Advances in Assimilation of Atmospheric Composition Observations

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NCAR/ASP Summer Colloquium
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Overview

- Background – Air quality issues and response
- Operational air quality forecasting
- ACOM air quality forecasting research
- WRF-Chem/DART quasi-real-time system
- Recent accomplishments:
  - Assimilation of CPSRs (retrieval full and partial profiles)
  - Constrained emissions
  - Joint assimilation of MOPITT and IASI CO CPSRs
  - Assimilation of MOPITT AOD
  - Quasi-realtime cycling applied to FRAPPE

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Background: Air Quality Issues and Response

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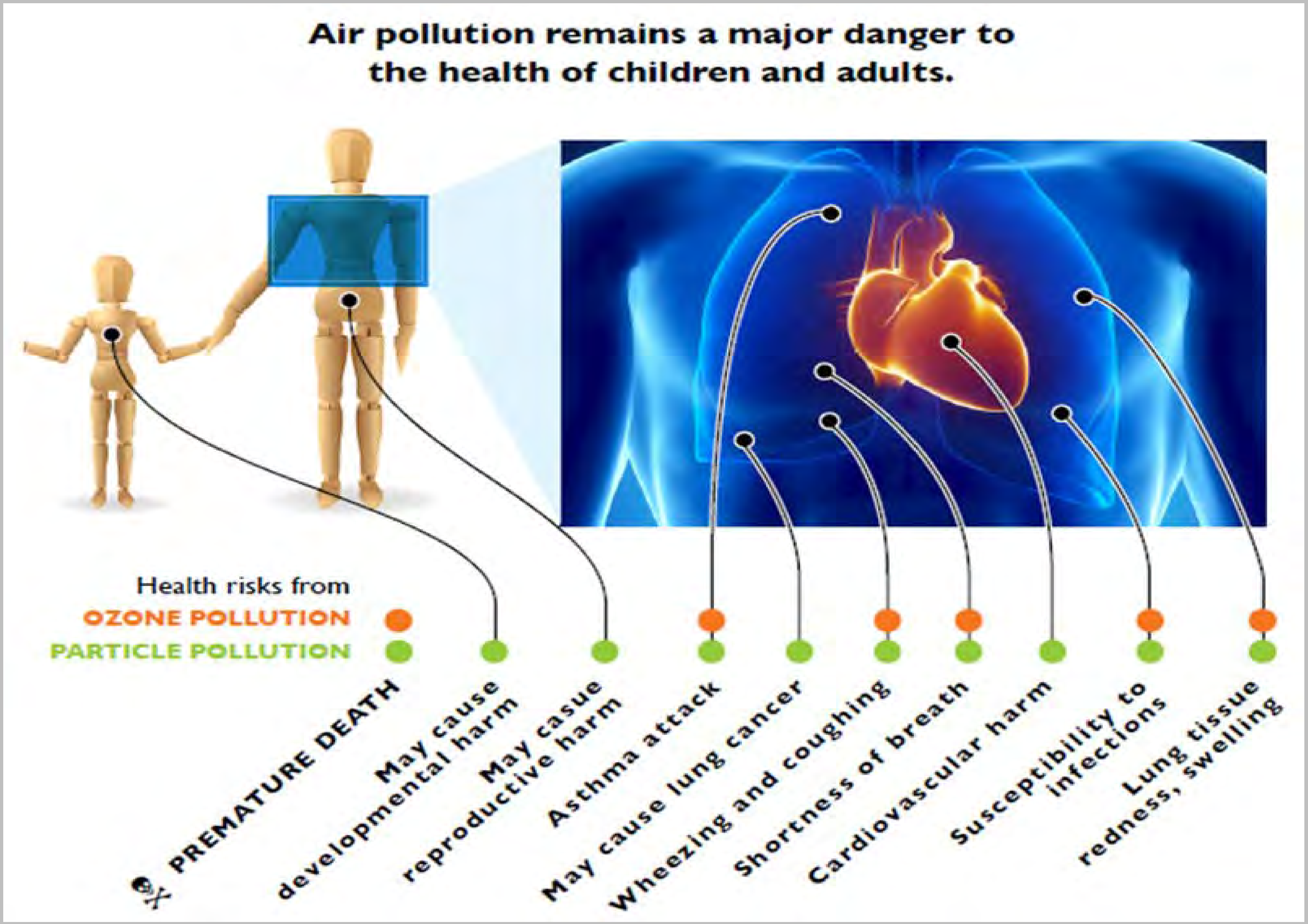
Health Impacts of Poor Air Quality



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What's the Cost of Poor Air Quality in the United States?

- ~$71 billion to ~$277 billion annually (0.7 – 2.8% of GDP)

Table 1
Gross annual damages ($billion/year)

Pollutant	Mortality	Morbidity	Agriculture	Timber	Visibility	Materials	Recreation	Total
$PM_{2.5}$	14.4	2.6	0	0	0.4	0	0	17.4
PM_{10}[1]	0	7.8	0	0	1.3	0	0	9.1
NO_x	4.4	0.8	0.7	0.05	0.2	0	0.03	6.2
NH_3	8.3	1.5	0	0	0.2	0	0	10.0
SO_2	16.1	2.9	0	0	0.4	0.1	0	19.5
VOC	9.6	1.8	0.5	0.03	0.2	0	0	12.1
Total	52.8	17.4	1.2	0.08	2.7	0.1	0.03	74.3

[1] PM_{10} represents coarse particles between 2.5 and 10 microns throughout the paper.

Muller and Mendelsohn: *J. Environ. Econ. Manage*. 54 (2007) 1-14.

What's Being Done to Address Poor Air Quality?

- US Clean Air Act: Passed in 1970, with major revisions in 1977 and 1990.
- Requires regulation of PM, O_3, SO_2, NO_2, CO, and Pb.
- Requires reduced emissions from motor vehicles and from new or expanded industrial plants.
- Provides authority to address emerging air pollution problems e.g., greenhouse gasses and climate change.
- 2014 – *Utility Air Regulatory Group v. EPA*
- 2016 – *Chamber of Commerce, et al. v. EPA*

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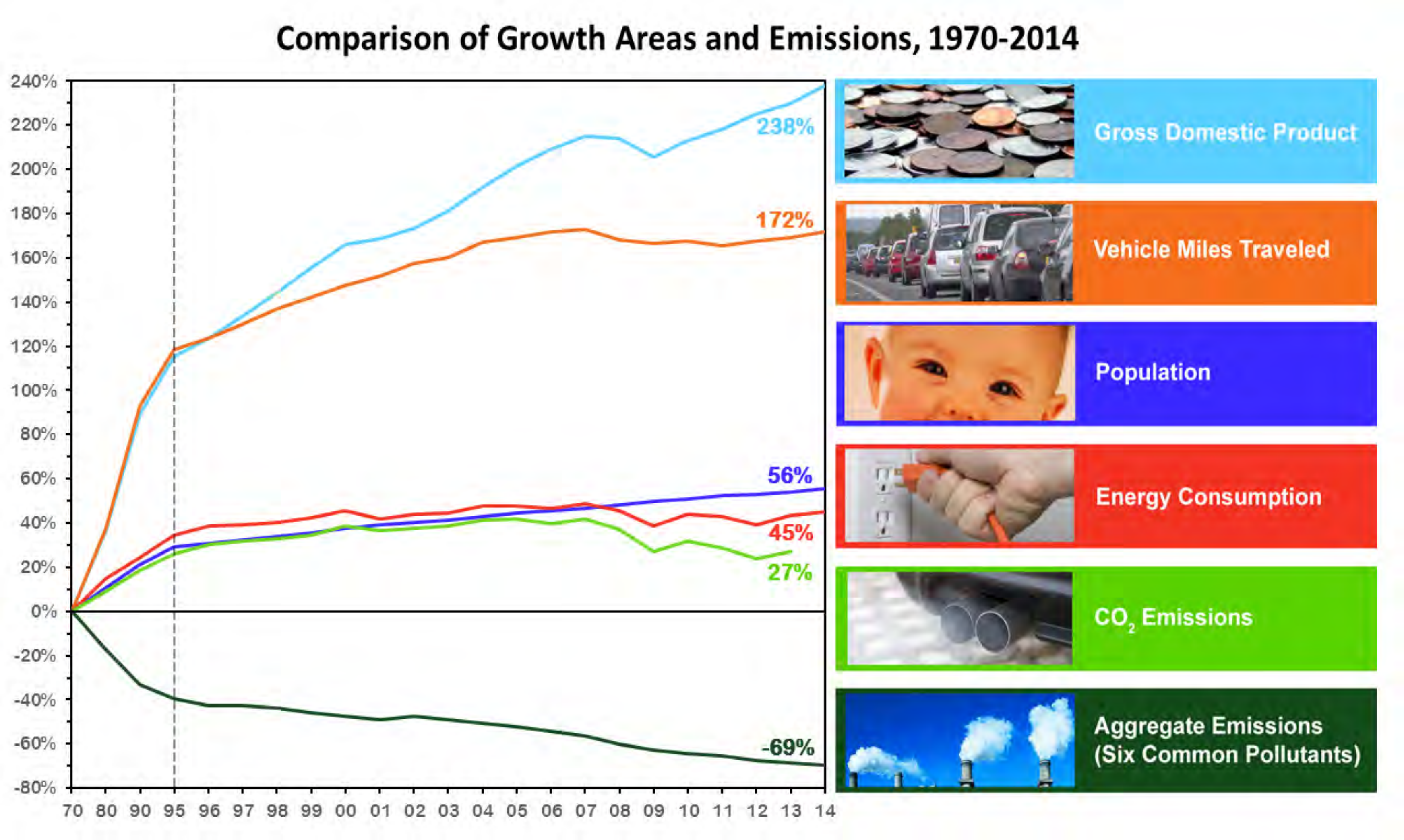
Has Air Quality Regulation Been Successful?



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Is this really Denver?

July 2015 – Denver Post

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Operational Air Quality Forecasting

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Western Europe: MACC/Copernicus

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About the Project
- Project Description
- More Details about the Project
- Sustainability of Services
- MACC-III Input Data
- Project Structure
- Partners

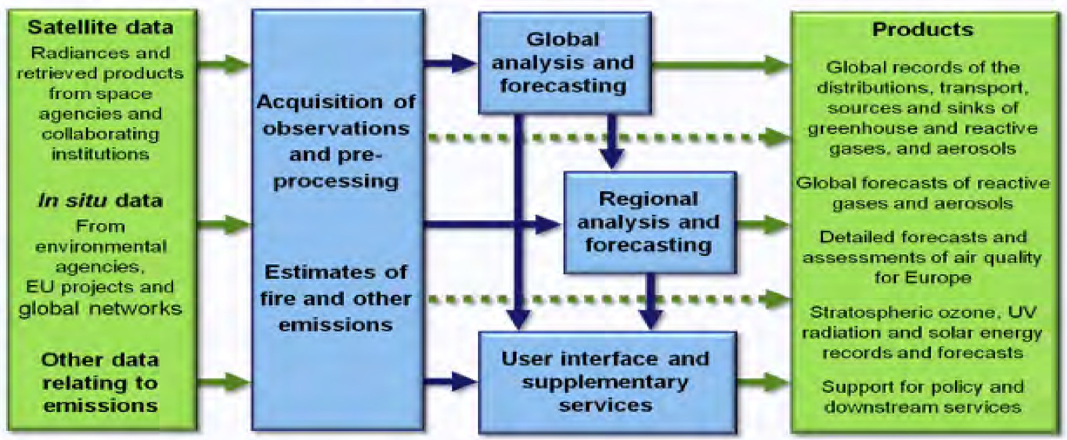
Today's Forecasts
- Reactive Gases
- Aerosols
- European Air Quality
- UV Index
- Ozone Layer
- CO2

Latest Analyses
- European Air Quality
- Fire Monitoring
- Reactive Gases
- Aerosols

Project Description

MACC-III - Monitoring Atmospheric Composition and Climate - Interim Implementation - is the current pre-operational Copernicus Atmosphere Service. MACC-III provides data records on atmospheric composition for recent years, data for monitoring present conditions and forecasts of the distribution of key constituents for a few days ahead.

MACC-II combines state-of-the-art atmospheric modelling with Earth observation data to provide information services covering European air quality, global atmospheric composition, climate forcing, the ozone layer and UV and solar energy, and emissions and surface fluxes.



Visit this page for more details about the project.

If you are interested in sustainability of the services please visit this page.

User Support
- Documentation
- Validation
- E-learning
- Mailing Lists
- Operational Info

Services
- Air Quality & Atmospheric Composition
- Climate Forcing
- Ozone Layer & Ultra-Violet Radiation
- Solar Radiation
- Emissions & Surface Fluxes

ACCESS CATALOGUE

MACC-III is a Coordination & Support Action (2014-2015) funded by the European Union under the Horizon 2020 Programme.
It is coordinated by the European Centre for Medium-Range Weather Forecasts and operated by a 36-member consortium.

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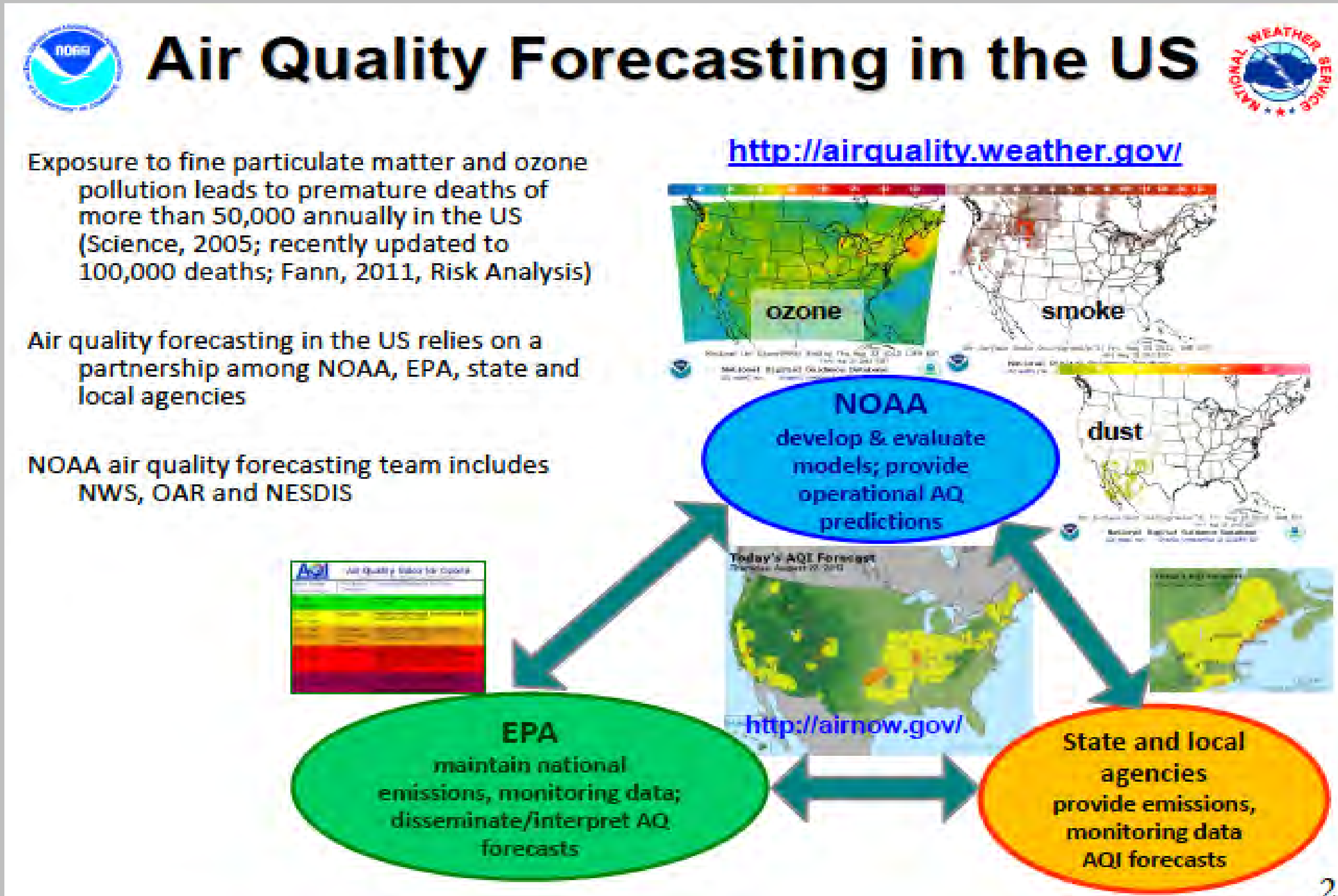
United States: NAM-CMAQ/HYSPLIT



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ACOM Air Quality Forecasting Research: OSSE for GEO, Emission Corrections, CAM-Chem/DART, and WRF-Chem/DART

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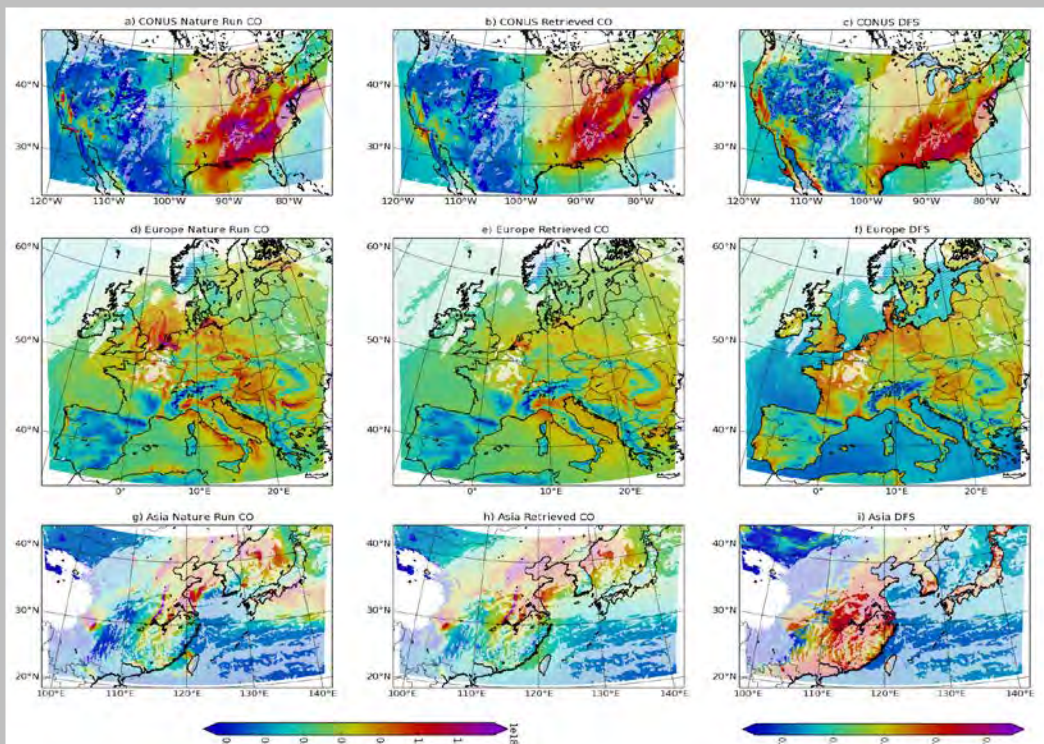
OSSE to evaluate a GEO constellation for Air Quality Prediction

Jérôme Barré, David Edwards, and Helen Worden

Simulated multispectral CO observation (Surface – 700 hPa)

Nature Run **“retrieved” CO** **DFS**

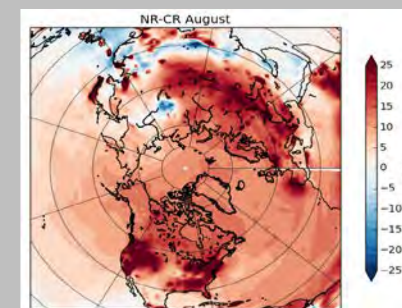


CO column **DFS**

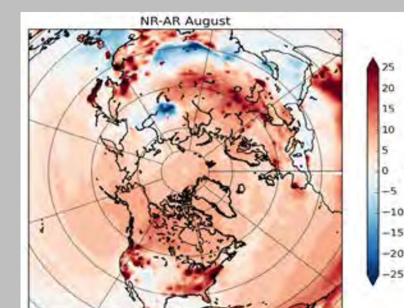
Barré et al., Atm. Env., 2015

Reduction in error from GEO observations

Nature – Control



Nature – Assim.



Barré et al., Atm. Env., under review, 2016

Ten-Year Reanalysis Based on Assimilation of MOPITT and IASI CO

Gaubert et al. (2016)

Assimilation of MOPITT and IASI CO with CAM-Chem/DART

Reanalysis of Chemical composition	DA method / Optimization	CO Observations	Model, DA chain	Additional observations	Coupling Met/Chem
Miyazaki et al. 2015	LETKF / Total CO emissions	MOPITT V6T, only 700 hPa level	CHASER-DAS	TES O3, MLS O3, HNO3, OMI NO2	Offline
Yin et al. 2015	4D-Var / Total CO emissions & Chemical production	MOPITT V6J, total CO columns	LMDz-INCA, PYVAR-SACS	Surface CH4, Methyl-Chloroform	Offline
Inness et al. 2013	4D-Var / CO concentrations	MOPITT V4, total CO colums	IFS-MOZART	IASI-CO, MLS O3, SCIAMACHY O3 and NO2…	Coupled
Gaubert et al. 2016	EAKF / CO concentrations	MOPITT V5J, CO profiles	DART/CAM-Chem	Conventional Met Obs	Online

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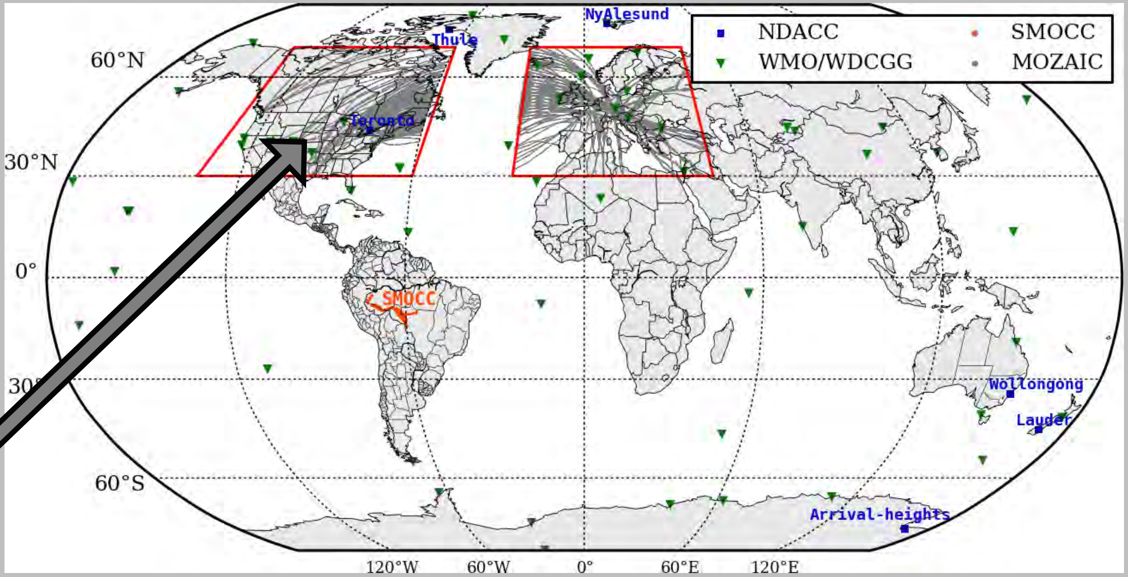
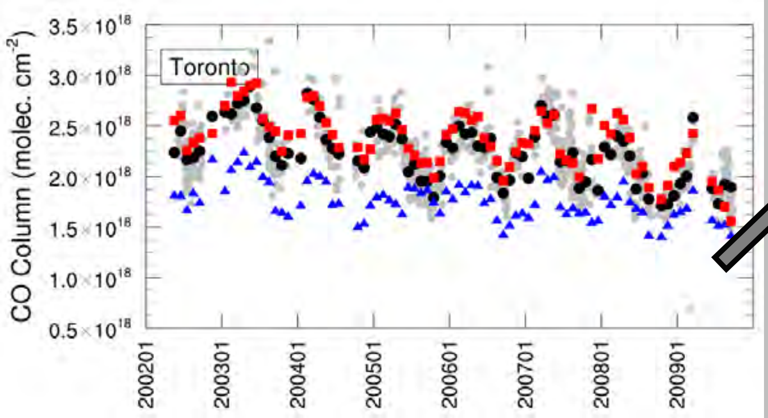
Needs to be validated against independent datasets

Improvement against the following independent observations:

- ➢ MOZAIC/IAGOS aircraft CO (grey lines)
- ➢ WMO/WDCGG surface CO observations
- ➢ NDACC/FTS total column retrieval
- ➢ Fields campaign





Gaubert et al. (2016)

- Observations, CO total columns (FTS)
- CAM-Chem run
- MOPITT-Reanalysis

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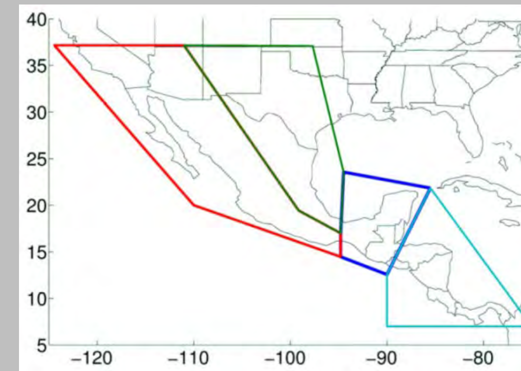
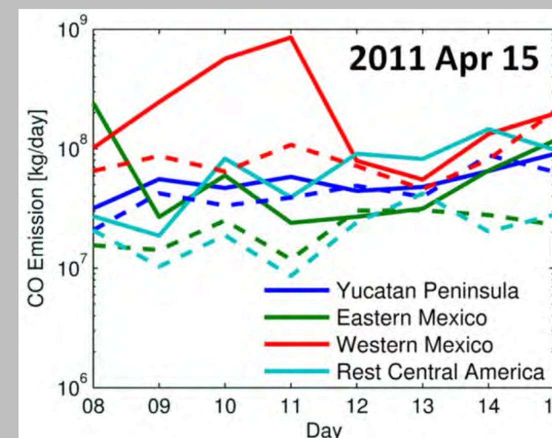
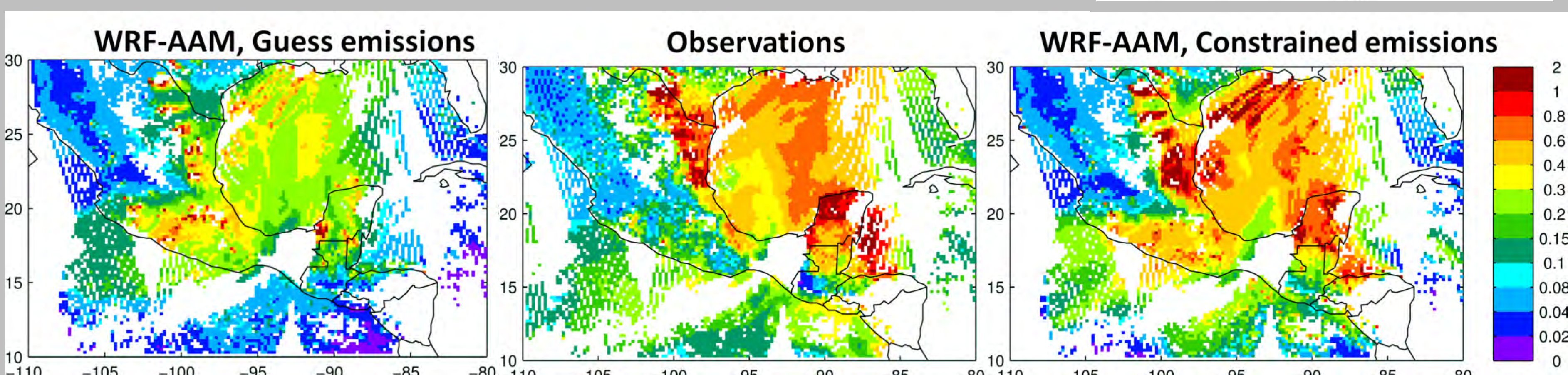
Constraining Biomass Burning Emissions for Assessing Smoke-Severe Weather Interactions

- WRF with aerosol-aware microphysics (AAM) (Thompson and Eidhammer, 2014) and WRF-Chem emissions.
- Inversion based on Saide et al. (GRL 2015b) using WRF tracers (no adjoint, no ensembles).
- Plans for using it operationally for the NASA ORACLES and NOAA FIREX field experiments
- Contact Pablo Saide (saide@ucar.edu) for more details.







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WRF-Chem/DART

- WRF-Chem – the Weather Research and Forecasting (WRF) model with online chemistry.
- DART – the Data Assimilation Research Testbed modified for assimilation of atmospheric composition observations.
  - MOPITT and IASI partial and total column CO
  - IASI partial and total column O3 (under development)
  - MODIS AOD and OMI NO2– under testing
  - AirNOW in situ observations – under testing
  - Emission constraints – State augmentation method – under testing
  - Assimilate as RETRs, QORs), and CPSRs
  - State variable localization (joint or independent assimilation)
  - Quasi-Realtime and dual-resolution cycling.

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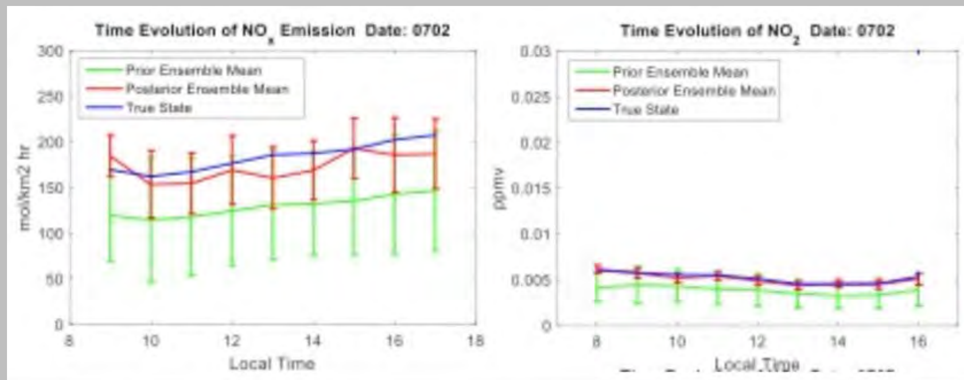
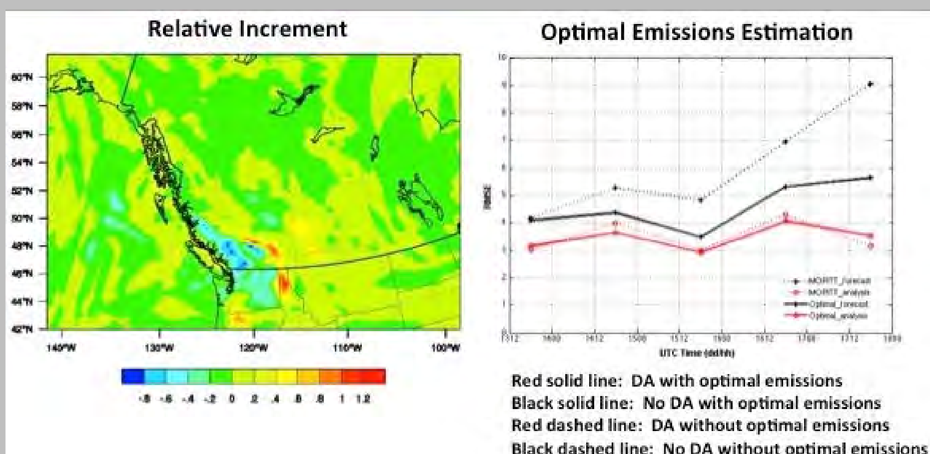
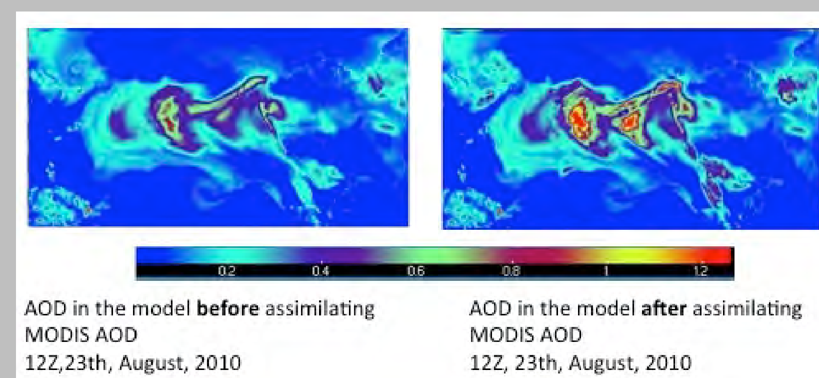
WRF-Chem/DART: Collaborations



Berkeley: Liu and Cohen
OMI NO2 and emission estimation

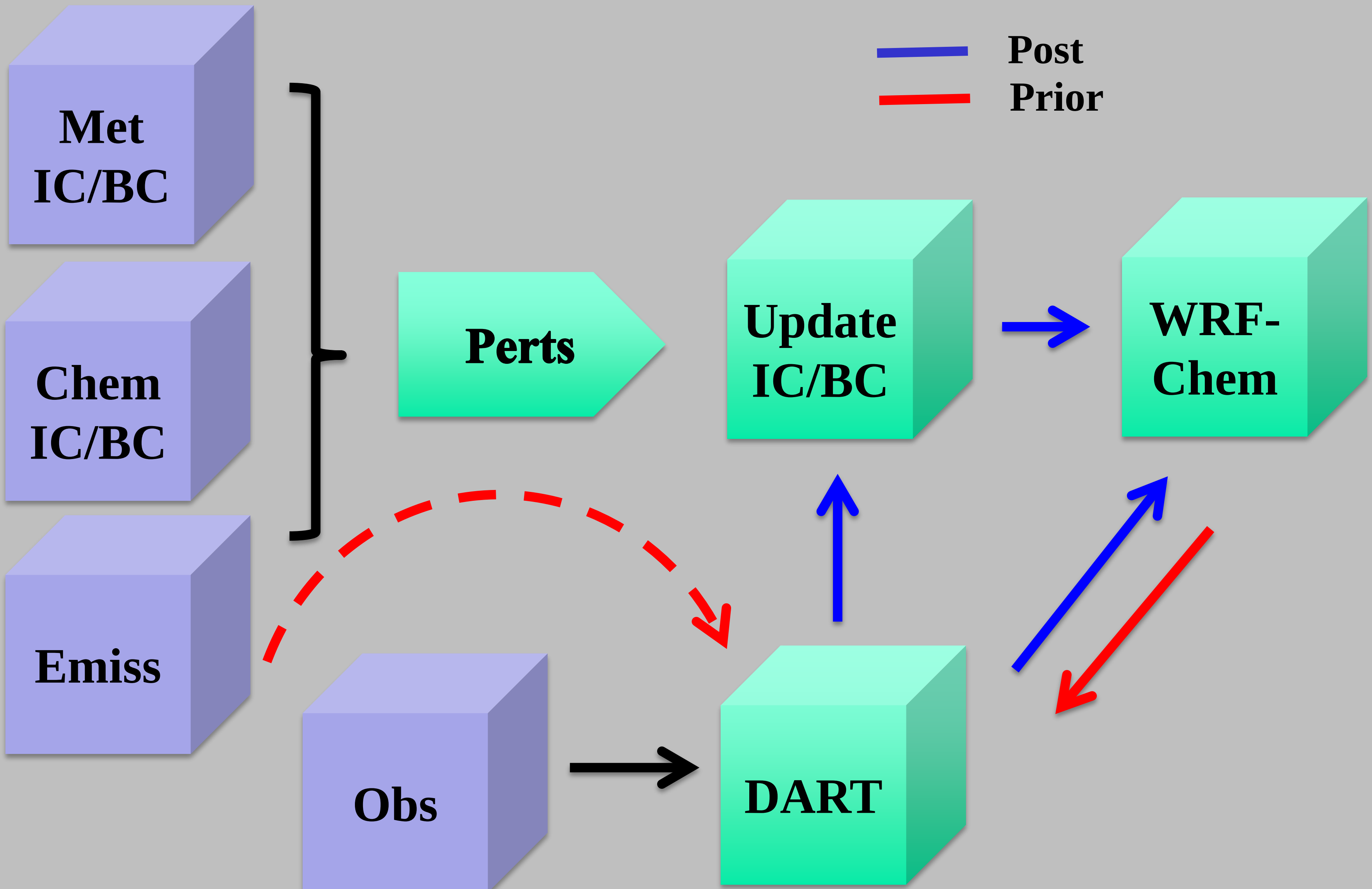


York Univ.: Miao and Chen
MOPITT total column CO and emission estimation



York Univ.: Liang and Chen
MODIS AOD

Real-Time WRF-Chem/DART Flow



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Efficient Chemical DA Forward Operators:

- Retrieval equation: $y_r = Ay_t + (I - A)y_a + \varepsilon$.
- Challenges include:
  - Large data volume with low information density.
  - Retrieval error covariance cross correlations.
  - Removing contribution of retrieval prior from the retrieval.
- Joiner and da Silva (1998) – assimilate phase space retrievals (remove retrieval prior and data compression).
- Migliorini et al. (2008) – assimilate quasi-optimal retrievals, $y_r - (I - A)y_a - \varepsilon = Ay_t$. SVD rotation based on E_m^2 and discard those modes whose forecast error variance singular values were significantly less than the transformed observation error variance (diagonalization, remove prior, and data compression).
- Mizzi et al. (2016a) – assimilate compact phase space retrievals (CPSRs) and Mizzi et al. (2016b) extend CPSRs to partial profiles.

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CPSRs: Retrieval Full Profiles

- $y_r - (I - A)y_a - \varepsilon = Ay_t$: A is singular and its leading left singular vectors span the domain.
- Project the quasi-optimal retrieval onto the leading left singular vectors of A: data compression.
- That transform reduces the number of observations from the dimension of the retrieval profile to the number of non-zero singular values.
- The transformed E_m^2 is non-diagonal: use an SVD diagonalization (Anderson, 2003; Migliorini et al., 2008).
- 1st SVD: $A = \Omega\Sigma\Psi^T = \Omega_0\Sigma_0\Psi_0^T$ - Compression Transform;

  2nd SVD: $\Omega_0^T E_m^2 \Omega_0 = \Pi\Lambda\Theta^T$ - Diagonalization Transform;

  Assimilate CPSRs:

$$\Pi^T\Lambda^{-1/2}\Omega_0^T(y_r - (I - A)y_a - \varepsilon) = \Pi^T\Lambda^{-1/2}\Sigma_0\Psi_0^T y_t.$$

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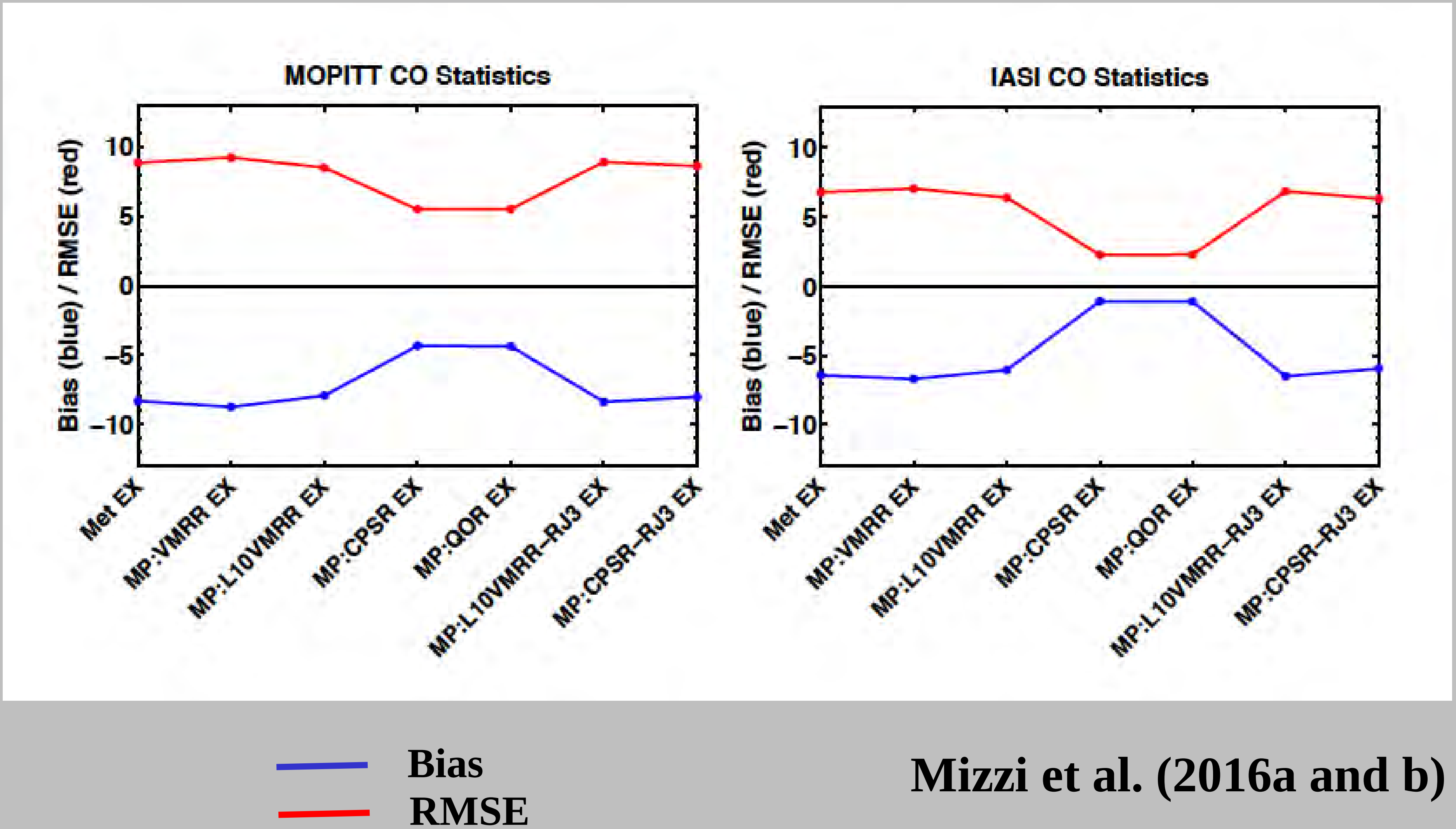
WRF-Chem/DART: Forecast Verification



Mizzi et al. (2016a and b)

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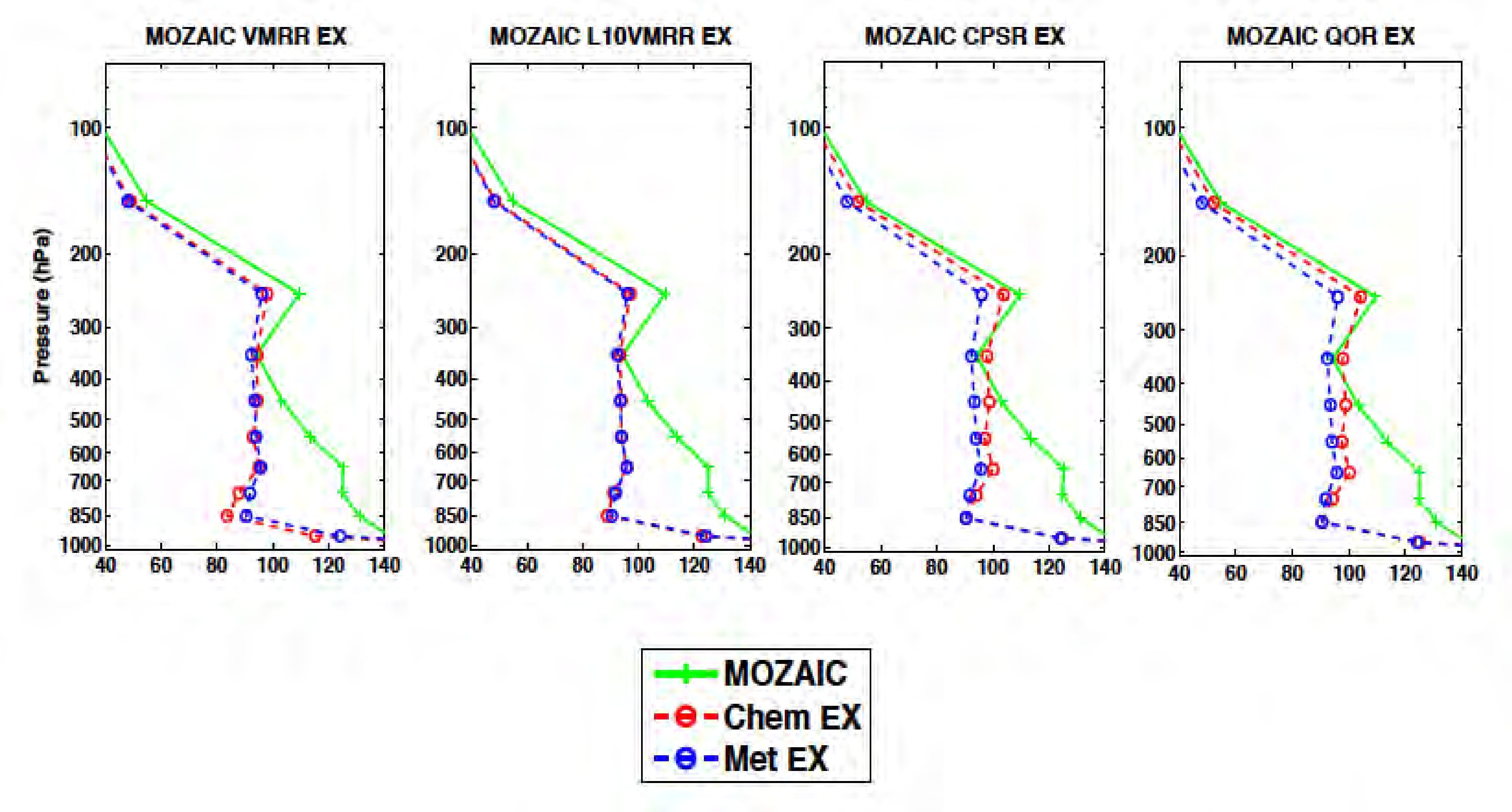
WRF-Chem/DART: Forecast Verification



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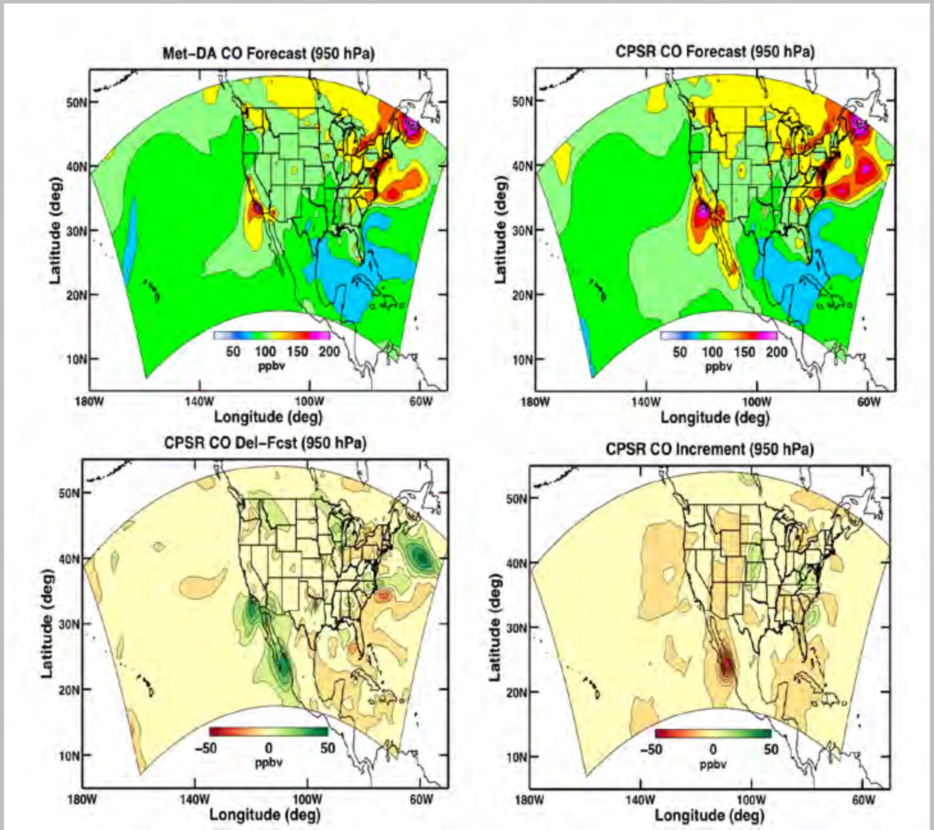

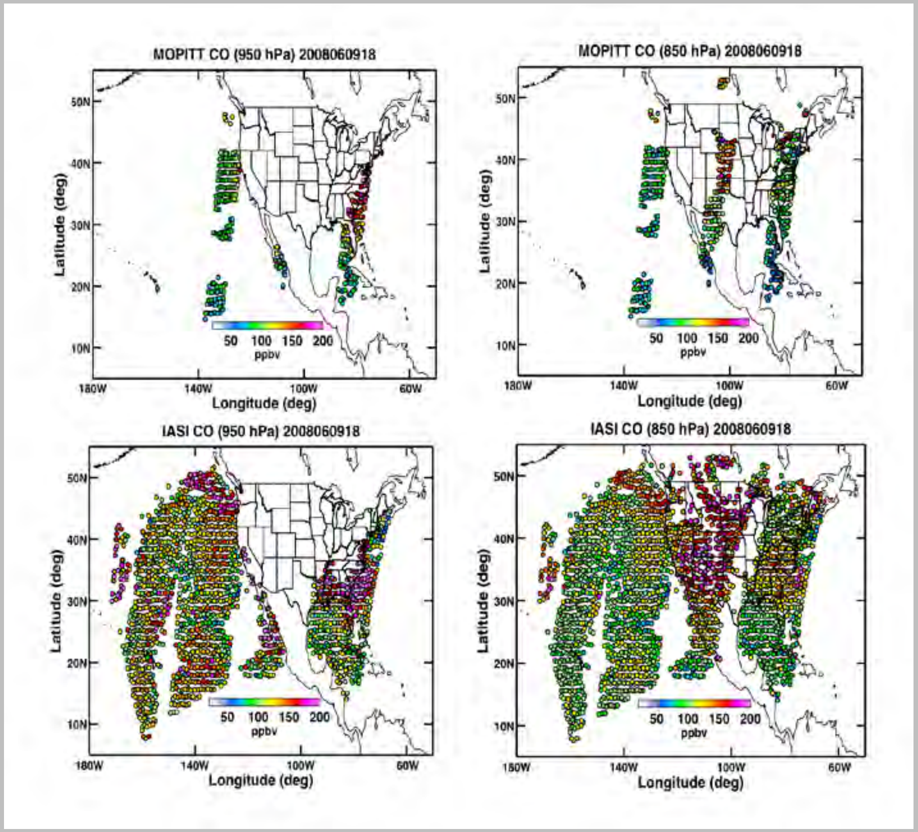

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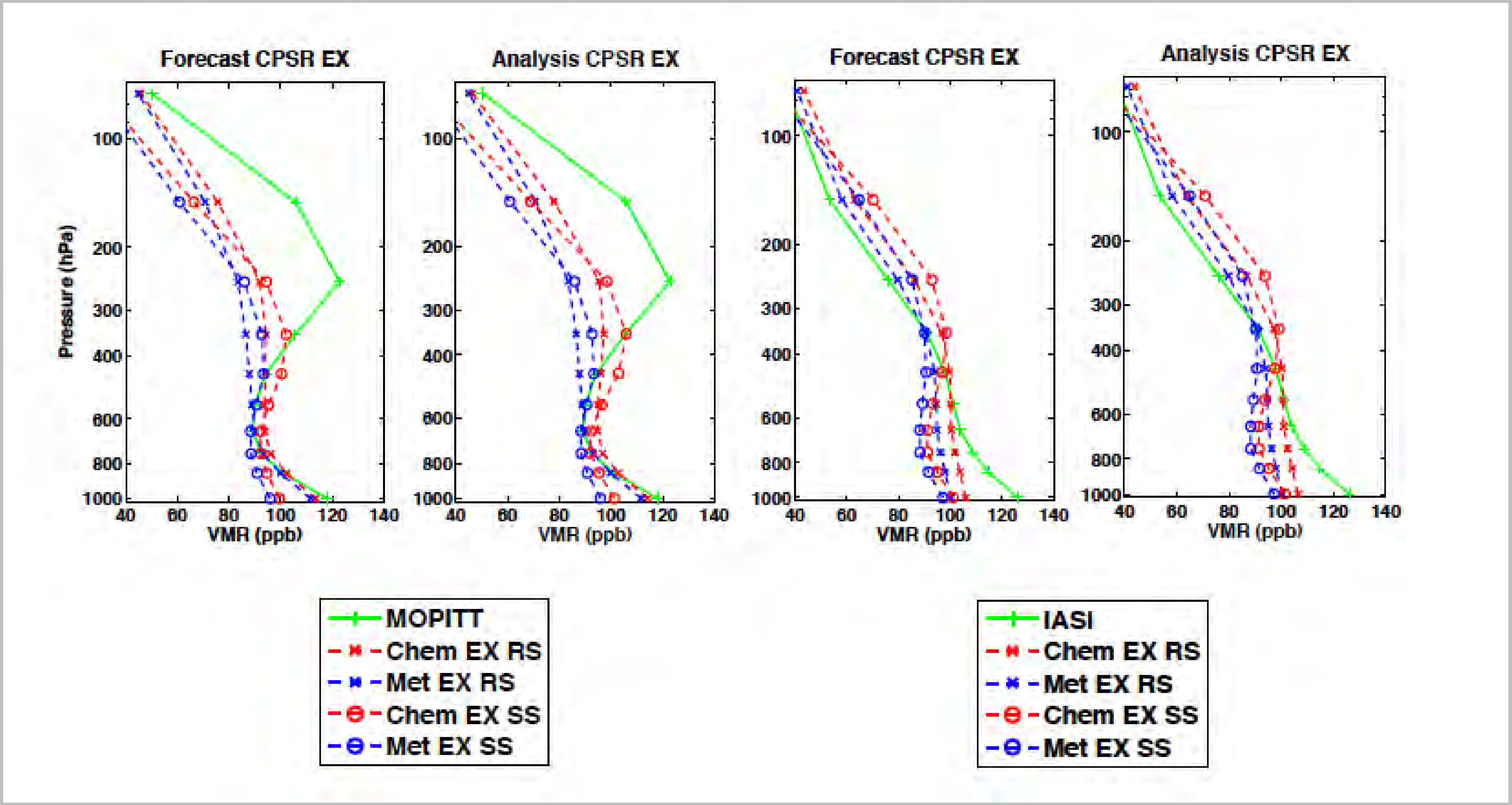
WRF-Chem/DART: Assimilation of Partial Profiles



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CPSRs: Retrieval Partial Profiles

- Mizzi et al. (2016b):

$$y_r - (I - A)y_a - \varepsilon = Ay_t$$

- Discard m elements of y_r. The resulting dimension is $n - m$.
- Discard the corresponding elements of y_a, rows of A, and rows and columns of E_m^2.
- A was square $(n \times n)$. It is now rectangular $(m \times n)$. Thus, this is called "CPSRs applied to rectangular systems." The dimension of E_m^2 is now $((n - m) \times (n - m)$.
- The rest of the derivation is similar to Mizzi et al. (2016a) because they used SVDs for the "compression" and "diagonalization" transforms.

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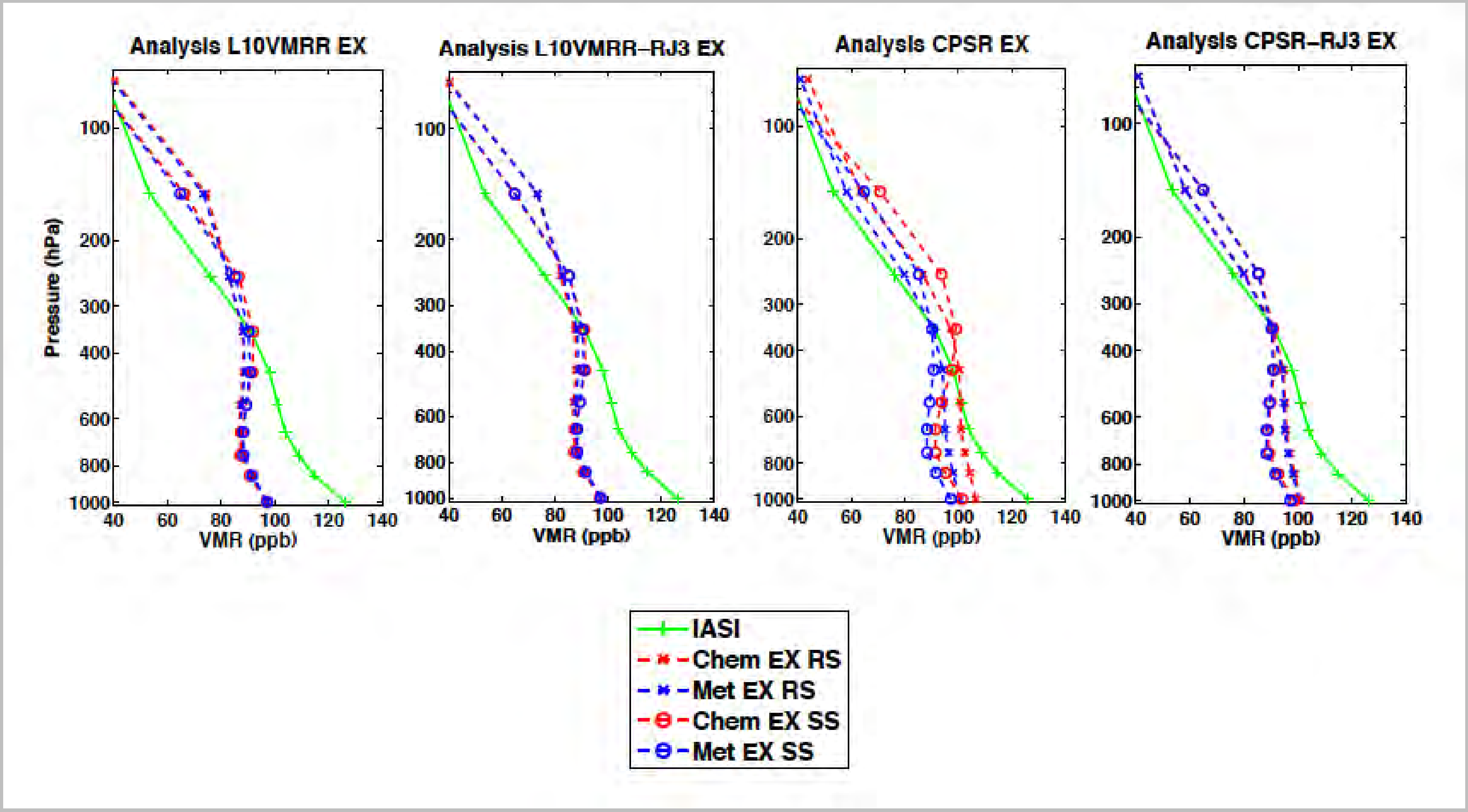
WRF-Chem/DART: Assimilation of Partial Profiles



Mizzi et al. (2016b)

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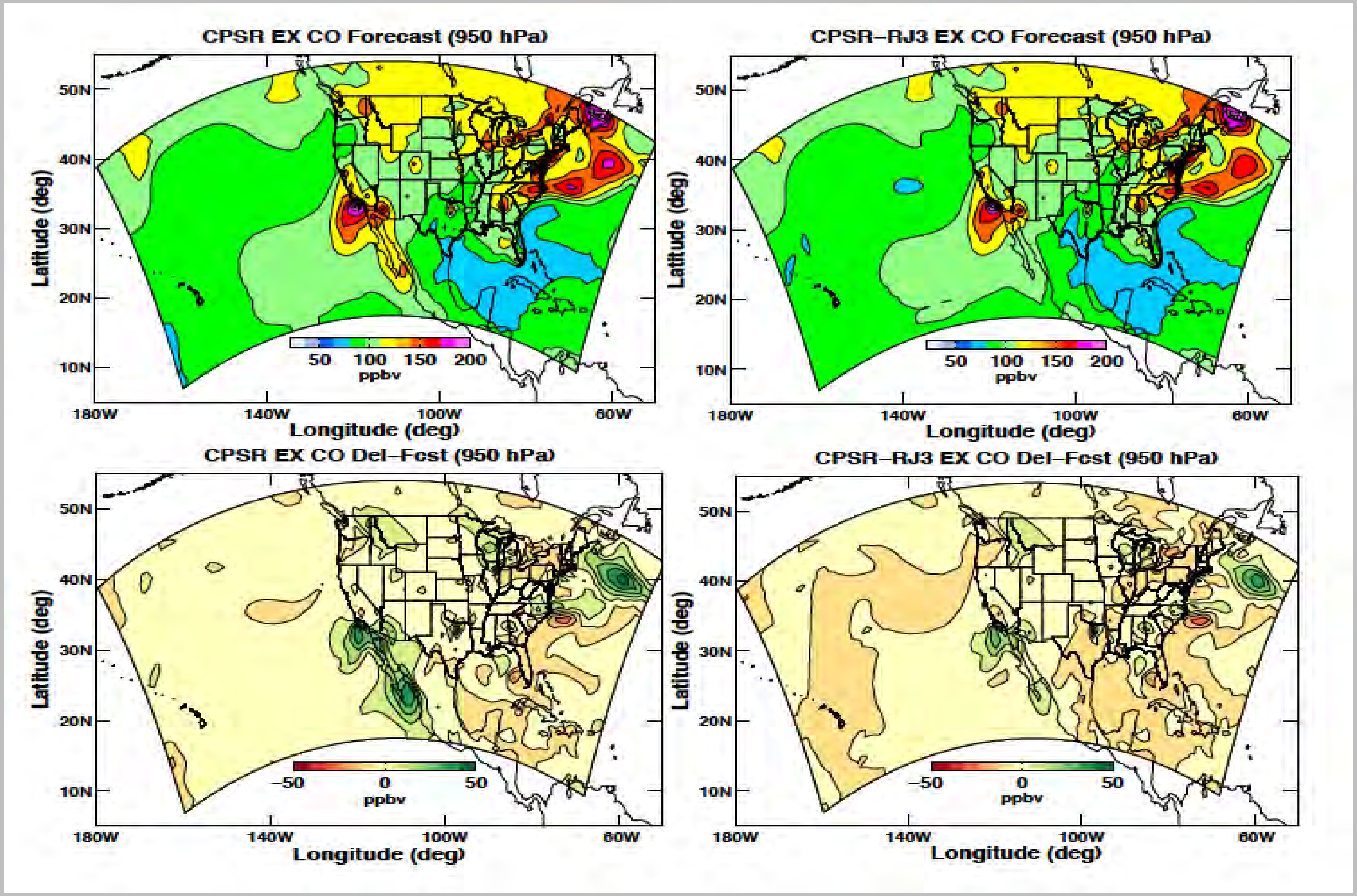
WRF-Chem/DART: Assimilation of Partial Profiles



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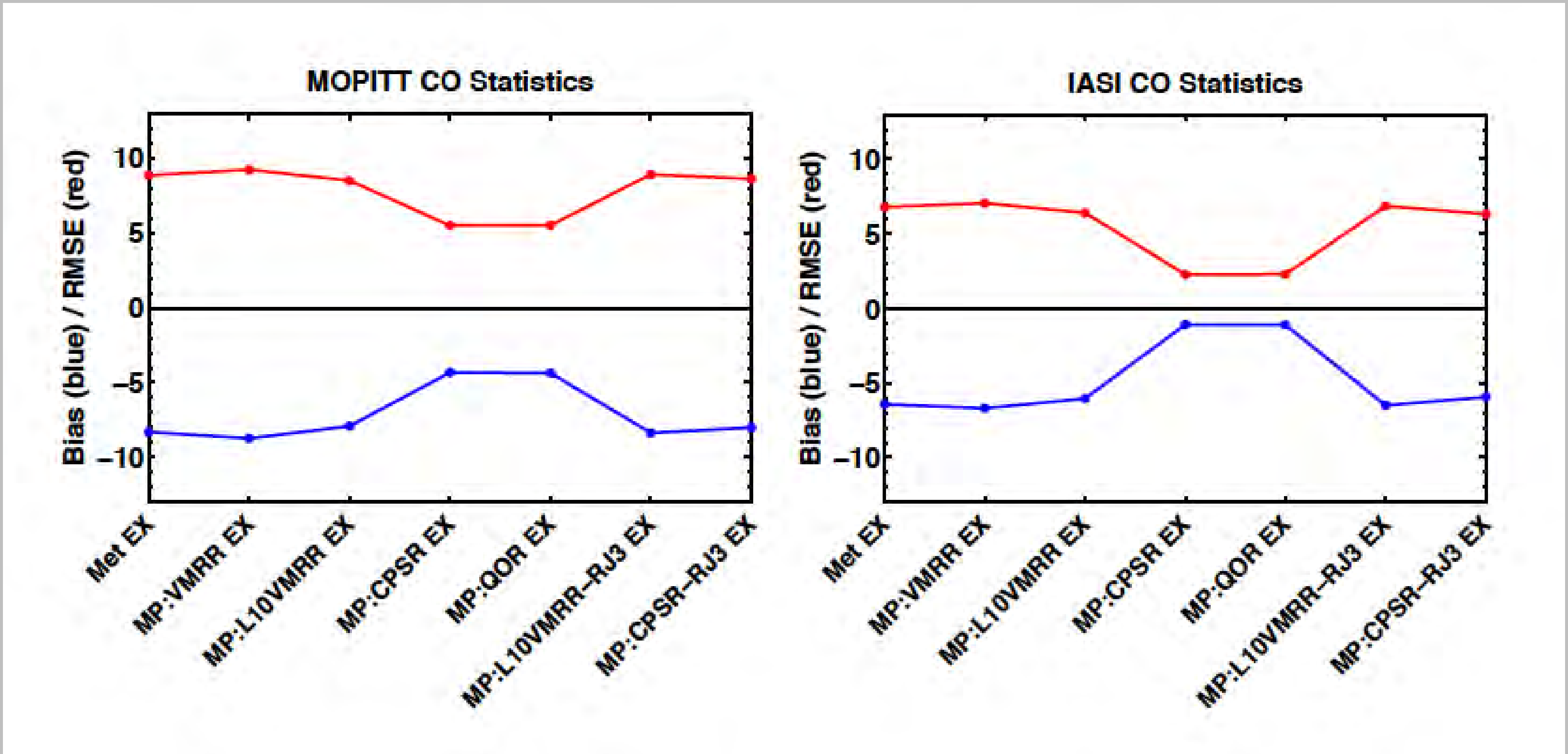
WRF-Chem/DART: Forecast Verification



Bias
RMSE

Mizzi et al. (2016a and b)

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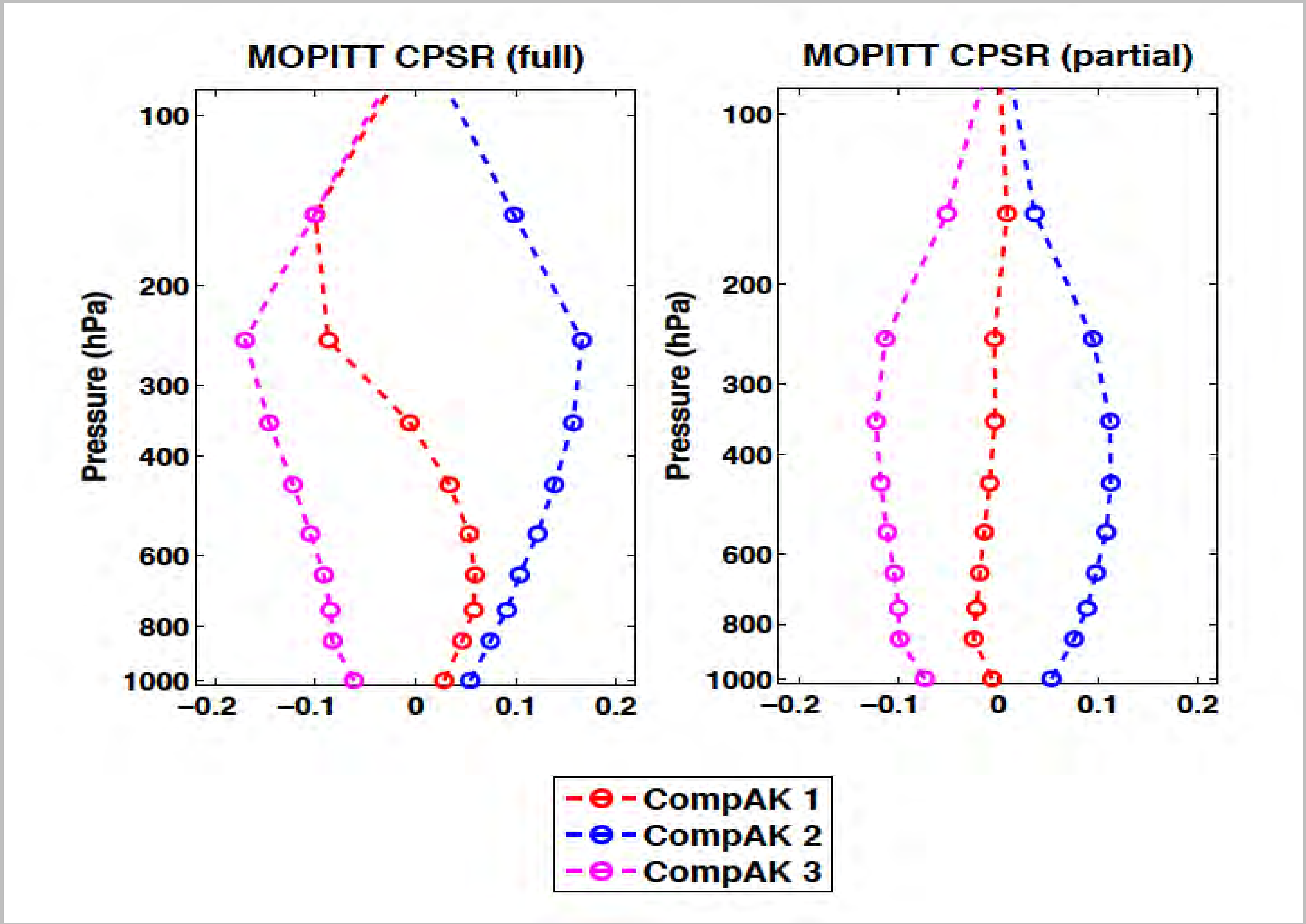
WRF-Chem/DART: Forecast Verification



Mizzi et al. (2016b)

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WRF-Chem/DART: Joint Assimilation of MOPITT and IASI CO CPSRs

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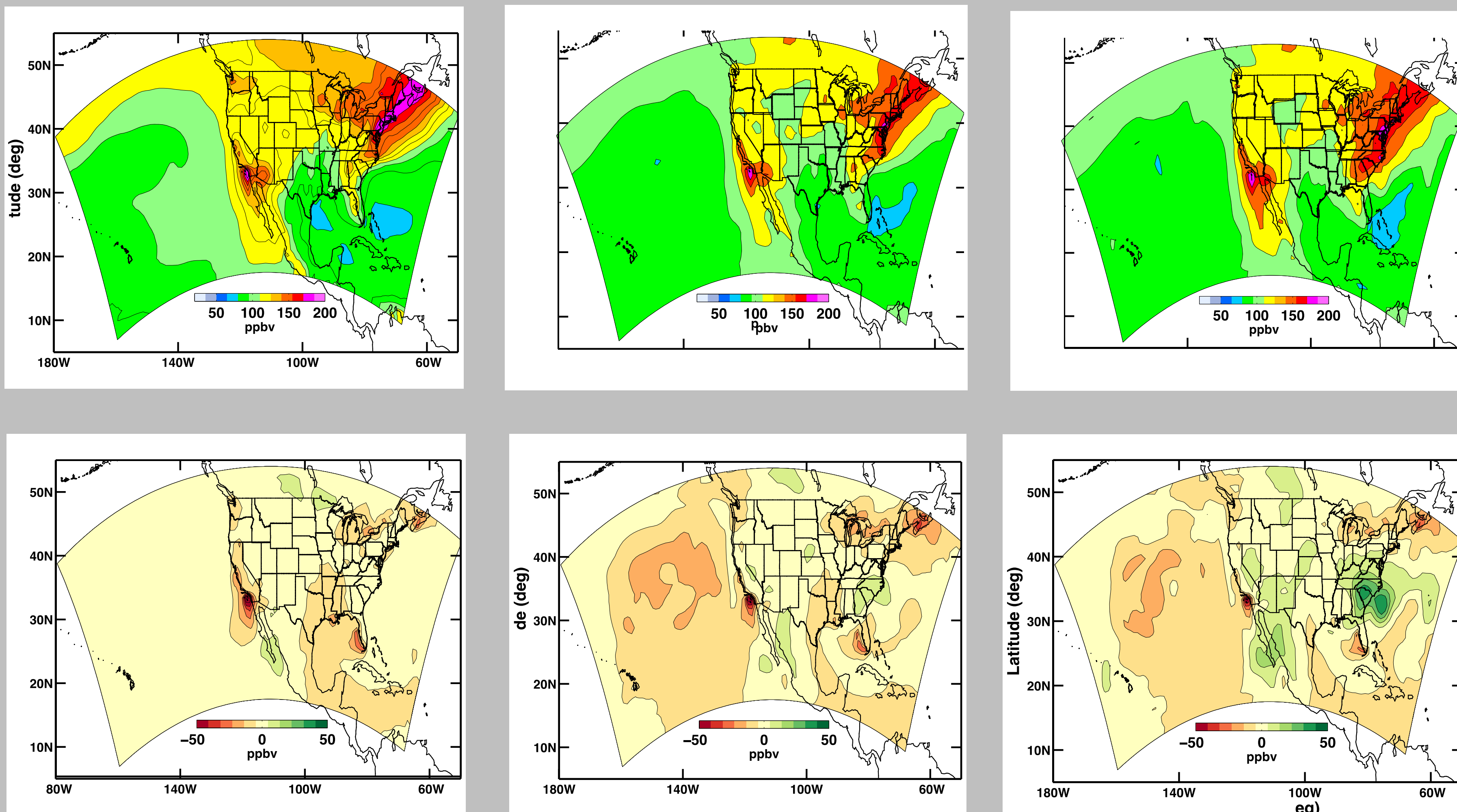
WRF-Chem/DART: Joint Assimilation



Mizzi et al. (2016c)

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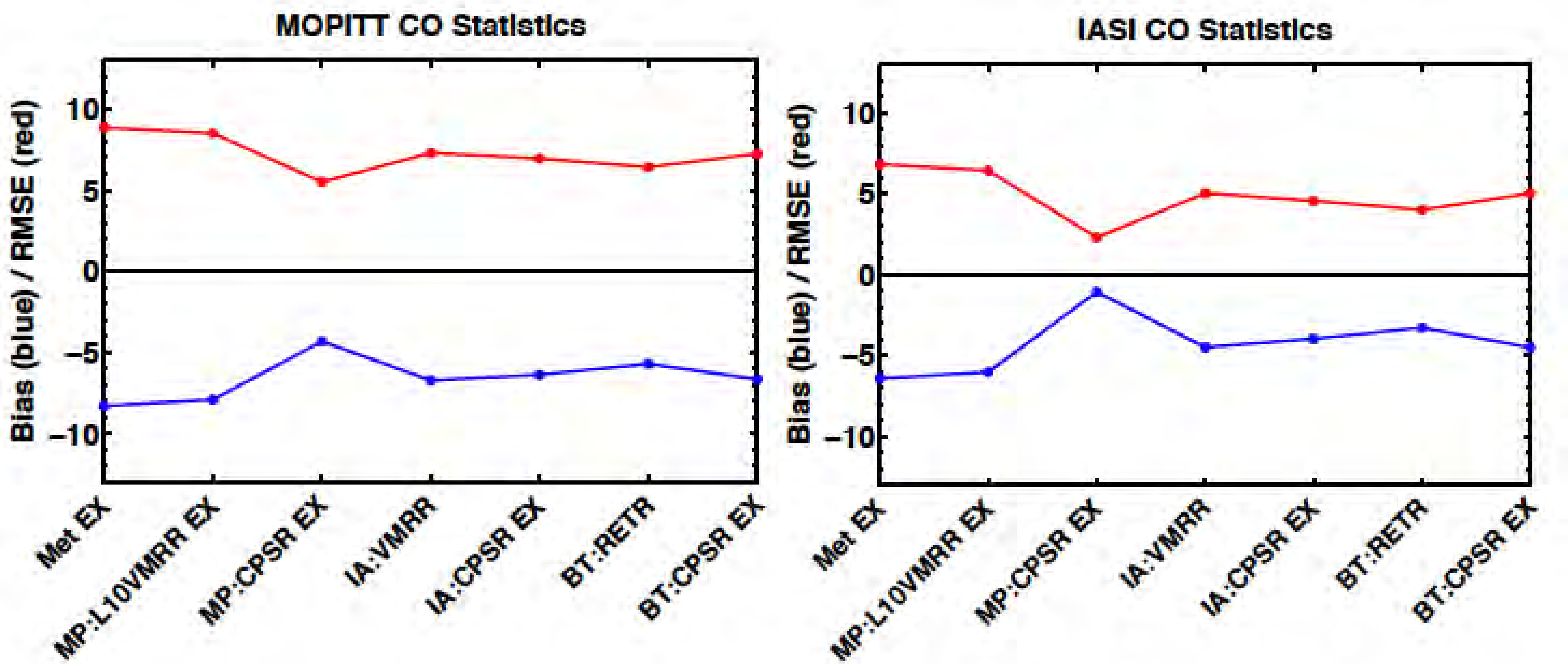
WRF-Chem/DART: Forecast Verification



Bias
RMSE

Mizzi et al. (2016b and c)

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WRF-Chem/DART: Illustration of Chem-DA Problems (Spread Collapse)

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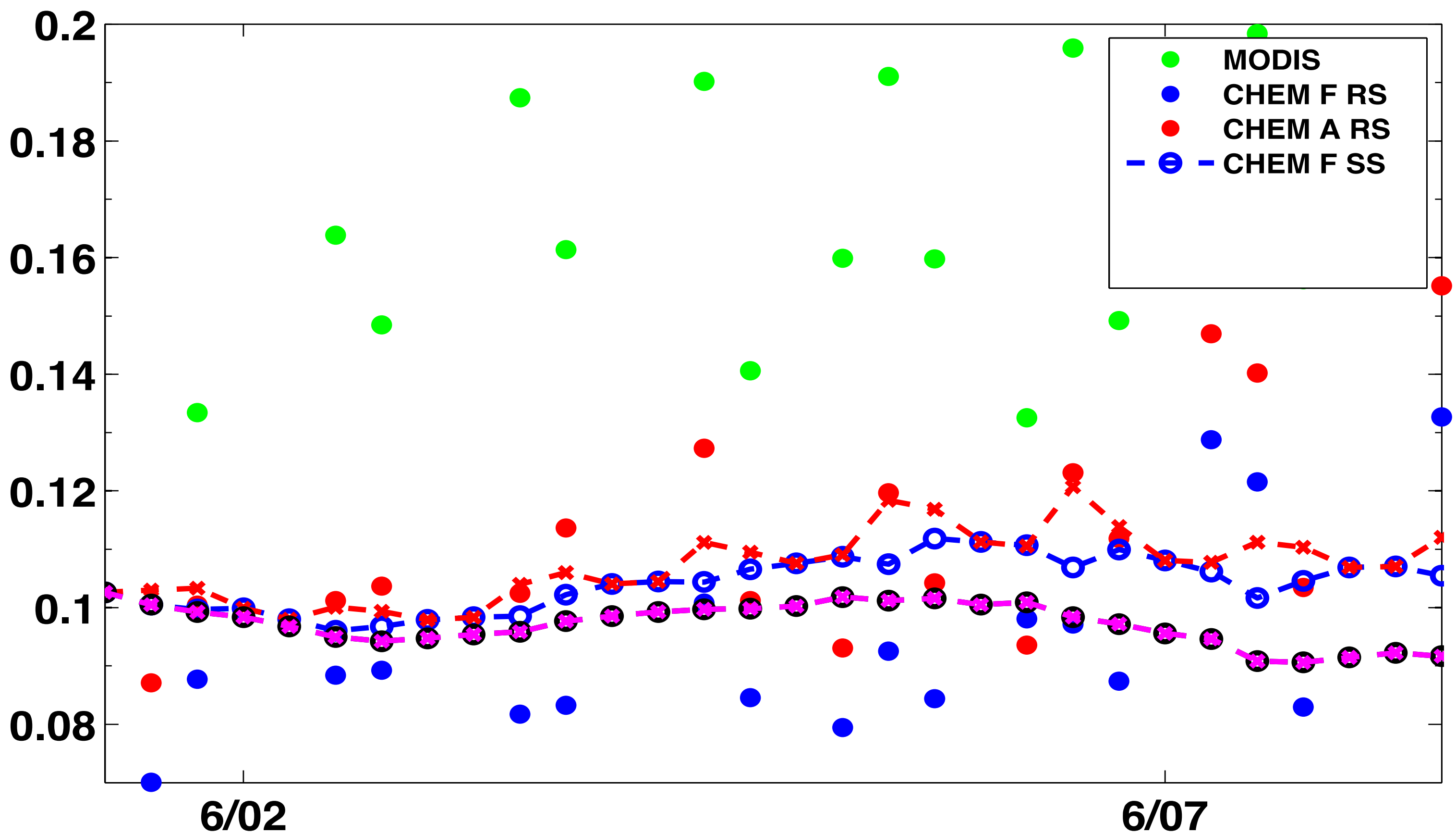
WRF-Chem/DART: MODIS AOD



Mizzi et al. (2016c)

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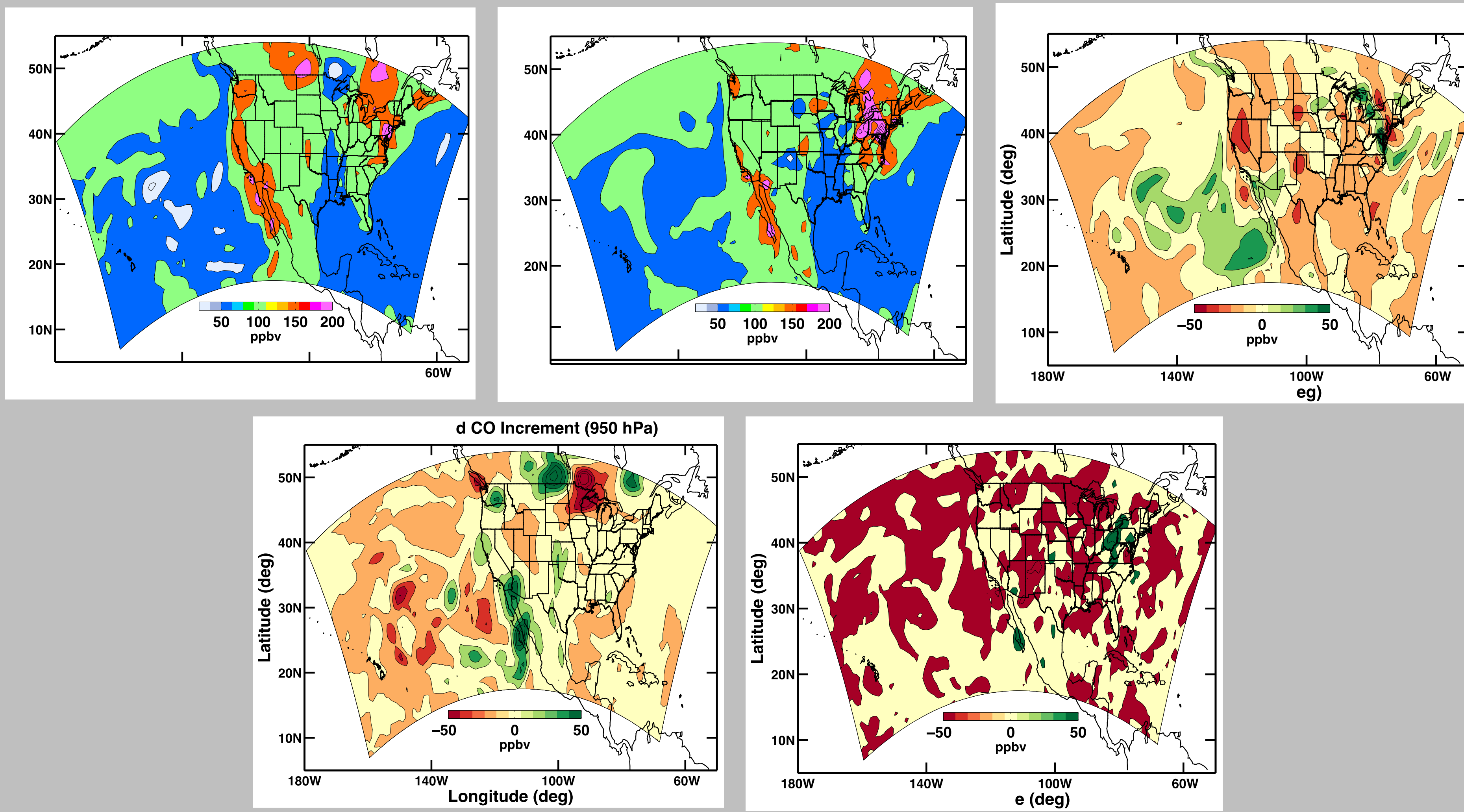
WRF-Chem/DART: Joint MOPITT. IASI and MODIS 18 UTC June 5, 2008



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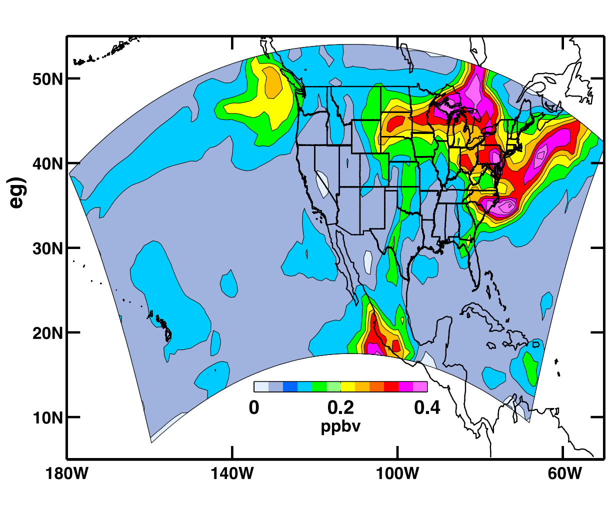

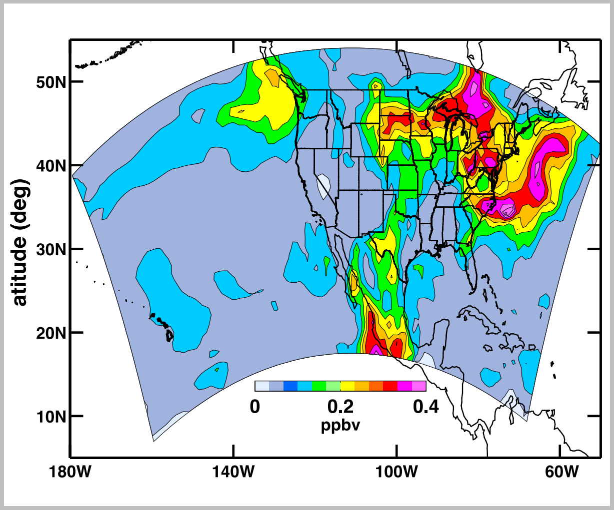

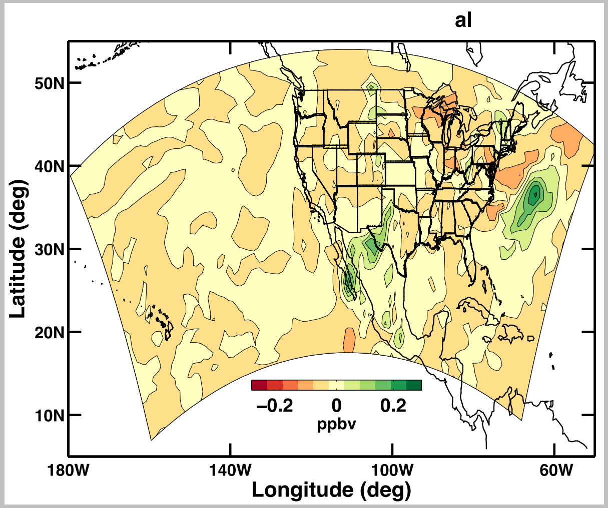

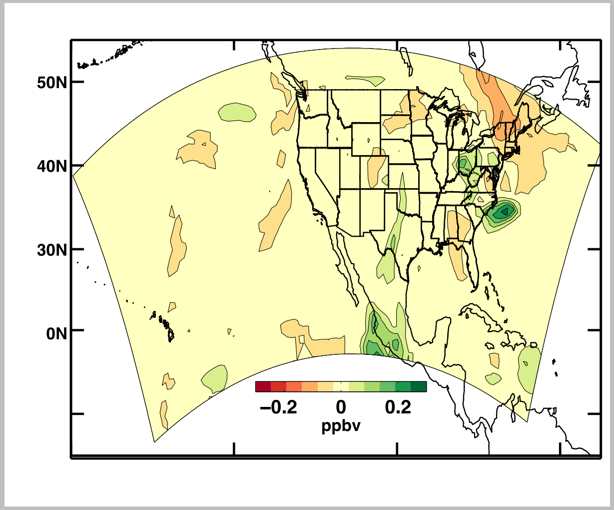

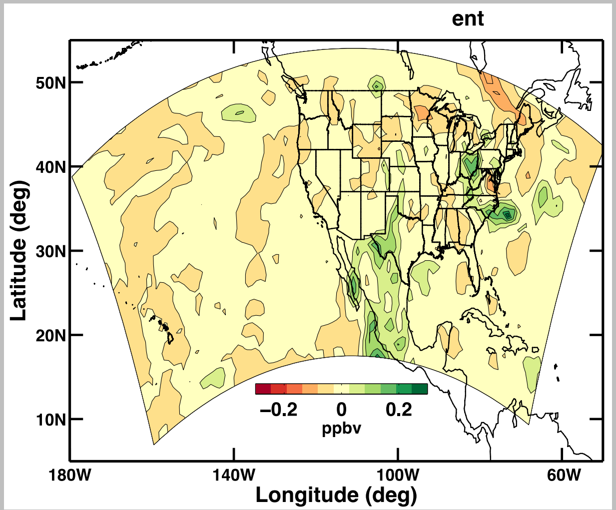

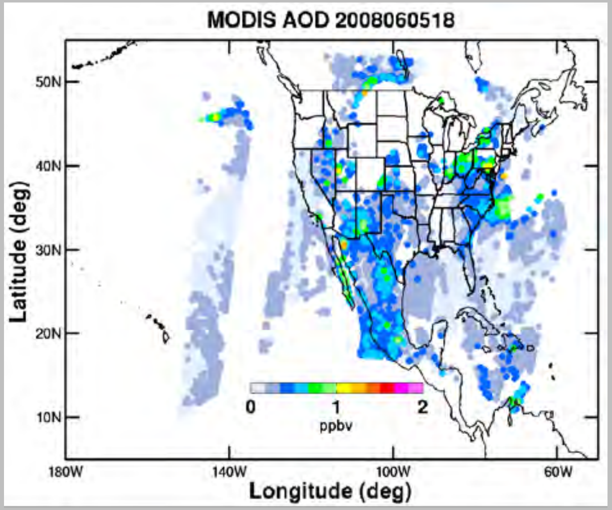

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Ensemble Kalman Filter

- Mitchell and Houtekamer (2001):

$$x_p = K\big(y - H(x_a)\big) + x_a$$

where $K = PH^T(HPH^T + R)^{-1}$ - P is the ensemble error covariance, R is the observation error covariance, and H is the forward operator mapping state variable x to observation y.

- **Problem:** undersampling can lead to spurious correlations in P.
- **Problem:** overfitting and cycling can lead to degeneracy/spread collapse.
- **Solution:** Localization – limit the spatial extent and/or state variable/observation correlations (reduce or set them to zero).
- **Solution:** Increase observation error to avoid overfitting
- **Solution:** Use prior or posterior covariance inflation.

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Ensemble Kalman Filter Least Squares Framework - Spread Collapse

$$\Delta \boldsymbol{x} = \left(\frac{\boldsymbol{cov}(\boldsymbol{x}, \boldsymbol{y})}{\boldsymbol{var}(\boldsymbol{y})} \right)^{1/2} \times \quad \Delta \boldsymbol{y}$$

x **-** the ensemble of state variables at a grid locations

y **-** the ensemble of expected observations at an observation location

$\boldsymbol{y} = \boldsymbol{H}(\boldsymbol{x})$ where $\boldsymbol{H}$ is the forward operator

$\Delta \boldsymbol{y}$ - the ensemble of expected observation increments

$\Delta \boldsymbol{x}$ - the ensemble of state variable increments

With spread collapse ***var(y)*** → 0

Anderson (2003)

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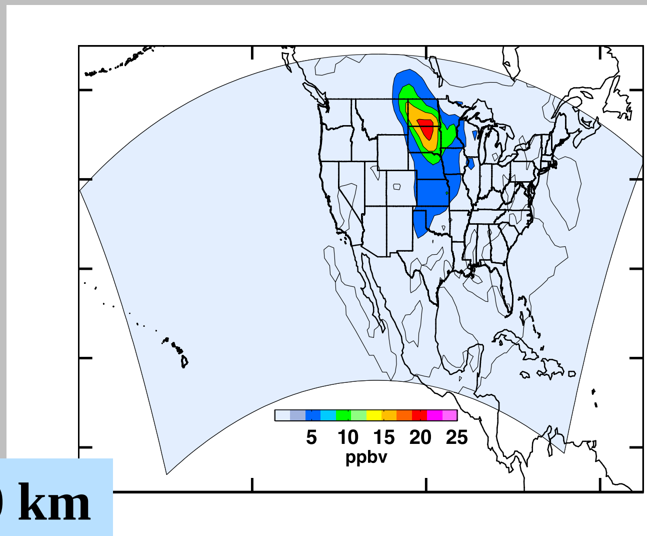
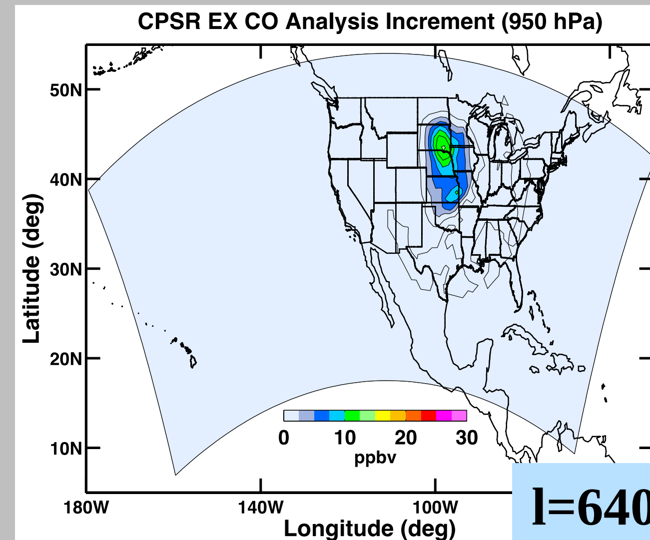
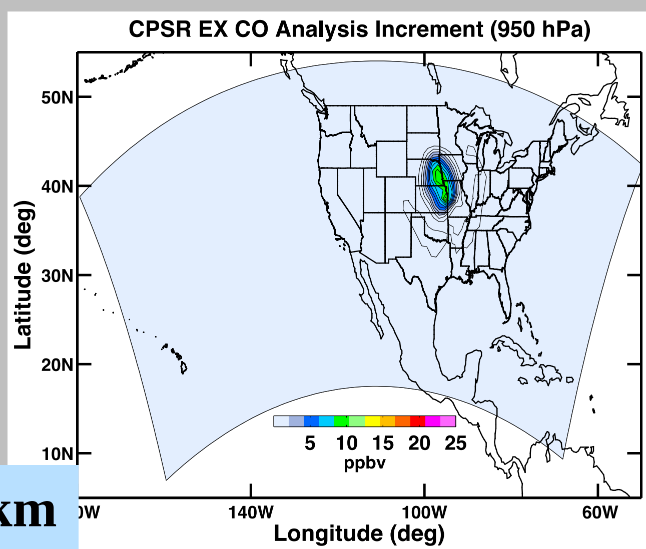
WRF-Chem/DART: Localization Examples



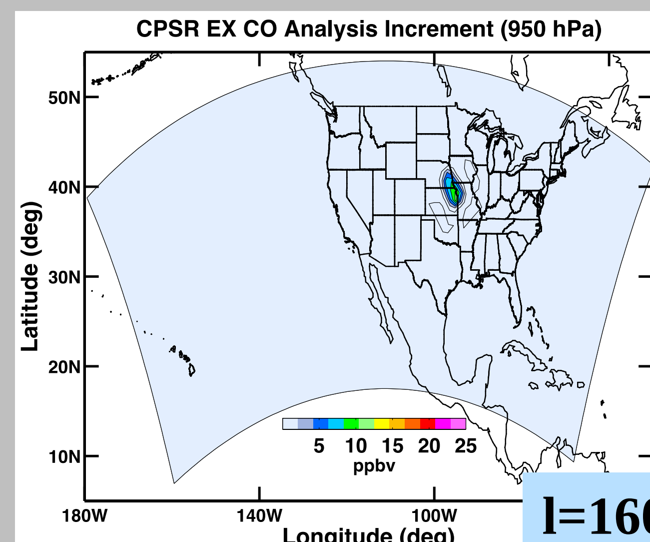
l=1300 km



l=640 km



l=320 km



l=160 km

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WRF-Chem/DART Applied to FRAPPE

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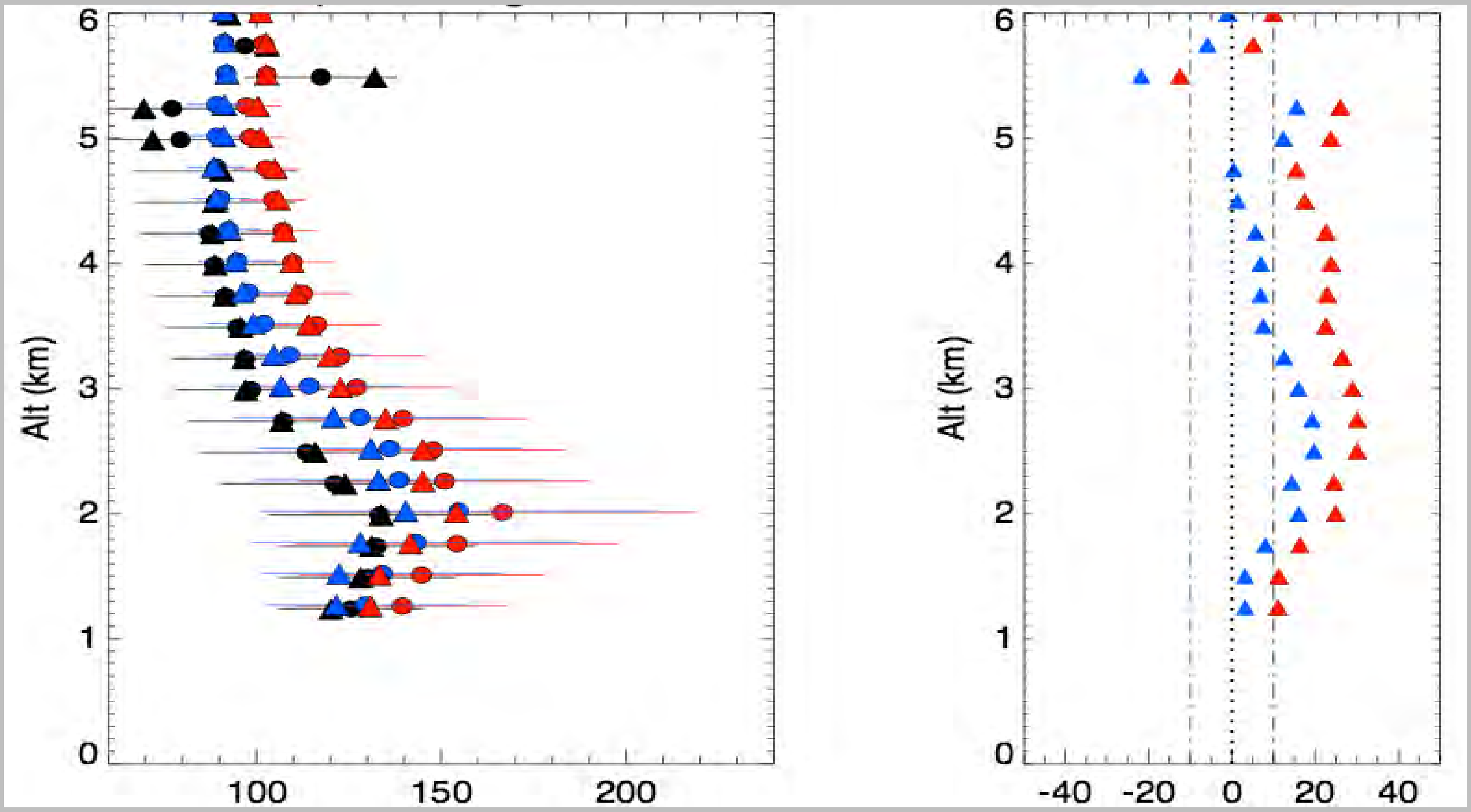
WRF-Chem/DART: FRAPPE (July 14 – 29, 2014)

● Met-DA ● Chem-DA ● Obs



CO (ppbv) (WRF-OBS)/OBS

● Mean ▲ Median

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WRF-Chem/DART: FRAPPE (July 27, 2014)

Met-DA

Chem-DA

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Summary:

- Poor air quality has substantial health and economic impacts.
- One approach to mitigation is accurate air quality forecasting.
- ACOM is working to improve air quality forecasting: OSSE for GEO, emission adjustments, real-time global/regional air quality forecasting/data assimilation, and more efficient forward operators.
- CPSRs improve air quality forecast skill at reduced computation costs (~35% reduction MOPITT, ~50% reduction IASI).

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