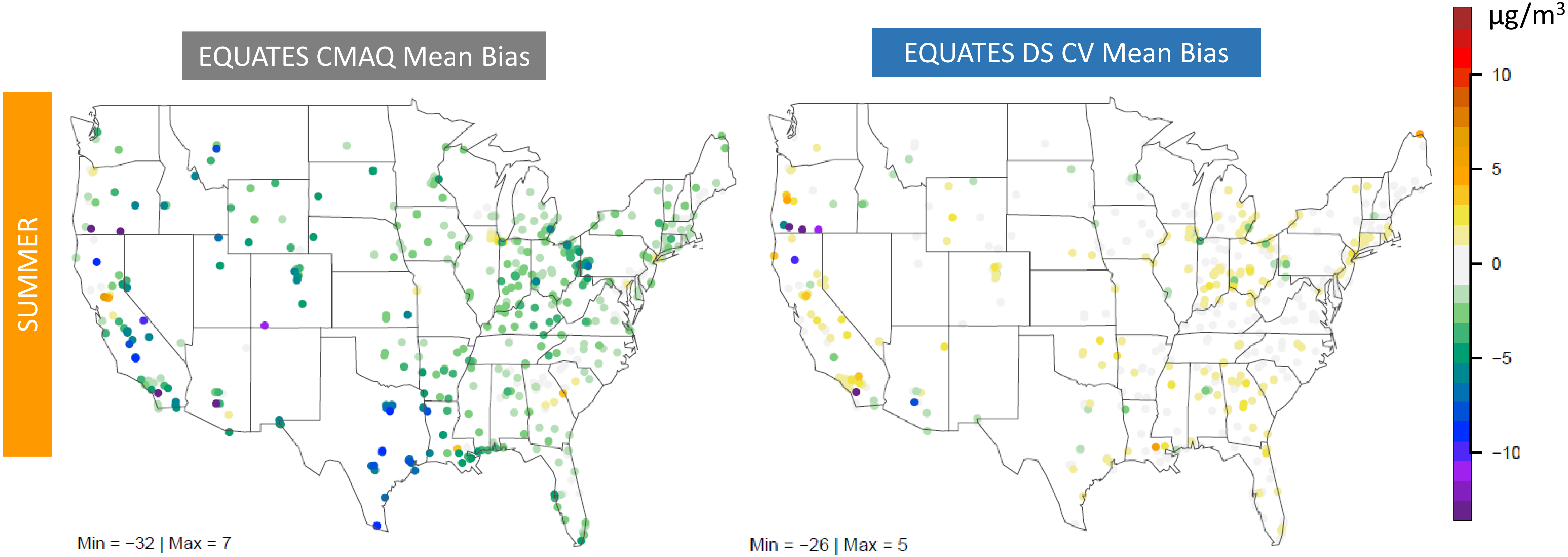


EQUATES DS has slightly lower *average* absolute error than CDC DS fused estimates for most regions and years.

$PM_{2.5}$ Results Summary

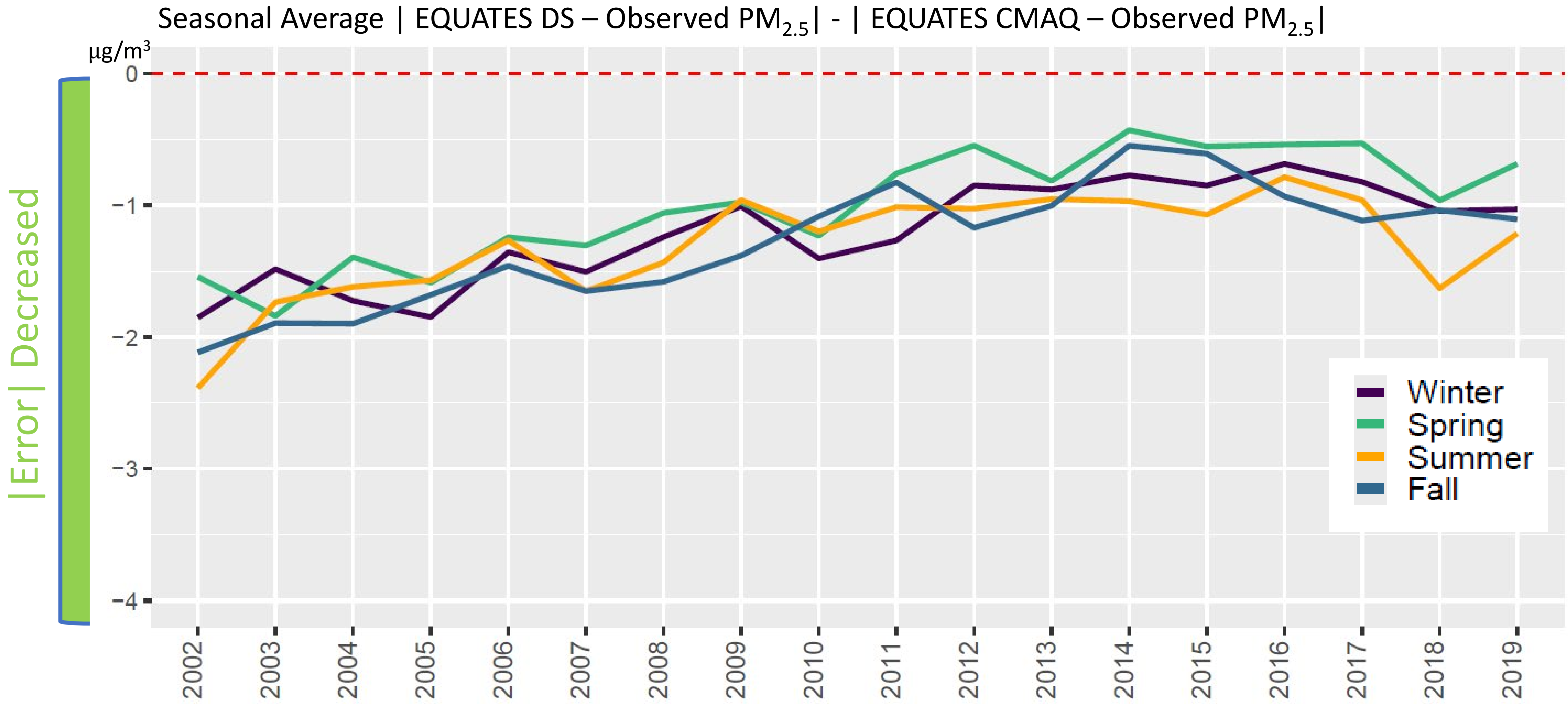
Decreased Bias using DS

2018 Summer Model – Obs. $PM_{2.5}$ Mean Bias



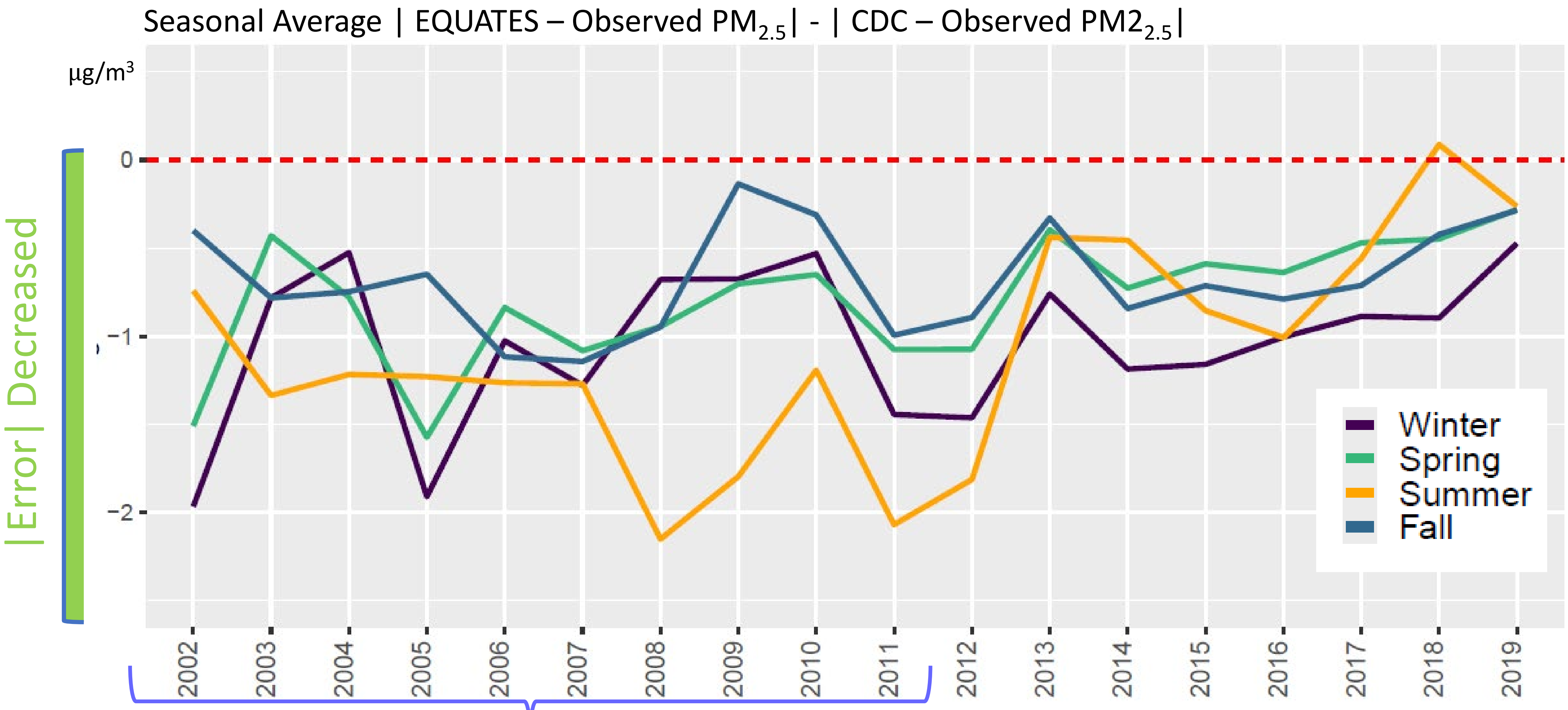
PM CV: Training sites = $PM_{2.5}$ from continuous FEM and daily filter; Prediction sites = 1-in-3-day and 1-in-6-day filter sites. The CV bias quantifies the error in the fused surfaces on the 2 out 3 days with the reduced PM network.

How different are the Fused and CMAQ $PM_{2.5}$ CV errors?



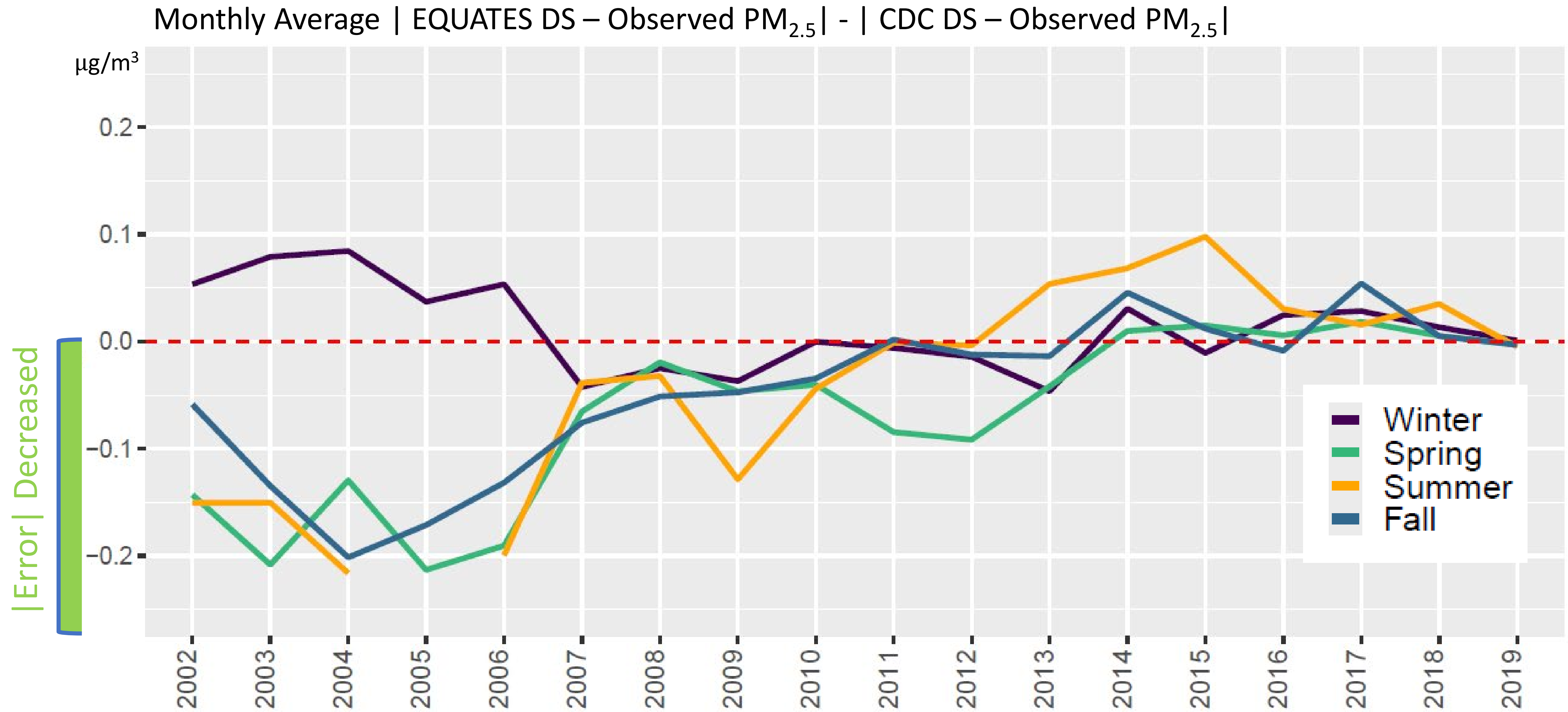
0.5 to 2.0 µg/m³ average decrease in absolute estimation error using DS compared to 'raw' CMAQ output.

How different are the EQUATES and CDC CMAQ $PM_{2.5}$ CV errors?



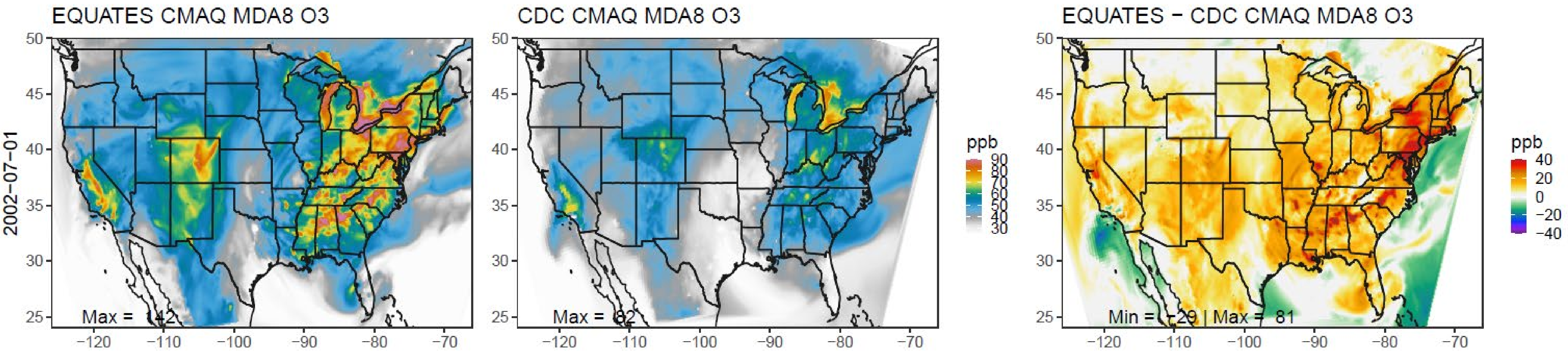
- **EQUATES error is 1-2 µg/m³ lower than CDC error for 2002-2012** in part due differences in CMAQ version.
- EQUATES uses CMAQv5.3.2 and the CDC simulations use CMAQ v4.6-v5.0.2 for 2002 -2012.
- There were substantial improvements in the modeled $PM_{2.5}$ seasonal patterns in CMAQv5.1 – CMAQv5.3.

How different are the EQUATES and CDC Fused $PM_{2.5}$ errors?



- EQUATES DS has slightly lower (.05 - 0.2 ug/m³) seasonal average error for 2002-2006 in Spring, Summer, Fall. These are the years where the CDC DS used a merged 12EUS and 36US domain.

Comparison of Daily Maps

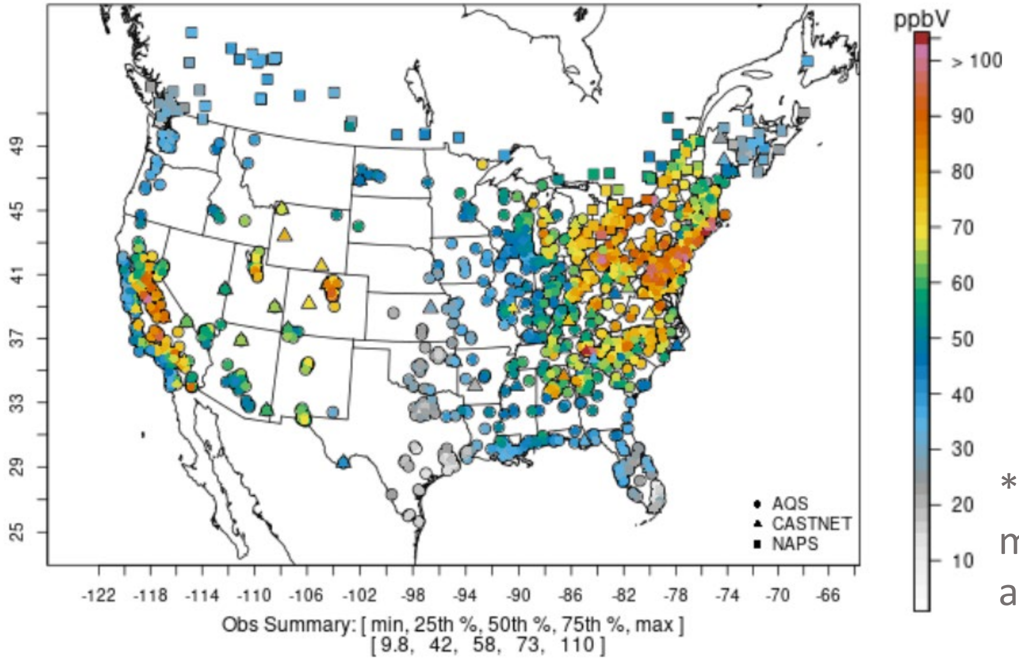


EQUATES vs CDC CMAQ MDA8 Ozone

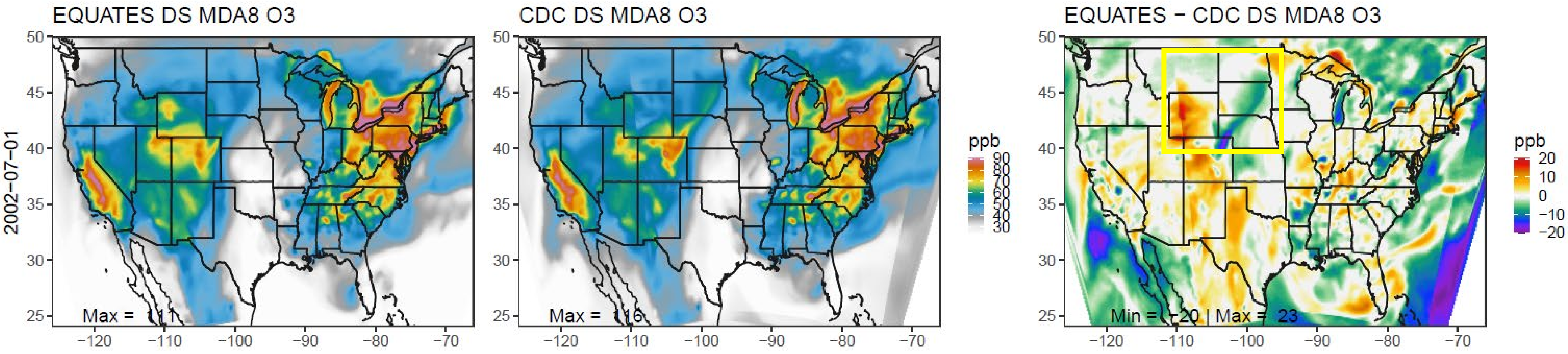
July 1, 2002 example

- Large differences in EQUATES and CDC CMAQ estimates due to differences in model inputs and configuration.
- EQUATES does a better job capturing peak ozone throughout the domain.

Observed MDA8 O_3 on 07/01/2002



*Observed and modeled color scales are slightly different

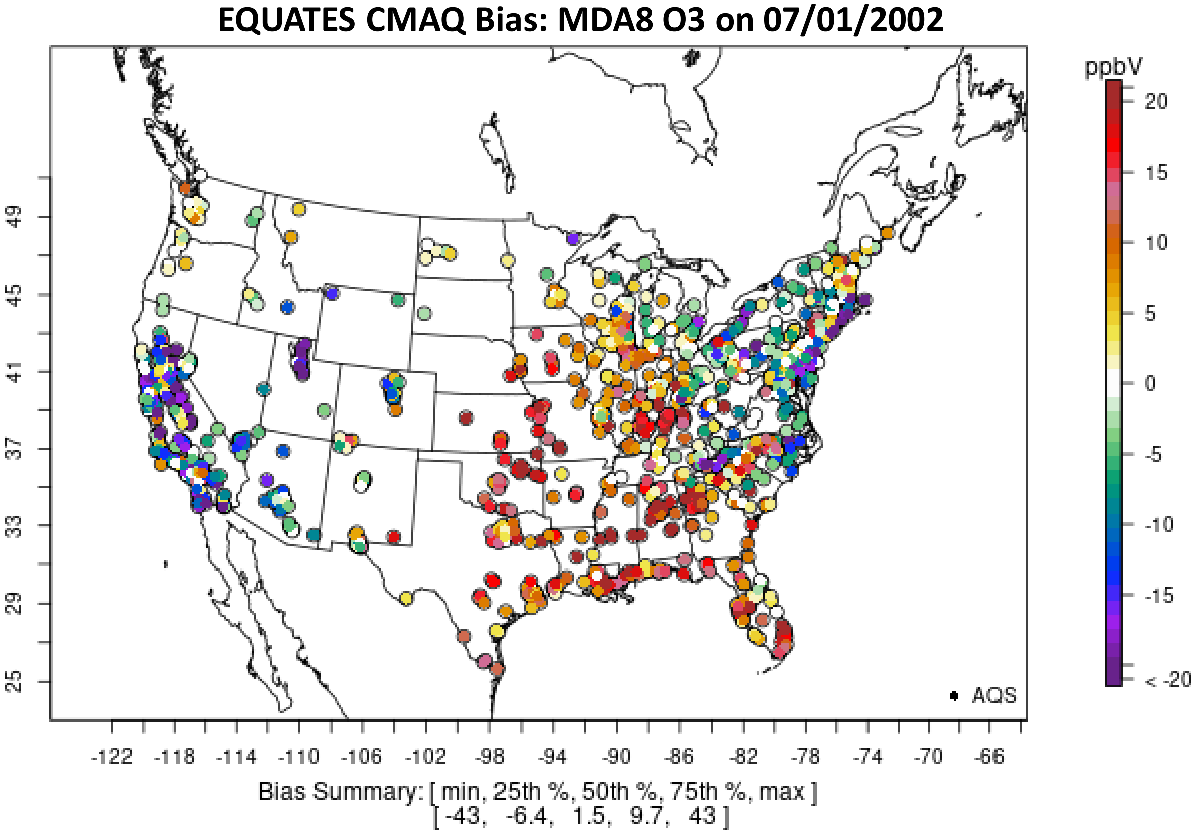


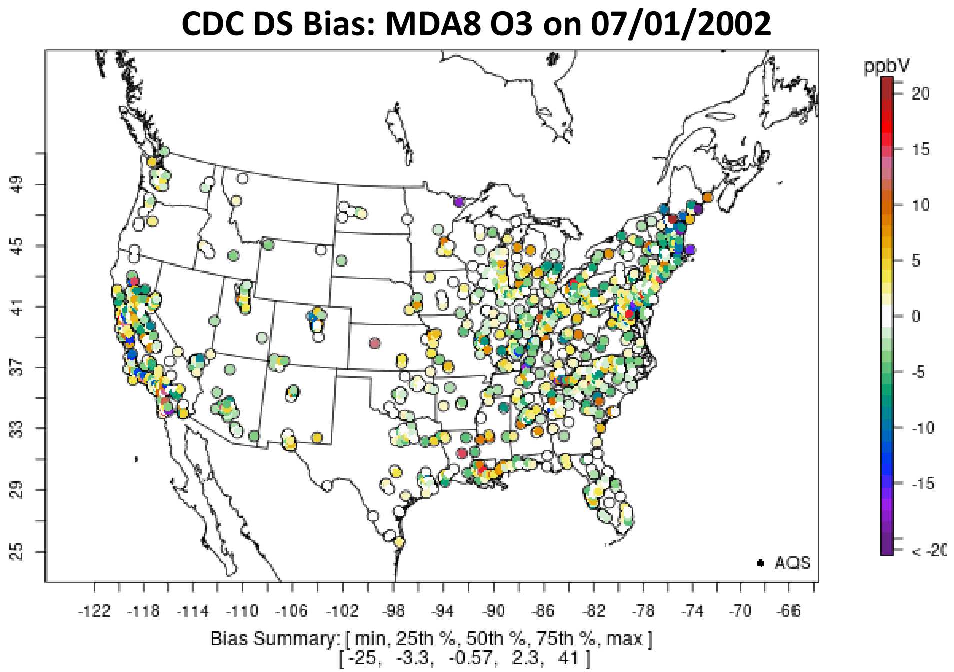
EQUATES vs CDC Fused DS MDA8 Ozone (July 1, 2002 example)

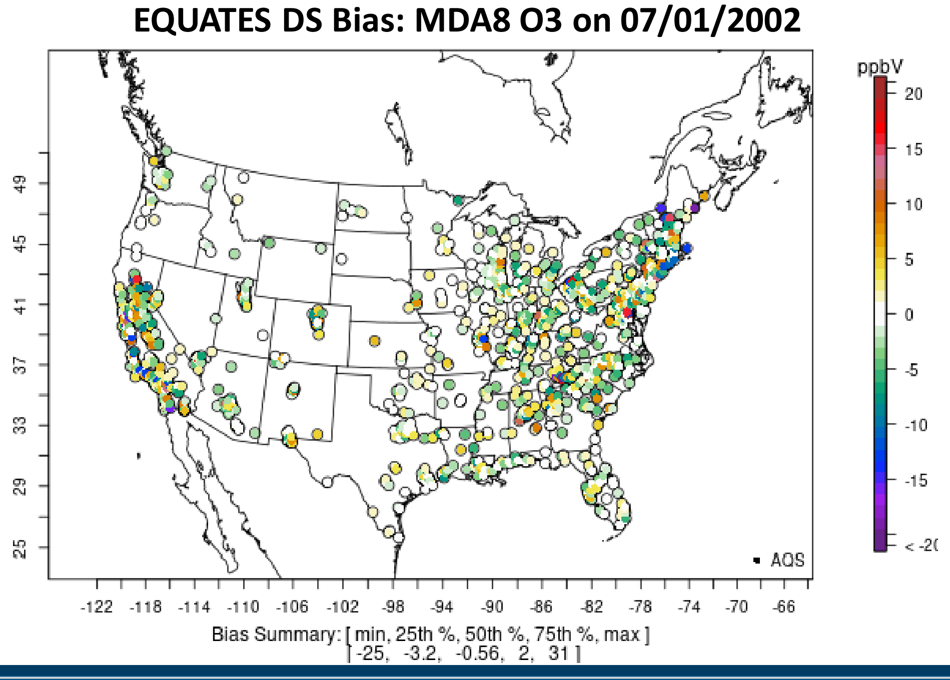
- Although EQUATES DS and CDC DS *average* cross validation errors were very similar, we still see substantial differences in the daily fused spatial fields(on the order of $\pm$ 20ppb for ozone).

→ The CMAQ data used in the data fusion does matter.

- Largest widespread differences in the Northern Rockies and Southwest where the ozone monitoring network is sparse.
- In these cases, improvements in the EQUATES CMAQ estimates, compared to CDC, will play a larger role in improving the fused surfaces.



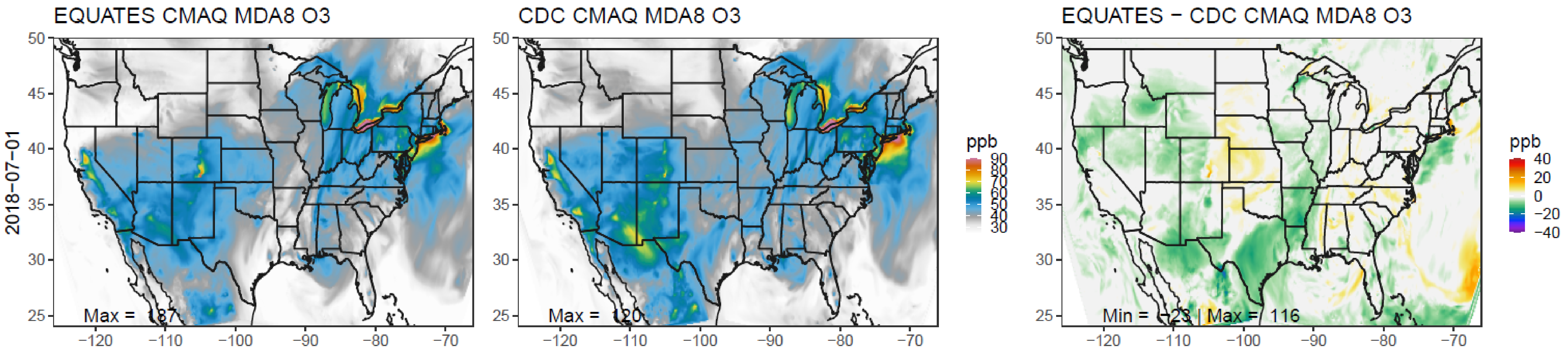




EQUATES CMAQ vs EQUATES DS vs CDC DS MDA8 Ozone Bias

July 1, 2002 example

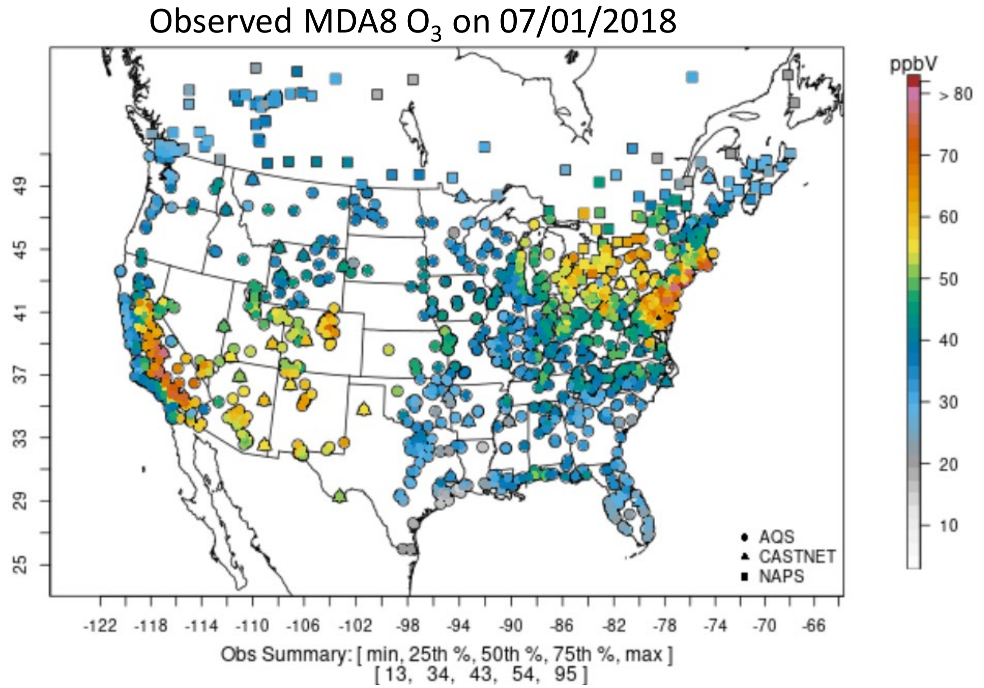
- Large over and underestimates in EQUATES CMAQ MDA8 O_3.
- Fused CDC and EQUATES surfaces reduce the bias (75% of the sites are within ± 3ppb)
- Fused surfaces can still have large bias (min = -25ppb, max= 41ppb)

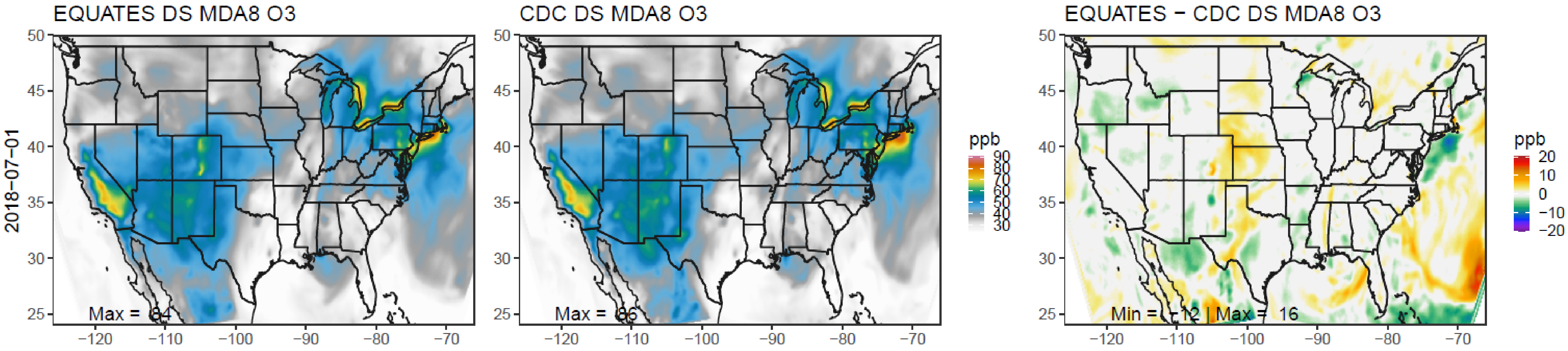


EQUATES vs CDC CMAQ MDA8 Ozone

July 1, 2018 example

- EQUATES and CDC CMAQ surfaces are much more similar than in 2002, due to similar model inputs and configuration.
- Both simulations miss peak ozone levels in the NE, Midwest, CA, and SW.
- EQUATES has more low bias in CA and the SW than the CDC simulation.





EQUATES vs CDC Fused DS MDA8 Ozone (July 1, 2018 example)

- Downscaled fused surfaces are much more similar than in 2002.
- Differences in the underlying CMAQ Modeling still show up as differences in the fused surfaces.

Main Take Aways

- As expected, **data fusion dramatically reduces bias** (and increases correlation) in spatial fields of $PM_{2.5}$ and MDA8 ozone in most cases.

DS fused ozone and $PM_{2.5}$ are an excellent estimate of air quality and should be preferentially selected over ‘raw’ model output for health studies when possible.

Main Take Aways

- Cross validation analysis shows DS fused surfaces can still have bias.

- What does this mean for applications using fused data, especially epidemiological studies?

  Recommend including evaluation of any model-based product in application studies. The implications of model bias/error on results will depend on the application including the regions, years, seasons of the study.

Main Take Aways

- Fused surfaces from two very different CMAQ simulations have very similar CV evaluation metrics when average over space and time.
- Large differences can still exist in the daily surfaces, particularly away from monitoring locations.

EQUATES DS provides the advantage of a consistent domain, model inputs and settings for all years (e.g., no discontinuities in early simulation years).

Next Steps

- Public release of EQUATES DS fused PM2.5 and MDA8 O_3 daily estimates (datasets for 12km x 12km gridded data, 2010 census tracts, 2010 zip codes).
- Release will include documentation of the CV methods and evaluation and comparison with CDC DS across regions and seasons.

Questions?

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