WRF-Chem/DART - A Regional Chemical Transport/ Ensemble Kalman Filter Data Assimilation System

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1. WRF-Chem/DART: An Introduction

WRF-Chem/DART is a community resource for real time chemical weather data assimilation/forecast research. It couples the Weather Research and Forecasting model (WRF) with online chemistry (WRF-Chem) and the Data Assimilation Research Testbed (DART). DART has been modified to include assimilation of *in situ* and remote/satellite observations of atmospheric composition. Specifically, WRF-Chem/DART assimilates:

- MOPITT and IASI total and partial column CO;
- IASI total and partial column O_3 (under development);
- OMI total column NO_2 (under testing); and
- MODIS AOD retrievals (under testing);
- AirNOW *in situ* observations (under testing);
- State variables localization;
- Constraining emissions with the State Augmentation Method (SAM); and
- Real-time scripting system;

WRF-Chem is a state-of-the-art numerical forecast model that simulates the emission, transport, mixing, and transformation of trace gases and aerosols simultaneously with meteorology. It is used for investigating regional air-quality, preparing field program analyses, and studying cloud-scale chemical interactions. WRF-Chem development is a collaborative effort between: NOAA/ESRL, DOE/PNNL, NCAR/ACOM, and various universities. It is well documented and contains an educational platform.

DART is a community resource for ensemble data assimilation research developed at NCAR/IMAGe. The Ensemble Adjustment Kalman Filter (EAKF) is DART's primary assimilation engine. DART contains other ensemble Kalman filters (EnKFs) as well as adaptive inflation, adaptive localization, and many data assimilation research utilities. DART is well documented and contains an interactive educational platform.

2. Recent Advances in WRF-Chem/DART

WRF-Chem/DART development is a collaborative effort between NCAR/ACOM, NCAR/IMAGe, and various universities. WRF-Chem/DART's recent advances include:

- Comparison of CPSR assimilation results with independent FRAPPE and IAGOS *in situ* observations and IASI CO retrievals;
- Extension of "compact phase space retrievals" (CPSRs) from assimilation of full retrieval profiles to assimilation of truncated retrieval profiles;
- Use of the the CPSR algorithm for analysis of retrieval assimilation results; and
- Quasi-realtime application of WRF-Chem/DART in FRAPPE/DiscoverAQ and PANDA.

3. CPSRs for Retrieval Partial Profiles

Mizzi et al. (2016) derived CPSRs for assimilation of full retrieval profiles, i.e., all elements of the retrieval profile, even bad observations were assimilated. Such bad observations should be discarded prior to the assimilation step to reduce: (i) computational costs; and (ii) analysis errors. Mizzi et al. (2017a) extend CPSRs to the assimilation of truncated retrieval profiles. Mizzi et al. (2017a) derive CPSRs the same way as Mizzi et al. (2016) except they discard known bad observations prior to application of the compression and diagonalization transforms. Their derivation is as follows:

The quasi-optimal form of the retrieval equation is

$$\mathbf{y_r} - (\mathbf{I} - \mathbf{A})\mathbf{y_a} - \boldsymbol{\varepsilon} = \mathbf{A}\mathbf{y_t}. \qquad (1)$$

where $\mathbf{y_r}$ is the retrieval profile (dimension n), $\mathbf{A}$ is the averaging kernel (dimension $n \times n$), $\mathbf{y_t}$ is the true atmospheric profile (unknown; dimension n), $\mathbf{I}$ is the identity matrix (dimension $n \times n$), $\mathbf{y_a}$ is the retrieval prior profile (dimension n), and $\boldsymbol{\varepsilon}$ is the measurement error in retrieval space (dimension n) with error covariance $\mathbf{E_m}$ – the measurement error covariance (dimension $n \times n$). We begin by discarding the m elements of $\mathbf{y_r}$ that are bad observations. The resulting dimension of the truncated retrieval profile $\mathbf{y_r}$ is $n - m$. We also discard the corresponding rows of $\mathbf{A}$, and the corresponding rows and columns of $\mathbf{E_m}$. The resulting dimensions are $(n - m) \times n$, and $(n - m) \times (n - m)$ respectively. Due to Mizzi et al. (2016)'s use of singular value decompositions (SVDs) for the compression and diagonalization transforms, the rest of the derivation is the unchanged. This approach reduces the computational cost of assimilating CPSRs beyond that obtained in Mizzi et al. (2016) by a factor of $(n - m)/n$.

4. Assimilation of Trace Gas Retrievals

Figure 1 based on Mizzi et al. (2016; 2017a) shows that assimilation of MOPITT CO CPSRs improves the CO forecast skill when compared to: (i) not assimilating CO observations (**Met EX**); and (ii) assimilating raw CO retrievals (**VMRR EX** and **L10VMRR EX**). Note: that VMRR denotes retrievals in volume mixing ratio (VMR) units, and L10VMRR denotes log_{10}(VMR) units.

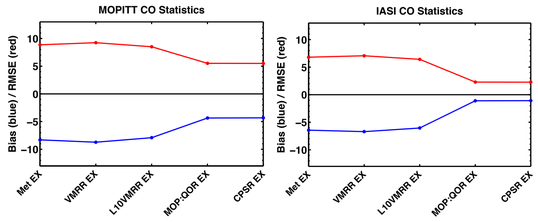

Figure 1: *Verification scores comparing CSPRs with other forward operator forms .*

Those results hold when compared against: (i) the assimilated observations (MOPITT CO - right panel); or (ii) independent observations (IASI CO - left panel). Phase space retrievals performs better than raw retrievals because the phase space transformations truncate the observation errors. **QOR EX** and **CPSR EX** perform similarly, but **CPSR EX** does so with a computational cost reduction of (∼35 %).

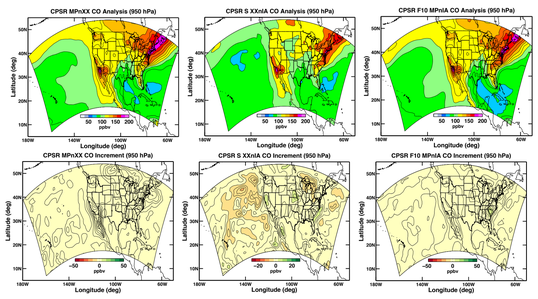

Figure 2: *Time average analyses (upper row) and increments (lower row) at 950 hPA for independent (**MPnXX**, **XXnIA**) and joint (**MPnIA**) assimilation of MOPITT and IASI CO CPSRs. The study period is June 1, 2008 00 UTC to June 10, 2008 00 UTC with cycling every 6 hrs.*

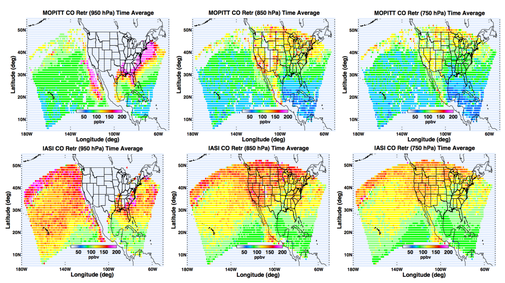

Figure 3: *Time average retrievals for MOPITT (upper row) and IASI (lower row).*

Figure 2 looks at the independent and joint assimilation of MOPITT and IASI CO CPSRs. The results from all experiments are similar, but the joint assimilation (**MPnIA**) results resemble the independent MOPITT (**MPnXX**) results more closely than the independent IASI (**XXnIA**) results due to the relative magnitude of the observation errors. Figure 3 shows the assimilated MOPITT and IASI CO retrievals at several pressure levels to account for topographic masking. Generally, the analyses and increments in Fig. 2 resemble the assimilated retrievals in Fig. 3.

Figure 4 shows vertical profiles for the same experiments. When compared against assimilated observations, Fig. 4 shows that the chemical assimilation experiments (**Chem EX**) perform better than the control experiment (**Met EX**) throughout the troposphere. When compared against independent (IASI) observations, the assimilation of MOPITT CO degrades WRF-Chem performance in the upper troposphere. That occurs because MOPITT CO may have a bias of ∼14 % above 250 hPa. That result highlights the need to remove bad observations from the retrieval profile.

Figure 5 shows results from discarding the biased MOPITT observations based on assimilation of raw retrievals (**L10VMRR-RJ3 EX**) and CPSRs (**CPSR-RJ3 EX**). The results show that: (i) both experiments behave similarly; (ii) discarding biased observations improves agreement with IASI in the upper troposphere (locally);

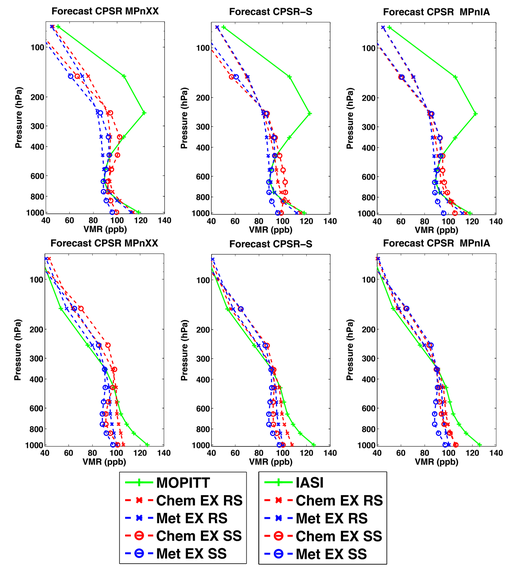

Figure 4: *Vertical profiles for independent and joint assimilation of MOPITT and IASI CO compared against MOPITT CO (upper row) and IASI CO (lower row). **RS** denotes retrieval space, and **SS** denotes state space.*

but (iii) degrades agreement in the middle and lower troposphere (remotely). Those remote impacts are troublesome and related to the non-local nature of the averaging kernel and phase space transform functions.

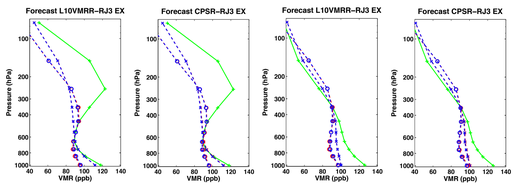

Figure 5: *Vertical profiles for experiments discarding MOPITT CO above 250 hPA compared with MOPITT CO (left two panels) and IASI CO (right two panels).*

5. Constrained Emissions

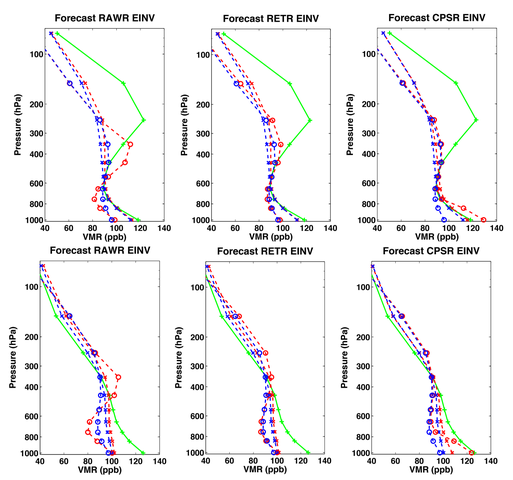

Figure 6: *Vertical profiles for experiments assimilating MOPITT CO with constrained emissions compared against MOPITT CO (upper row) and IASI CO (lower row).*

Mizzi et al. (2016) concluded that the WRF-Chem emissions are likely: (i) too high in polluted areas; (ii) too low in non-polluted areas; and (iii) the near-surface horizontal averages are dominated by the non-polluted areas. In this section we use the state augmentation method (SAM) to adjust those emissions. SAM uses ensemble cross-correlations between the expected observations and emissions to adjust the emissions during the assimilation step. Figure 6 shows results from those experiments. Generally, the constratined emissions are most sensitive to VMR retrievals (**RAWR EINV**) and CPSRs (**CPSR EINV**). Those sensitivities are present when compared to the assimilated (MOPITT) or independent (IASI) observations. The near-surface improvements are most apparent for **CPSR EINV** and are consistent with the conclusions of Mizzi et al. (2016) because there are emission: (i) reductions in polluted ares; (ii) increases in non-polluted areas; and (iii) the near-surface averages are increased.

6. Real Time WRF-Chem/DART Applied to FRAPPE

One goal of WRF-Chem/DART is issuing real time chemical weather forecasts. To that end we are collaborating with Dr. Gabriele Pfister of NCAR/ACOM to apply WRF-Chem/DART in quasi-real time to FRAPPE. For that application we use 30 ensemble members and dual-resolution cycling where: (i) ensemble data assimilation and forecasting occur on a 15 km grid; and (ii) deterministic high-resolution air quality forecasting occurs on a 3 km grid with cycling every 6 hrs and assimilation of MOPITT CO. Our FRAPPE study period is July 14, 2014 to Aug 5, 2014. Preliminary results are shown in Figs. 7 and 8.

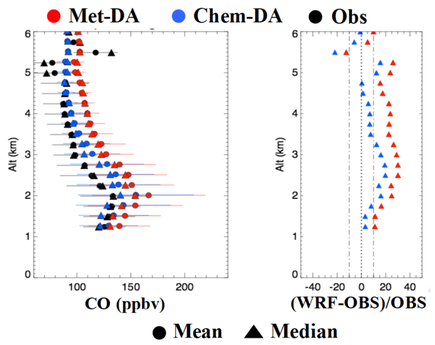

Figure 7: *Vertical profiles of CO forecast statistics based on FRAPPE in situ observations.*

Figure 7 shows vertical profiles of the mean and median on the left and relative error on the right. Both panels show that assimilating MOPITT CO (**Chem-DA**) yields significant improvements in the WRF-Chem CO forecasts compared to the control experiment (**Met-DA**).

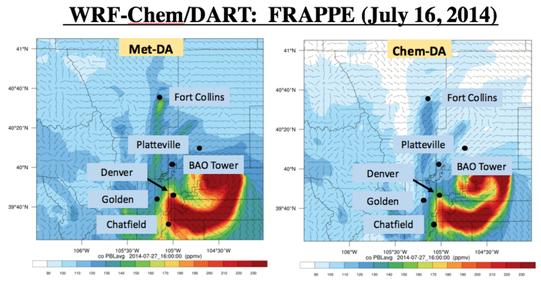

Figure 8: *Real Time WRF-Chem/DART Control (Met-DA) and Chemical Data Assimilation (Chem-DA) Fine Grid Forecasts.*

Figure 8 compares the **Met-DA** and **Chem-DA** fine grid forecasts (vertically averaged for the boundary layer). We chose this day because it shows the CO-trapping effect of the Denver Cyclone. Generally, the results are similar, but **Chem-DA** shows reduced magnitude and spatial extent for the cyclone feature. Those results are consistent with the conclusions of Mizzi et al. (2016) which suggest that the WRF-Chem emissions are too strong in polluted areas.

7. More Information

For information on using WRF-Chem/DART or on chemical data assimilation in general, contact Dr. Arthur P. Mizzi by e-mail at mizzi@ucar.edu or by phone at 303-497-8987.

8. References

Mizzi, A. P., A. F. Arellano, D. P. Edwards, J. L. Anderson, and G. G. Pfister: 2016, Assimilating compact phase space retrievals of atmospheric composition with WRF-Chem/DART: A regional chemical transport/ensemble Kalman filter data assimilation system. *Geosci. Model Dev.*, **9**, 1-14.

Mizzi, A. P., D. P. Edwards, and J. L. Anderson: 2017a, Assimilating compact phase space retrievals (CPSRs): Comparison with independent observations (MOZAIC *in situ* and IASI retrievals) and extension to truncated retrieval profiles. (*under internal review*).

Mizzi, A. P., X. Liu, A. F. Arellano, J. Liang, R. C. Cohen, Y. Chen, D. P. Edwards, and J. L. Anderson: 2017b, Assimilating compact phase space retrievals (CPSRs): Joint assimilation of MOPITT and IASI CO as CPSRs and MODIS AOD as raw retrievals with constrained emissions. (*in preparation*).