Status/Updates of CAM4/5 Chemistry

Available Chemical Mechanisms, CAM4

Bulk Aerosol Model (BAM):

Includes Black Carbon, Organic Carbon, Sea Salt, Dust, SO_2, SO_4, H_2O_2, DMS
(prescribed monthly fields of O_3, OH, HO_2, NO_3, N_2, O_2)

BAM and tropospheric chemistry (trop_mozart):

Tropospheric mechanism, 103 species (MOZART: *Emmons et al., 2010*)
Stratospheric chemistry is prescribed: (O_3, NO_x, HNO_3, CH_4, CO,N_2O, N_2O_5, H_2O)
Emissions, Dry/Wet Deposition

Tropospheric/ stratospheric chemistry (trop-strat mozart):

Tropospheric and Stratospheric mechanism including
stratospheric heterogeneous reactions, more than 150 species, about 300 reactions
(Lamarque et al., 2012)

Status/Updates of CAM4/5 Chemistry

Updates (November Release):

CAM4-BAM and trop. chemistry + SOA chemistry and MEGAN:

new species (BENZENE and XYLENE) + new reactions

Setup to run with MEGAN2.0 (interactive with the land model, hydrocarbons emissions vary depending on the land type)

Model of Emissions of Gases and Aerosols from Nature (MEGAN)

CAM5 Chemistry

Modal Aerosol Model (MAM3/7) and tropospheric chemistry

Tropospheric Chemistry (SO_2, DMS, H_2SO_4) with MAM3/7 to calculate the aerosol modes

MAM3/7 and tropospheric/ stratospheric chemistry:

Tropospheric Chemistry (SO_2, DMS, H_2SO_4) with MAM3/7 to calculate the aerosol modes, no changes to the stratospheric chemistry

MAM3 Specified Dynamics (SD) run with tropospheric chemistry

for Polar Model Intercomparison Project (POLMIP) (results will be presented).

NESL

NSF

Updates for both CAM4/5 Chemistry

- Updates of the chemical scheme to JPL2010
- Updates on a few tropospheric rate constants
- Rate approach added to pre-processor
- Remove organic halogen surrogates (better description of organic species)
- Updated heterogeneous polar chemistry (stratosphere only)
- rhminh for the stratosphere (dehydration issue)
- New SAD dataset (testing heating rates)

- SE/FV dynamical core comparison: on-going tracer tests based on SD configuration
- kPP mechanism Box Model or SCAM w/ chemistry

-> Create version for CCMI simulations

CAM4 / CAM5 with Chemistry

Simone Tilmes, *Jean-Francois Lamarque, Louisa Emmons, Steve Arnold, Xiaohong Liu, Po-Lun Ma, Jushua Schwarz, HIPPO team*

- Differences in chemistry due to meteorology (clouds, precipitation, temperatures)
- **Differences in chemistry due to differences in aerosols and coupling with chemistry**

Model Runs: CAM4-BAM, CAM5-MAM3/7

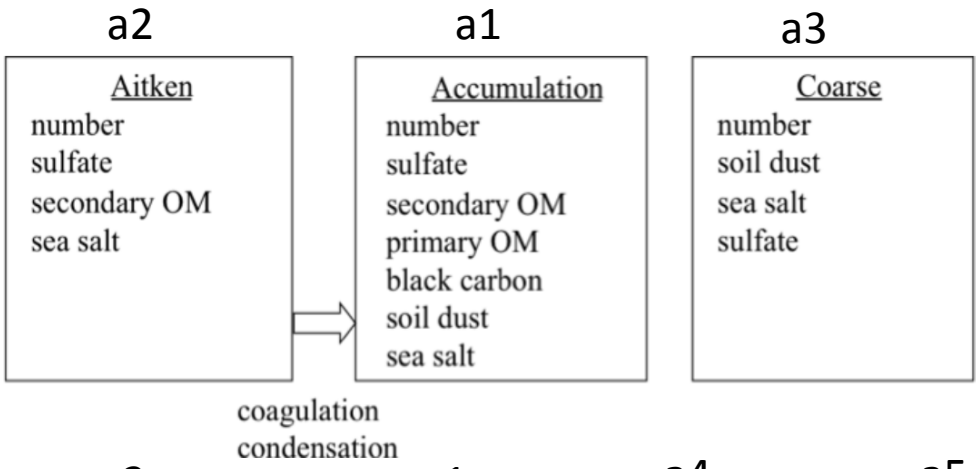
Tropospheric/stratospheric chemical mechanism for all simulations, to the most part same emissions.

Online (year 2000)	**CAM4-BAM**	**CAM5-MAM3**	**CAM5-MAM7**
CH_4 LIFETIME (yr)	8.2	9.1	9.0
CO LIFETIME (yr)	0.14	0.15	0.15
Lightening NO_x (TgN/yr)	4.4	4.6	4.6

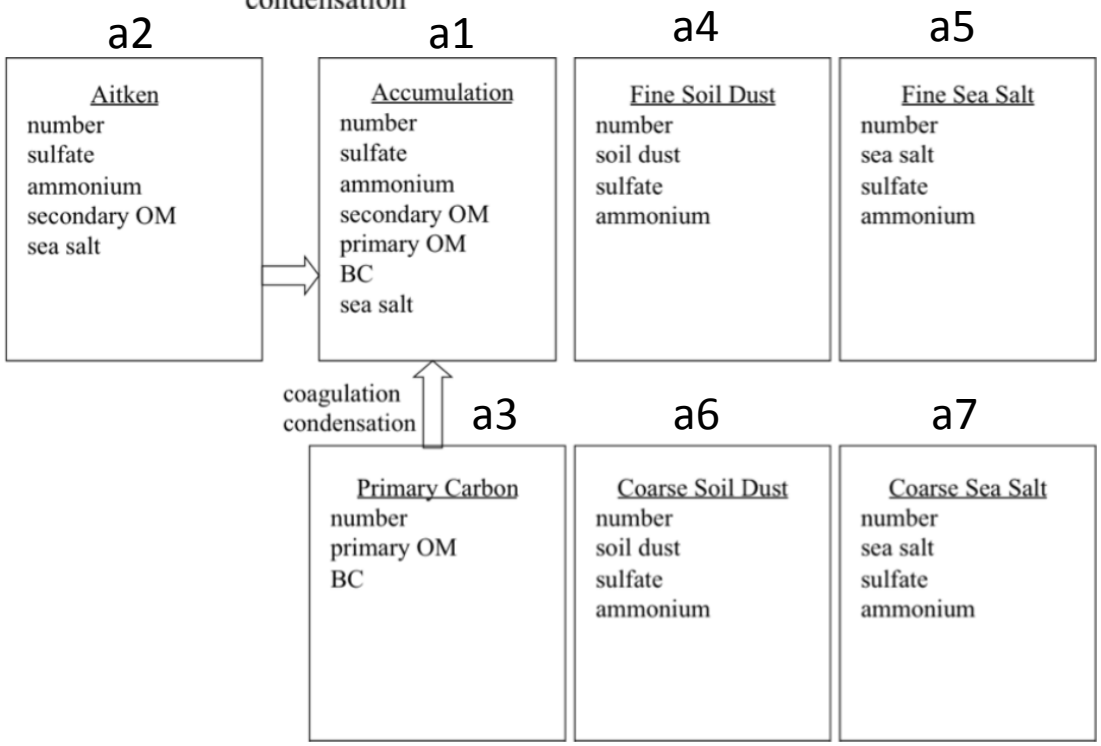
SD Runs (2008)	**CAM4-BAM**	**CAM5MAM3**	**CAM5MAM3 (without Het_{H2O2})**
CH_4 LIFETIME (yr)	7.9	9.7	9.5
CO LIFETIME (yr)	0.14	0.16	0.15
Lightening NO_x (TgN/yr)	6.8	4.3	4.3

Aerosols: CAM5 Modal Aerosol Model (MAM3/7)

MAM3



MAM7



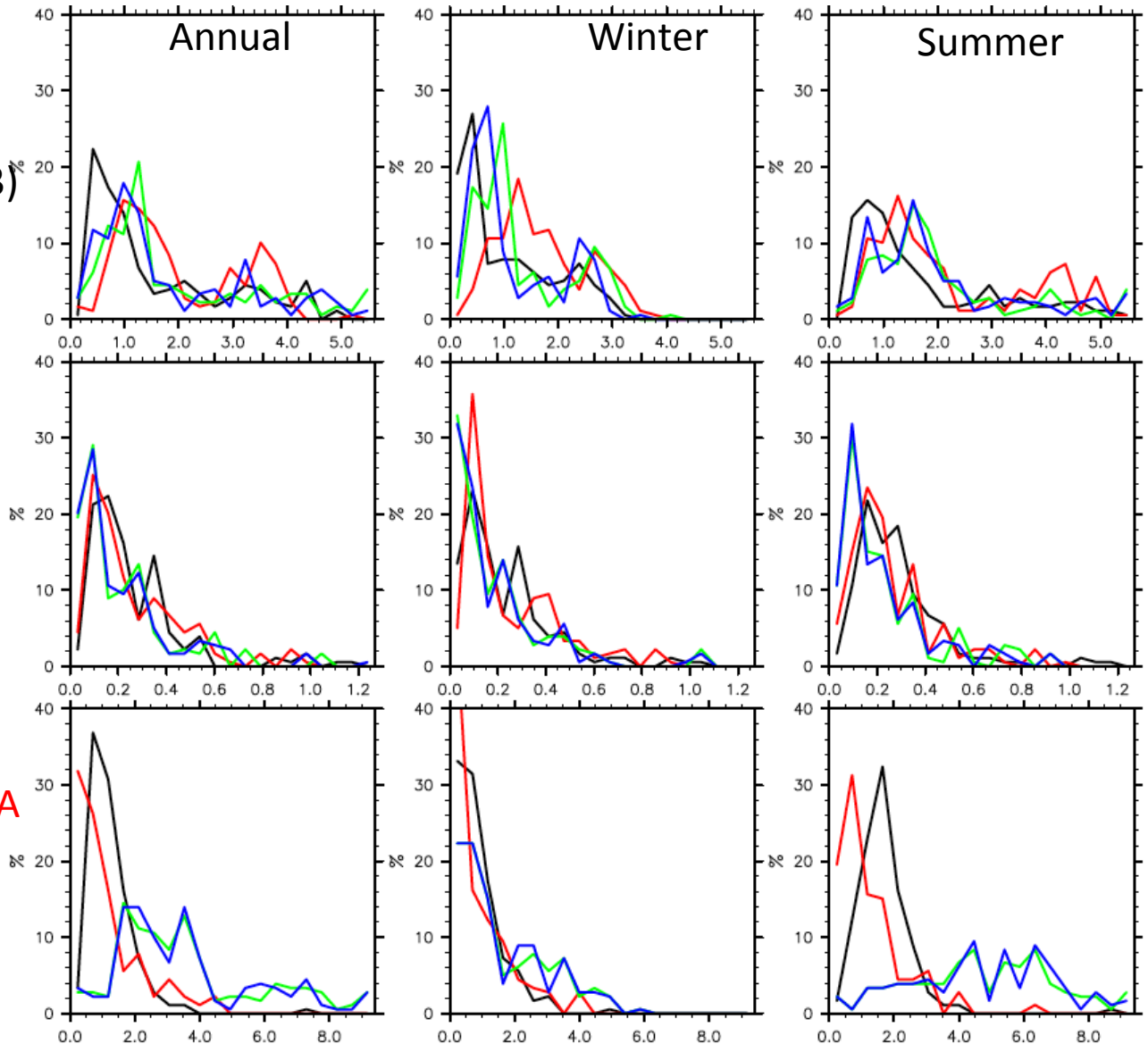
Liu et al., 2011

Differences in Aerosols, CAM4 and CAM5

Sulfate:
SO_4
SO_4 (a1,a2,a3)
SO_4 (a1,a2, a4-7)

BC:
CB1, CB2
BC (a1)
BC (a1, a3)

OC:
CB1, CB2, SOA
pom (a1, a3), soa (a1, a2)
pom (a1, a3), soa (a1, a2)



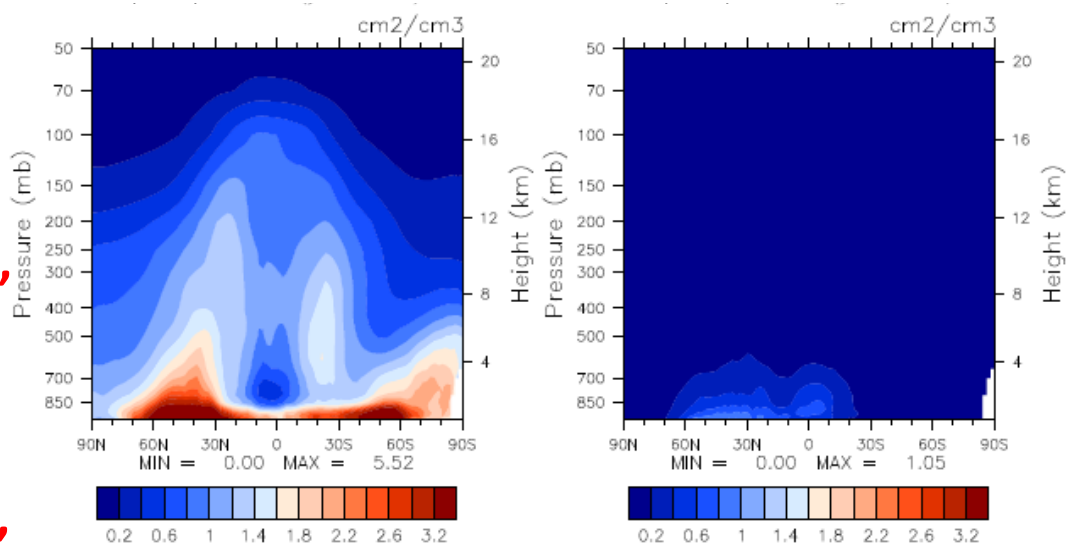
IMPROVE
CAM4-BAM
CAM5-MAM3
CAM5-MAM7

Surface layer concentration (mg/m^3)

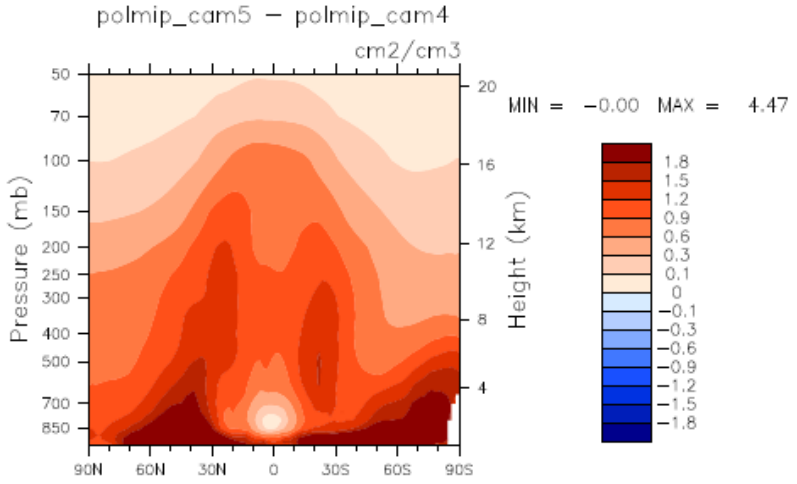
Differences in Surface Area Density (SAD)

CAM5: (Aitken_mode) MAM3: so4_a2, soa_a2, ncl_a2

MAM7: so4_a2, nh4_a2, soa_a2, ncl_a2



CAM4-BAM: sfc_sulf + sfc_nit + sfc_oc + sfc_soa + sfc_bc



SAD is much larger in CAM5-MAM due to the inclusion of ncl_a2. For MAM7 primary organic carbons are not included

Tropospheric Heterogeneous Reactions

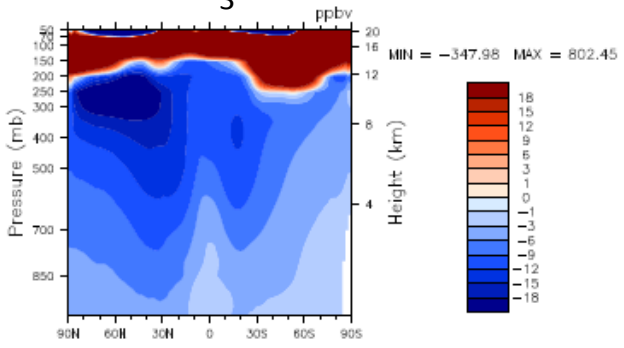
CAM4-BAM
CAM5-MAM

- [usr_N2O5_aer] N2O5 -> 2 * HNO3
- [usr_NO3_aer] NO3 -> HNO3
- [usr_NO2_aer] NO2 -> 0.5*OH + 0.5*NO + 0.5*HNO3
- CB1 -> CB2 ; 7.10e-6
- OC1 -> OC2 ; 7.10e-6
- [usr_SO2_OH] SO2 + OH -> SO4
- [usr_SO2_OH] SO2 + OH -> H2SO4
- DMS + OH -> SO2 ; 9.60e-12, -234.
- [usr_DMS_OH] DMS + OH -> .5 * SO2 + .5 * HO2
- DMS + NO3 -> SO2 + HNO3 ; 1.90e-13, 520.
- NH3 + OH -> H2O ; 1.70e-12, -710.
- [usr_HO2_aer] HO2 -> 0.5*H2O2

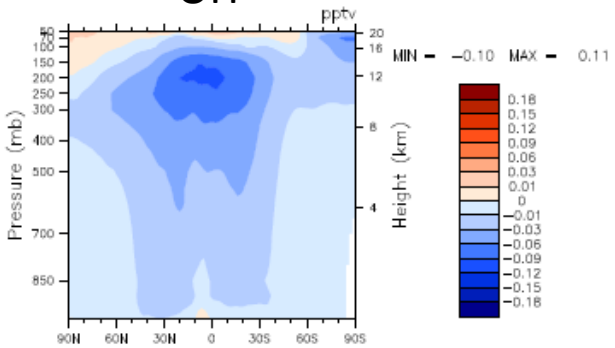
Increased SAD will have an impact on Chemistry

Differences: CAM5-MAM3 - CAM4-BAM

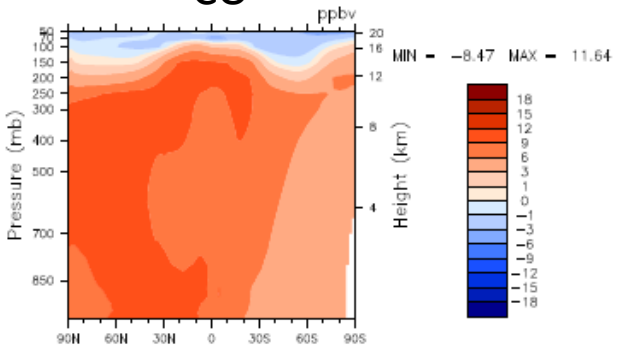
O_3



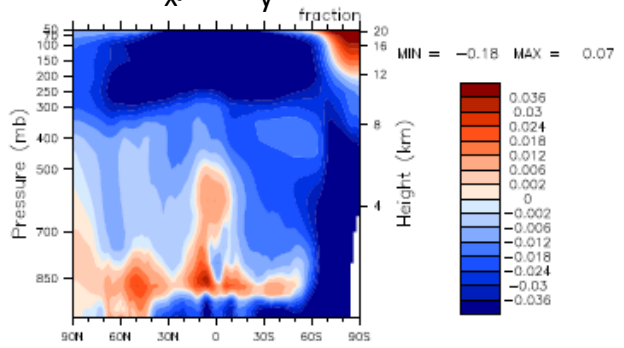
OH



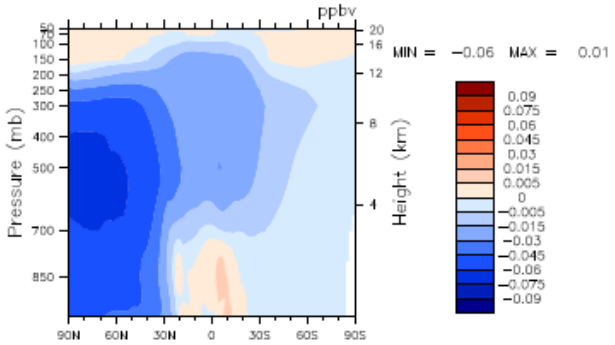
CO



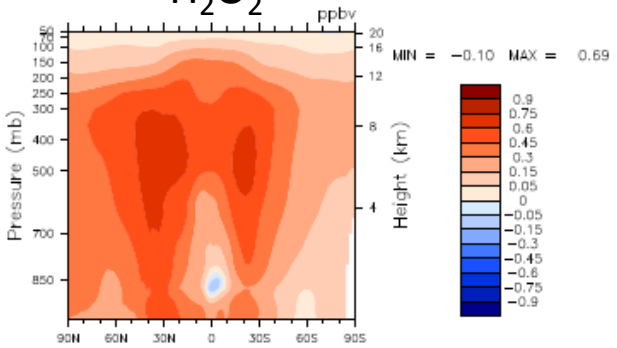
NO_x/NO_y



PAN



H_2O_2

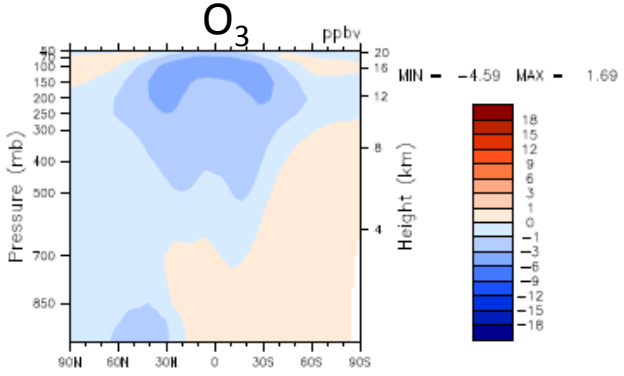


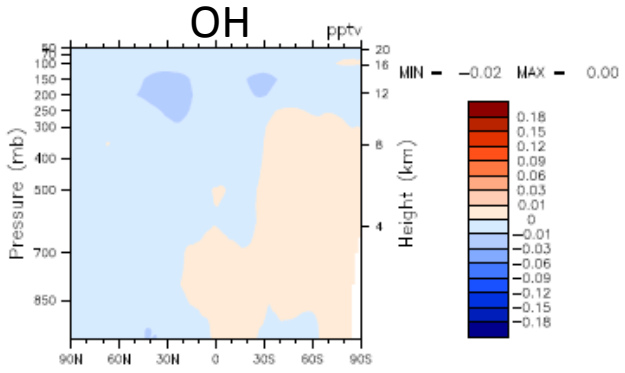
Increase SAD results in: - at night more N_2O_2 converted to HNO_3 -> decrease in NO_x/NO_y

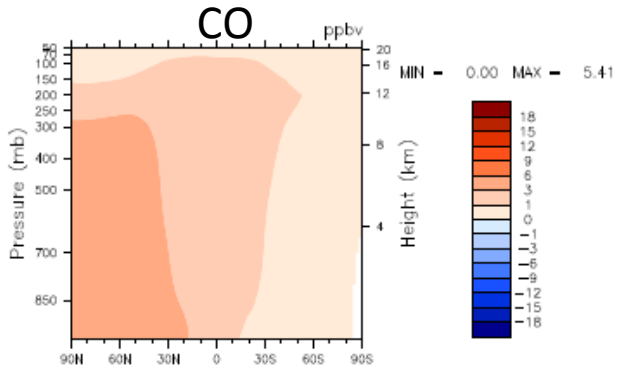
- less NO_2 from N_2O_2 by sunrise -> less PAN formation
- Less NO_x -> less OH -> more CO (increased CH_4 lifetime)

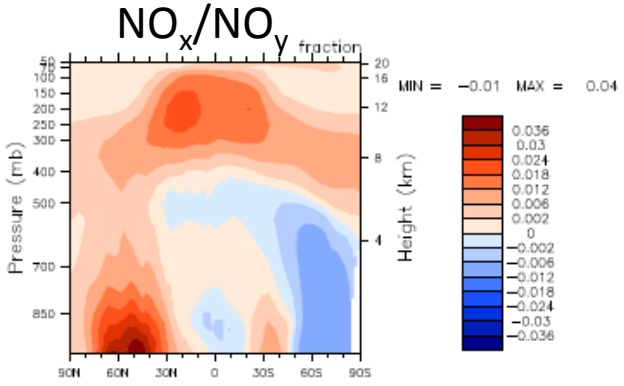
- more H_2O_2 formation

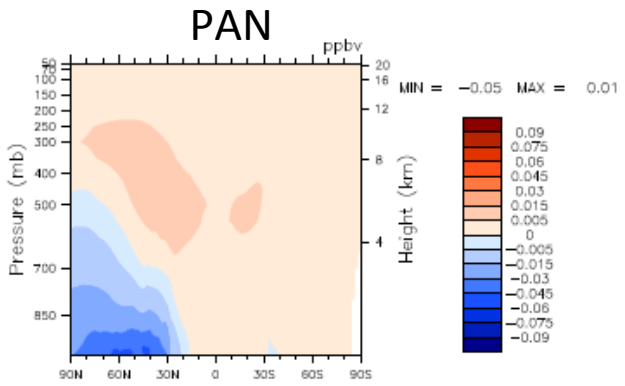
CAM5-MAM3 - CAM5-MAM3 (no HET_{H2O2})

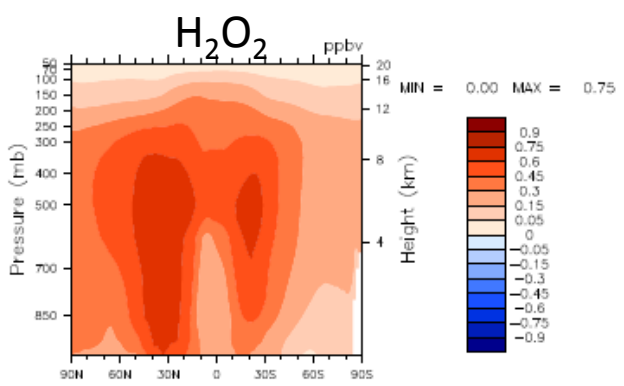












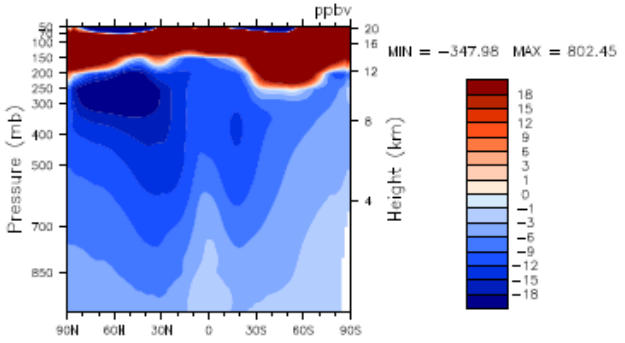
Importance of Reaction HO_2 -> 0.5*H_2O_2
Reduced HO_2 -> less OH with consequences for CO and NOx/NOy

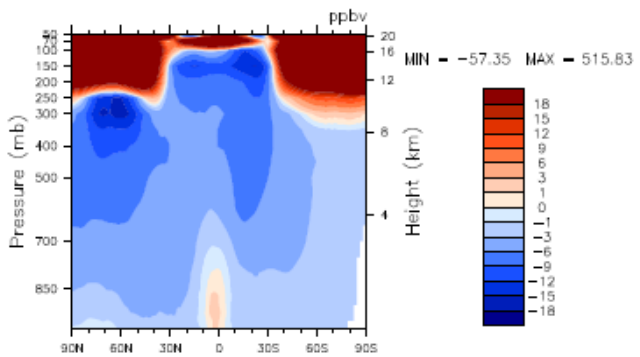
Differences: CAM5-MAM3 - CAM4-BAM

Specified Dynamics

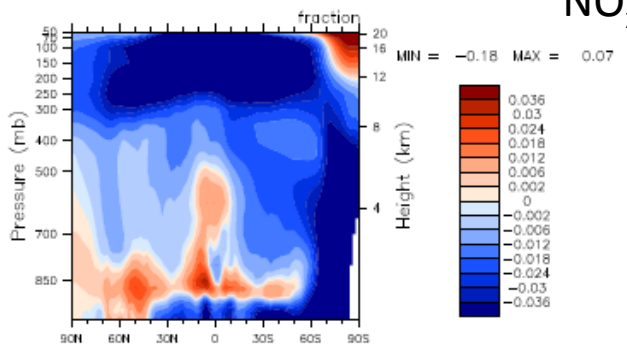
Online

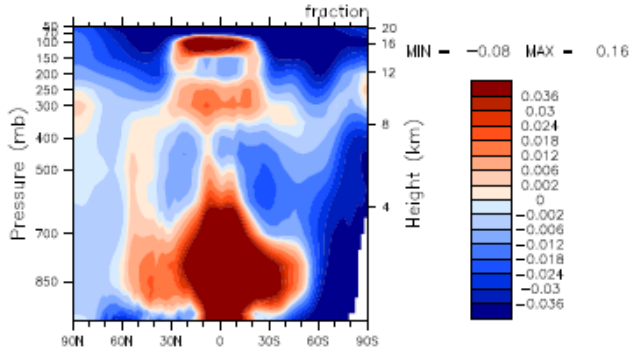
O_3





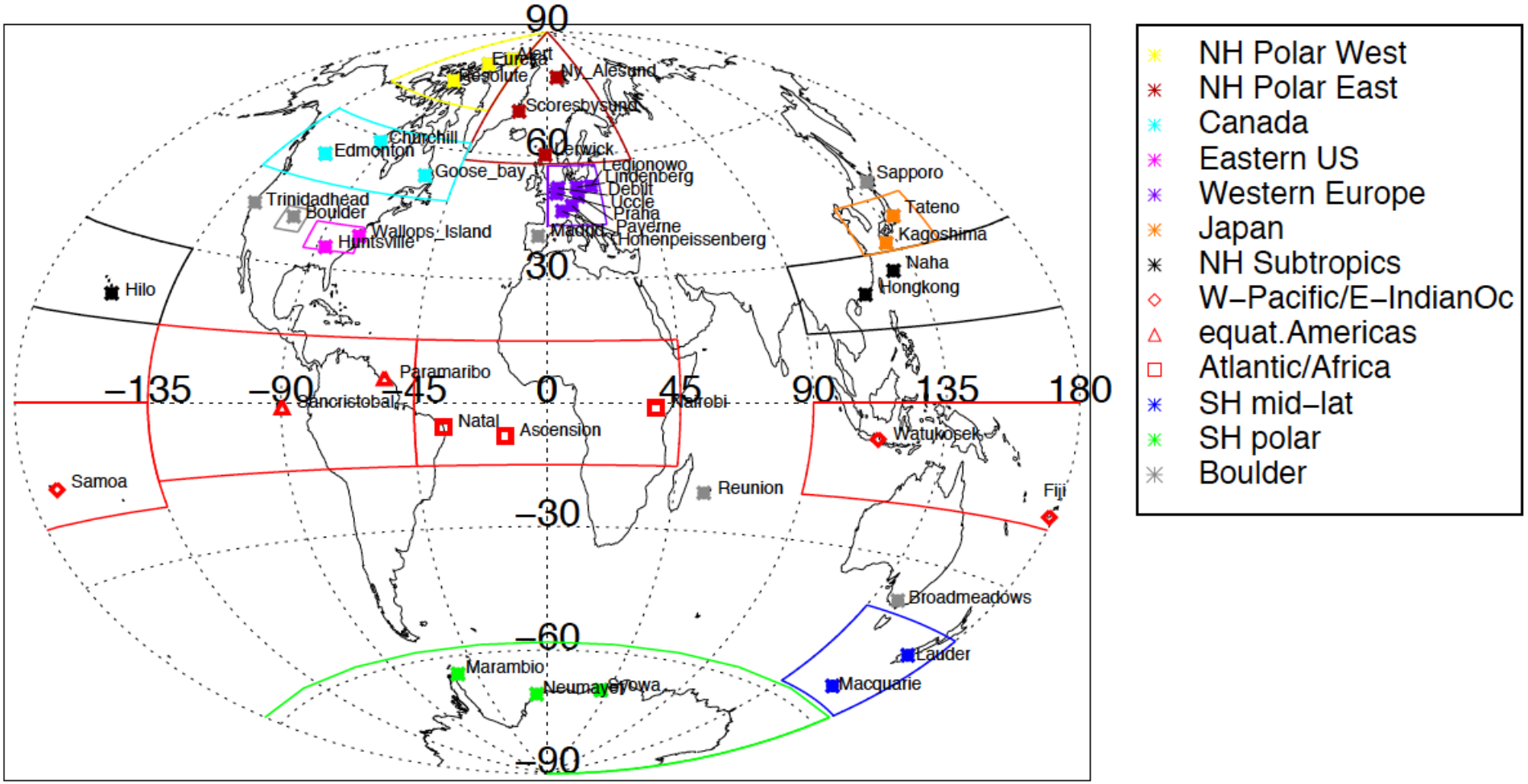
NO_x/NO_y





SD and online results are different!!! Differences in meteorology important.

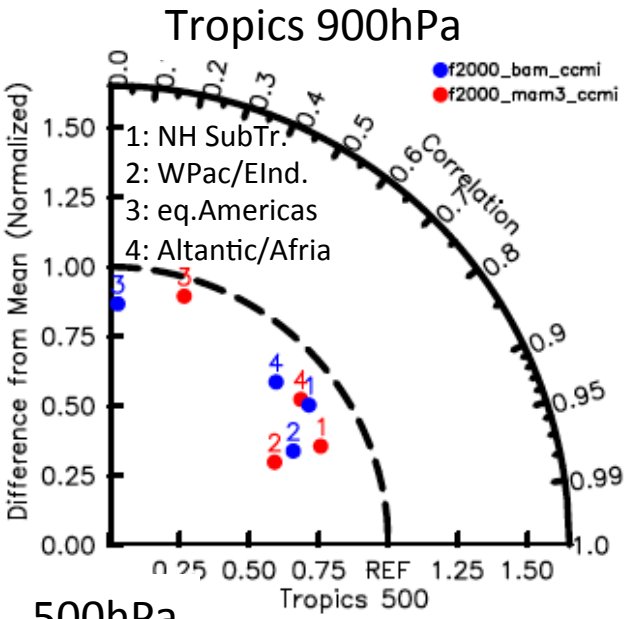
Comparisons with Ozonesondes

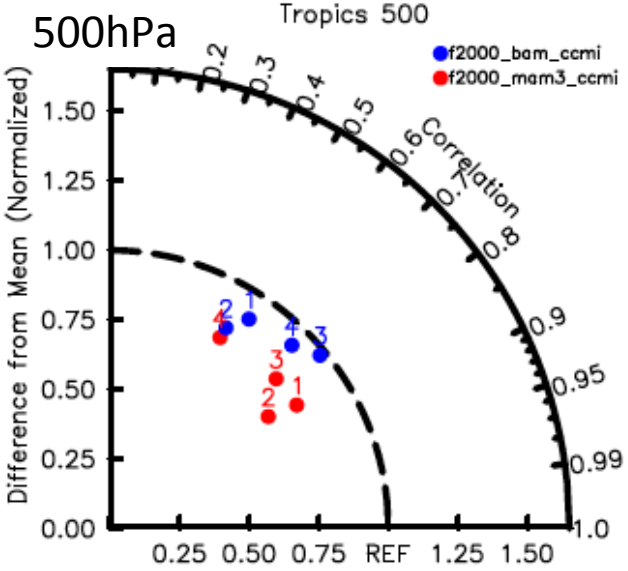


Tilmes et al., 2012

CAMChem-BAM
CAMChem-MAM3

Comparison to Ozonesondes

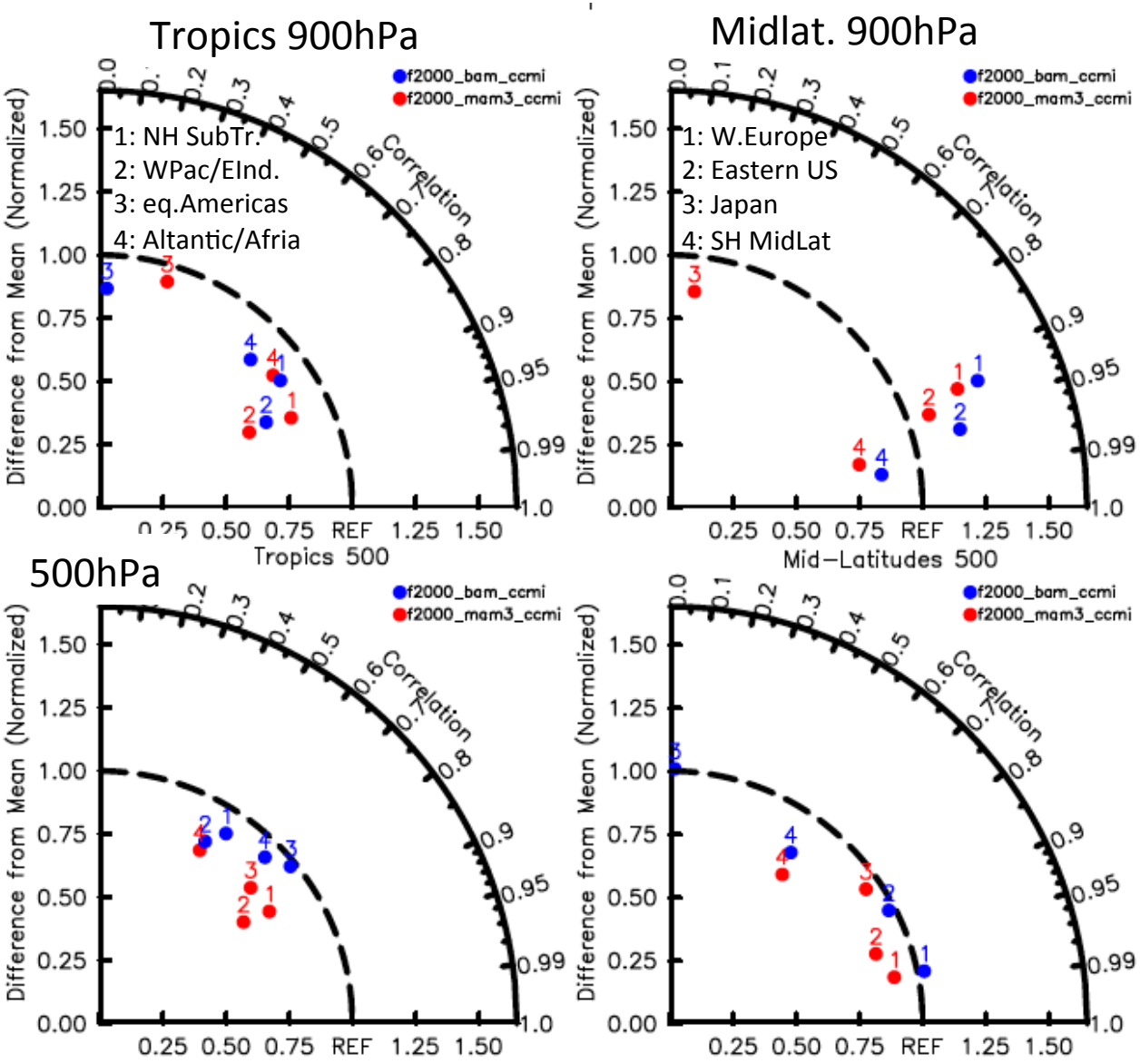




Differences from the mean

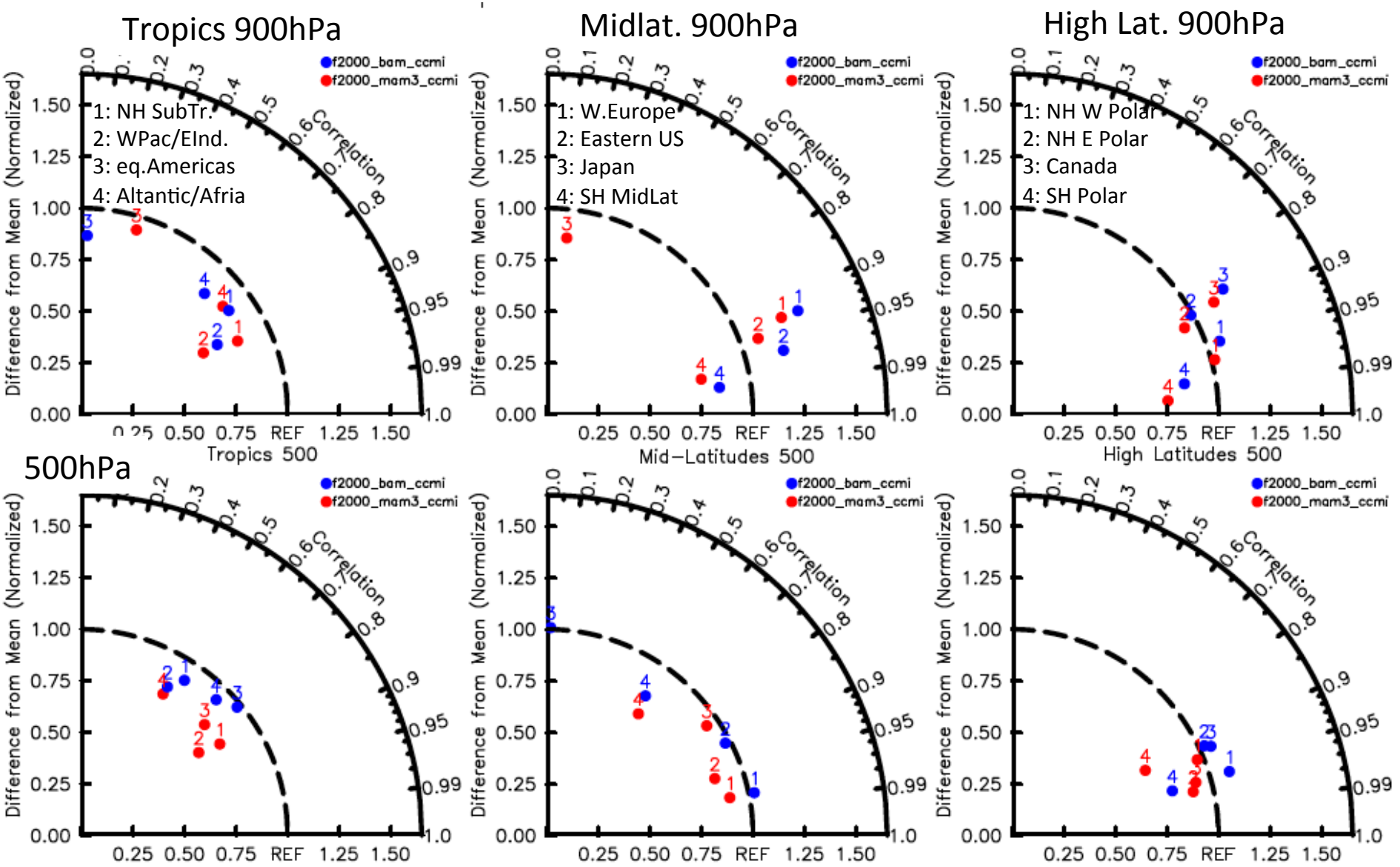
CAMChem-BAM
CAMChem-MAM3

Comparison to Ozonesondes



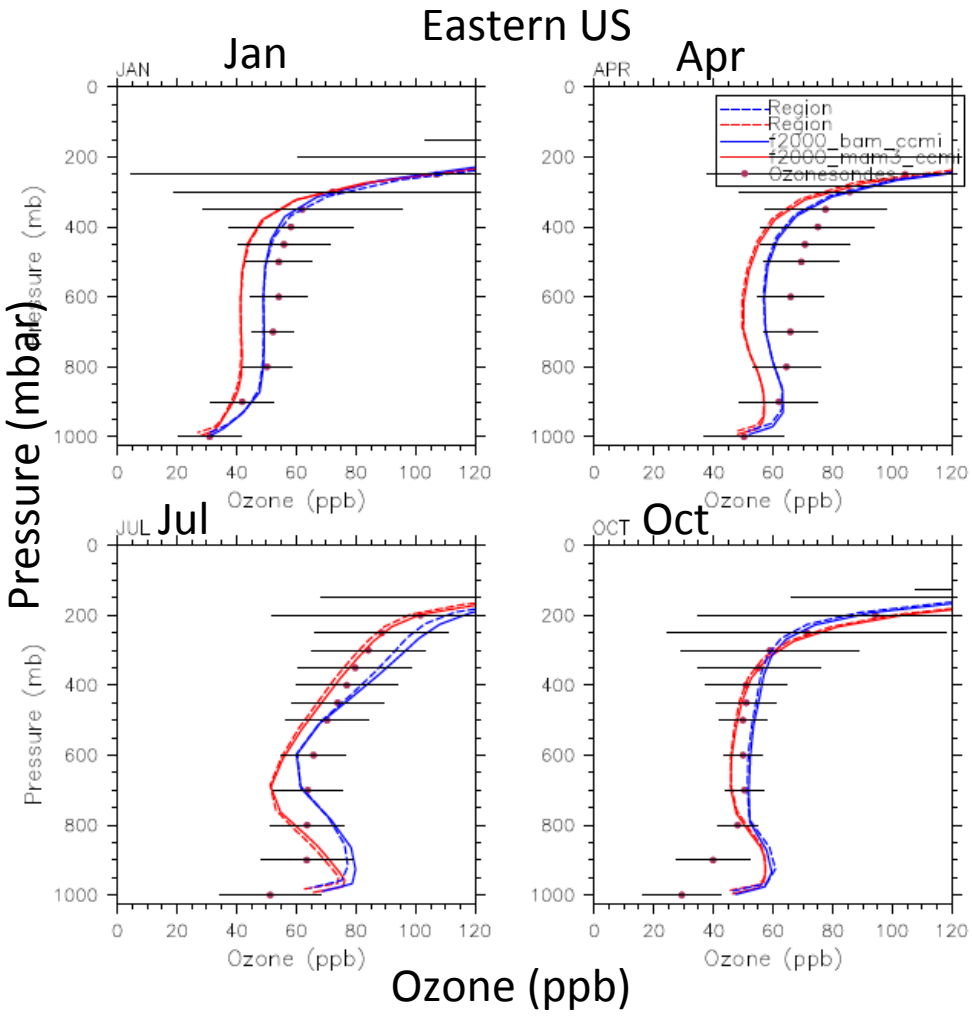
CAMChem-BAM
CAMChem-MAM3

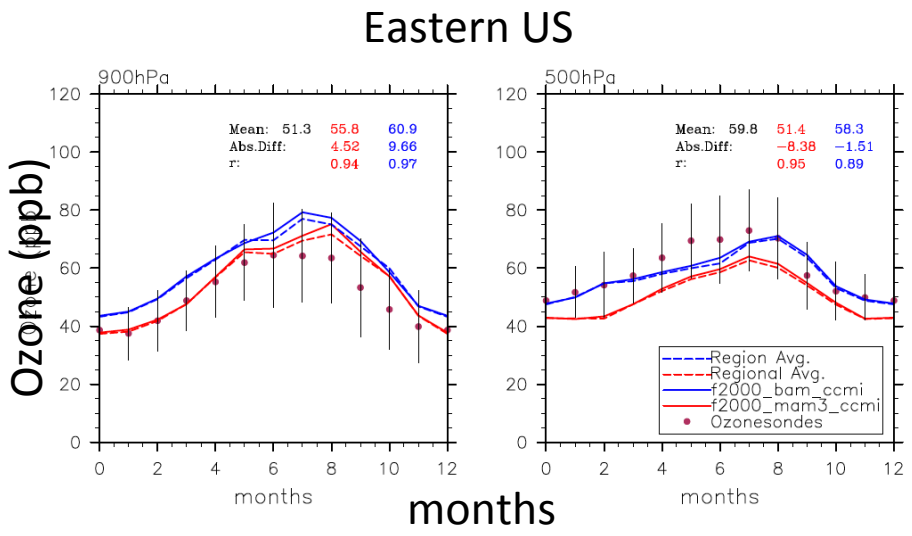
Comparison to Ozonesondes



CAMChem-BAM
CAMChem-MAM3

Comparison to Ozonesondes





CAM5-MAM3:

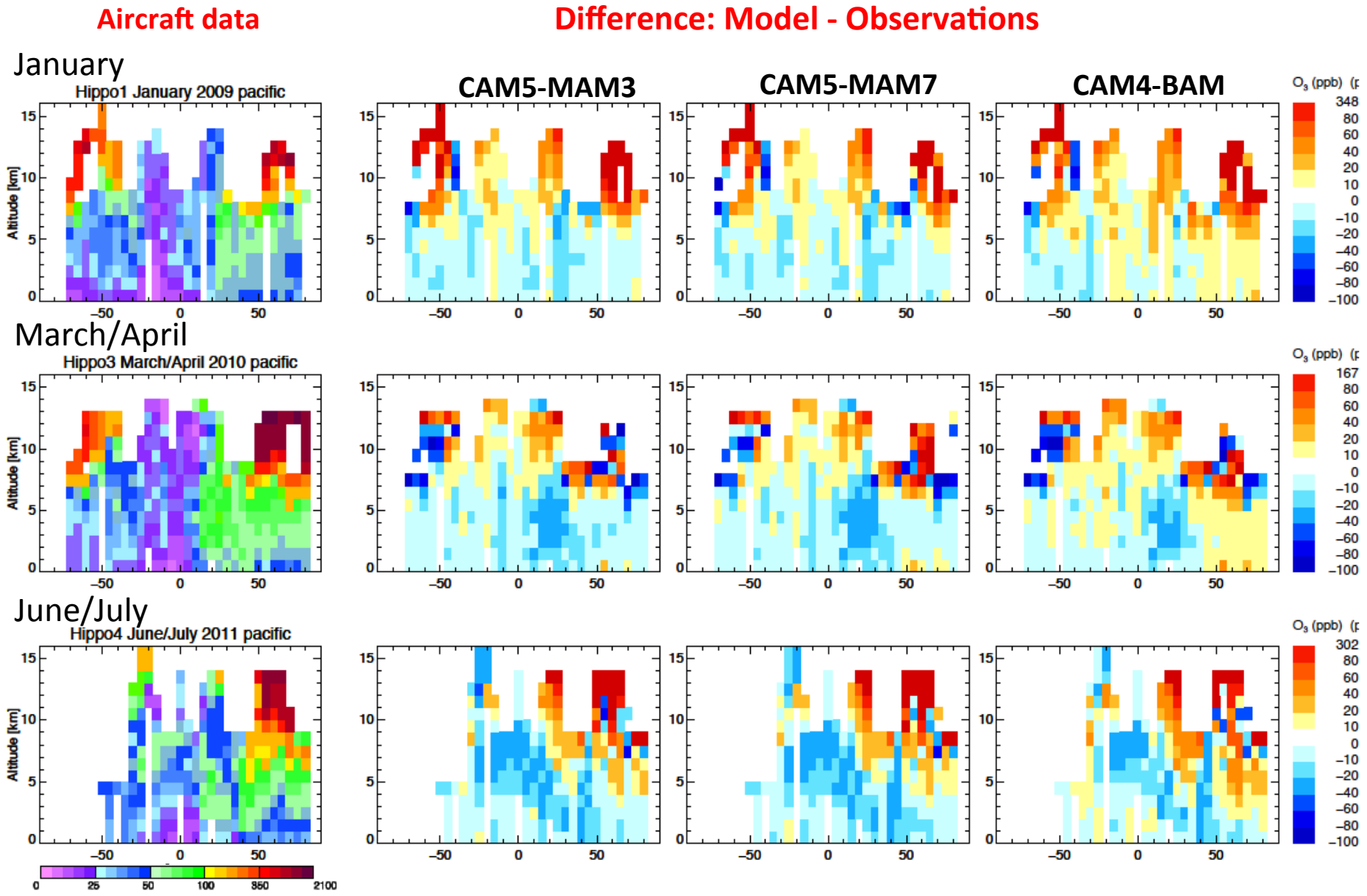
- Improvement of high bias at 900hPa,
- Slightly smaller in the troposphere

Comparisons with HIPPO

Flight paths for all five Missions

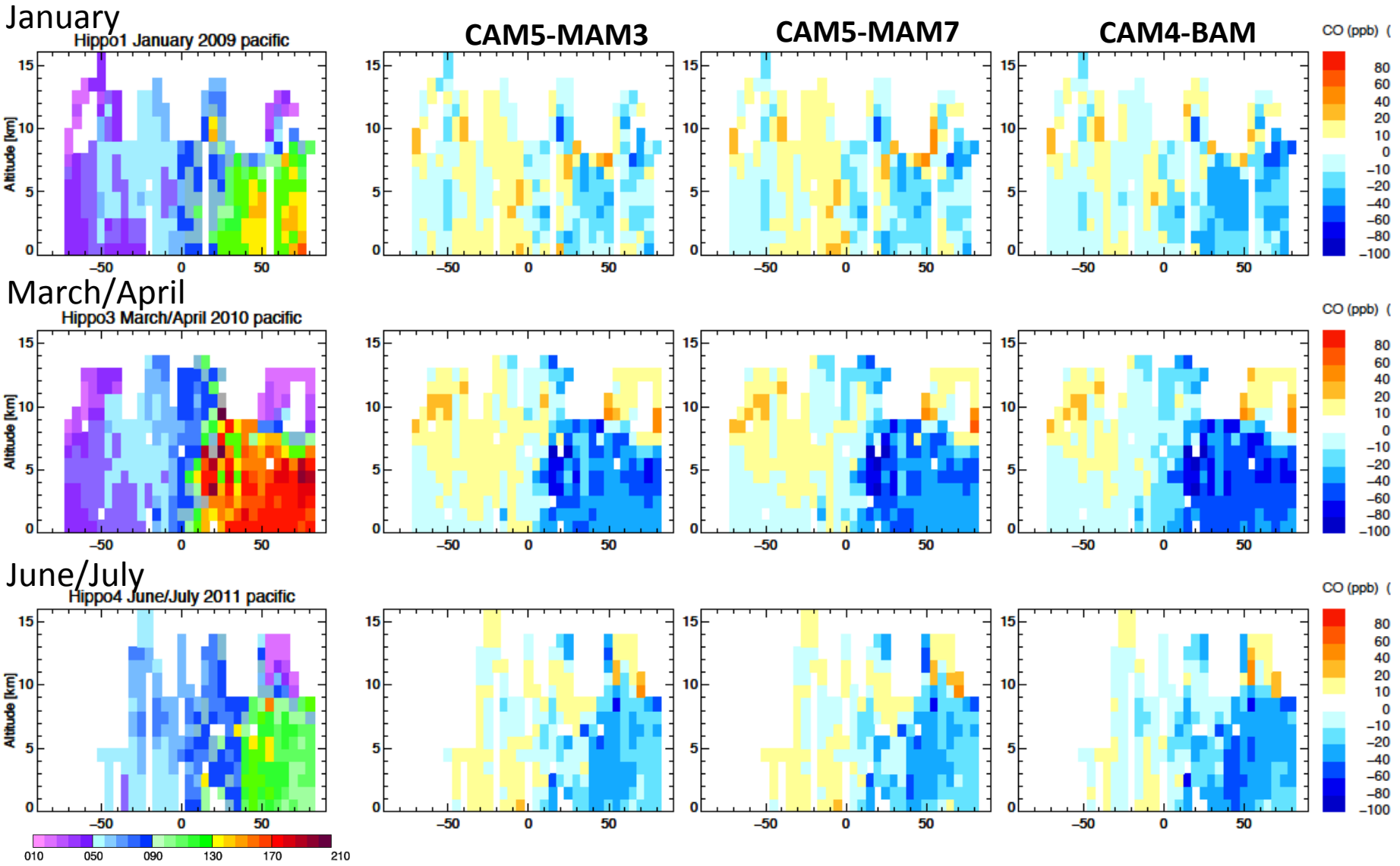
HIPPO1: January 2009
HIPPO2: November 2009
HIPPO3: March/April 2010
HIPPO4: June/July 2011
HIPPO5: August/Sep 2011

Climatological Comparison to HIPPO: Ozone

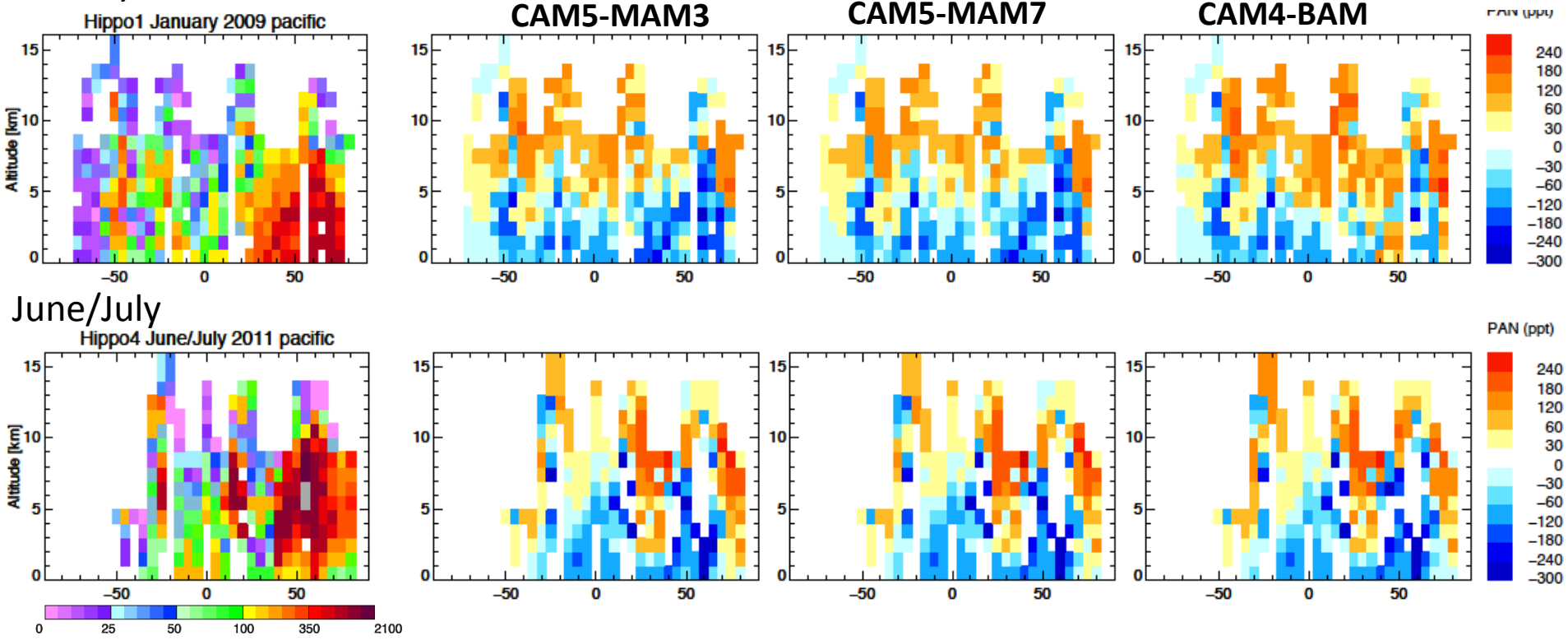


Climatological Comparison to HIPPO: CO

Aircraft data | **Difference: Model - Observations**



Climatological Comparison to HIPPO: PAN



Climatological Comparison to HIPPO: BC

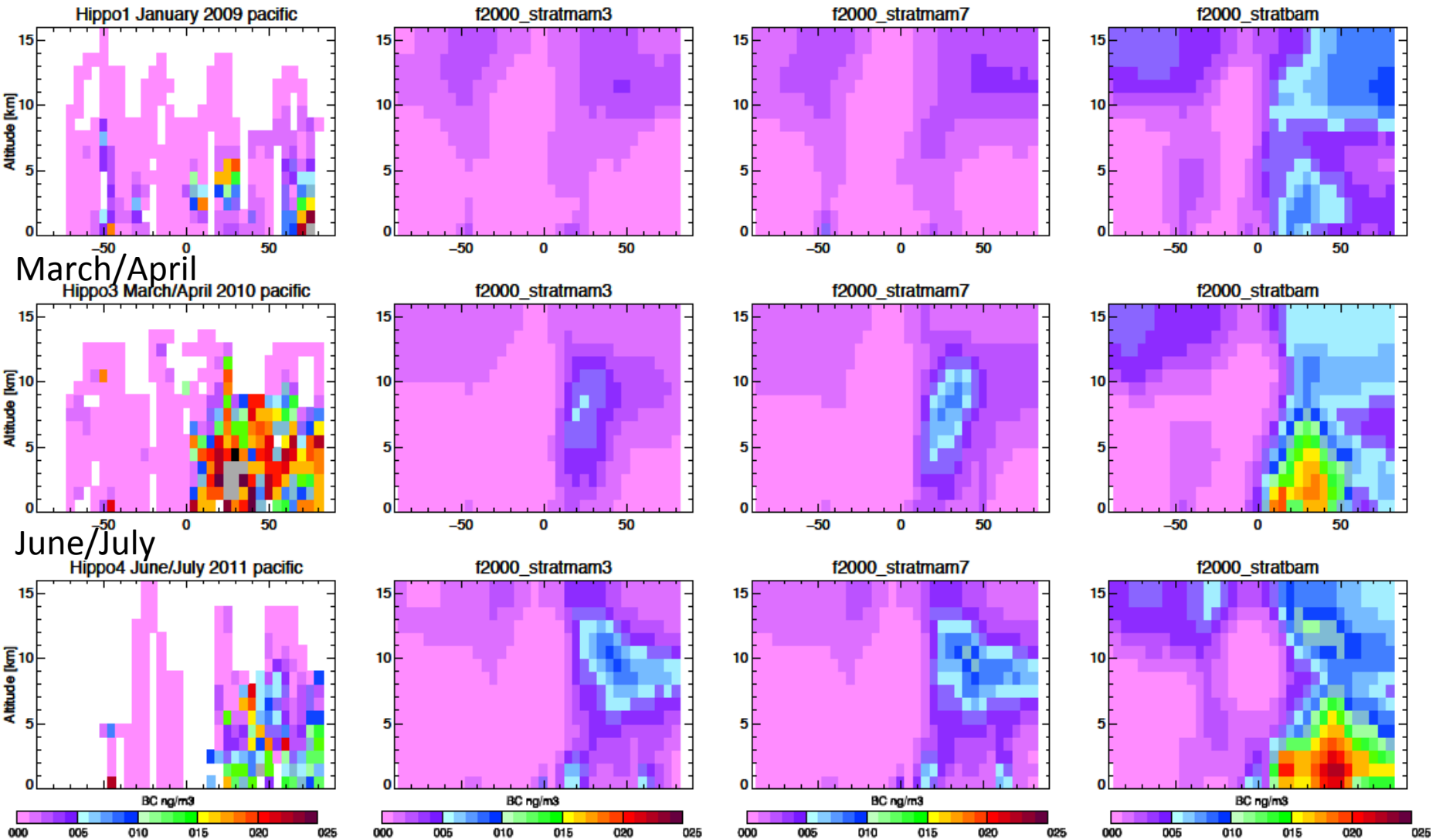
Aircraft data

Model Results

January

March/April

June/July



Summary/Conclusions

Modal Aerosol Model (MAM3/7):

- SAD calculation based on particles denoted to the Aitken mode, including sea salt -> large SAD
- NH_4NO_3 is not included yet, SOA not coupled

Consequences for the chemistry:

- Increased heterogeneous reactions, change in NOx/NOy,
- Decrease in OH, CH_4 lifetime, PAN, increase in CO

Comparison to observations:

- Ozone in CAM5-MAM slightly low in the troposphere
- PAN too low at the surface, too high in the upper troposphere
- BC too high in the stratosphere (add BC fix?)
- Not all HIPPO data might be suited for climatological comparison