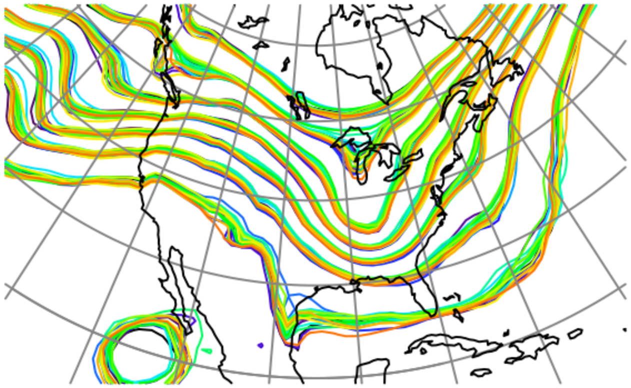

A Unified DART Ensemble Data Assimilation Capability for CAM(-CHEM), WACCM, and WACCM-X

Kevin Raeder, for
DART: Jeff Anderson, Tim Hoar, Nancy Collins, Johnny Hendricks
CSEG: Alice Bertini, Mariana Vertenstein, Steve Goldhaber, Jim Edwards
And: Nick Pedatella (HAO), Benjamin Gaubert (ACOM),
Raffaele Montuoro (CIRES, TAMU).

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Outline

1) Context
2) Motivation and Examples of Tools
3) Examples from WACCMX and CAM-Chem
4) Summary

1) Goal

Make Data Assimilation Research Testbed (DART) tools immediately usable in the development and evaluation of CAM-based models, and in process studies.

DART = Ensemble Kalman Filter
= CAM ensemble forecasts
+ Bayesian statistical correction by observations

Strategy

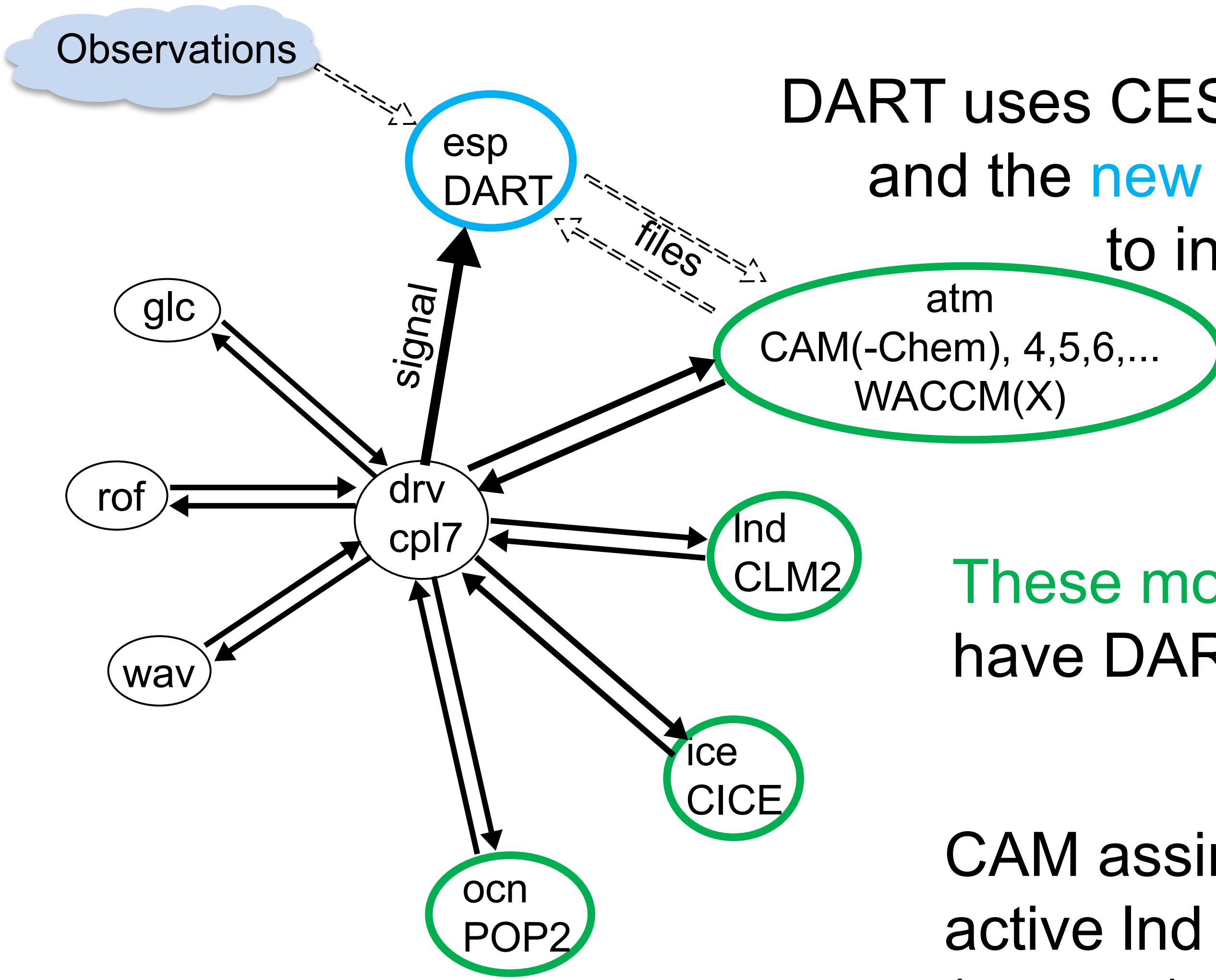
- ✓ Merged DART SourceMods into the CESM trunk.
- ✓ Adopted CESM file naming convention for CAM+DART output.
- ✓ Developed pre-tag testing of β versions of CESM2-CAM-FV, focused on features needed by DART.

Result

Eliminated the post-tag steps of updating, verifying (and often fixing) the interface between CESM and DART.

When a tag is released, it should be usable with DART

DART⟺ CESM



DART uses CESM infrastructure and the new ESP component to interface to model components.

These models have DART interfaces

CAM assimilations have active lnd and ice (not ocn) components

DART Uses New and Old CESM capabilities

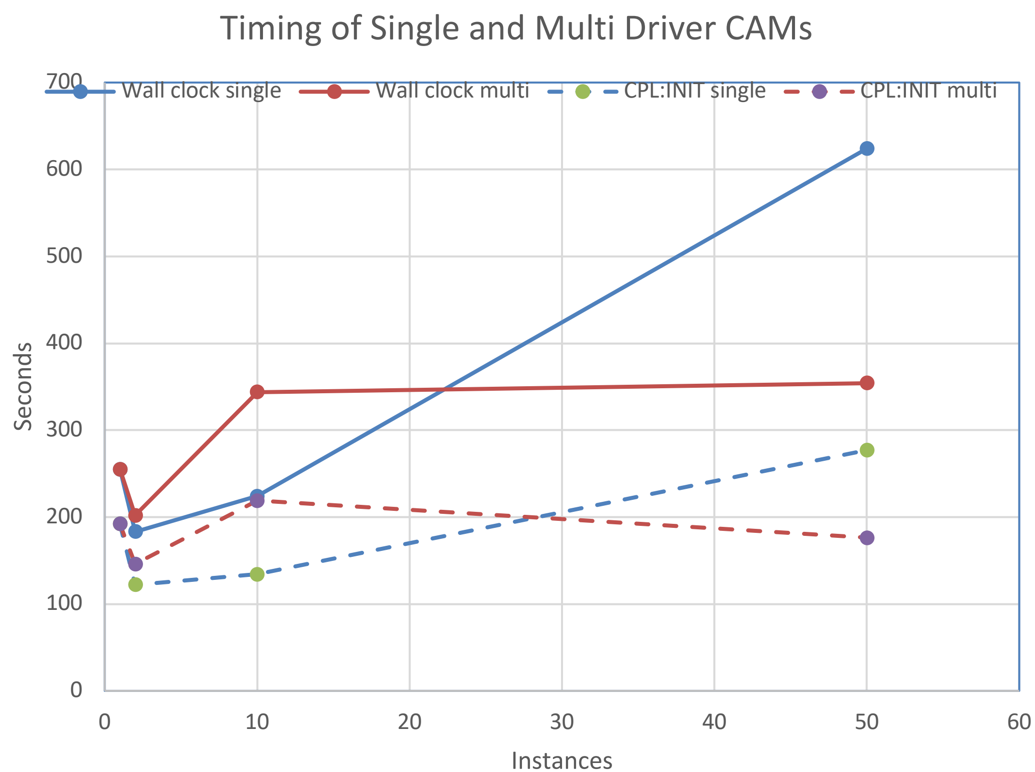
- Multi instance (ensemble forecasts)
- Multi driver (Montuoro)
- Multi component
- Pause-resume (first version)
- st_archive and naming convention accommodates DART

Multi-instance CAM wallclock

drv = 1

drv = # instances

nodes/instance = constant



2) Examples of Model Evaluation Tools

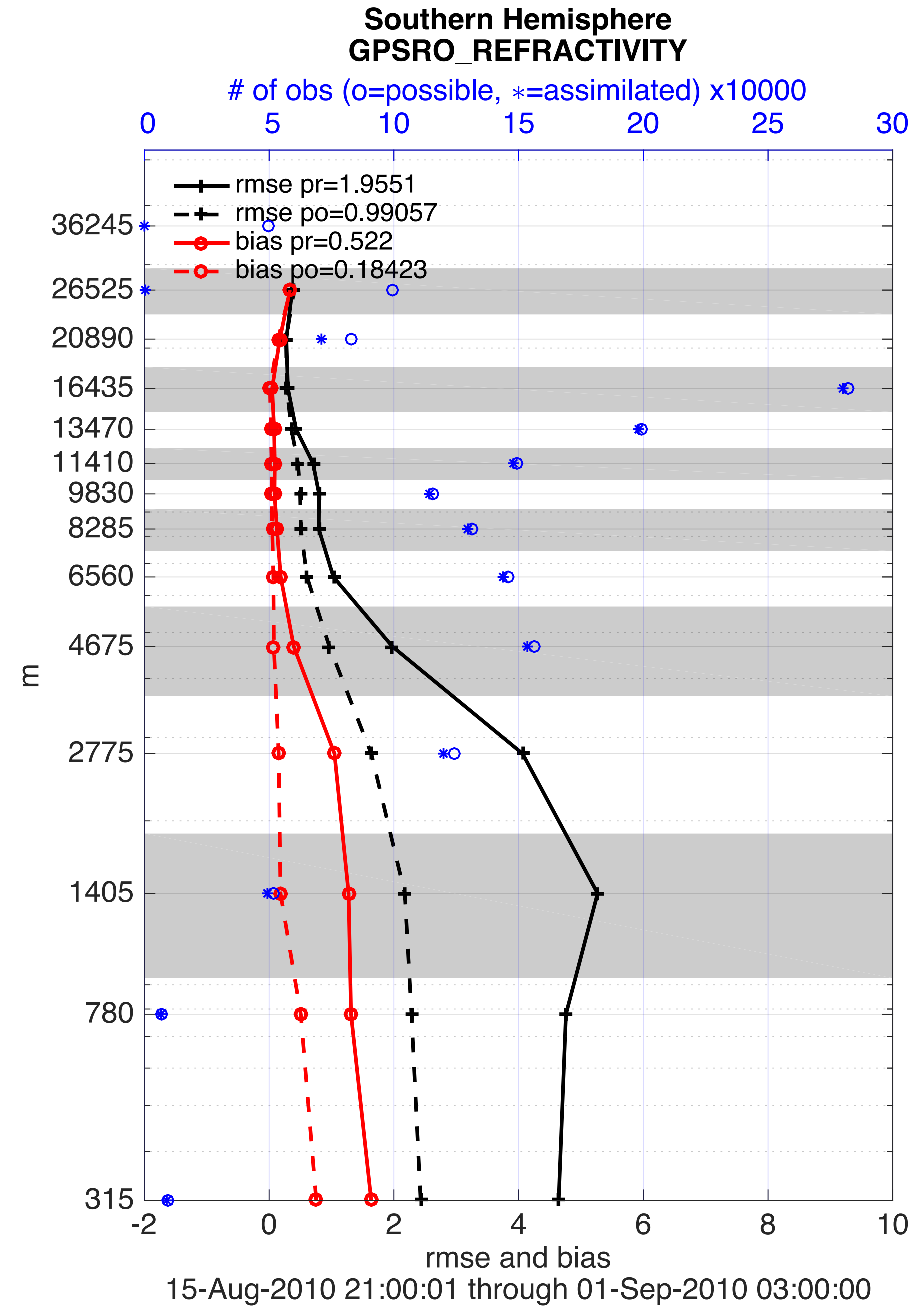
Evaluate CAM State in "Observation Space"

Use CAM state to generate an estimate of an observation.
E.g. interpolate the T field to the location of a thermometer.
Or 10^6 thermometers . . .

T measurement may, or may not,
have been used in the assimilation.

"Obs Space" Profile

Calculate index of refractivity from CAM's T, Q, ... and compare against COSMIC GPS measurements.



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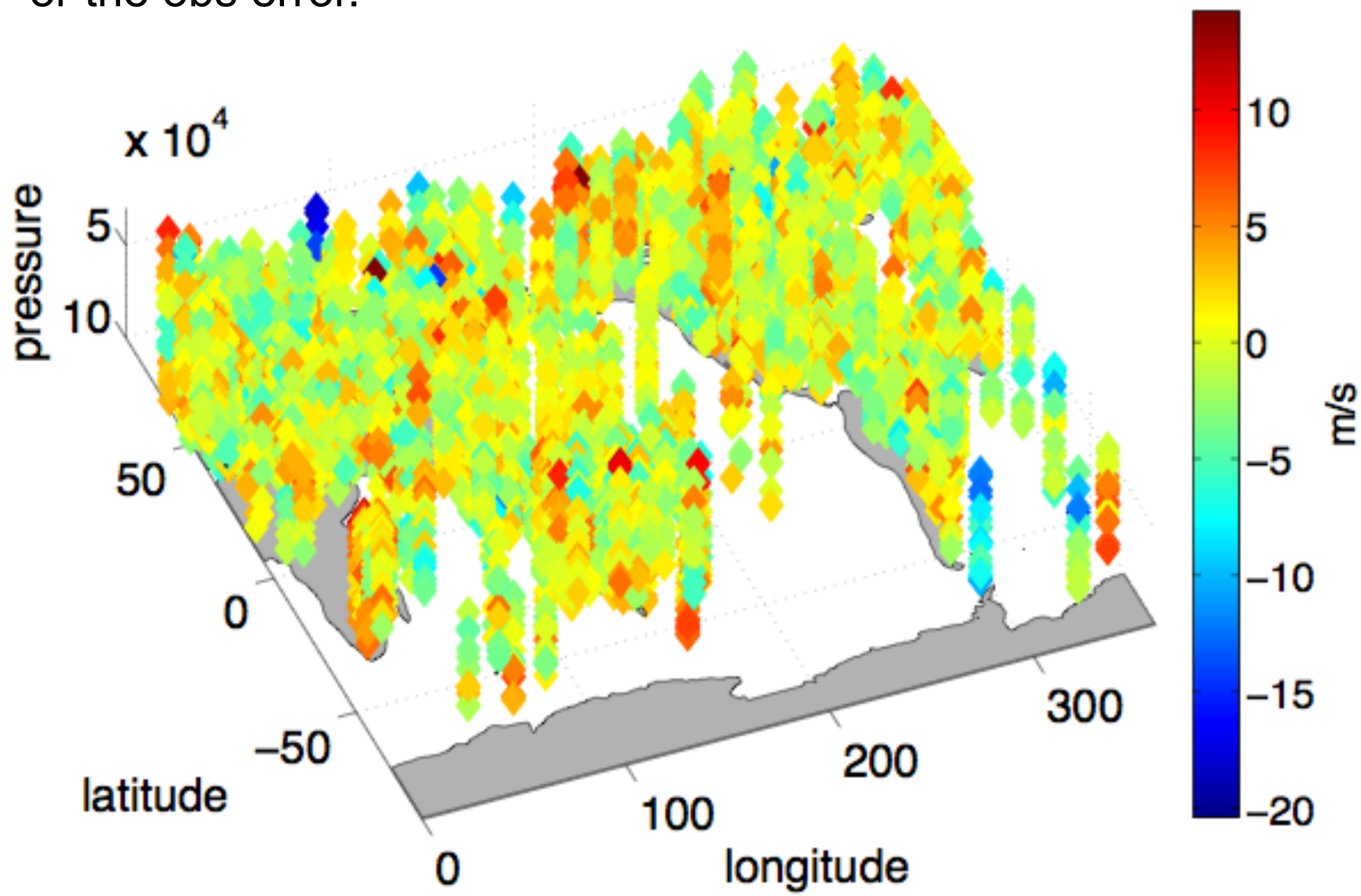
Model Biases at Observation Locations

- Matlab script generates the model bias at each obs location, here U from radiosondes.
- Bias can be absolute units, or normalized by the obs value, or the obs error.



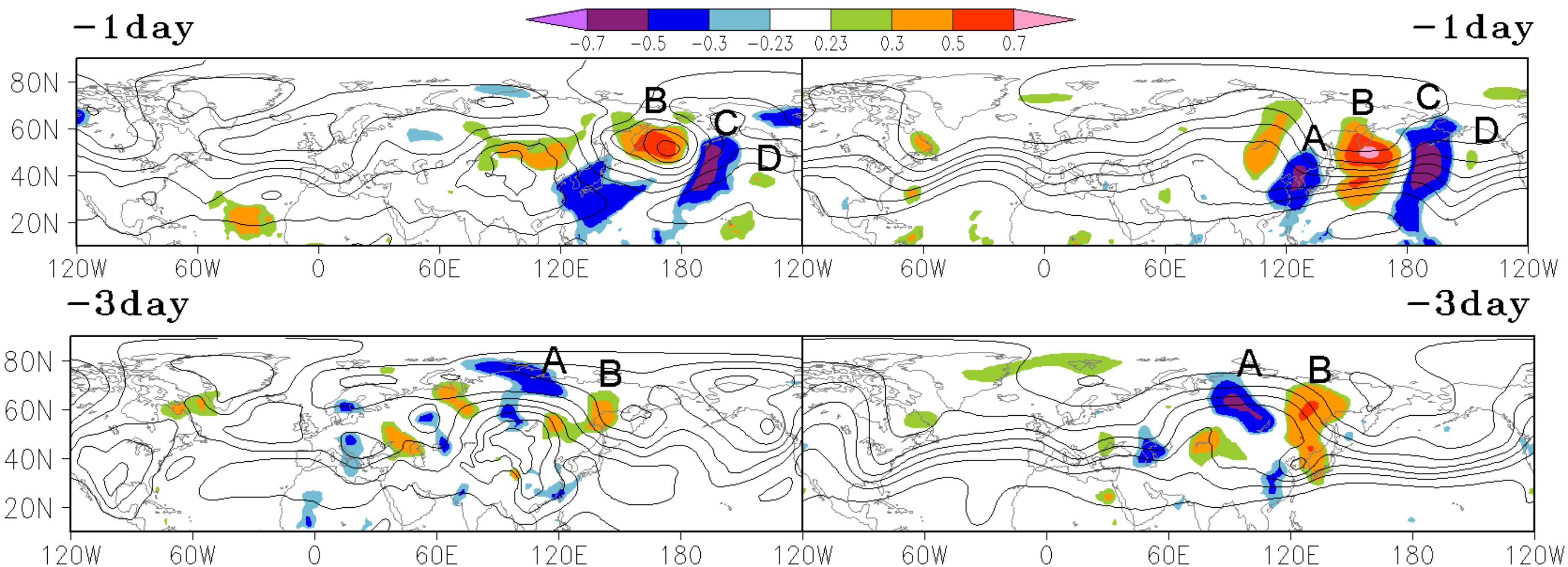
Ensemble-based Sensitivity Studies

Chang, et al. 2012, Medium Range Ensemble Sensitivity Analysis of Two Extreme Pacific Extratropical Cyclones

$$"sensitivity" = \frac{\mathrm{cov}(\mathbf{J_M}, \mathbf{x_{iM}})}{\sqrt{\mathrm{var}(\mathbf{x_{iM}})}\sqrt{\mathrm{var}(\mathbf{J_M})}}$$ = correlation

$\mathbf{J_M}$=cyclone minimum pressure at a chosen time

$\mathbf{x_{iM}}$= Sea Level Pressure $\mathbf{x_{iM}}$= 300 hPa Z



3) Example of Model Evaluation and Process Study with WACCMX

Analysis and Hindcast Experiments of the 2009 Sudden Stratospheric Warming in WACCMX+DART

N. M. Pedatella, H.-L Liu, D. R. Marsh, K. Raeder, J. L. Anderson, J. L. Chau, L. P. Goncharenko, and T. A. Siddiqui

Journal of Geophysical Research - Space Physics

WACCMX+DART analysis fields reproduce the middle and upper atmosphere variability during the 2009 major sudden stratospheric warming (SSW) event better than the specified dynamics WACCMX.
This leads to WACCMX+DART better representing the downward transport of chemical species from the mesosphere into the stratosphere following the SSW.

WACCMX Overview

WACCMX 2.0 = union of WACCM 4.0 and TIE-GCM. *Liu et al.* [2017]
Chemical, dynamical, and physical processes necessary to model the troposphere, stratosphere, mesosphere, thermosphere and ionosphere.

126 vertical levels, from the surface to 4.1×10^{-10} hPa (~500-700 km).
Varying vertical resolution of roughly 1.1-3.5 km in the lower atmosphere, 0.25 scale height above 0.96 hPa (~50 km).

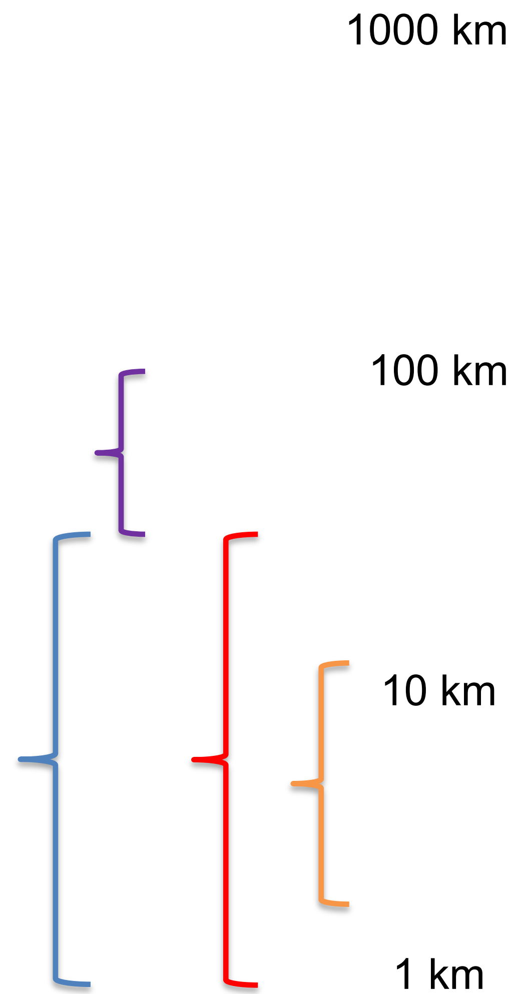
Forced with realistic solar and geomagnetic conditions:

- Geomagnetic activity = the Heelis empirical convection pattern [*Heelis et al.*, 1982], driven by the three hour geomagnetic K_p index, at high-latitudes.
- Solar irradiance using the models of *Lean et al.* [2005] and *Solomon and Qian* [2005].
- Added forcing of the migrating semidiurnal lunar tide (M 2) based on *Pedatella et al.* [2012].
- Historical Greenhouse gases and ozone depleting substances.

Assimilation Overview

DART is used to constrain the lower and middle atmosphere variability:
The WACCMX ionosphere is not directly constrained by observations.
It is responding to forcing from the constrained lower atmosphere, as well as solar forcing.

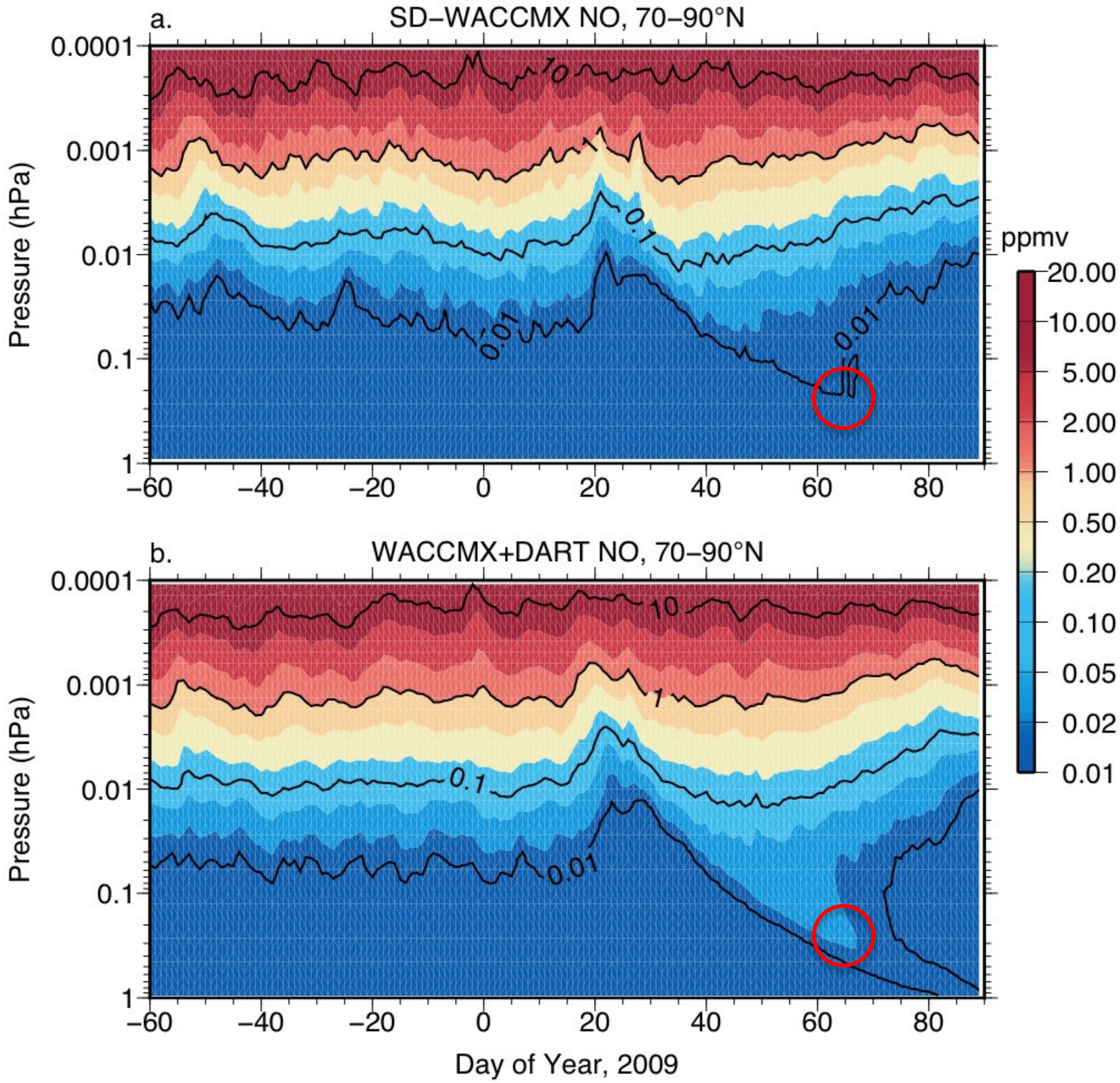
- ✓ Aircraft and radiosonde temperatures and winds,
- ✓ Satellite drift winds,
- ✓ Constellation Observing System for Meteorology, Ionosphere, and Climate (COSMIC) refractivity,
- ✓ Temperatures from Aura Microwave Limb Sounder (MLS) and Thermosphere Ionosphere Mesosphere Energetics Dynamics (TIMED) satellite Sounding of the Atmosphere using Broadband Emission Radiometry (SABER).



The MLS and SABER temperatures are assimilated up to $1 \times 10-3$ hPa (~95 km) and $5 \times 10-4$ hPa (~100 km), respectively.

Zonal mean nitric oxide (NO) during November 2008-March 2009 averaged between 70-90∘N in (a) SD-WACCMX and (b) WACCMX+DART.

SD NO < 0.01
DART NO > 0.02



Ongoing Investigation

This improved downward transport of NO may still be an underestimate.
The remaining NO deficit may be from:

- still underestimating the downward transport,
- errors in chemical reaction rates,
- the precipitating auroral electrons have a fixed characteristic energy of 2 keV,
- the pattern of precipitation is highly idealized,
- no production of NOx by medium energy (up to 1 MeV) electrons in the mesosphere.

Improving the characterization of these processes is the subject of ongoing research.

Increments added to the model state by assimilation generate small scale waves,
-> spurious mixing, reduction of O/N_2 and e^- density.
But damping waves reduces tides, which are already too weak.
Ongoing research to find the best solution, if they are actually spurious.

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3) Example of Model Development and a Process Study with CAM-Chem

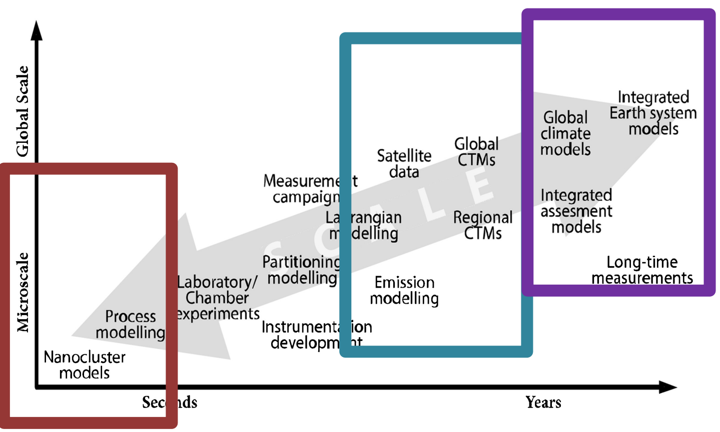
Chemical Weather Feedback on Chemical Climate

bridging the scales using Data Assimilation and CESM

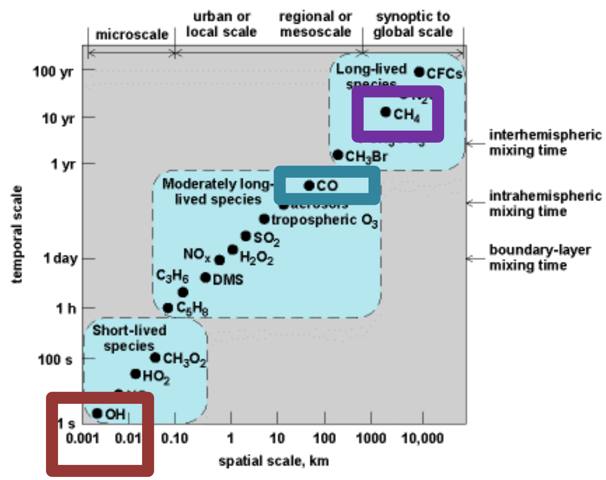
Benjamin Gaubert & many co-authors
Atmospheric Chemistry Observations & Modeling Laboratory (ACOM)

CH_4-O_3-CO-NOx-OH chemical coupled system: Scale interaction

- OH radical is a highly reactive gas lifetime < 1 second, dOH/dt = f(CO, CH_4)
- CO has a moderate lifetime ~1 to 3 Months, dCO/dt = f(OH)
- CH_4 has a long lifetime ~10 years, dCH_4/dt = f(OH)



Suni et al., Anthropocene, 2015



Seinfeld and Pandis, ATMOSPHERIC CHEMISTRY AND PHYSICS: From Air Pollution to Climate Change, 2006

$$\frac{\mathrm{d}[\mathrm{CH_4}]}{\mathrm{d}t} = S_{\mathrm{CH_4}} - R_5$$

$$\frac{\mathrm{d}[\mathrm{CO}]}{\mathrm{d}t} = S_{\mathrm{CO}} + R_5 - R_6$$

$$\frac{\mathrm{d}[\mathrm{OH}]}{\mathrm{d}t} = S_{\mathrm{OH}} - R_5 - R_6 - R_7.$$

Prather, Lifetimes and time scales in atmospheric chemistry, 2007

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Understanding CO spatial variability and trends: Observations

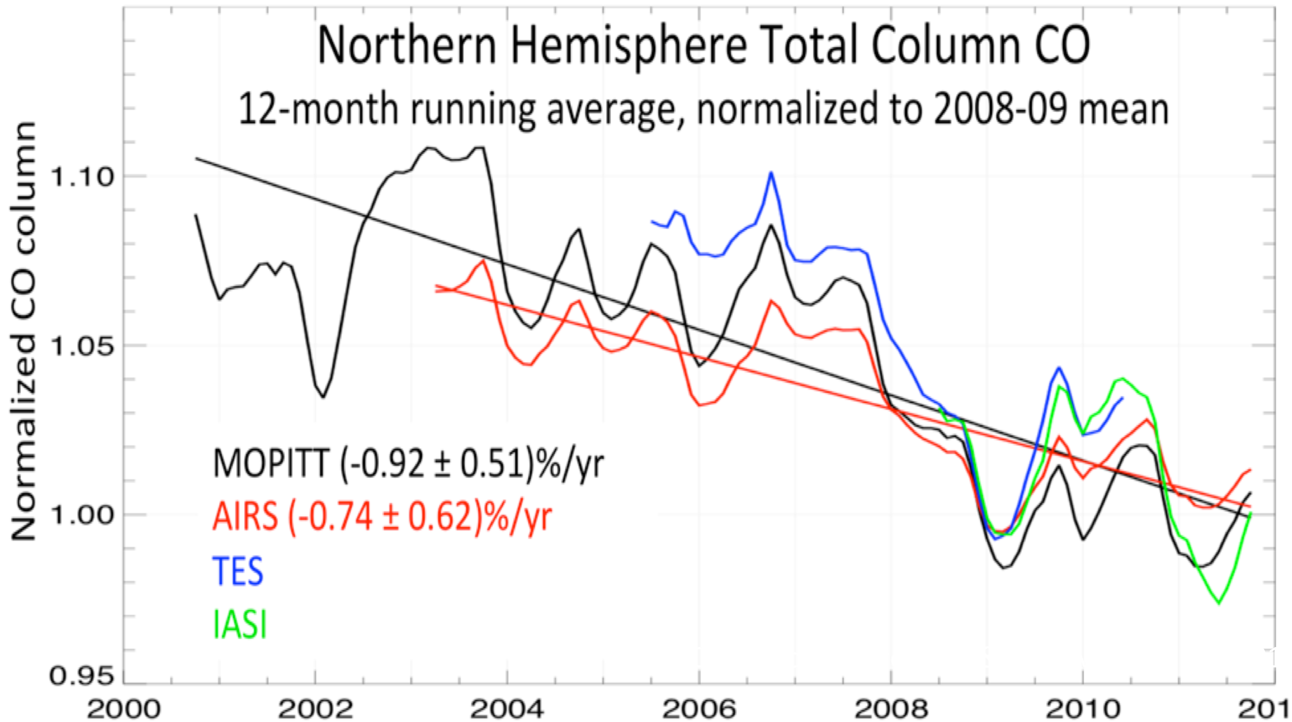
The 2000's onward: the satellite era

Time series of satellites instruments measuring CO:

- ✓ **MOPITT** (TIR-NIR) 2000-2022
- ✓ **SCIAMACHY** (NIR) 2002-2007
- ✓ **TES** (TIR) 2004-2010
- ✓ **AIRS** (TIR) 2002-2008
- ✓ **IASI** (TIR) a,b,c 2006-2023
- ✓ **CrIS** (TIR) 2011-2026
- ✓ **TROPOMI** (NIR) 2017-2024

12-month running averages for N. Hemisphere total column CO measurements normalized by the 08/2008–07/2009 average CO column for each instrument.

H. Worden et al., ACP 2013



NSF

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Comparison of Earth system models with MOPITT

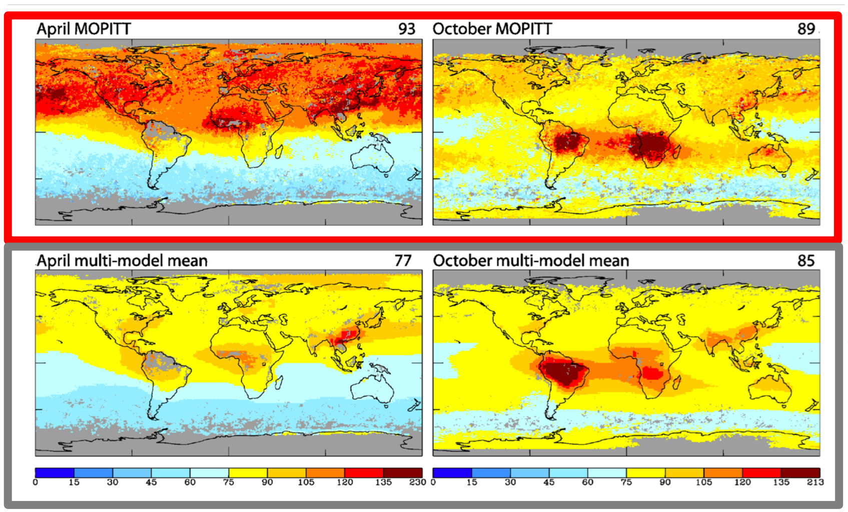


Figure 1. MOPITT and multimodel CO (ppbv). (top) MOPITT observations from 2000 for April (left) and October (right) for the 500 hPa retrieval level. (bottom) Equivalent fields for the multimodel ensemble average when all the S1 simulations are sampled with the MOPITT averaging kernel and a priori CO profiles. Values in the top right corner are the global mean area-weighted CO (ppbv). Grey areas indicate no data.

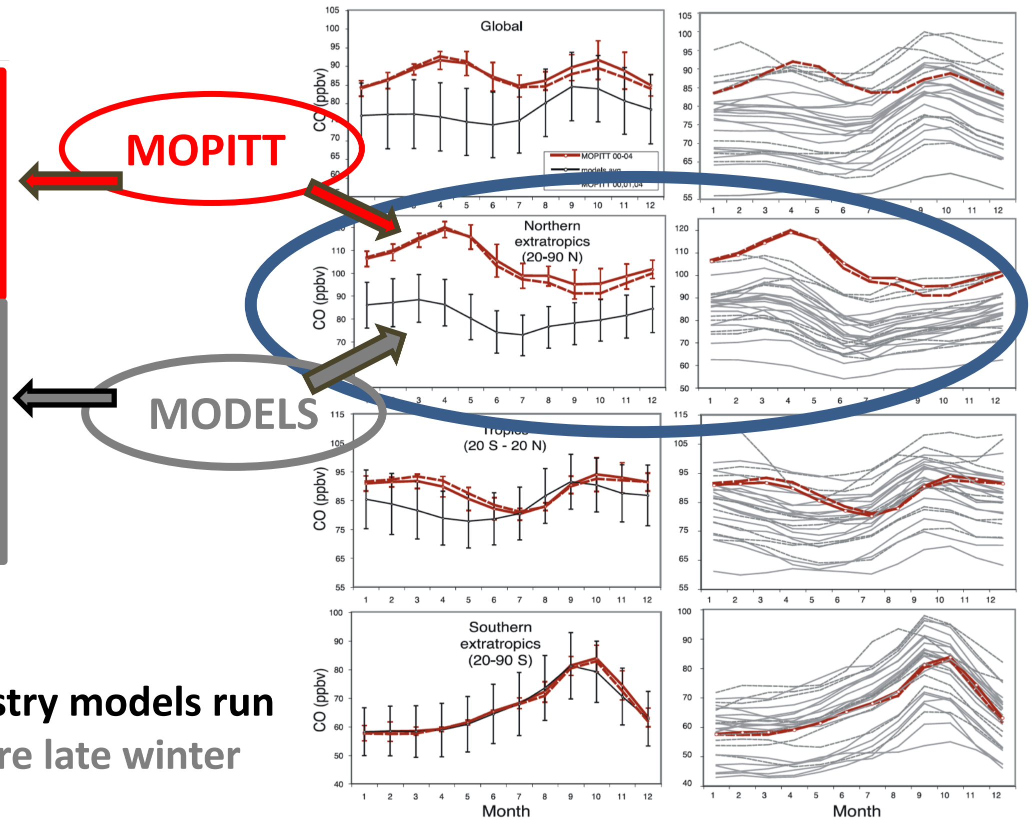


Figure 3. Annual cycle of CO in observations and in the models for the MOPITT 500 hPa retrieval level. MOPITT data (red) include averages over the entire 2000–2004 period (solid line) and excluding 2002 and 2003 (dashed line), and include the standard deviation over 2000–2004. Model results (black) show the (left) S1 (2000 control) multimodel model mean and standard deviation and (right) results from each individual model, with dashed lines among the individual models indicating those models with methane lifetimes outside the TAR range.

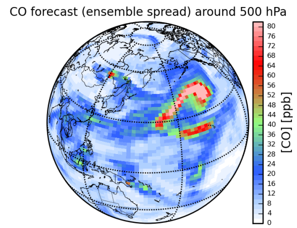
- **Shindell et al. (2006): 26 atmospheric chemistry models run**
  - ✓ Underestimation of the northern hemisphere late winter build up of CO
  - ✓ Location and magnitude and timing of BB events in October
  - ✓ Bias in CO can lead to bias in CH_4 lifetime

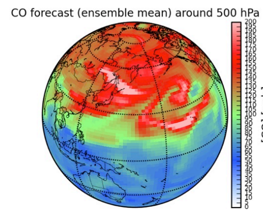
CESM/CAM-CHEM

- CESM122 / CAM4 / 1.9°x2.5°
- MOZART tropospheric chemistry (explicit OH calculation)
- Prescribed surface CH4
- MEGAN / FINN / RCP8.5 emissions

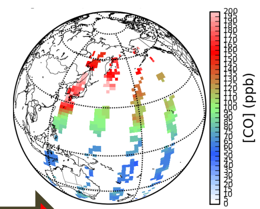
30 CAM-Chem forecasts

- Ensemble of emissions (and update of CO tags)
- Ensemble of transport
- Ensemble of deposition (land model)
- Ensemble of Chemistry



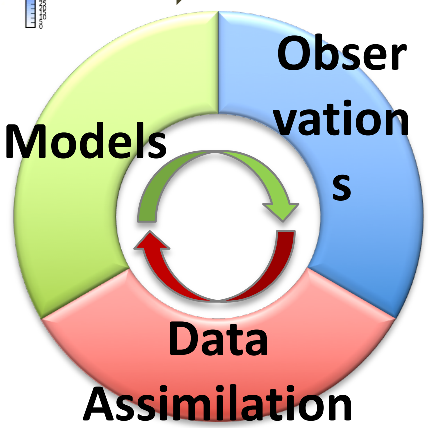


MOPITT obs around 550hPa

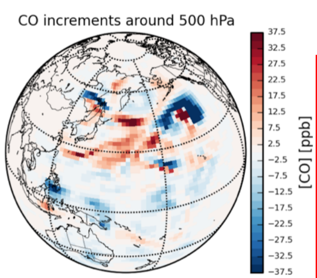


Observations

- Meteorological observations
  - DART/CAM (Raeder et al. 2012)
- MOPITT V5J daytime retrieval
  - DART/CAM-Chem (Barré et al. 2015)



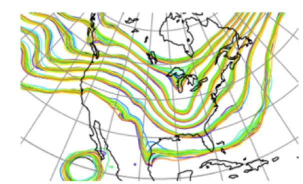
Ensemble of optimized initial conditions every 6 hours

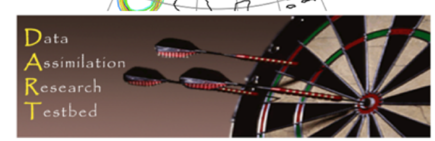


Data Assimilation Research Testbed (DART)

Anderson et al. (2009)

- [CO] inferred by MOPITT
- P, T, U, V, Q inferred by Meteorological observations
- Space and time additive inflation / Spatial localization





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Reanalysis of MOPITT observations

- **MOPITT-Reanalysis (2002-2013):**
  - Assimilates Meteorological and MOPITT-CO every 6 hours
  - Assimilation of CO updates only the CO concentrations and CO tags
  - Ensemble of 30 CAM-Chem simulations (Explicit OH calculation)

- **DART-Control (2002-2003): same setup to quantify MOPITT impacts**
  - Assimilates Meteorological ~~and MOPITT-CO every 6 hours~~
  - Ensemble of 30 CAM-Chem simulations (Explicit OH calculation)
  - Only difference with the MOPITT-Reanalysis is CO

Same meteorology (DART) One Assimilates MOPITT

- **Control-Run (2002-2013):**
  - CAM-Chem nudged to MERRA reanalysis

- **Control-SCO (2002-2013):**
  - CAM-Chem nudged to MERRA reanalysis,
  - replace CO fields every 24 hours,
  - only difference with Control-Run is CO

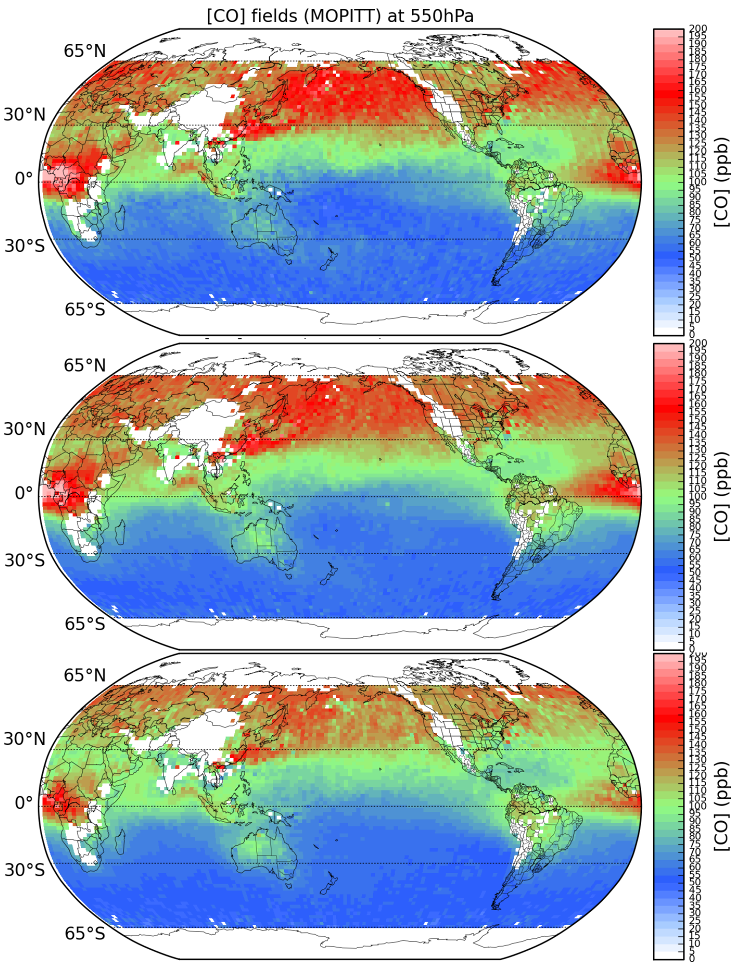
Same meteorology (MERRA) One has CO forced to MOPITT Reanalysis

Impact of CO assimilation

MOPITT Obs on CAM grid

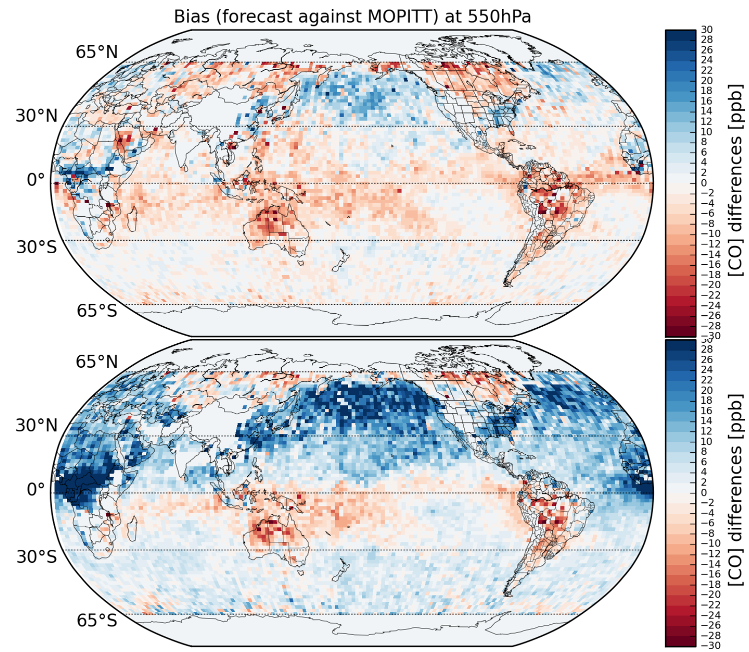
MOPITT Reanalysis

DART-Control



DJF 2002/2003

MOPITT-Reanalysis minus MOPITT



DART-Control minus MOPITT

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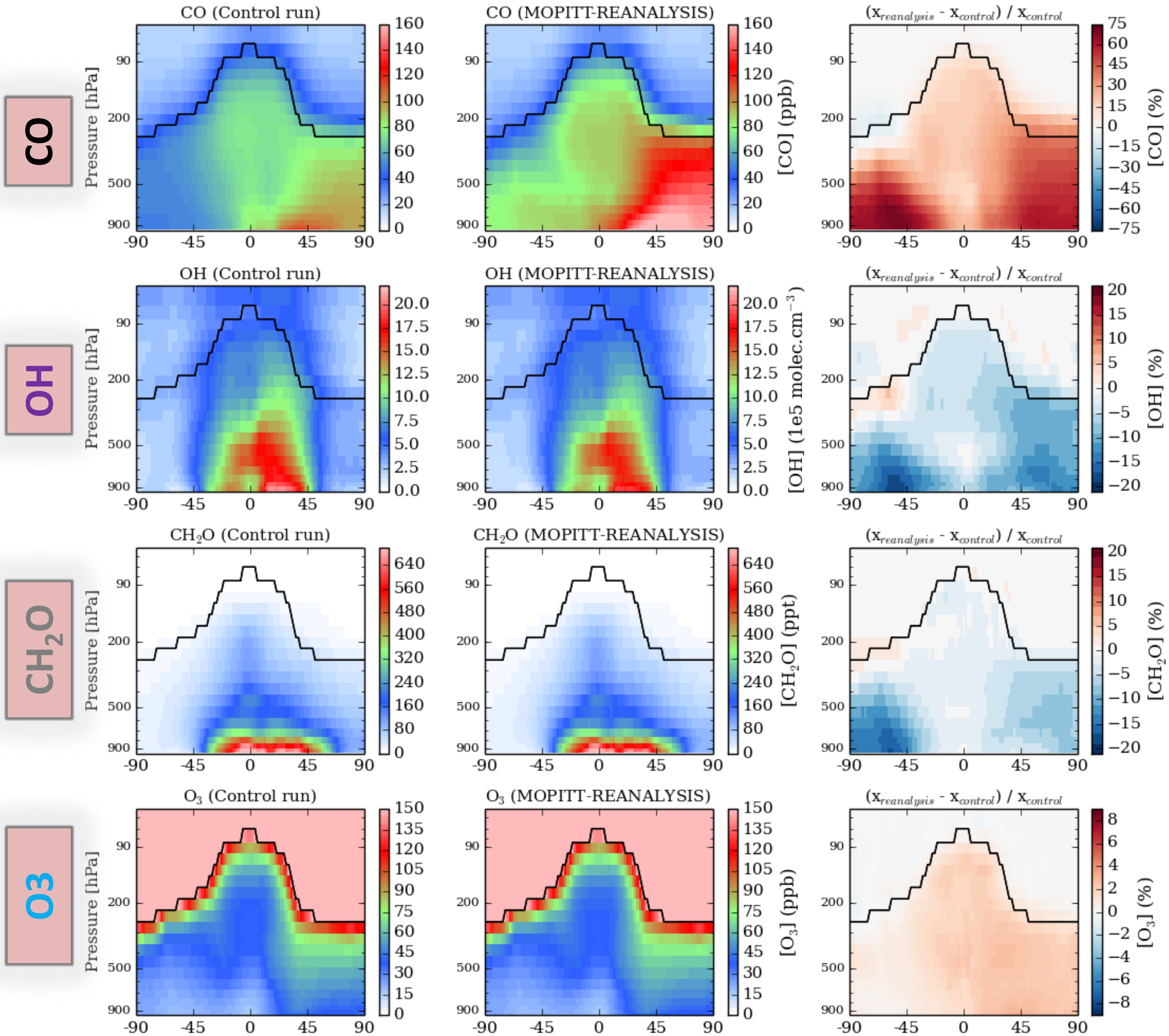
Impact of CO assimilation, 1 Year 2002/2003



Increase in CO by assimilation leads to lower OH levels

- ❖ **Increase primary compounds lifetime, including CH_4**
- ❖ **Decrease secondary pollutant production**
- ❖ **5–10% enhancement of Northern Hemisphere O_3, where NOx are available**
- ❖ **Large increase in H_2O_2**

$$\frac{d[CO]}{dt} = S_{CO} + R1 - R2$$

$$R2 = k_2[CO][OH]$$

$$\frac{d[OH]}{dt} = S_{OH} - R1 - R2 - R3$$

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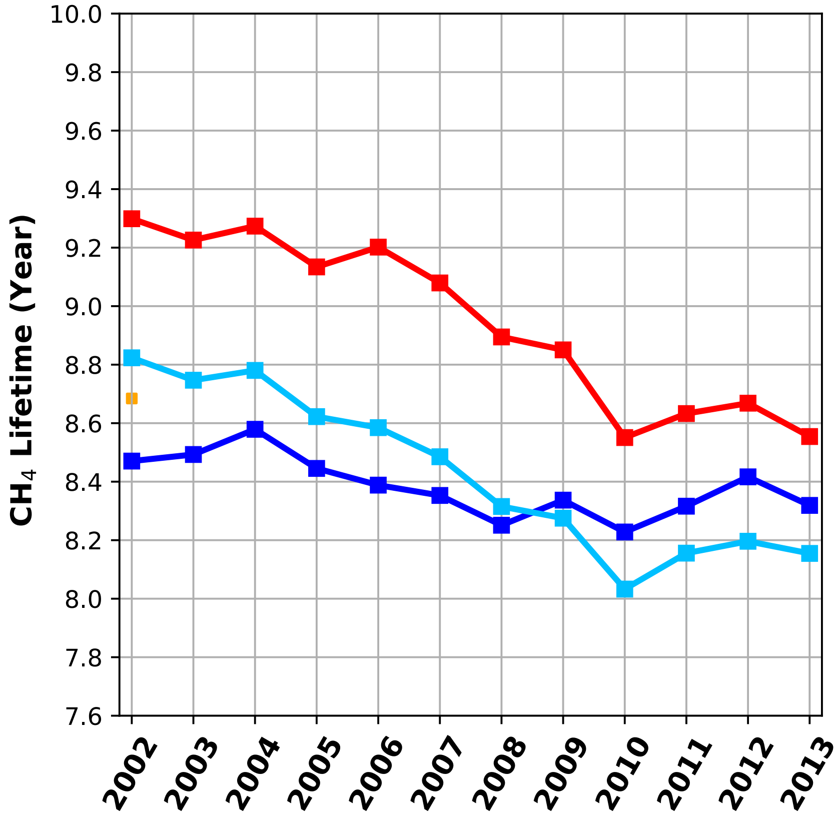
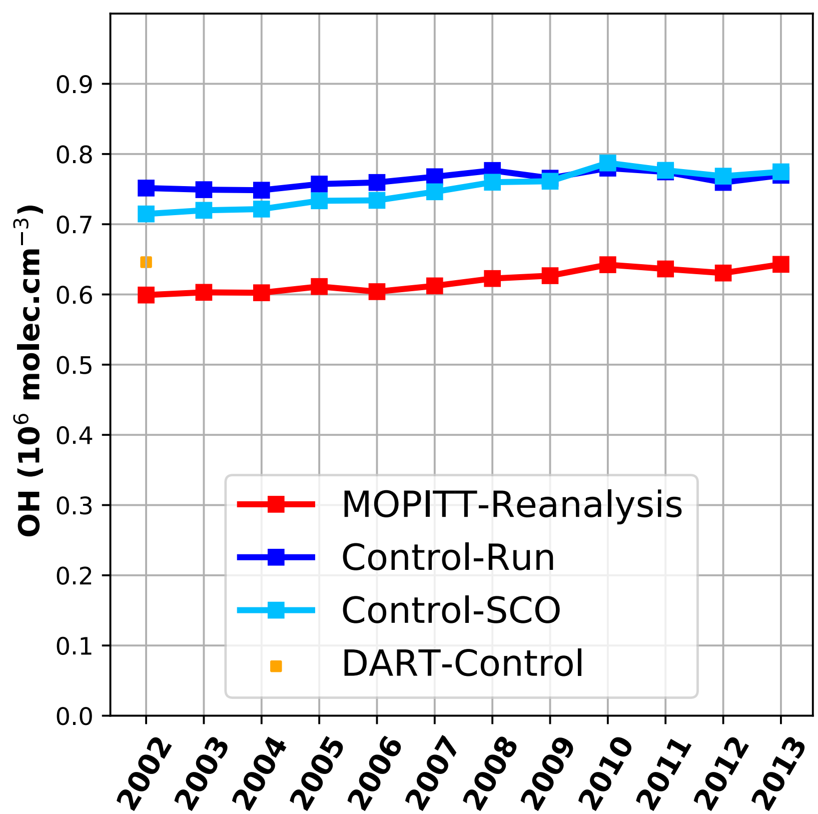
Chemical response from CO changes over time

1) Decrease in CO; Decrease in CO +OH reaction;
2) Decrease in CH_4 lifetime / increase in OH

11 Years





The shorter CH_4 lifetime is not due to a change in meteorology

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Summary

- Despite a rather good knowledge of underlying processes, the emissions, chemical coupling and scale interactions leads to model uncertainties

- The synergistic use of MOPITT CO measurements and model simulation in a data assimilation framework allowed us to:
  - Quantify the negative trend in anthropogenic emission.
  - Quantify the negative trend in Biomass Burning emission.
  - Isolate a positive trends in the chemical production from increase in CH_4 and related chemical feedbacks.

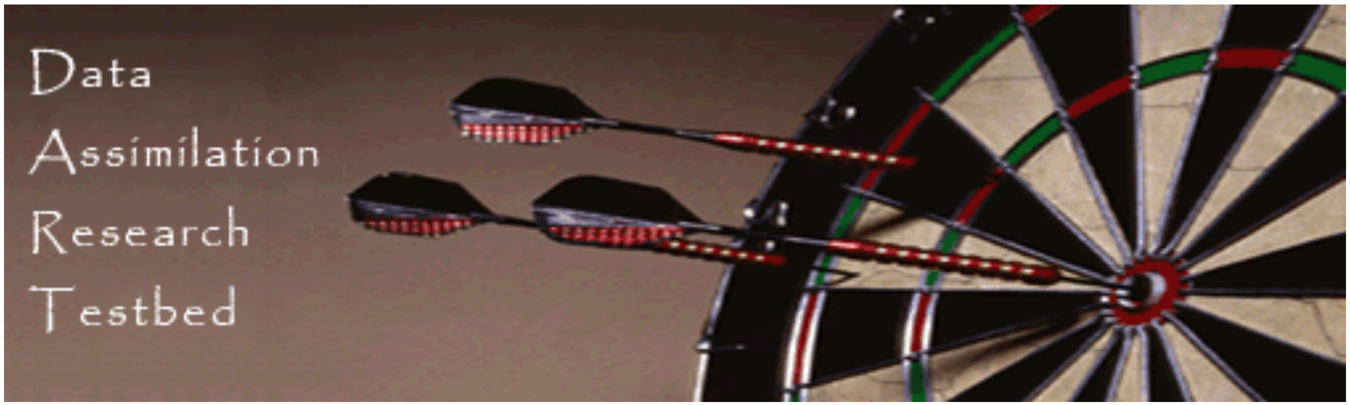
- A better knowledge of the CO budget leads to an improve understanding of the CH_4 budget, both in terms of chemical sink, the CH_4 lifetime, and in terms of BB sources
  - Climate and air quality cobenefits of reducing emissions

4) Wrap-up

CAM+DART:

- ✓ has been incorporated into β-tag testing to make it usable at release,
- ✓ provides state-of-the-art data assimilation tools to assist with CAM model development efforts,
- ✓ helps identify model deficiencies,
- ✓ efficiently focuses almost any model version(s) on an actual synoptic situation.
- ✓ eliminates uncertainty from foreign model bias, interpolation error.

Learn more about DART at:



www.image.ucar.edu/DAReS/DART

Anderson, J., Hoar, T., Raeder, K., Liu, H., Collins, N., Torn, R., Arellano, A., 2009: *The Data Assimilation Research Testbed: A community facility.* BAMS, **90**, 1283—1296, doi: 10.1175/2009BAMS2618.1

Even More Options

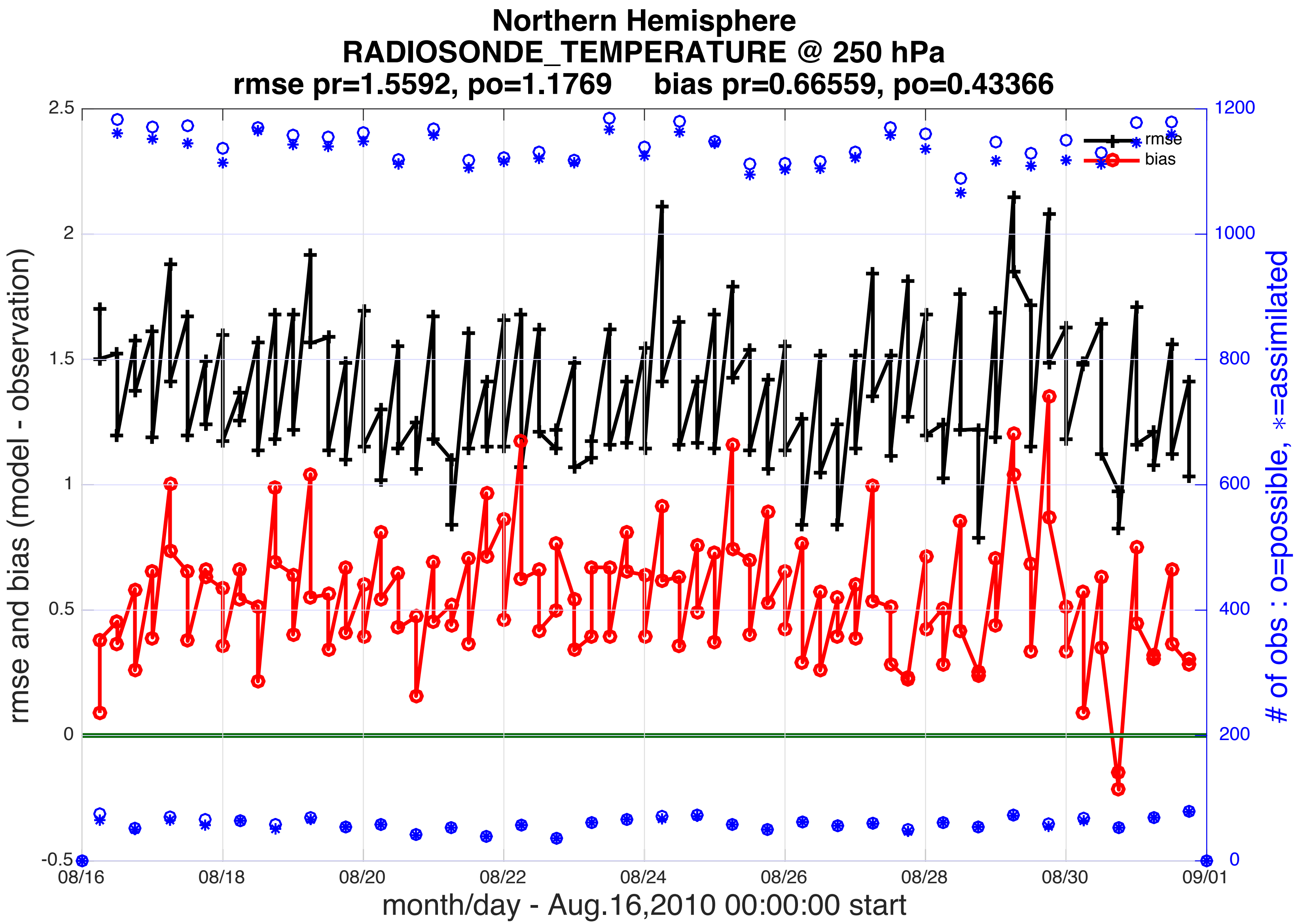
+ Any CAM model state (from CAPT, a climate run, ...) can be compared directly to observations.
+ More focused and detailed than anomaly correlations.
  "T is biased relative to radiosonde observations north of 50N, but the winds are not".
+ The model state can be compared to any observations assimilated by NCEP (even radiances), and more, by calculating the model estimates of the observations during the forecast.

All Flavors of CAM-FV Can Be Evaluated

- ✓ CAM-Chem
- ✓ WACCM(-X)
- ✓ Virtually any version such as CAM4, 5, yours, ...

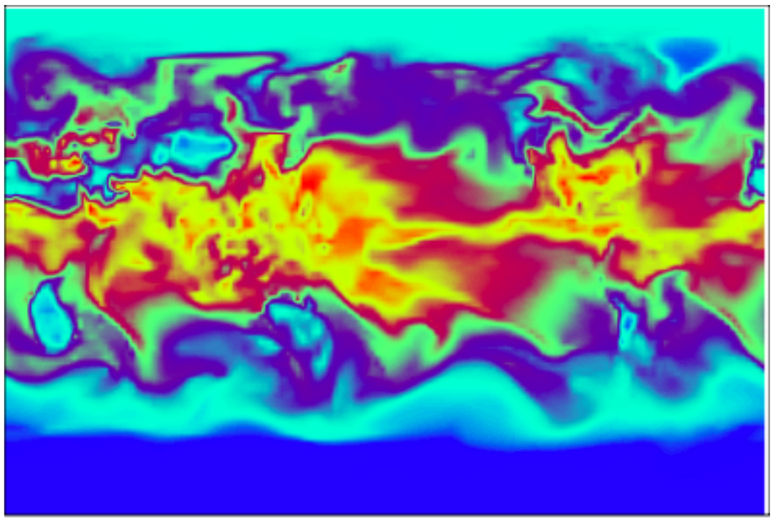
- ❑ CAM-SE; interface probably needs updating.
- ❑ MPAS-A; can be developed from existing pieces (easily? Zarzycki, Ha).

"Obs Space" Time Series



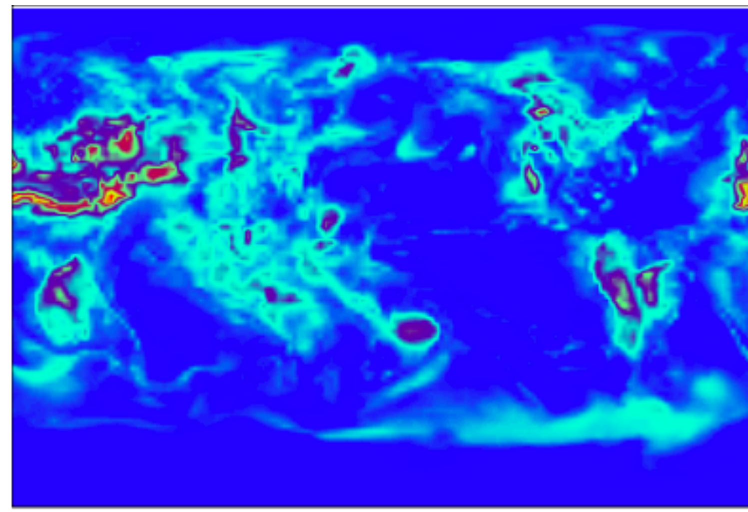
Ensemble Mean (analysis) and Spread (confidence)

Q level=30 Mean



posterior ensemble state
Range of Specific humidity: 6.61214e-06 to 0.0217079 kg/kg

Q level=30 spread

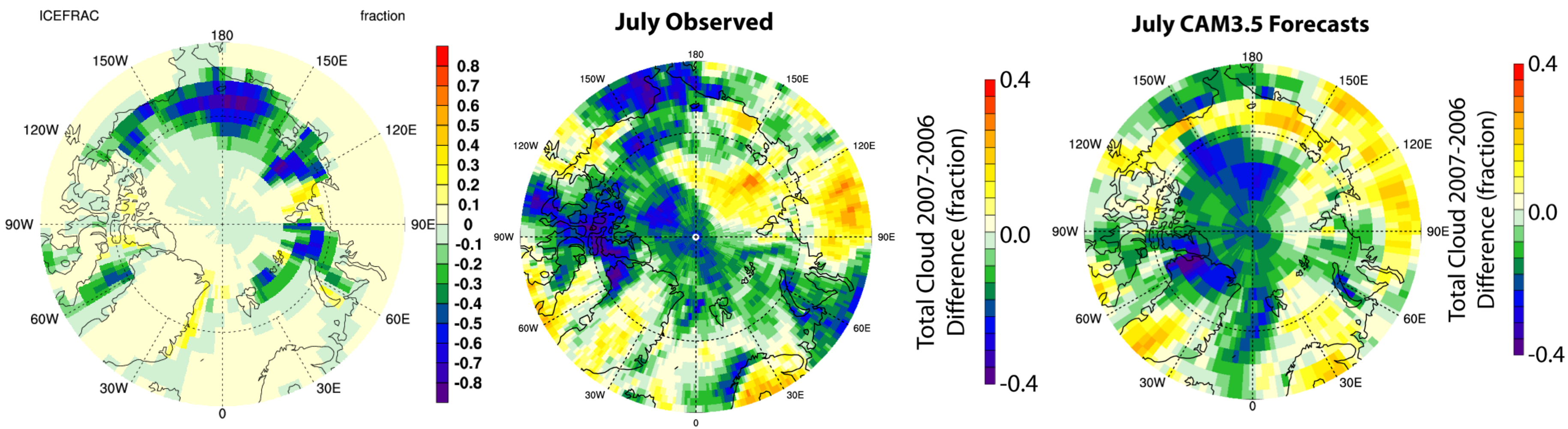


posterior ensemble state
Range of Specific humidity: 2.05892e-05 to 0.00680974 kg/kg

Change in spread during a forecast is a diagnostic of model error growth.

Initial Conditions for Process Studies

Kay, et al. 2009; Cloud response to the 2007 Arctic sea ice loss in CAM3.5 and CAM4

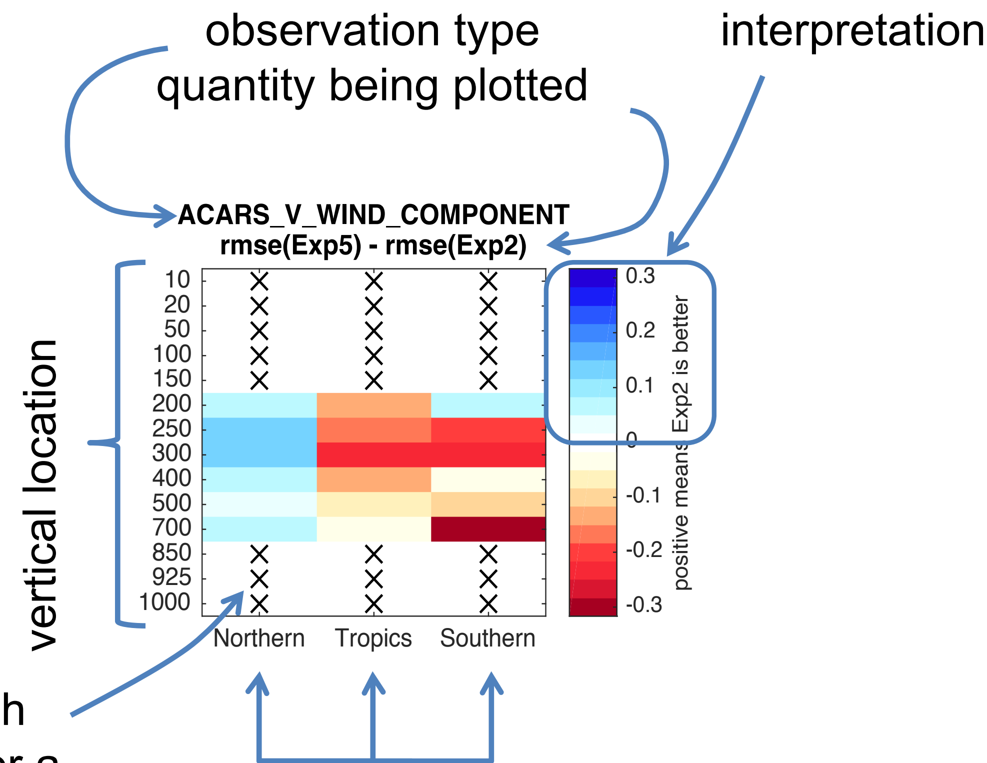


CAM3.5 has an unrealistic feedback between stratus clouds and sea ice because stratus clouds are only diagnosed over open water.

+ On CAM's native grid -> no interpolation or foreign model error to wonder about.
+ Analysis error estimate comes for free from ensemble spread; varies with location, time, and field.
+ Analyses can be generated with study-focused observation sets.

“Obs Space” Comparison of 2 CAMs

Performance of 2 CAMs compared against the observations successfully assimilated by both models.



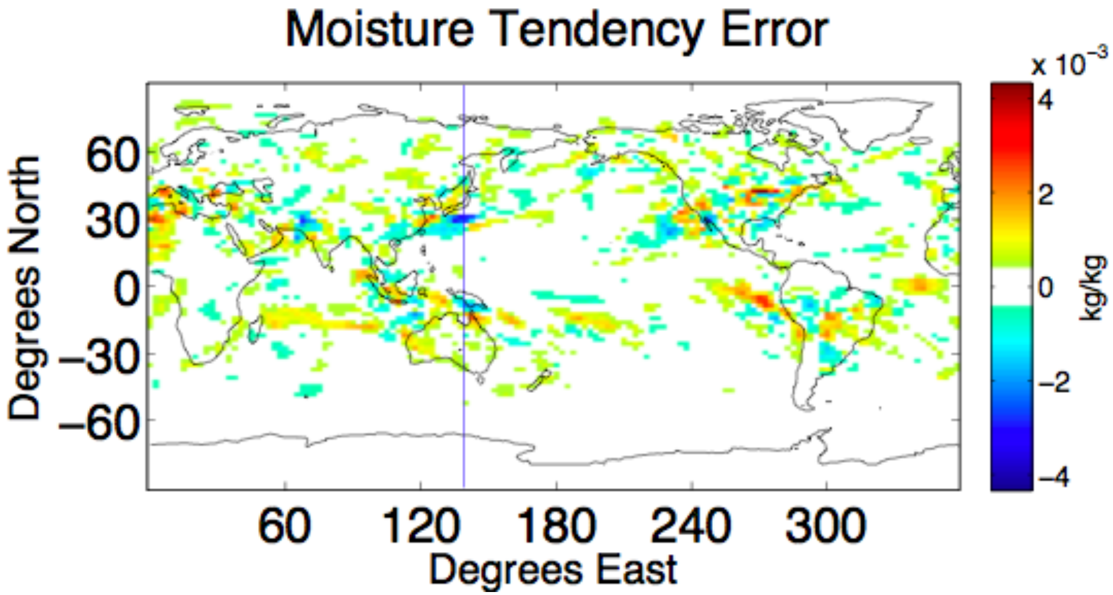
‘X’ = not enough observations for a judgment.

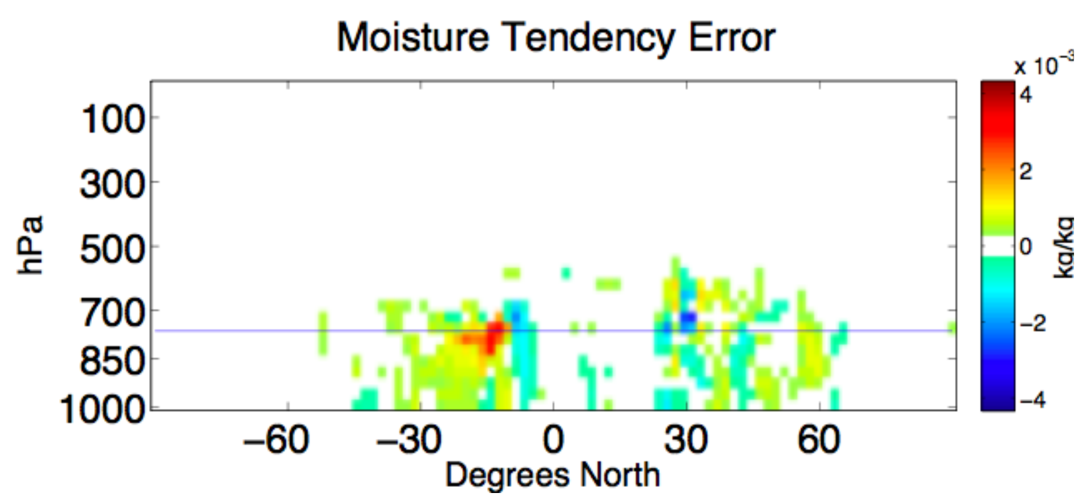
Regions

Northern: 20-90N
Tropics: 20S-20N
Southern: 90S-20S

Tendency Errors

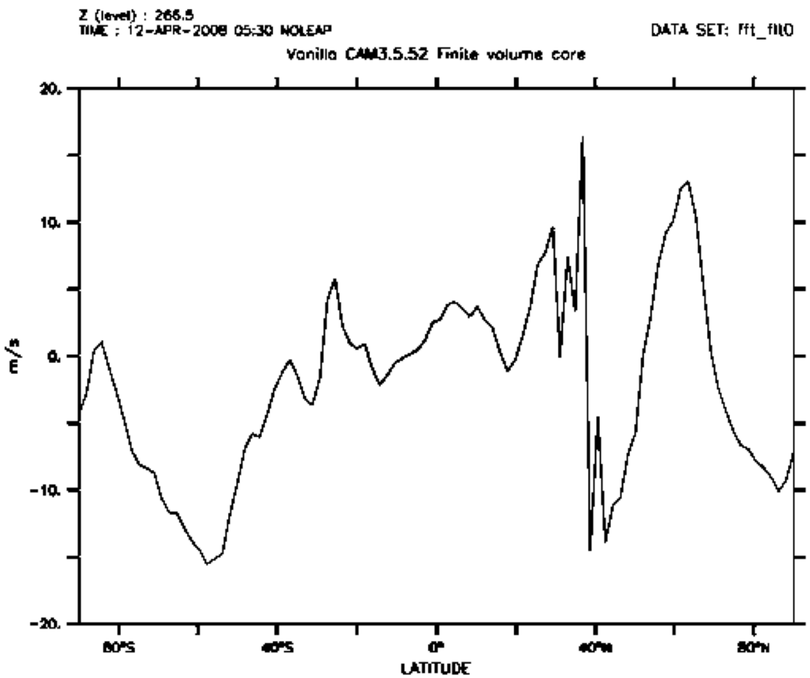
DART-CAM can provide time-averaged tendency errors of the state variables over short periods. These have significant correlation with model bias as measured from long climate runs. Shown is a 6-day average of 6-hour Q tendency errors from July 2003.
This highlights areas where CAM wants to stray from reality.



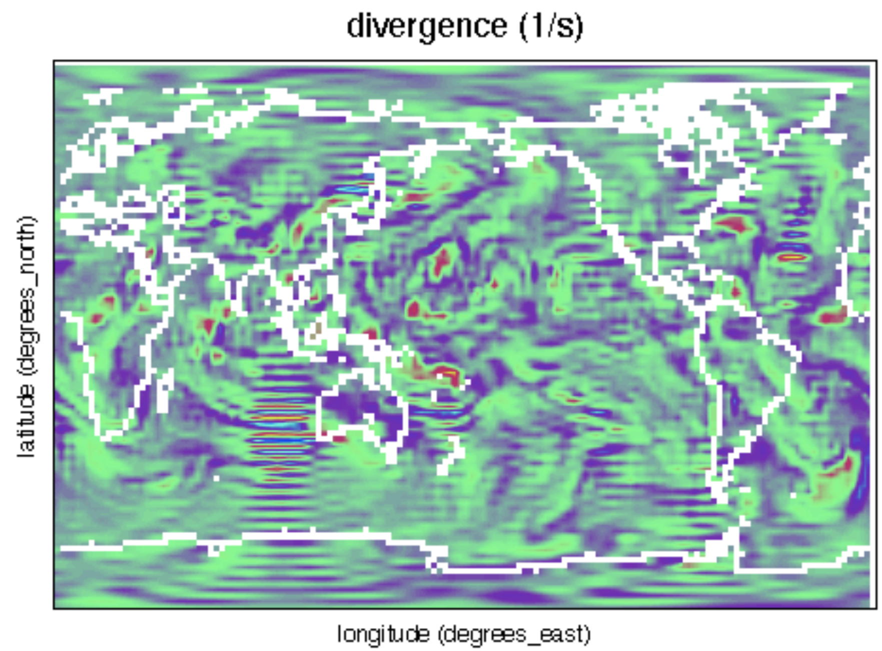


FV dy-core noise (circa 2008)

- First noticed in DART-CAM assimilations.
- Seen in free-running FV CAM, even on the cubed-sphere grid (Lauritzen).



Meridional wind (V) for free running CAM. Sporadic intermittent noise is especially visible at upper level v winds.



Divergence field in free running CAM at model level 10 (around 200 hPa). Noise visible throughout the run.

3) Making These Tools Available

- Tools exist.
- Bottleneck; making DART work with chosen CESM+CIME.
- The Fix; Develop pre-β tag testing of CESM2-CAM-FV in the context of DART.
- CAM will be first implementation.
- Other components will use it as a template.
- They will need forcing files from CAM+DART → new reanalysis.

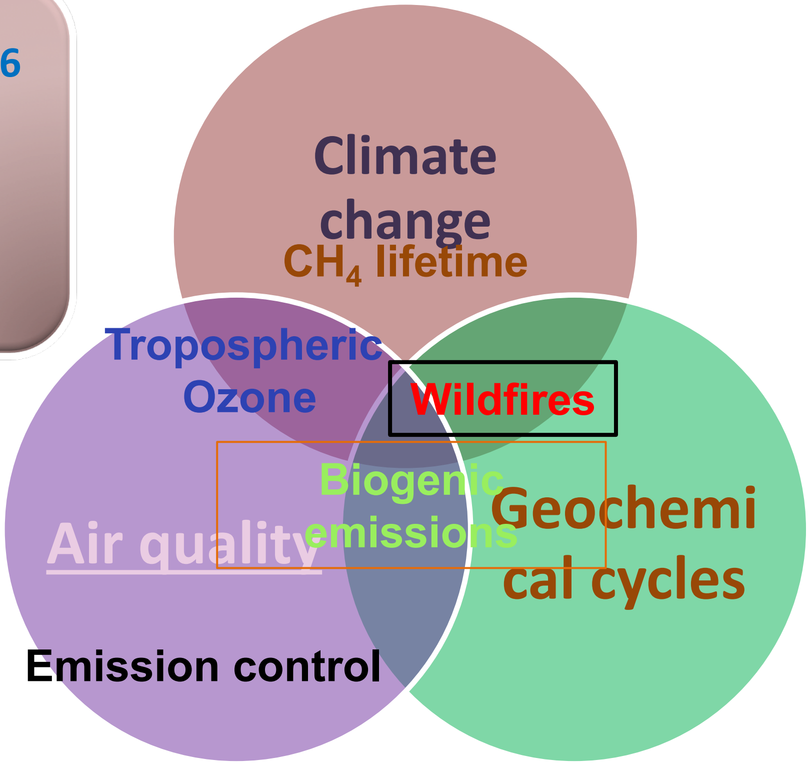
Proposed Testing Procedure

1. Run a DART+CESM setup script to
   A. build a small ensemble, low resolution, sparse observation case
   B. stage input files
   C. set namelist values (both DART and CESM)
2. First forecast + assimilation cycle.
   A. 1-24 hours, depending on the component
   B. DART can start from a single model state;
      perturbs it to make an ensemble (or tell CESM to).
3. 2 more assim cycles in 1 job to test the
   A. multi-cycle capability
   B. interim restart file management
   C. st_archive for history and restart files
4. Set up and run a large ensemble (~100), 1-degree case for
   A. 1 cycle = 1-24 hours, depending on the component.
   B. Still small observation set.
5. Repeat some steps for CAM variants

Why CO ? Atmospheric composition, Air quality & Climate

- **Indirect radiative forcing of 0.23 W.m^{-2} [0.16 to 0.30 W.m^{-2}], IPCC, Stocker et al. (2013)**
  - ✓ CO_2 precursor (0.09 W.m^{-2})
  - ✓ Controlling CH_4 lifetime (0.07 W.m^{-2})
  - ✓ Precursor of tropospheric ozone (0.08 W.m^{-2})

- **Important for Air Quality and Chemistry**
  - ✓ Indicator of combustion efficiency, from anthropogenic and wildfires sources
  - ✓ Track pollution plumes
  - ✓ oxidative capacity and photochemical smog

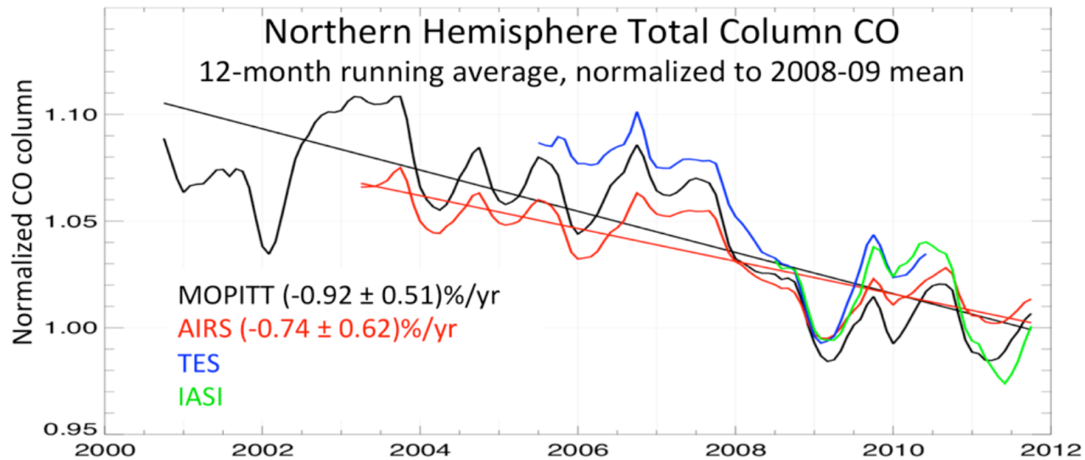


Understanding CO spatial variability and trends: Observations

The 2000's onward: the satellite era

Time series of satellites instruments measuring CO:

- ✓ **MOPITT** (TIR-NIR) 2000-2022
- ✓ **SCIAMACHY** (NIR) 2002-2007
- ✓ **TES** (TIR) 2004-2010
- ✓ **AIRS** (TIR) 2002-2008
- ✓ **IASI** (TIR) a,b,c 2006-2023
- ✓ **CrIS** (TIR) 2011-2026
- ✓ **TROPOMI** (NIR) 2017-2024



12-month running averages for N. Hemisphere total column CO measurements normalized by the 08/2008–07/2009 average CO column for each instrument.

H. Worden et al., ACP 2013

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Impact of CO assimilation, 1 Year 2002/2003

CO

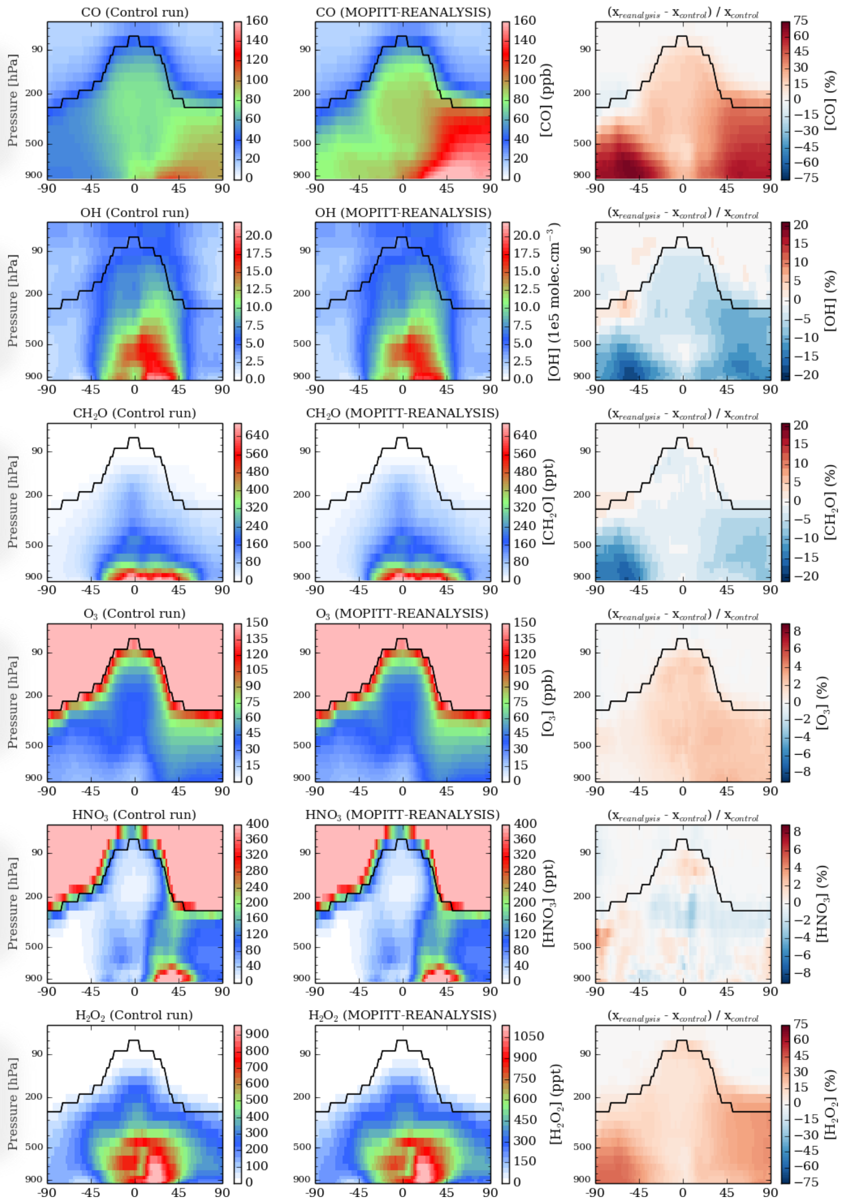
OH

CH_2O

O3

HNO3

H2O2



- **Increase in CO by assimilation leads to lower OH levels**
  - **Increase primary compounds lifetime, including CH_4**
  - **Decrease secondary pollutant production**
  - **5–10% enhancement of Northern Hemisphere O_3, where NOx are available**
  - **Large increase in H_2O_2**

$$\frac{d[CO]}{dt} = S_{CO} + R1 - R2$$

$$R2 = k_2[CO][OH]$$

$$\frac{d[OH]}{dt} = S_{OH} - R1 - R2 - R3$$

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