Ensemble Forecasting/Assimilation/Emissions Estimation with WRF-Chem/DART: Accomplishments, Lessons Learned, and Future Plans

A. Mizzi, C.-H. Hsu, M. Johnson, B. McDonald, R. Kumar, D. Henze, and J. Anderson

NASA Ames Research Center/BAERI

NOAA Chemical Systems Laboratory/CIRES

CU Boulder/MecE

(arthur.p.mizzi@nasa.gov)

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Overview

- ✔ WRF-Chem/DART
- ✔ Lessons learned
- ✔ Future projects

arthur.p.mizzi@nasa.gov

WRF-Chem/DART

Introduction to WRF-Chem/DART

- ✔ A regional chemical weather forecast/ensemble data assimilation system based on WRF-Chem and DART using the ensemble adjustment Kalman filter and the state augmentation method.
- ✔ Assimilates MOPITT and IASI CO, IASI O_3, MODIS AOD, OMI O_3, NO_2, SO_2, TROPOMI CO, O_3, NO_2, SO_2, and proxy TEMPO O_3, NO_2 total/partial column and/or profiles retrievals, and AirNow *in situ* observations.
- ✔ Working on interface with NASA JPL's MOMO-Chem/LETKF and NASA GMAO's GEOS-CF and NU-WRF- Chem systems.
- ✔ Working to assimilate OMI HCHO; TROPOMI HCHO, and CH_4; TES CO, O_3, CO_2, CH_4, and NH_3; CrIS CO, O_3, CH_4, NH_3, and PAN; GOME2A and SCIAMACHY NO_2; and MLS O_3 and HNO_3 total/partial column and/or profile retrievals.
- ✔ Working to assimilate GOES LFCs, AOD total column retrievals, and JSAHs; VIIRS PM and AOD total column retrievals; and TROPOMI AOCHs.
- ✔ Collaborators throughout North America, Asia, and Western Europe are working on operational AQ forecasting; assimilation of NO_2, CO_2, NH_3, CH_2O with dynamic/realtime emissions estimation in response to events like COVID.

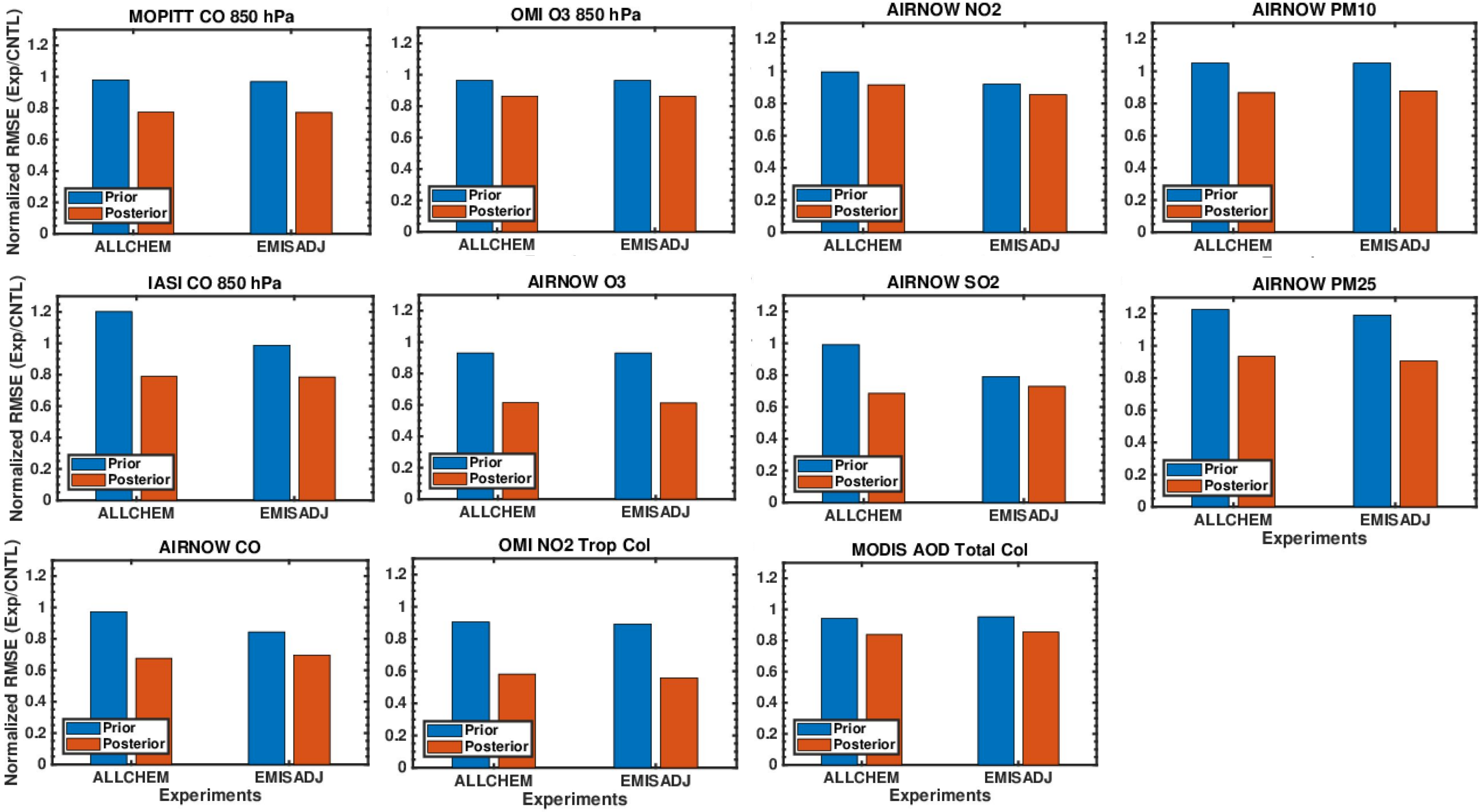
arthur.p.mizzi@nasa.gov

FRAPPE Application
(Illustration of WRF-Chem/DART Capabilities)

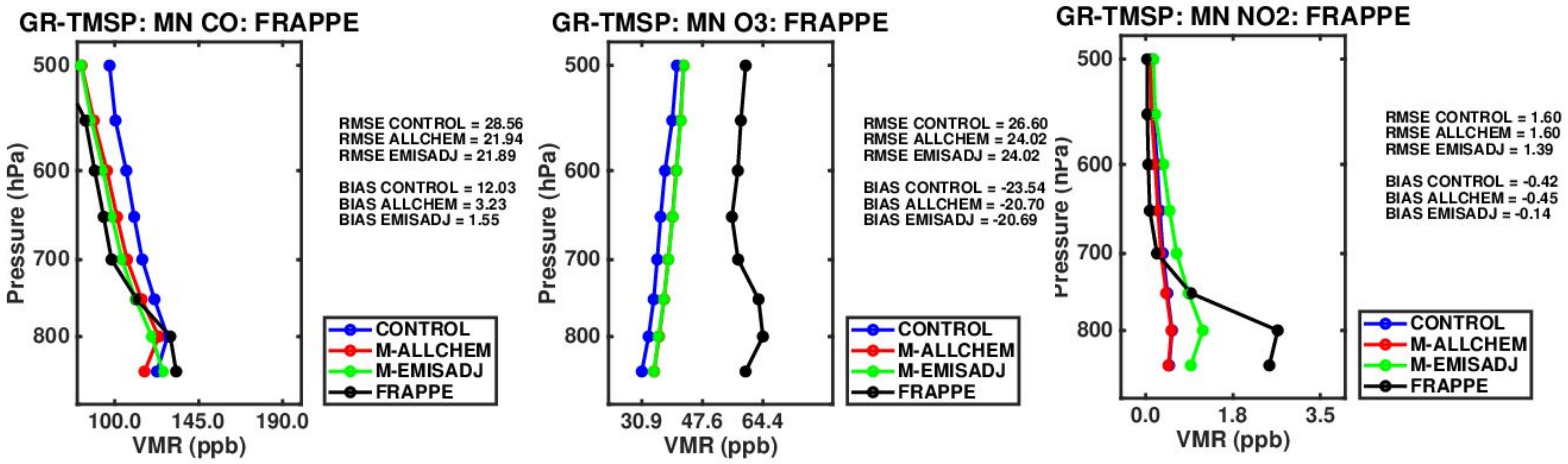
FRAPPE Application

- ✔ FRAPPE (Front Range Air Pollution and Photochemistry Experiment) – Discover AQ – Investigated air pollution in the Colorado Front Range during July and August 2014.
- ✔ Three experiments:
  - **CONTROL** - assimilate only conventional meteorology observations;
  - **ALLCHEM** – same as CONTROL except also assimilate chemistry observations (MOPITT and IASI CO profile; MODIS AOD total column; OMI O_3 profile and NO_2, tropospheric column retrievals and AQS CO, O3, NO2, SO_2, PM10, and PM2.5 in situ observations); and
  - **EMISADJ** – same as **ALLCHEM** except include 'top-down' emissions estimation.
- ✔ Assimilation terms and skill metrics:
  - **Increment** – the assimilation posterior minus the assimilation prior;
  - **Difference** – the **ALLCHEM** or **EMISADJ** result minus the **CONTROL** result;
  - **Emissions Factor** – the emissions posterior divided by its prior; and
  - **NRMSE** – the 'normalize root mean square error' defined as the **ALLCHEM** or **EMISADJ** RMSE divided by the **CONTROL** RMSE.

FRAPPE: NRMSE for Assimilated Observation Types

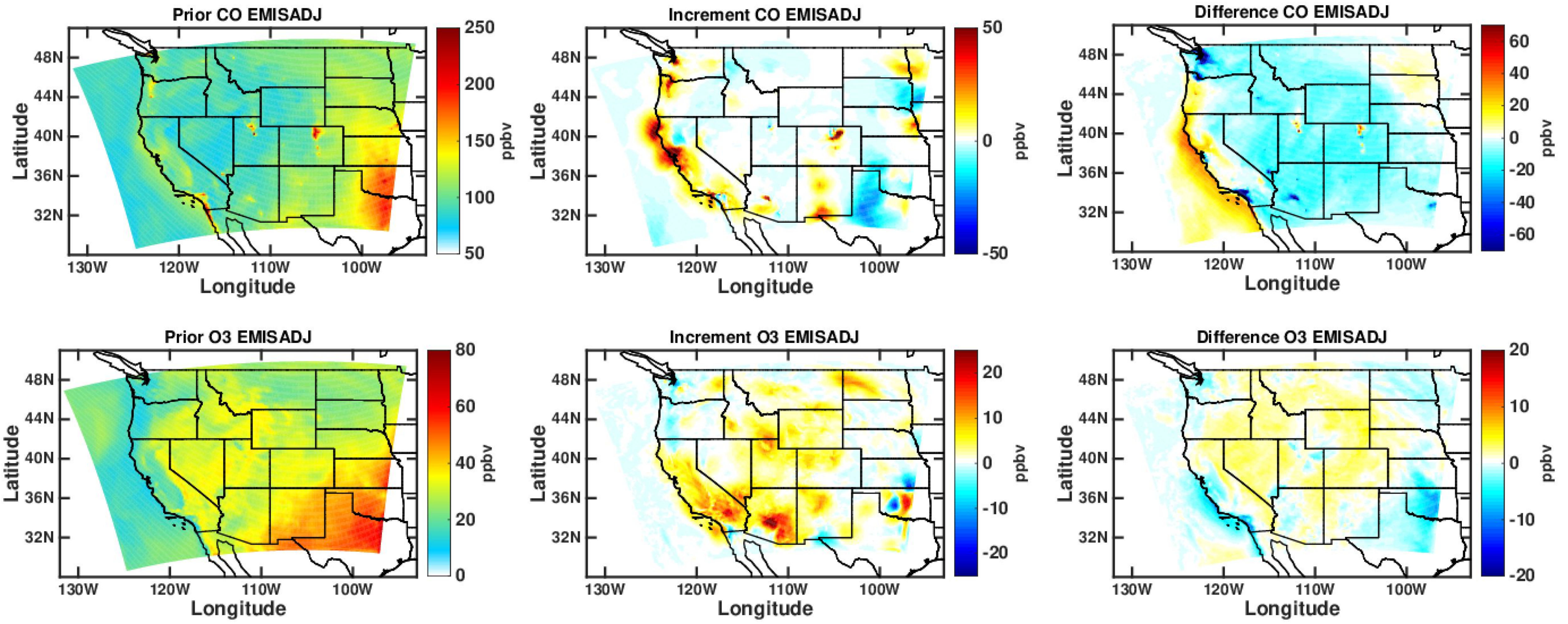


FRAPPE Comparison (Spatiotemporal Summation)
(FRAPPE Dates: 7/17, 7/20 7/21, 7/22, and 7/23)



- Chemical data assimilation and dynamic emissions estimation improve forecast compared to **CONTROL** based on comparison with FRAPPE aircraft profile observations.

FRAPPE: Selected Trace Gas Maps July 23, 2014 18 UTC



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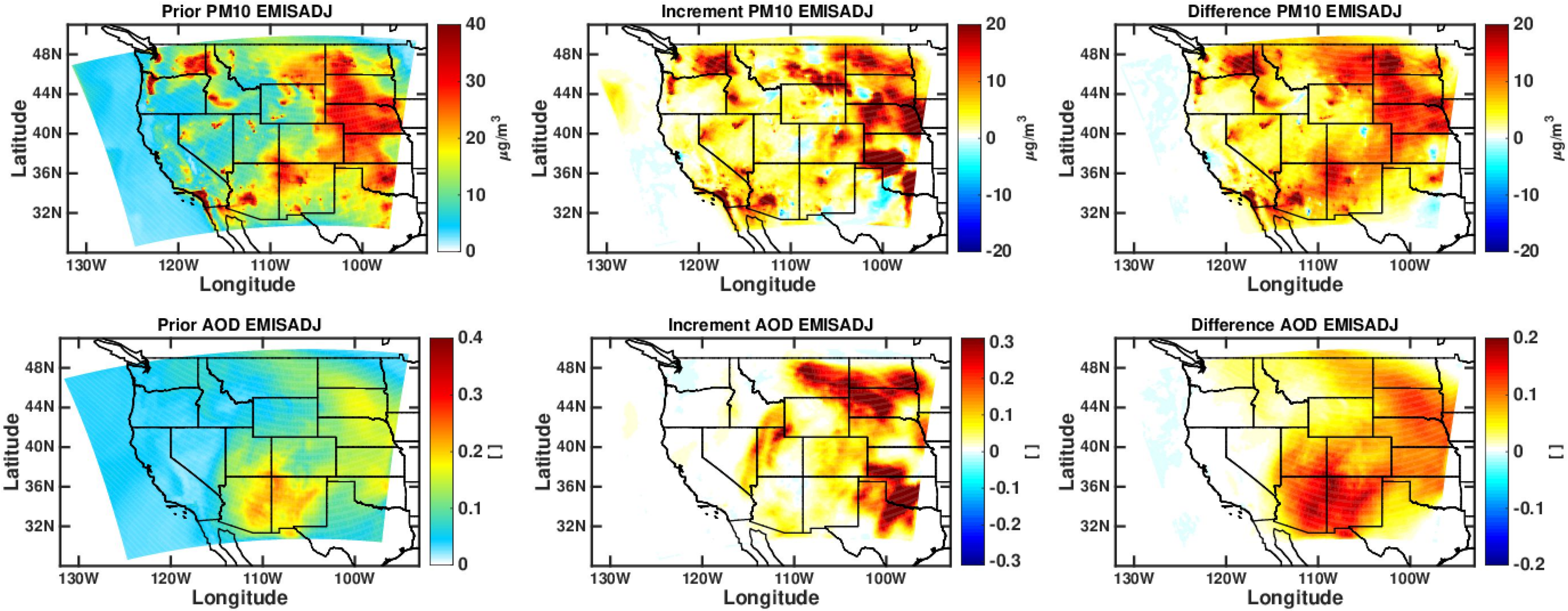
FRAPPE: Selected Aerosol and AOD Maps July 14, 2014 18 UTC



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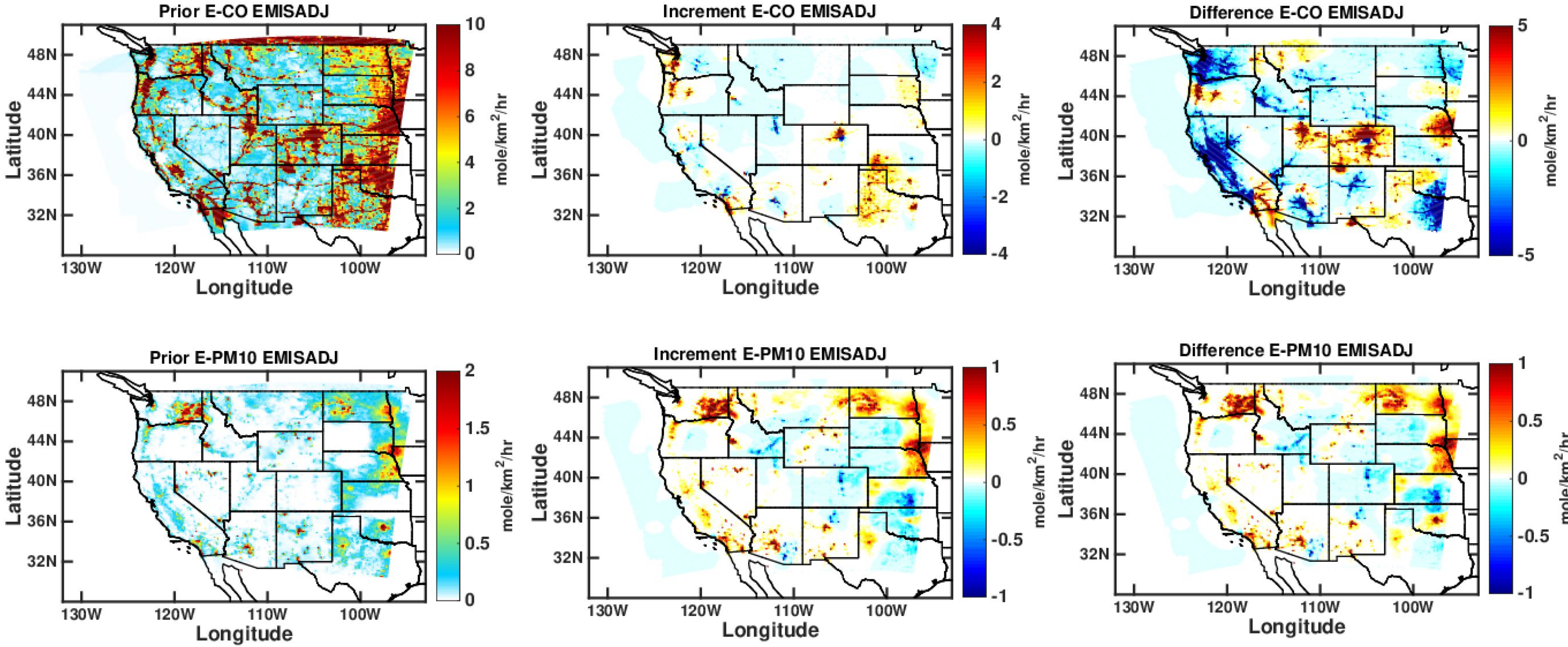
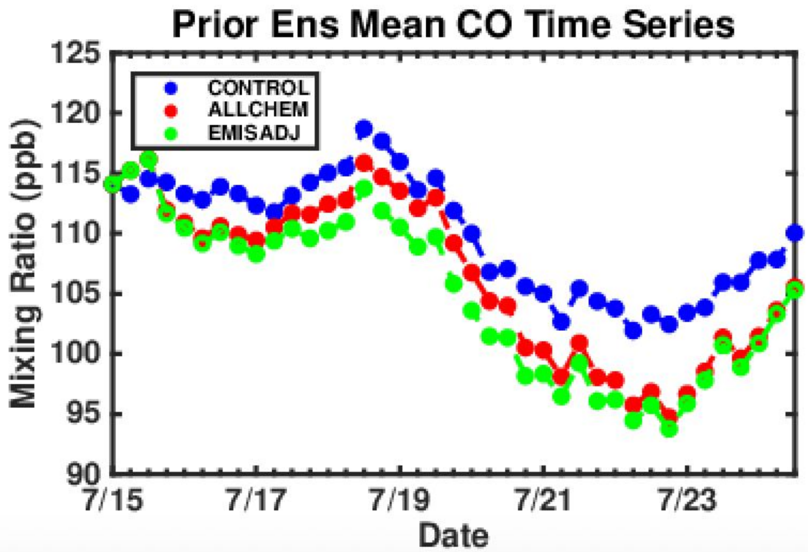
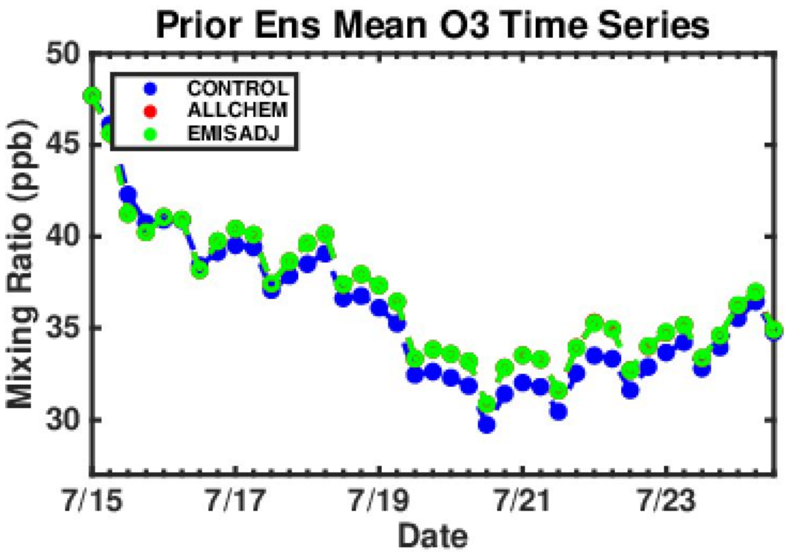
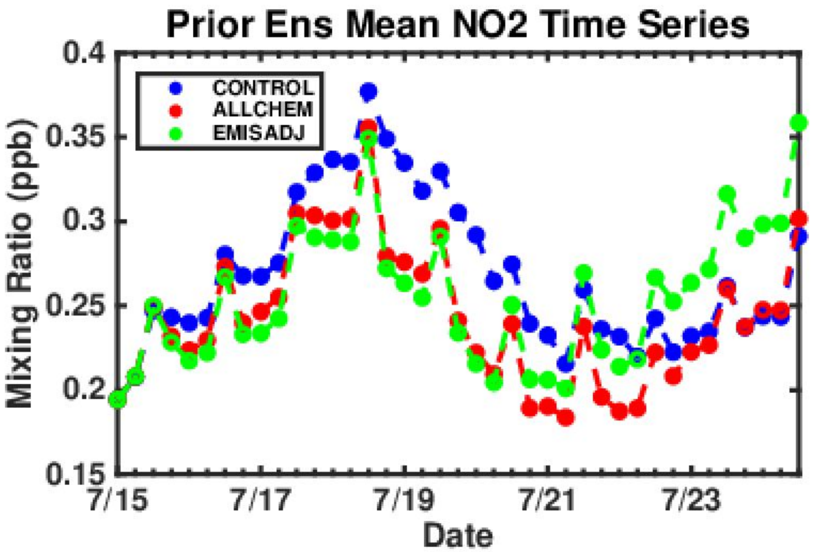
FRAPPE: Selected Emissions Maps July 23, 2014 18 UTC

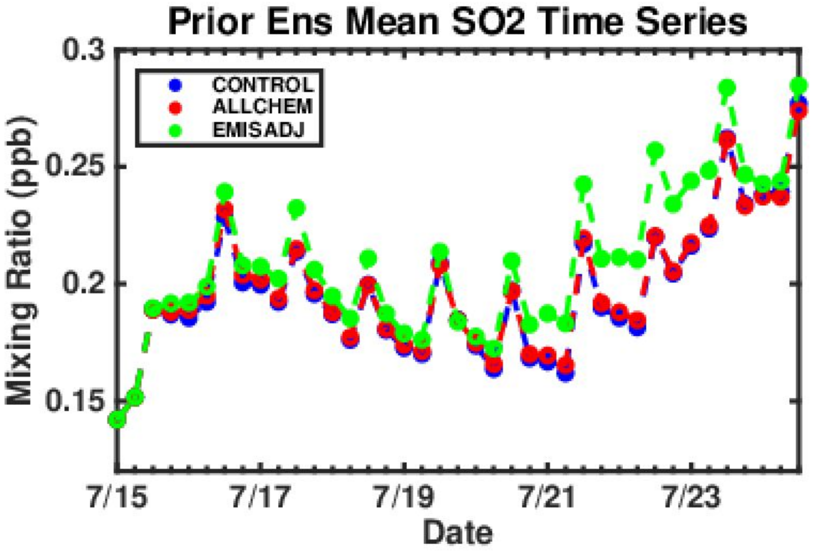


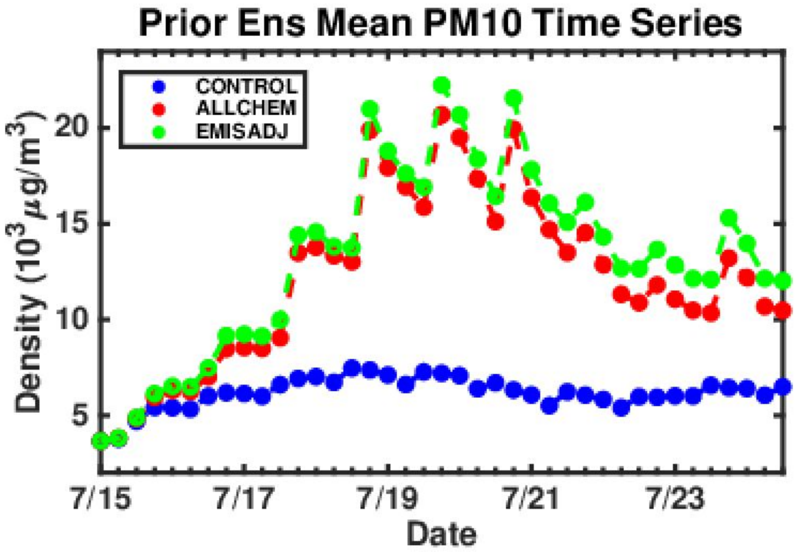
FRAPPE: Criteria Pollutant Timeseries

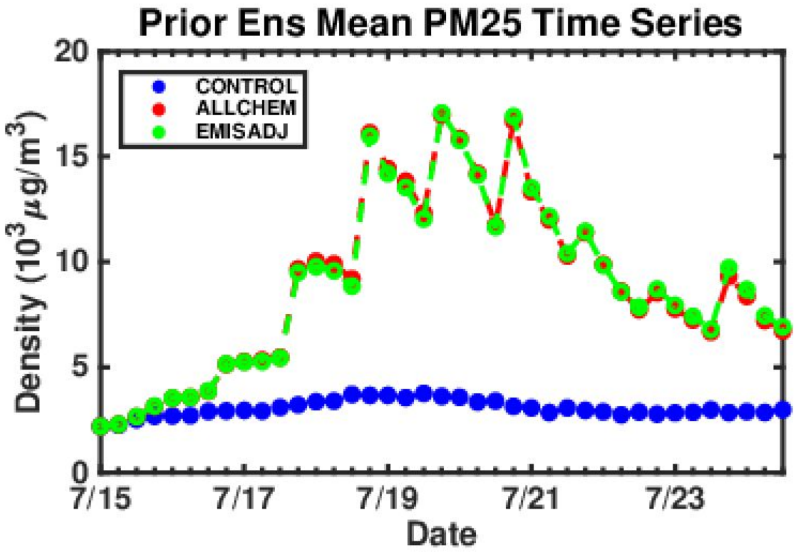




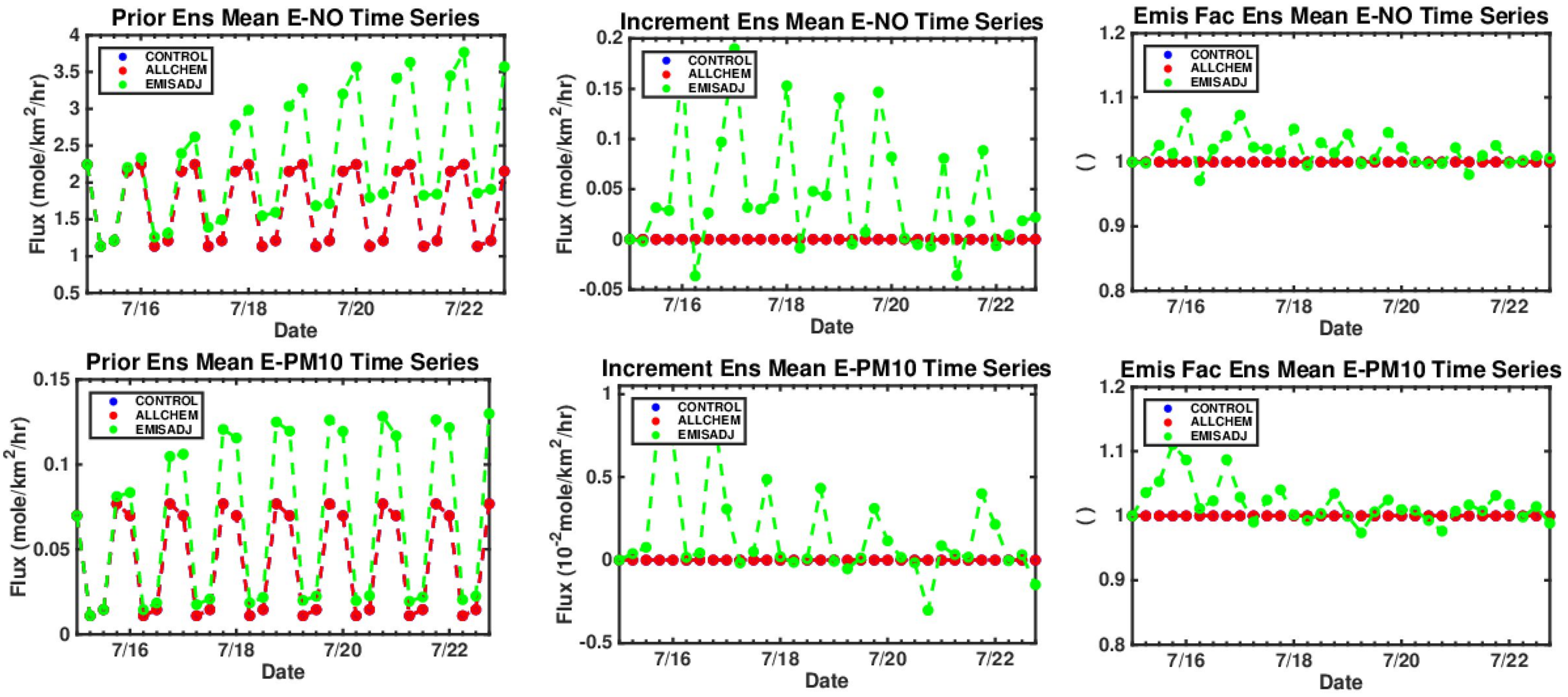








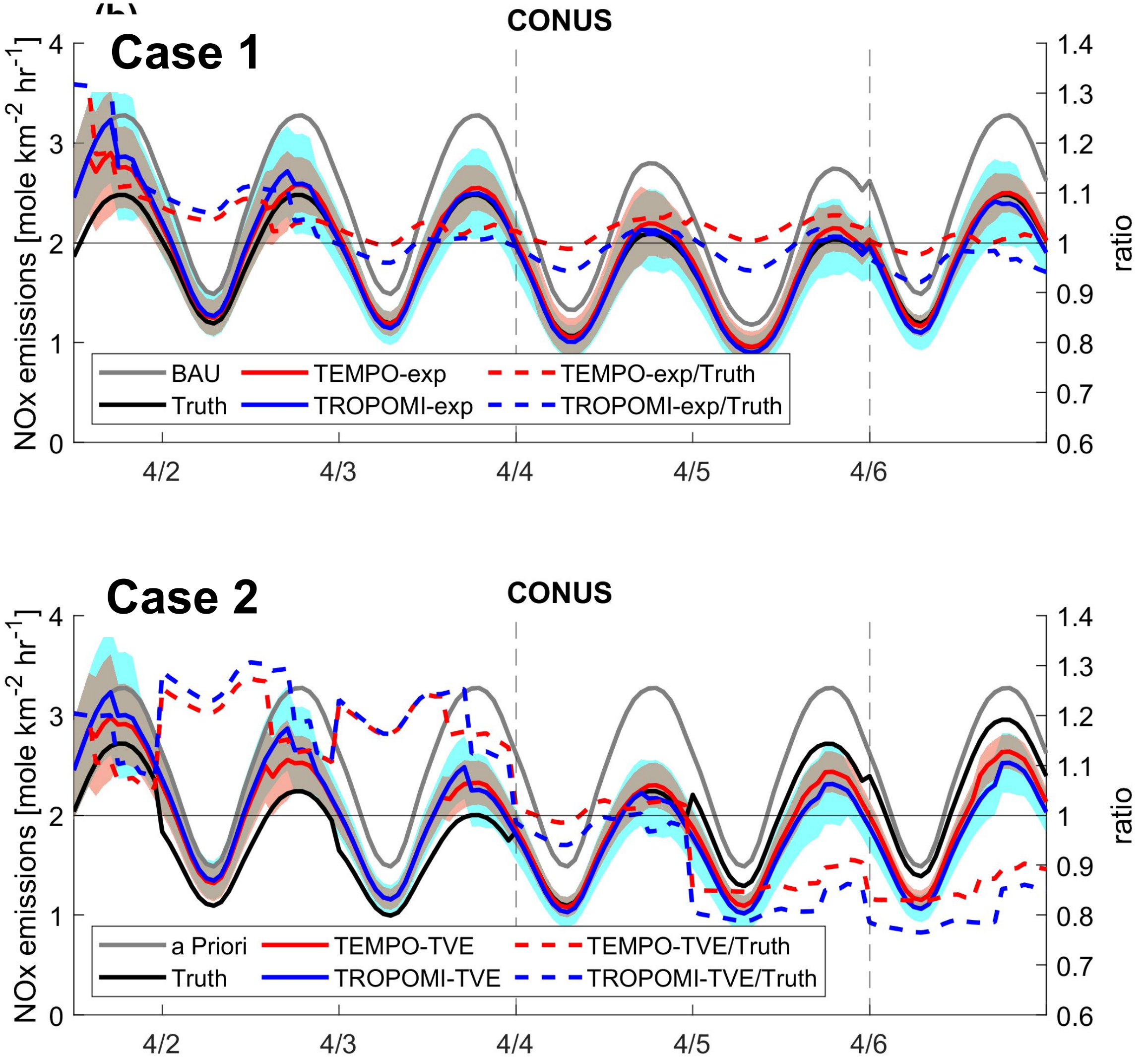
FRAPPE: Selected Criteria Pollutant Emissions Timeseries

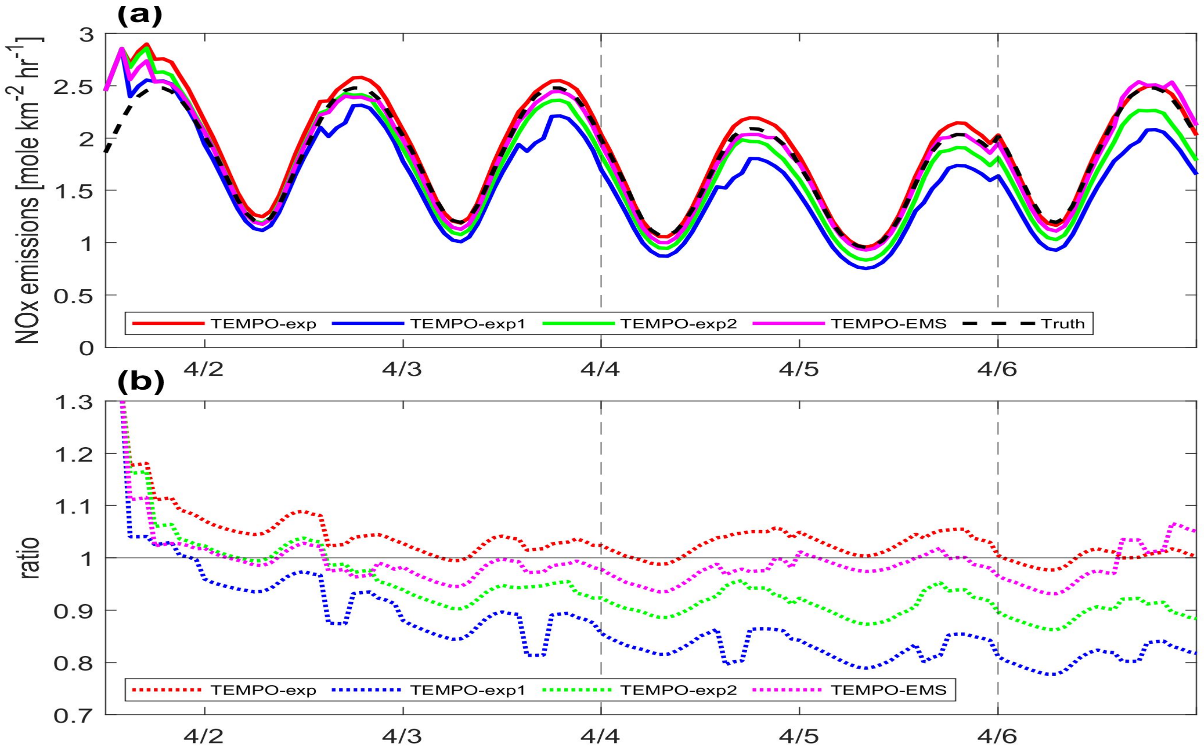


COVID OSSEs
(Assimilate synthetic TEMPO and TROPOMI NO_2 tropospheric columns)

TROPOMI and TEMPO NO_2 OSSEs to Recover COVID Period Emissions

Univ. of Colorado – Hsu and Henze; NOAA/CSL – McDonald: Hsu et al. (2023)





- TEMPO recovers COVID emissions twice as fast as TROPOMI.
- Using more cycles with shorter observation windows improves forecast skill by assimilating more observations and reducing impact of unrepresentative observations.

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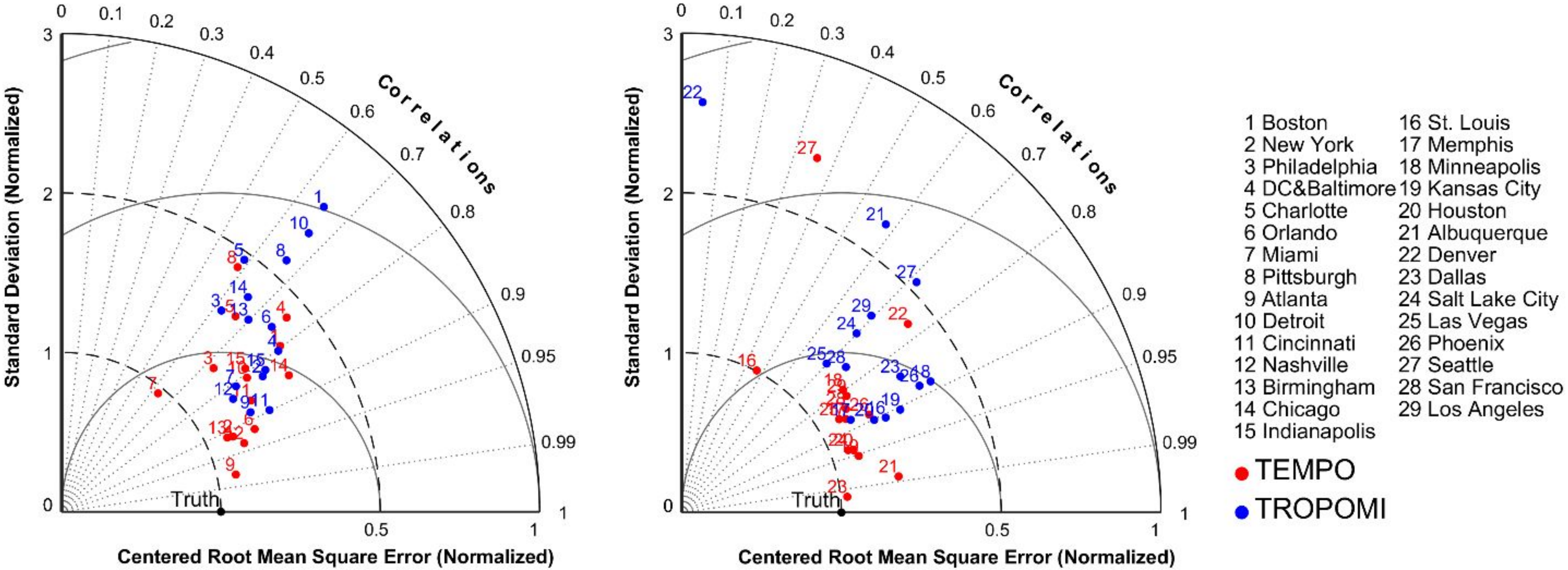
Taylor Diagram for Selected Urban Areas



- TEMPO performs better than TROPOMI in most urban areas.

Lessons Learned

Lessons Learned from 10 Years with WRF-Chem/DART

- ✔ Atmospheric composition forecasting/assimilation/emissions estimation is computational expensive. The advent of GEO platforms and increased assimilation of retrieval profile will make the computational costs even more challenging.
- ✔ The algorithm for generation of the chemical initial, lateral, and upper boundary conditions, and emissions matters. Without the appropriate spread or ensemble error lateral, vertical, and temporal ensemble error correlation length scales, the results can be problematic.
- ✔ Chemical species and most emissions are positive definite quantities that are commonly distributed log-normally. The Gaussian assumption underlying ensemble assimilation methods and clamping can cause problematic results.
- ✔ When a log-normal transform for chemistry variables, it is necessary to generate the spread after the log-normal transform. Similarly, the inflation needs to be evaluated/applied after the transform.
- ✔ Dynamic emissions estimation improves forecast skill and predictability.

Lessons Learned from 10 Years with WRF-Chem/DART cont.

- ✔ Assimilation of profile retrievals as opposed to column retrievals, and joint assimilation of satellite retrievals with surface *in situ* measurements improve forecast skill.

- ✔ The advent of geostationary platforms like GEMS, TEMPO, Sentinel-4, and GeoXO will revolutionize the volume of atmospheric composition observations. To account for the large volume of observations, use more of the observations, reduce the number unrepresentative observations during transition periods, it will be necessary to:
  - Reduce the number of observations to be assimilated. Thinning is preferred over super-obbing because the later can introduce bias; and
  - Use smaller cycling periods and observation windows.

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Future Plans

Ongoing and Proposed Applications

- ✔ NOAA/CSL, NASA/ARC, and CU Boulder/Mec-E are collaborating on COVID OSSEs top demonstrate that assimilation of synthetic TEMPO NO_2 tropospheric column retrievals can recover the COVID period emissions from 'business as usual' (BAU) emissions more accurately and more quickly than assimilation of synthetic TROPOMI NO_2 tropospheric column retrievals. We are extending this to assimilation of actual TEMPO and TROPOMI retrievals and comparison of results from: (i) no log transform, (ii) log transform, and (iii) a non-Gaussian form to the EAKF (EAKF-NG).
- ✔ Under a NASA ROSES ACMAP funded project, we are preparing a 20-year Tropospheric Atmospheric Composition and Emissions Reanalysis 2005 - 2024 (TRACER-I) as a regional complement to NASA/JPL's Tropospheric Chemistry Reanalysis II (TCR II).
- ✔ NOAA/CSL, NASA/ARC, and CU Boulder/Mec-E are collaborating on a FIREX-AQ Williams Flat fire OSSE to study the recover of wildfire emissions from assimilation of satellite retrievals. This project is funded in part by a NOAA C4 grant.
- ✔ NOAA/CSL, NASA/ARC, and CU Boulder/Mec-E are also collaborating on a greenhouse gas (GHG) OSSE over Los Angeles.