WRF-Chem/DART: Introduction, Application, Verification, and Compact Phase Space Retrievals (CPSRs)

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Boulder, CO 80301

 # NCAR/Atmospheric Chemistry Observations and Modeling Laboratory, Boulder, CO

WRF-Chem/DART: Introduction

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WRF-Chem/DART

- **WRF-Chem/DART** – a regional chemical weather forecast/ensemble data assimilation system (ensemble adjustment Kalman filter) developed by NCAR/ACOM and NCAR/IMAGe.
- **WRF-Chem** – the Weather Research and Forecasting (WRF) model with online chemistry.
- **DART** – the Data Assimilation Research Testbed (a flexible software environment for exploring different ensemble data assimilation methods, models, and observations).

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WRF-Chem/DART cont.

- **WRF-Chem/DART:**
  - ✓ Assimilates MOPITT and IASI CO total and partial column retrievals, IASI O_3 total and partial column retrievals (under development), OMI total column NO_2 retrievals, MODIS total column AOD retrievals, and AirNow and PANDA *in situ* observations.
  - ✓ Assimilates chemical species mixing ratios or log of mixing ratios.
  - ✓ Assimilates partial column retrievals as raw (RETRs), quasi-optimal (QORs), and compact phase space retrievals (CPSRs).
  - ✓ State variable localization to enable joint, independent, and specified correlation assimilation of meteorology and/or chemistry observations.
  - ✓ Uses State Augmentation Method (SAM) to obtain emission updates from assimilation of chemistry observations.

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WRF-Chem/DART cont.

- **WRF-Chem/DART:**
  - ✓ WRF-Chem/DART repository download link: https://svn-dares-dart.cgd.ucar.edu/DART/tags/wrf-chem.r11690
  - ✓ Sample input/output data:
    - Go to NCAR ftp site at ftp.ucar.edu
    - Go to ../pub/mmm/mizzi
    - Get the PANDA_REAL_TIME_DATA.tar file. This is the input data and directory structure.
    - Get the real_PANDA_RETR_VARLOC.tar file. This is the sample output data and directory structure.
  - ✓ WRF-Chem/DART Users' Guide is not available so collaboration is recommended/necessary.

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WRF-Chem/DART cont.

- **WRF-Chem/DART Applications:**
  - ✓ Being applied to 2008 Case Study (NCAR/ACOM – Mizzi, Arellano, Edwards, and Anderson); FRAPPE/Discover AQ (NCAR/ACOM – Mizzi, Pfister, and Edwards; UC-Berkley – Cohen and Liu), and PANDA (NCAR/ACOM – Mizzi, MPI-M – Brasseur and Bouarar, and Nanjing Univ. – Wang).
  - ✓ **2008 Case Study** – CONUS domain with western extension; 100 km (101x41x34) resolution; June 1 – June 30, 2008; 20-member ensemble; assimilate MOPITT and IASI CO as RETRs and CPRs and MODIS AOD as RETRs; real time scripting.
  - ✓ **FRAPPE/Discover AQ** – Western US nested domain with 15 km (180x140x37) and 3 km (321x291x37) resolutions; data assimilation on coarse grid; July 14 – August 3, 2014; 30-member ensemble; assimilate MOPITT CO as RETRs; real time scripting.

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WRF-Chem/DART cont.

- **WRF-Chem/DART cont:**
  - ✓ **KORUS AQ** –Korea/Southeast Asia nested domain with 15 km (140x140x37) and 3 km (231x231x37) resolutions; data assimilation on coarse grid; April 20 – June 14, 2016; 20-member ensemble; assimilate MOPITT CO and MODIS AOD; real time scripting.
  - ✓ **PANDA** – Central and East Asia nested domain with 60 km (150x112x37) and 20 km (148x157x37) resolutions; 10-member ensemble; assimilation on coarse grid; quasi-real time; assimilate MOPITT (development and testing).

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FRAPPE Application

(Assimilate MOPITT CO as RETRs, AirNow CO and O3 *in situ* observations, and emissions adjustment)

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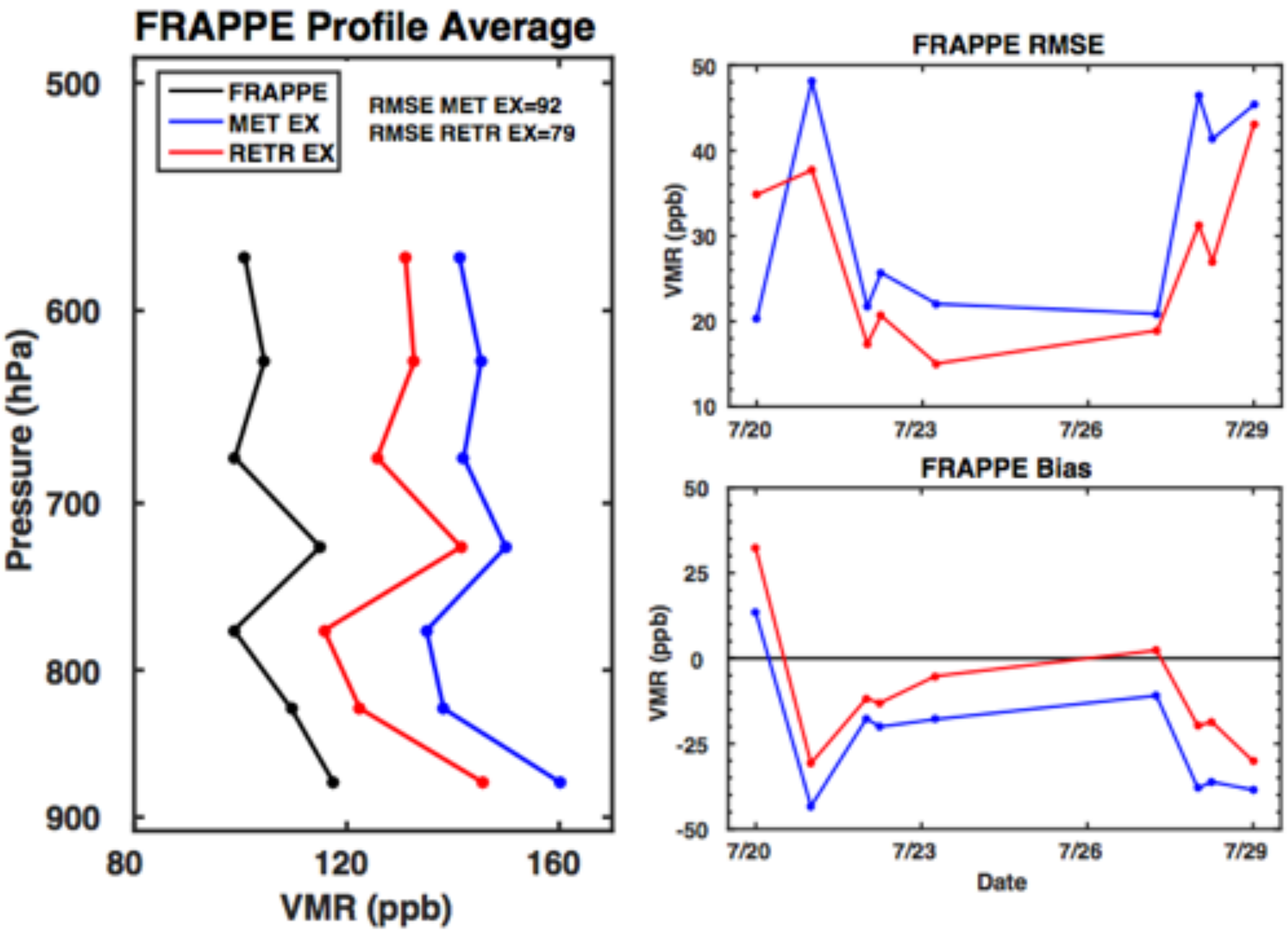
FRAPPE Application

July 2014



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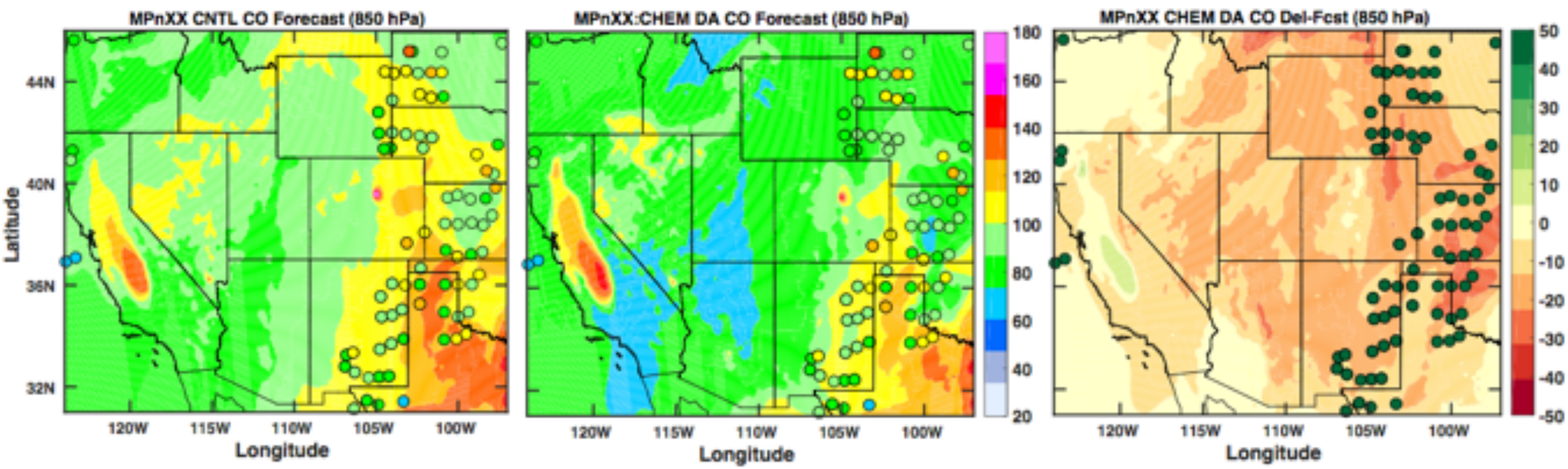
FRAPPE Application (MOPITT CO RETRs)

July 21, 2014 18 UTC



Met Ex **RETR Ex** **Met Ex – RETR Ex**

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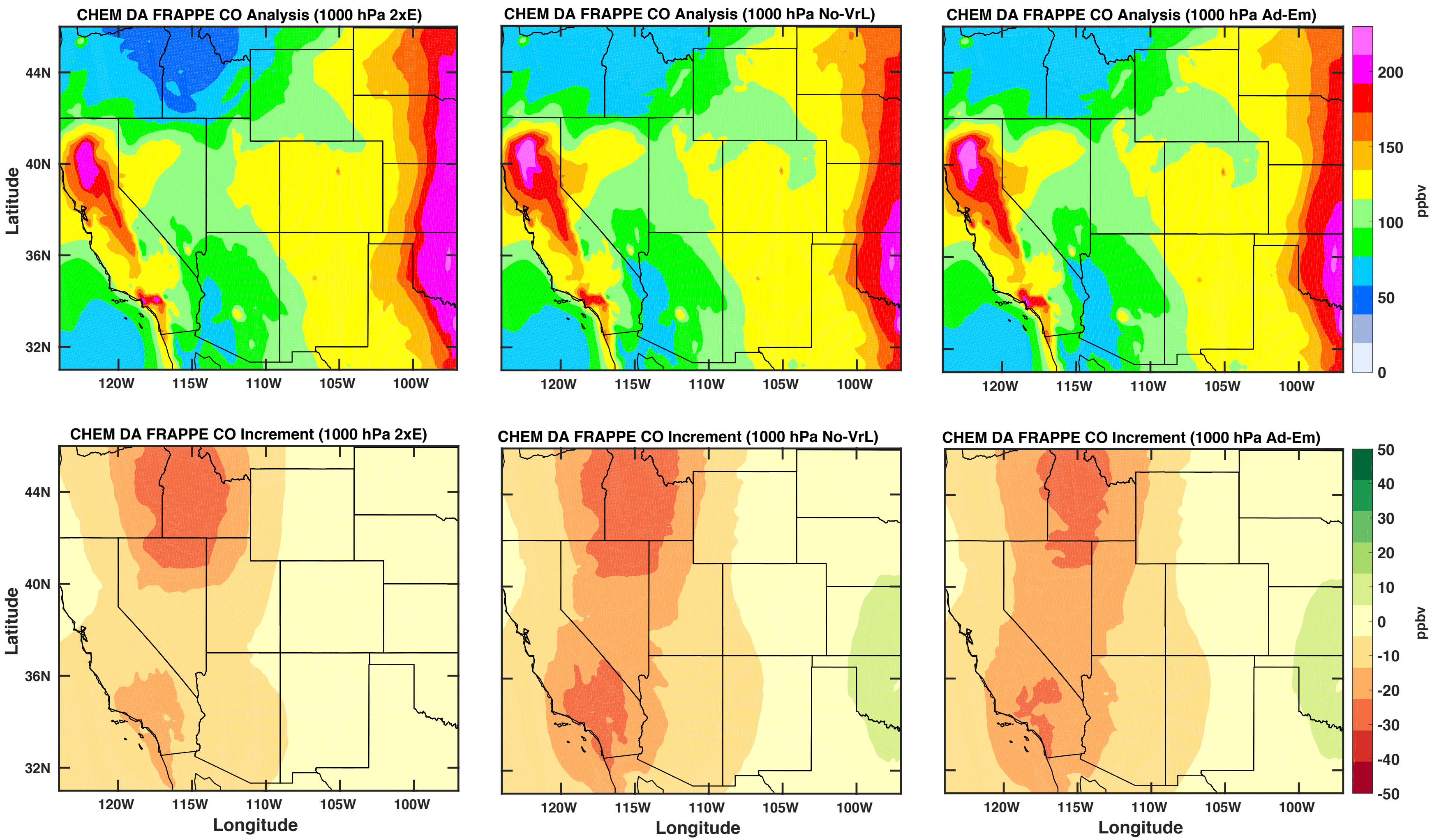
FRAPPE Application (MOPITT CO RETRs)

July 20, 2014 18 UTC



RETR Ex　　No State Variable Loc　　No Loc and Adj Emiss

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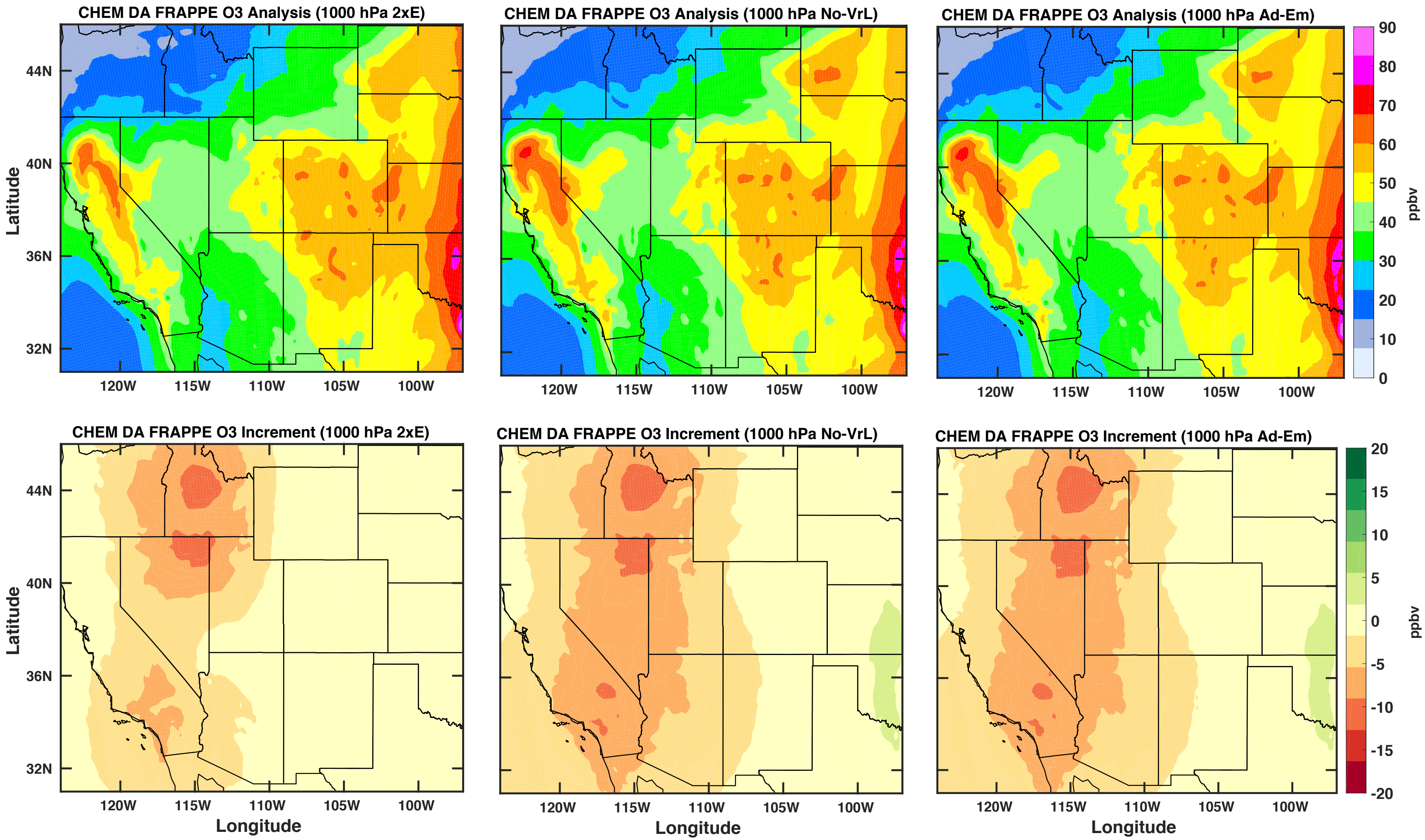
FRAPPE (MOPITT CO RETRs)

July 20, 2014 18 UTC



RETR Ex | **No State Variable Loc** | **No Loc and Adj Emiss**

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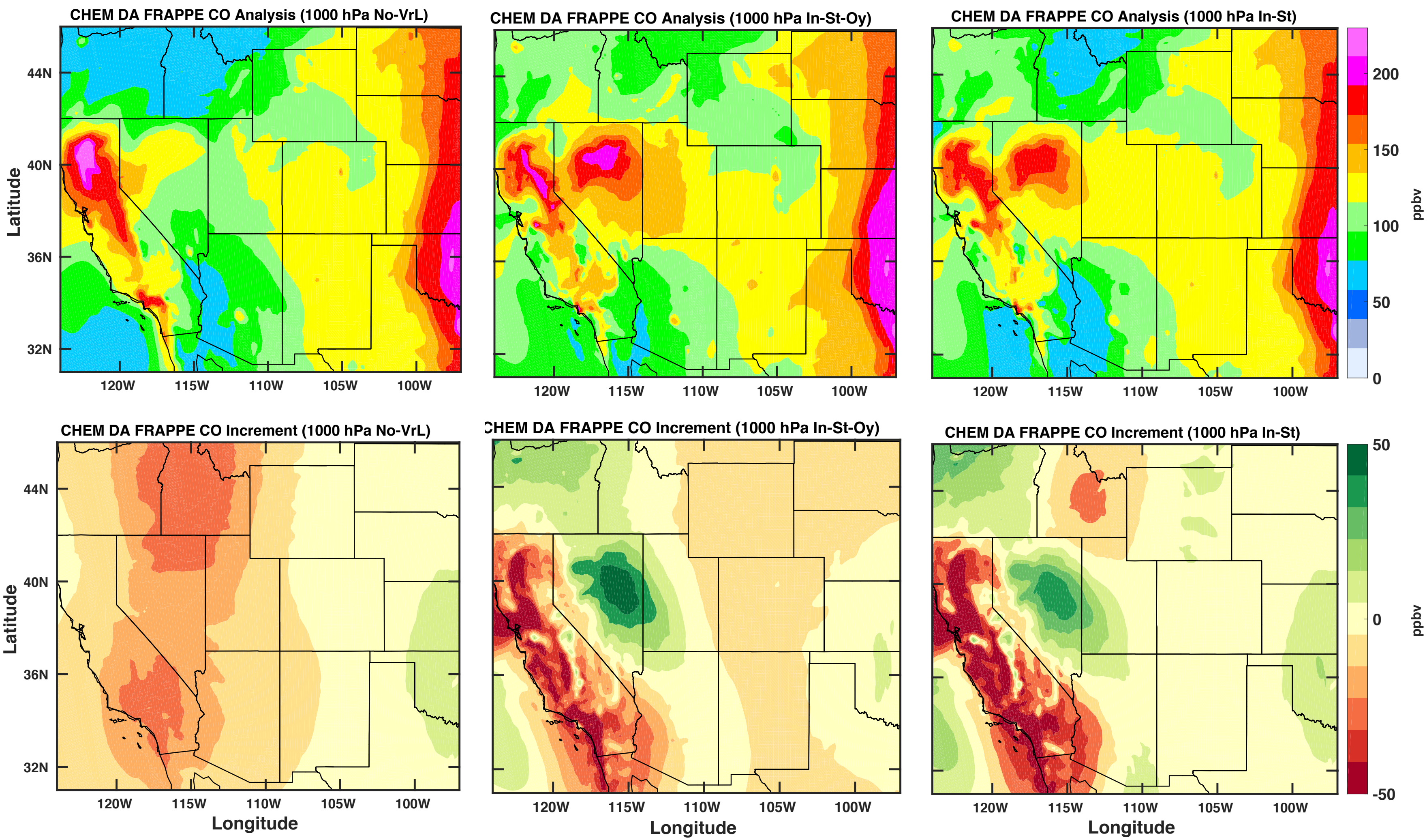
FRAPPE (MOPITT CO and AirNow CO, O3)

July 20, 2014 18 UTC



No State Variable Loc | **In Situ** | **No Loc and In Situ**

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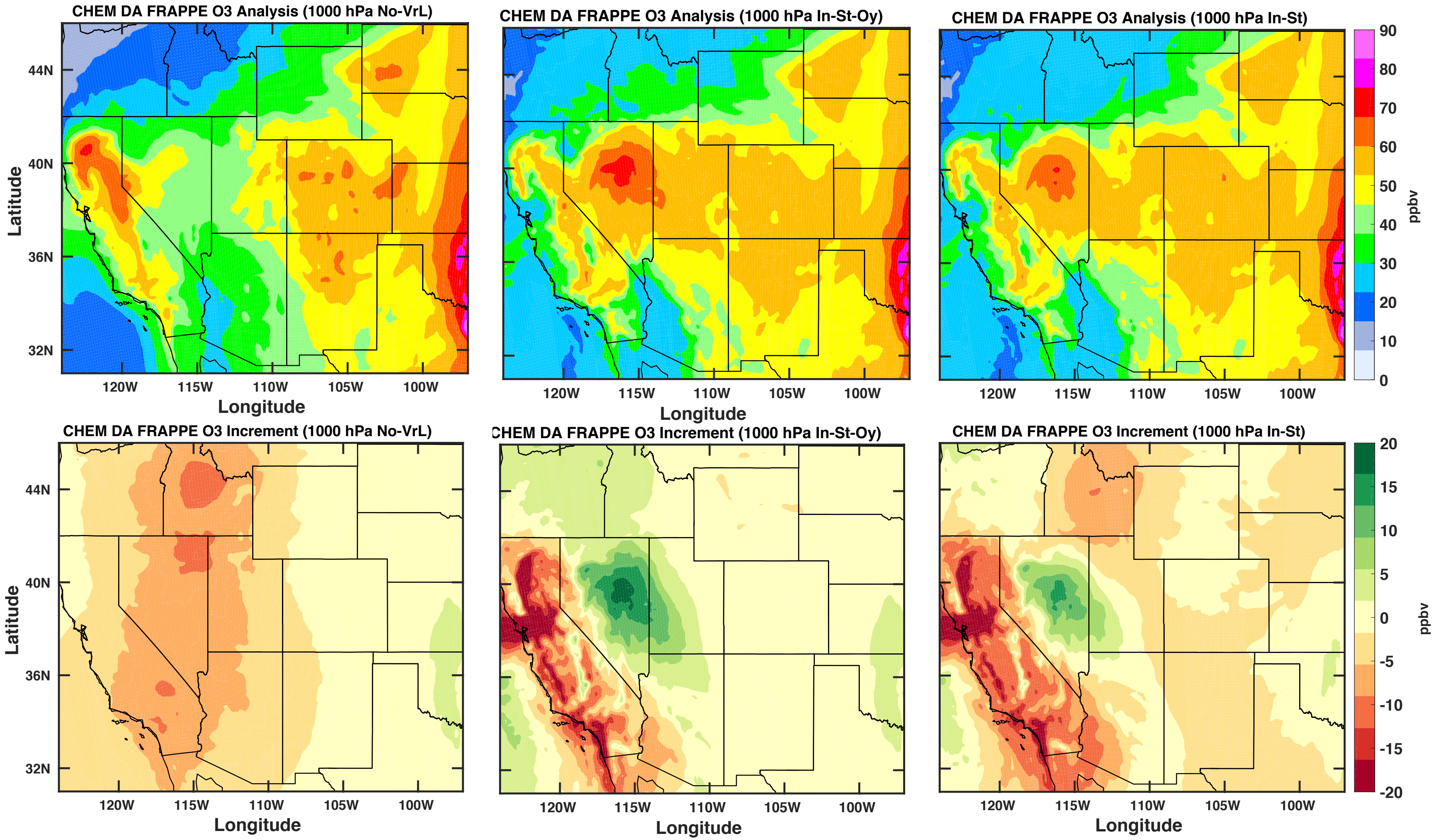
FRAPPE (MOPITT CO and AirNow CO, O3)

July 20, 2014 18 UTC



No State Variable Loc In Situ No Loc and In Situ

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KORUS Application
(Assimilate MOPITT CO and MODIS AOD)

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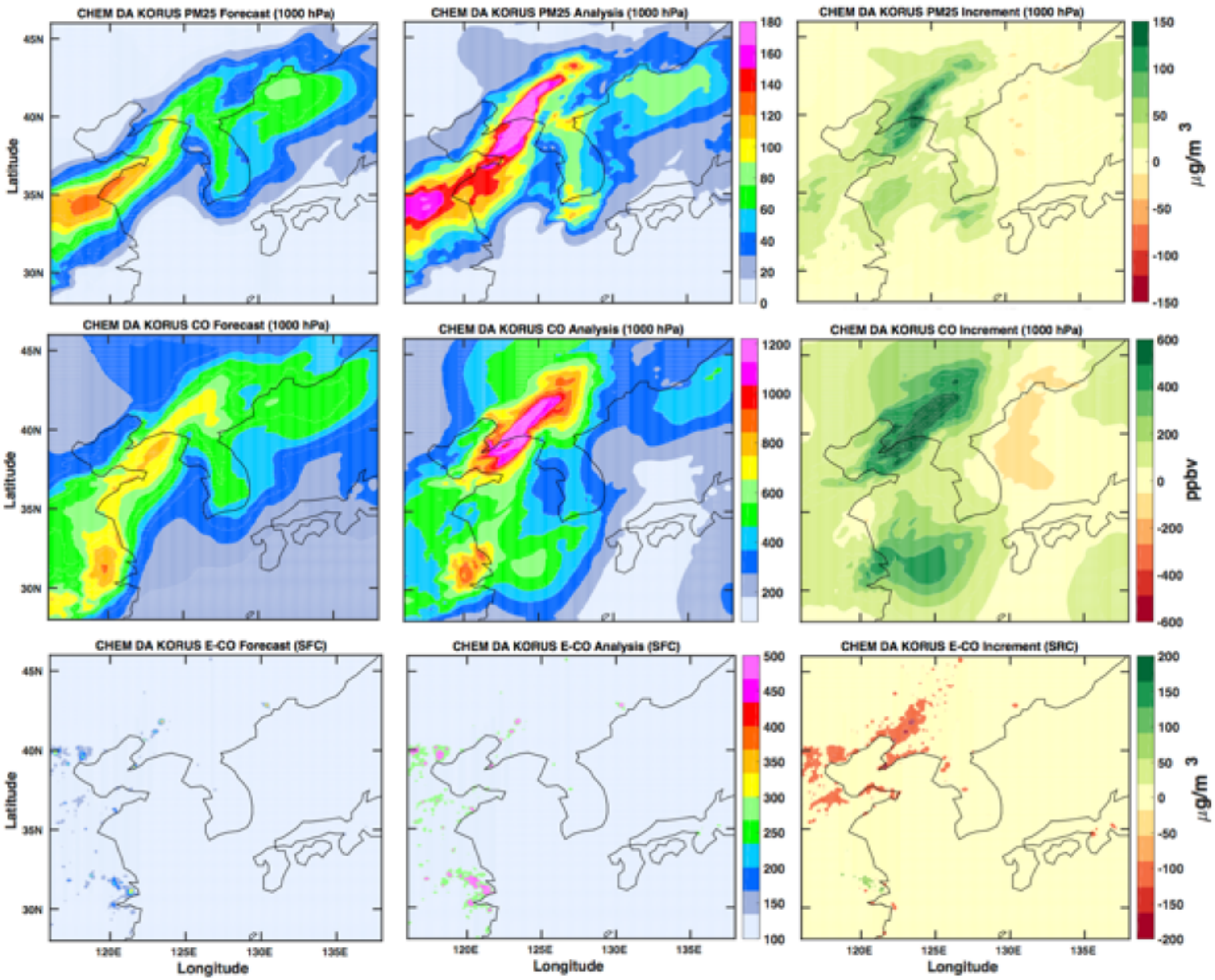
KORUS (MODIS AOD)

May 25, 2016 06 UTC



Assimilated species

Interspecies adjustment

Emissions adjustment

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Compact Phase Space Retrievals (CPRS): Full Retrieval Profiles

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CPSRs: Full Retrieval Profiles

- $y_r = A y_t + (I - A) y_a + \varepsilon \Rightarrow y_r - (I - A) y_a - \varepsilon = A y_t$ where A is singular and its leading left singular vectors span its range.
- Project the quasi-optimal retrieval onto the leading left singular vectors of A: data compression step.
- 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): diagonalization step.
- 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:

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

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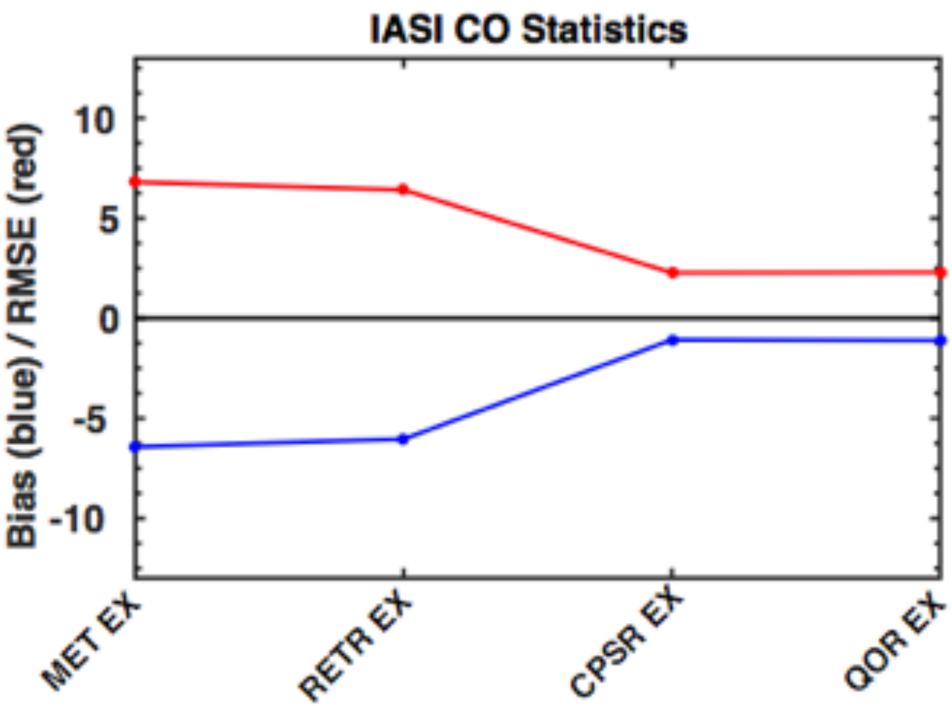
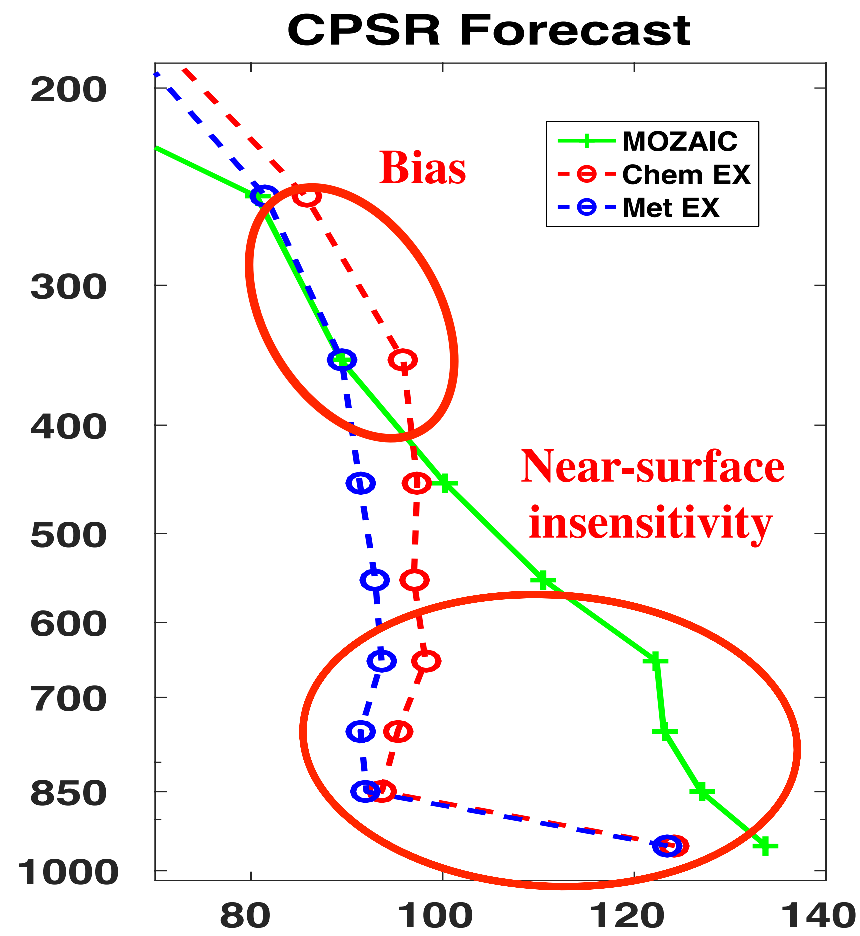
18

2008 Case Study: Forecast Verification





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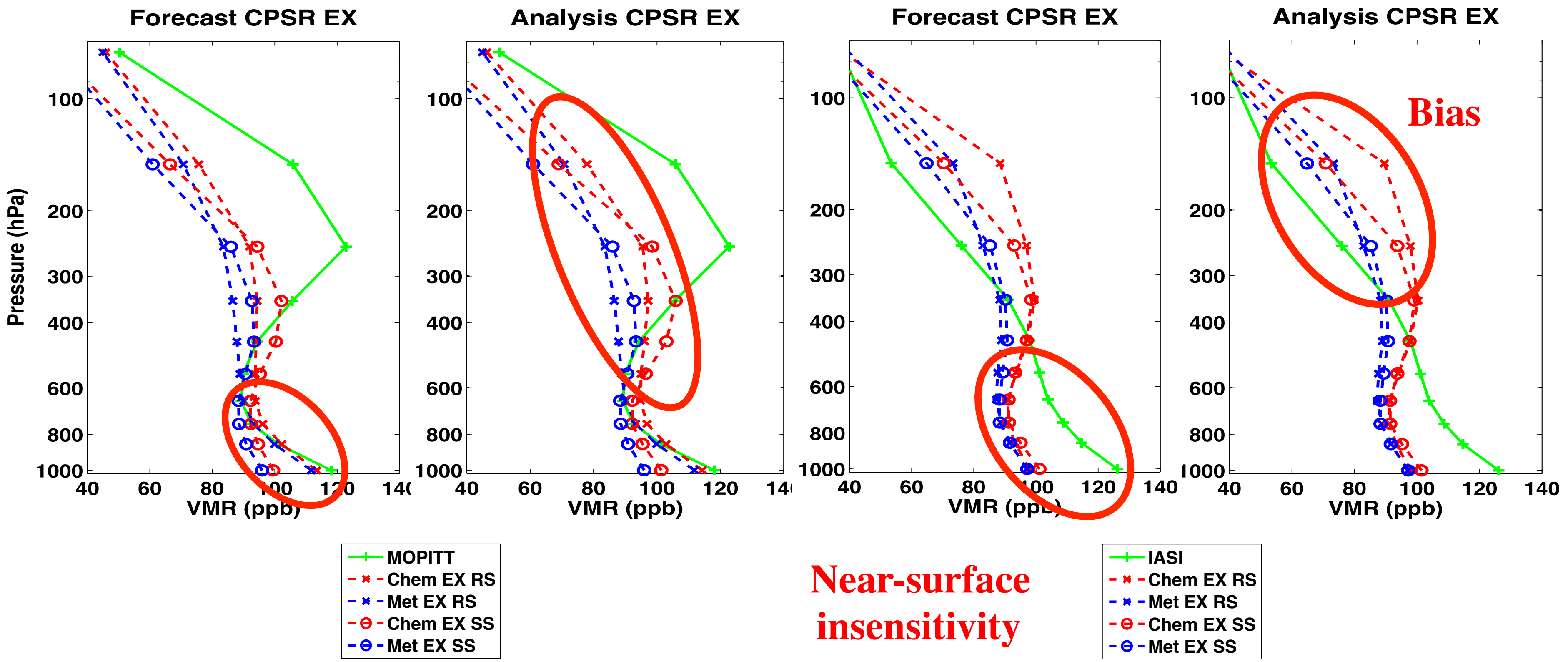
Vertical Profiles (Full Retrieval Profiles)



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Why do CPSRs loose near-surface sensitivity?

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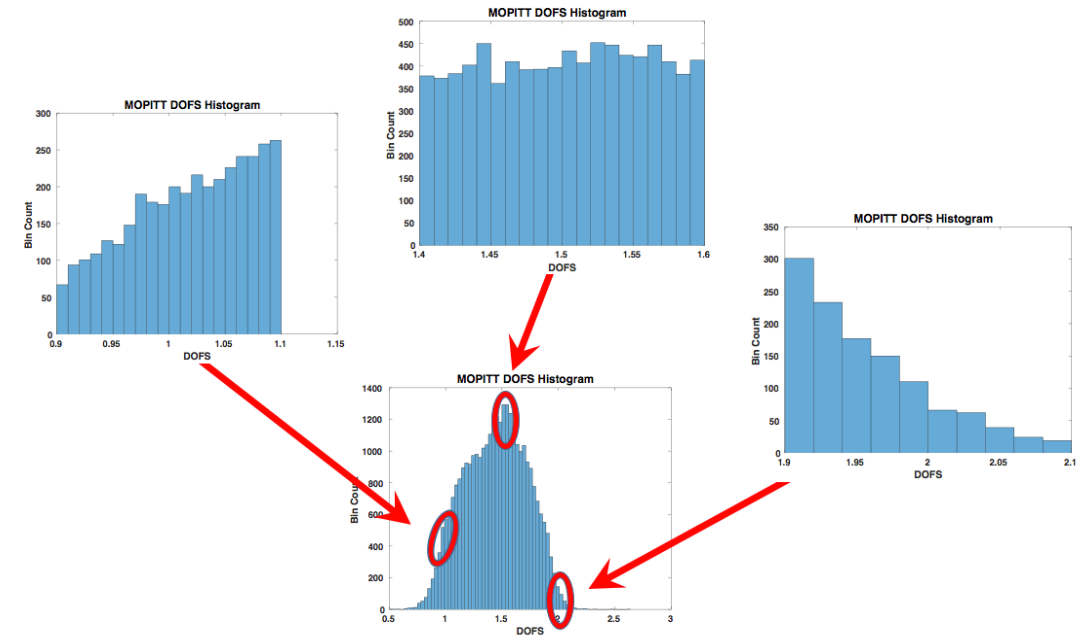
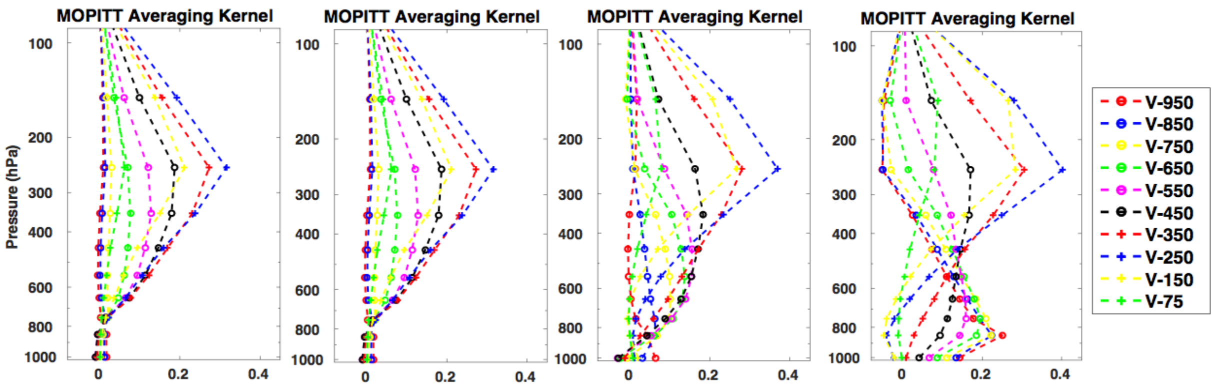
Dependence on DOFs

MOPITT DOFS Histograms





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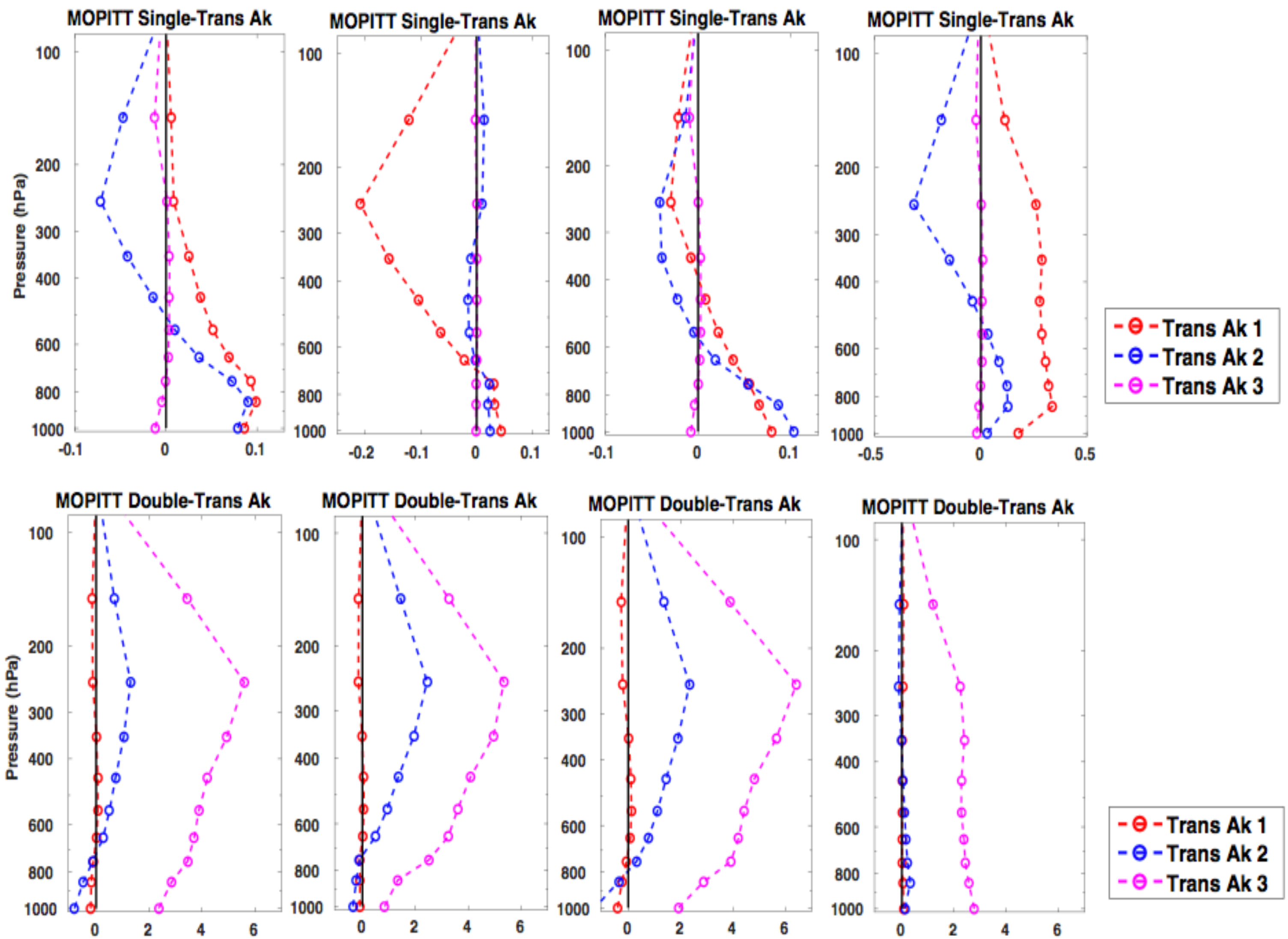
Dependence on DOFS



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Summary and Conclusions

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Summary and Conclusions

- Presented an introduction to and summary of the current status of WRF-Chem/DART - a regional, quasi-real-time chemical weather forecast/ensemble data assimilation system.

- Present results from the application of WRF-Chem/DART to: (i) 2008 Case Study, (ii) FRAPPE/Discover AQ, and (iii) KORUS AQ. Those results show that:

  - Assimilation of CO RETRs improved analysis fit and forecast skill when compared to not assimilating chemistry observations when compared to independent observations (*in situ* and retrievals)

  - Assimilation of CO CPSRs improved fit/skill when compared to assimilating CO RETRs at reduced computational costs when compared to independent observations (*in situ* and retrievals).

  - When we allowed interspecies adjustments (assimilation of observed chemical species adjusted unobserved chemical species) and turned off state variable localization (meteorological observations adjusted chemical species and vice versa) we obtained reasonable/consistent analyses and increments (not verified).

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Summary and Conclusions cont.

- When we turned on emissions adjustments we found reasonable/consistent adjustments to the analyses (not verified).

- Introduced/discussed ”compact phase space retrievals” (CPSRs) as applied to full and truncated partial-column retrieval profiles.
- Used an analysis of the compressed and rotated averaging kernels to explain why the assimilation of MOPITT CO showed little-to-no adjustment in the lower troposphere for CPSRs in the 2008 Case Study.

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References

- Mizzi, A. P., A. F. Arellano, D. P. Edwards, J.L. Anderson, and G. G. Pfister: 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, 2016.
- Mizzi, A. P., D. P. Edwards, and J. L. Anderson: Assimilating compact phase space retrievals (CPSRs): Comparison with independent observations (MOZAIC in situ and IASI retrievals) and extension to assimilation of retrieval partial profiles. [*under internal review*], 2017a.
- Mizzi, A. P., X. Liu, A. F. Arellano, J. Liang, R. C. Cohen, Y. Chen, D. P. Edwards, and J. L. Anderson: 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*], 2017b.

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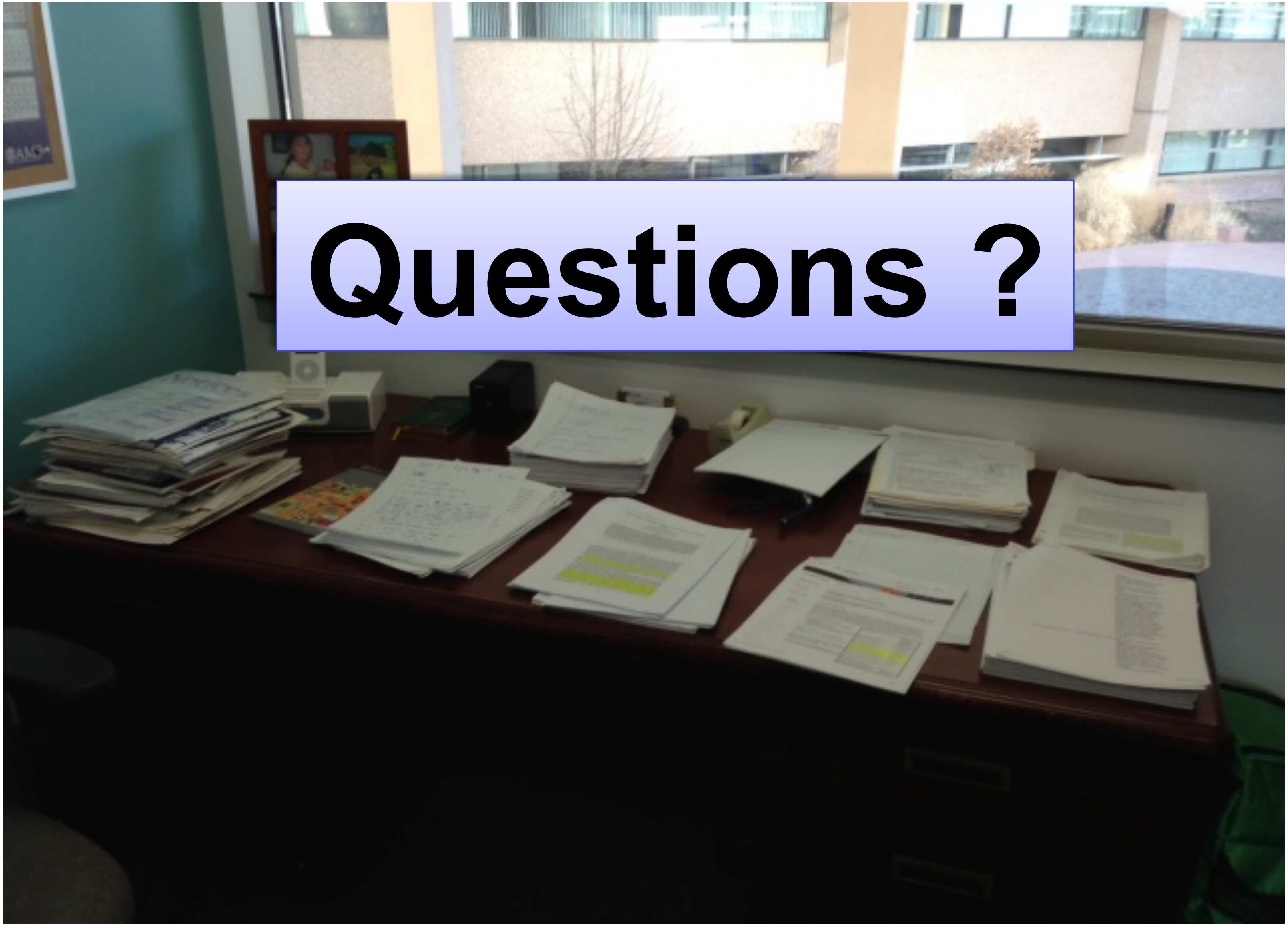

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Addressing the Bias: Extension of Compact Phase Space Retrievals (CPRS): Truncated Retrieval Profiles

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CPSRs: Extension to Truncated Retrieval Profiles

- Mizzi et al. (2017a):

$$y\downarrow r - (I - A) y\downarrow a - \epsilon = A y\downarrow t$$

  - ✓ Discard m elements of y_r. The resulting dimension is $n-m$.
  - ✓ Discard the corresponding rows of A, and the corresponding rows and columns of E_m (resulting dimension $(n-m)\times(n-m)$).
  - ✓ A was a square $n\times n$ matrix. It is now a rectangular $(n-m)\times n$ matrix. Thus, assimilation of retrieval partial profiles is called "CPSRs applied to rectangular systems."
  - ✓ The rest of the derivation follows Mizzi et al. (2016) due to their use of SVDs for the "compression" and "diagonalization" transformations.

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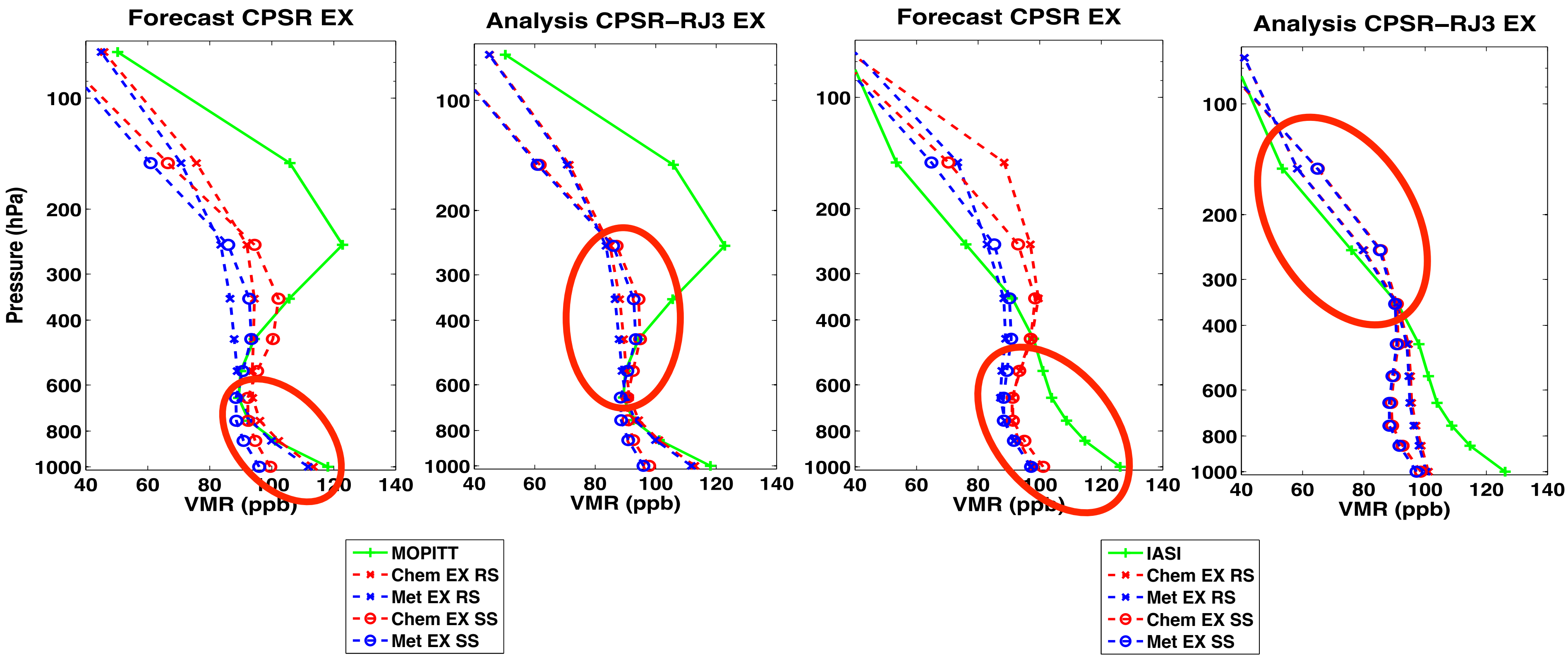
Vertical Profiles (Truncated Retrieval Profiles)



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