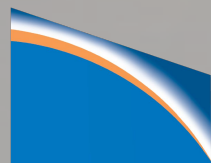


A Comparison Between the MOZART-T1S and MOZART-T4S Chemical Mechanisms

Shawn Honomichl, Simone Tilmes, and Rebecca Buchholz

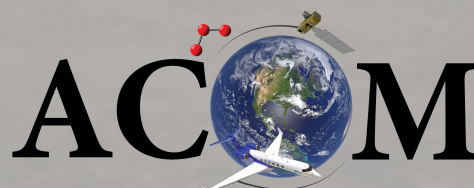
AMWG Winter Meeting

5 February, 2024



NCAR

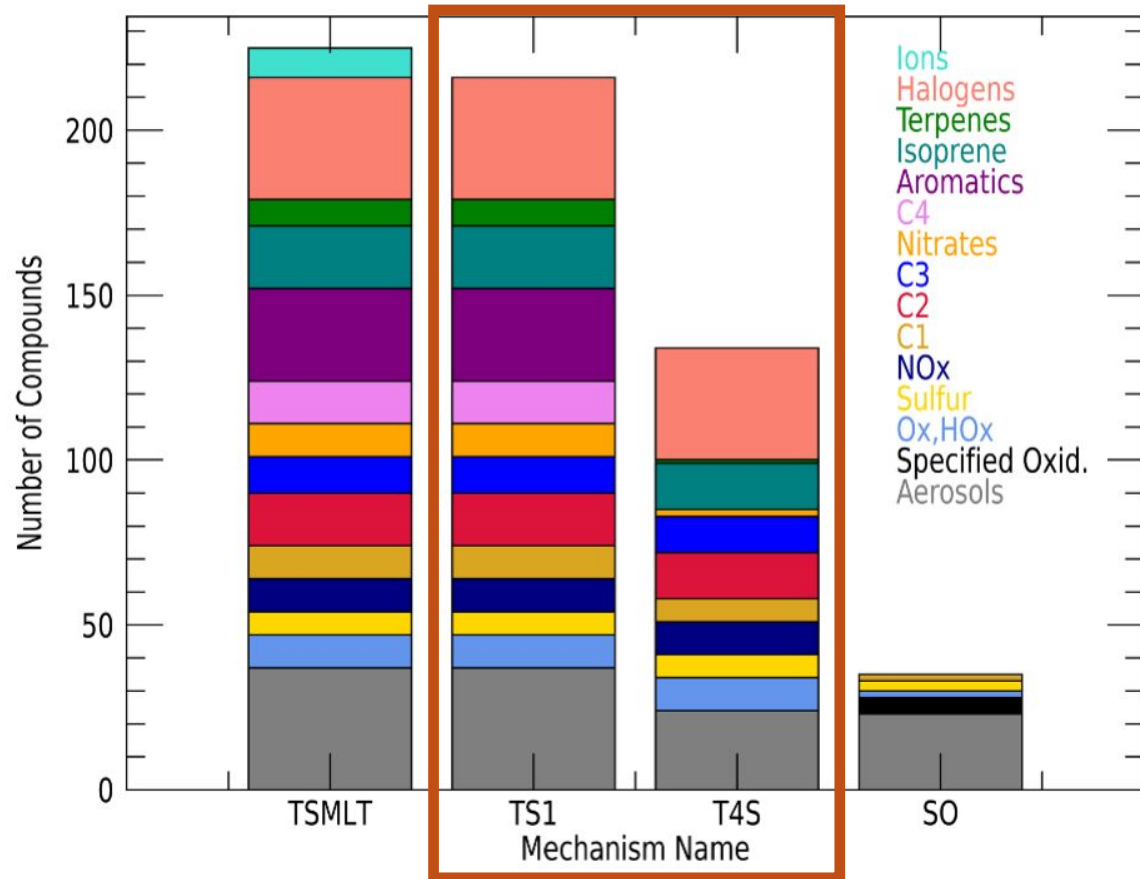
NATIONAL CENTER FOR ATMOSPHERIC RESEARCH



Atmospheric Chemistry Observations & Modeling Lab

Chemical Mechanisms

Compounds in CESM Mechanisms



| Name | Description | # tracers | # reactions |
|---------------------|--|-----------|-------------|
| T1MA (TSMLT) | T1 with stratosphere, mesosphere, lower thermosphere chemistry | 234 | 583 |
| T1S (TS1) | T1 with comprehensive stratospheric chemistry and full sulfur chemistry | 231 | 528 |
| T4S | T4 with comprehensive stratospheric chemistry, no odd F, C>3 hydrocarbons simplified | 141 | 364 |
| SO | Specified Oxidants, with GHGs | 31 | 12 |

- Expectation for T4S Compared to T1S:
 - Lower cost
 - Faster running simulations
 - Similar chemistry, budgets, & biases.

- T4S may be a better choice if Bullet 1 holds true & you don't need the species that are excluded.

Model Setup

3 Different Model Runs (T1S, T4S, T4Sr2)

Setup (T1S/T4S):

- CESM Tag: **cesm3_0_beta02**
- Free Running
- ne30.pg3
- Mid Top (80 km top)
- 93 Vertical Levels
- CAM7 Physics
- MAM5 Aerosols
- 1980– 2015 (1995-2011)

Setup (T4Sr2 Run):

- Same as the other setup with following exception:
 - CESM Tag: **cesm3_0_beta04**
 - **Updated Dust Tuning**
 - **Moving Mountain GW Scheme**

Timing, Costs, and Stability

Timing (T1S/T4S):

- T1S: 2.7 simulated years per day on 26 nodes
- 2.75 sim yrs/day on 28 nodes (Default)
 - 31876 pe-hrs/simulated_year
- T4S: 3.9 simulated years per day on 24 nodes
- 4.0 sim yrs/day on 26 nodes (Default)
 - 18569 pe-hrs/simulated year

T4S ~ 1.4 times faster than T1S

Timing (T4Sr2):

- 4.0 sim yrs/day on 26 nodes
19930 pe-hrs/simulated year

Stability (T1S/T4S):

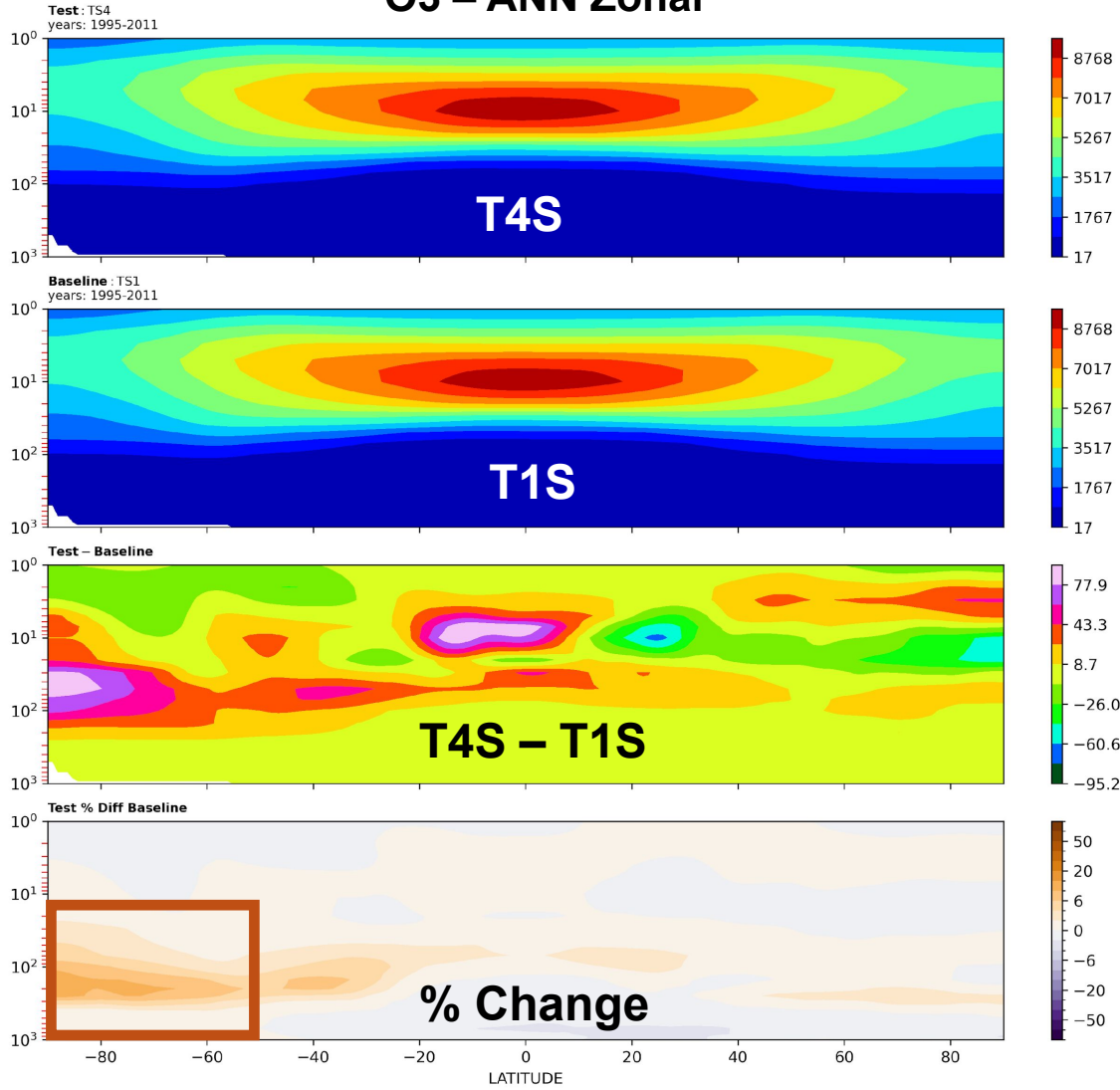
- No stability issues on T1S run
- Had to adjust time step (se_nsplitt) a couple of times on the T4S run

Stability (T4Sr2):

- No major stability issues.
 - More stable than the other T4S run

Ozone – Climatology (1995-2011)

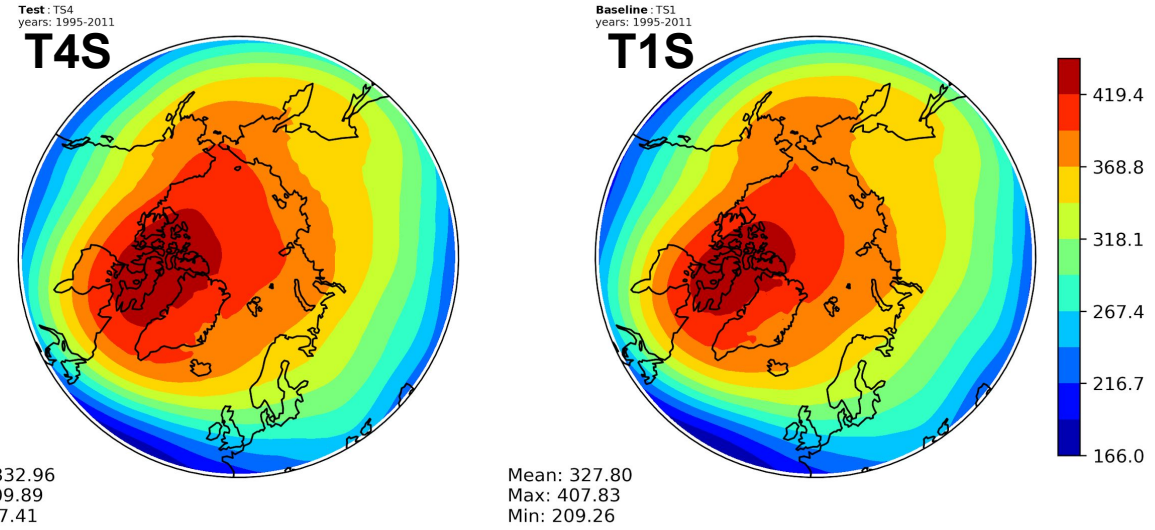
O3 – ANN Zonal



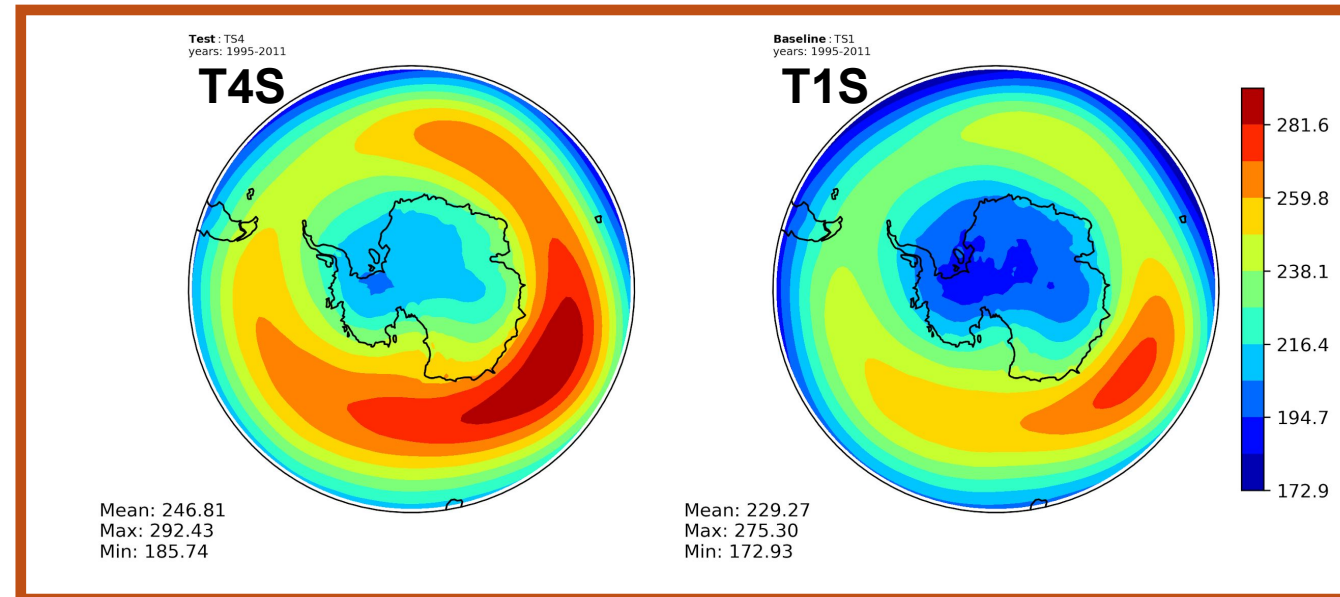
Largest deviation in the southern hemisphere polar UTLS.

- T4S about 17 ppbv (10%) higher

O3 – 200 hPa – ANN – NH Polar



O3 – 200 hPa – ANN – SH Polar

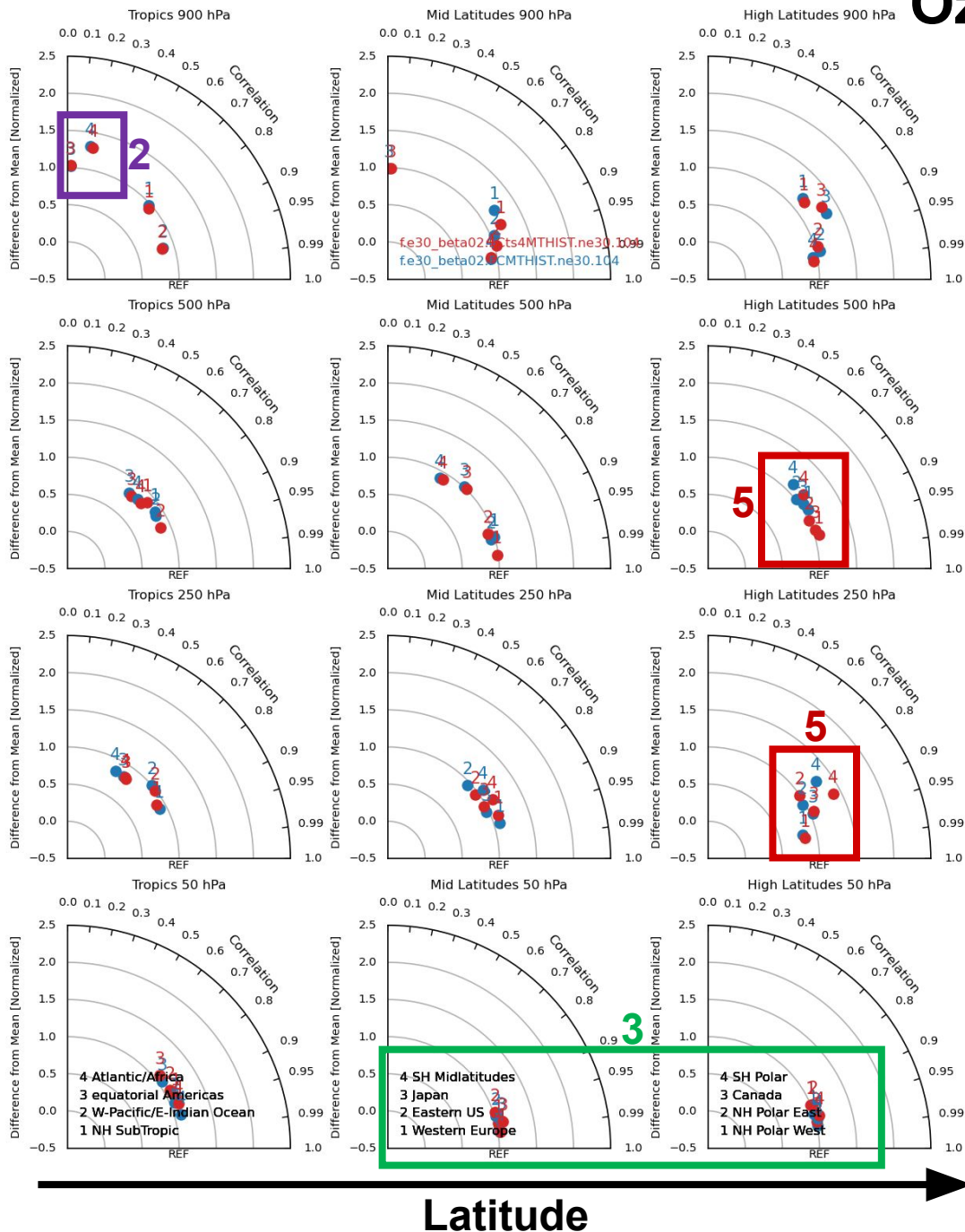


Ozone – Taylor Diagrams

- Left to right: Tropics, Mid Lat, High Lat
- Top to Bottom: 900, 500, 250, and 50 hPa

- Red Dots: T4S
- Blue Dots: T1S

1. Correlations increase with altitude.
2. Worst correlations: **low level tropics**
3. Best correlations: **Mid/High latitude stratosphere**
4. T1S & T4S similar placements.
5. SH Polar: **T4S correlation slightly higher than T1S at 50 and 250 hPa**

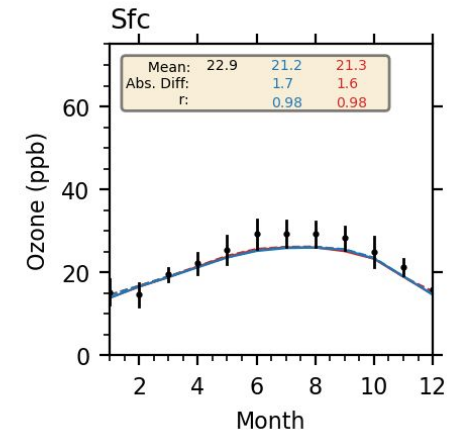
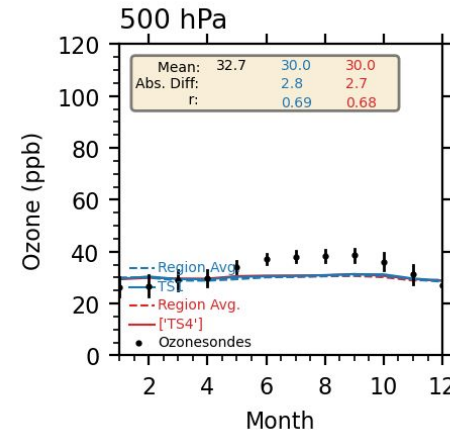
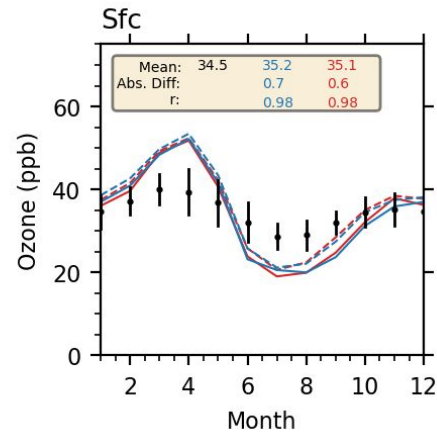
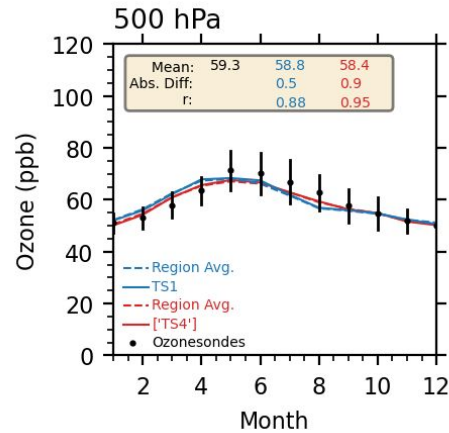
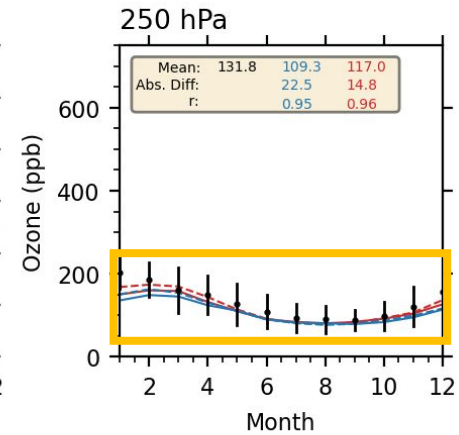
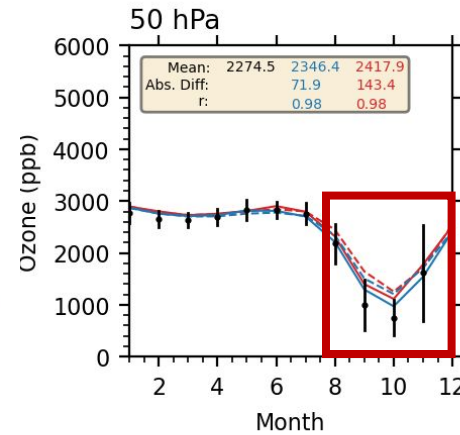
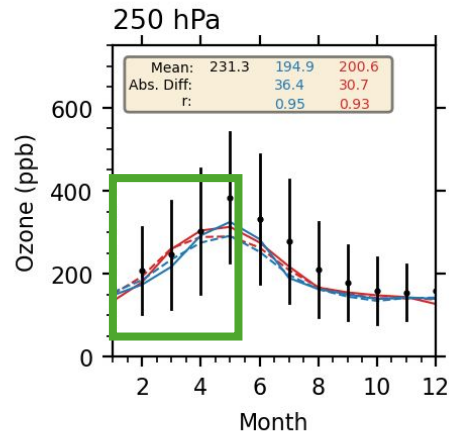
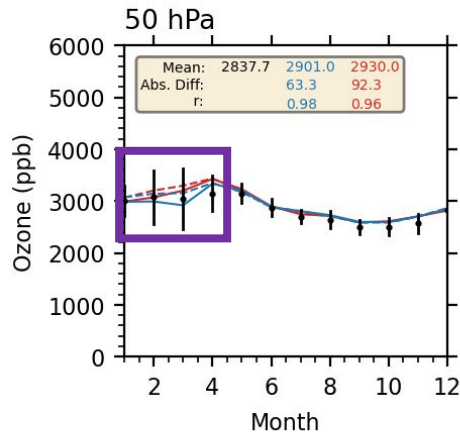


Solid: Point Avg
Dashed: Regional Avg

Ozone – Seasonal Cycle

NH Polar

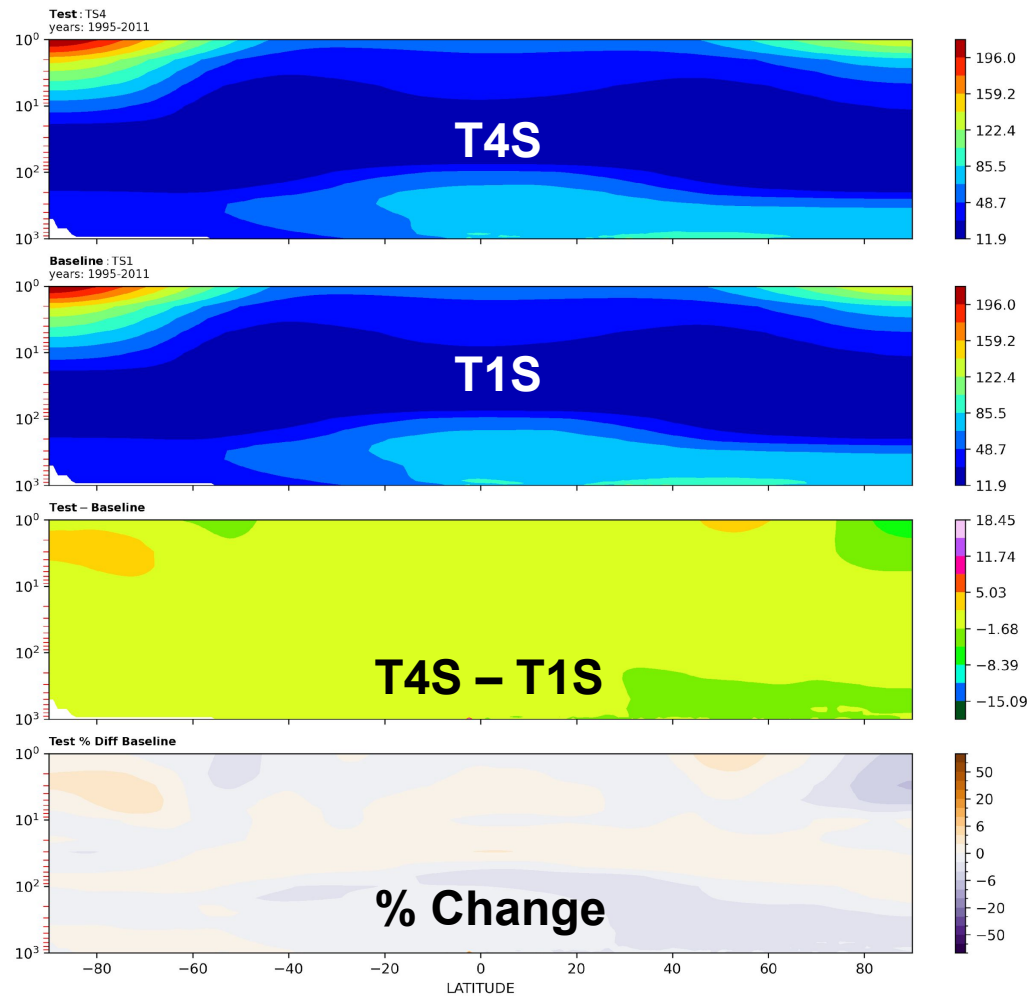
SH Polar



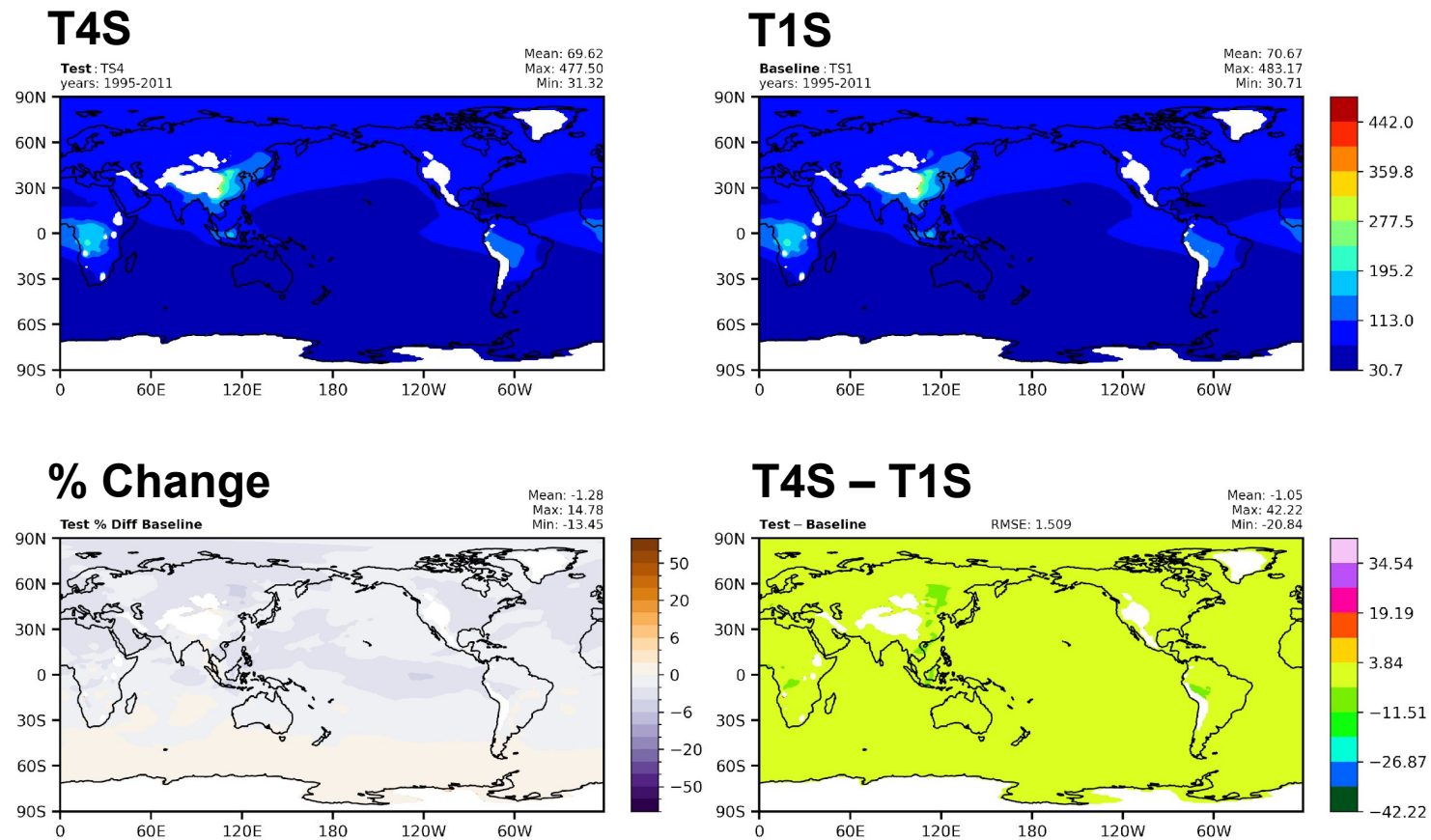
- SH lower stratosphere departure occurs primarily in SH summer months.
- Other notable areas:
 - NH 50 hPa early part of year.
 - NH 250 early part of year.
 - SH 50 hPa end of year.

Carbon Monoxide

CO – ANN Zonal



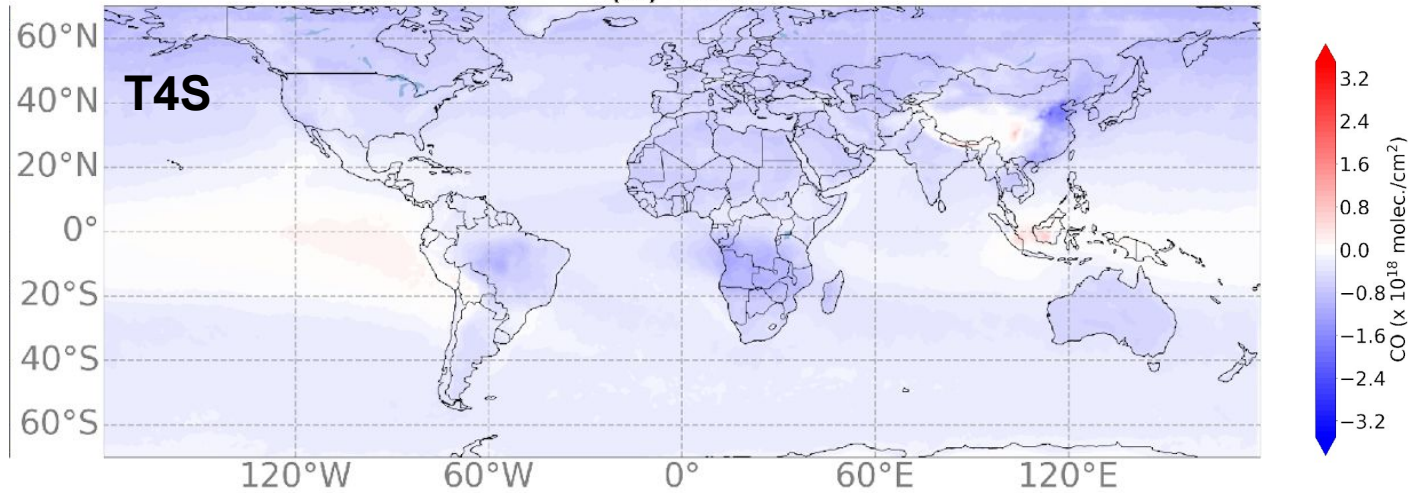
CO – 850 hPa ANN Map



No Significant differences in CO!

Carbon Monoxide – Total Column Difference from MOPITT

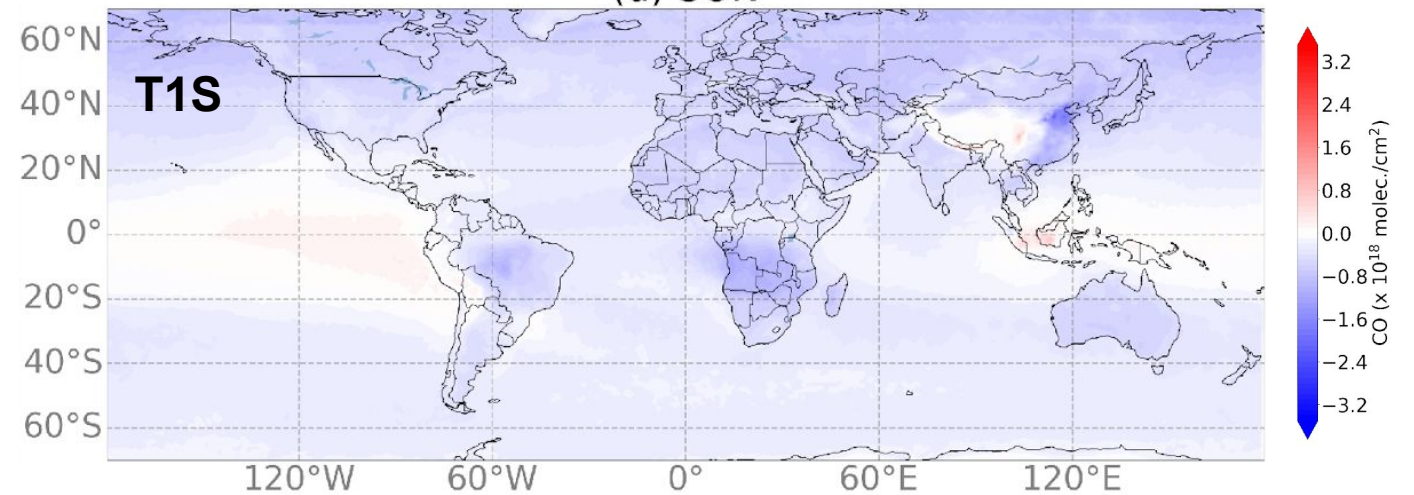
(d) SON



Longitude

Model - MOPITT

(d) SON



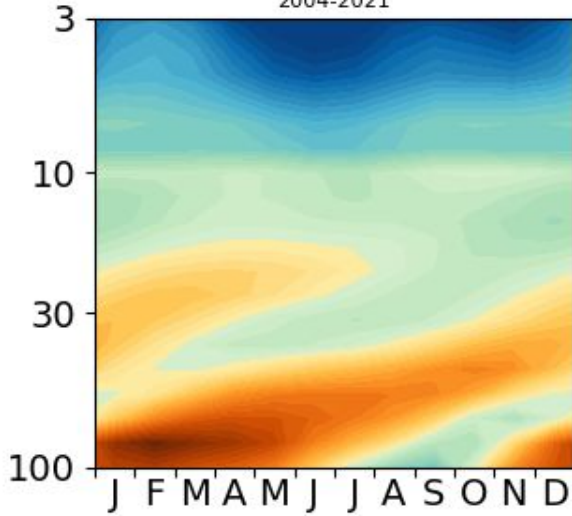
Longitude

**CO low bias on both the T4S
and T1S runs**

Tape Recorder

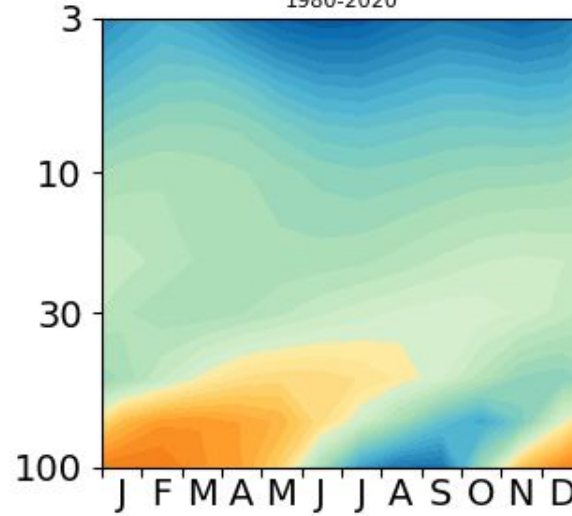
MLS

2004-2021



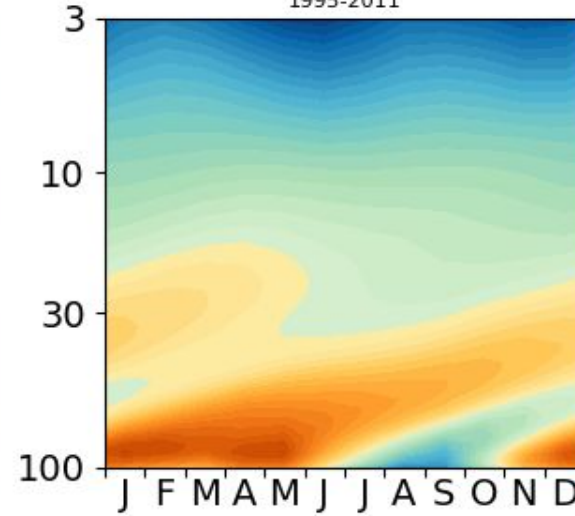
ERA5

1980-2020



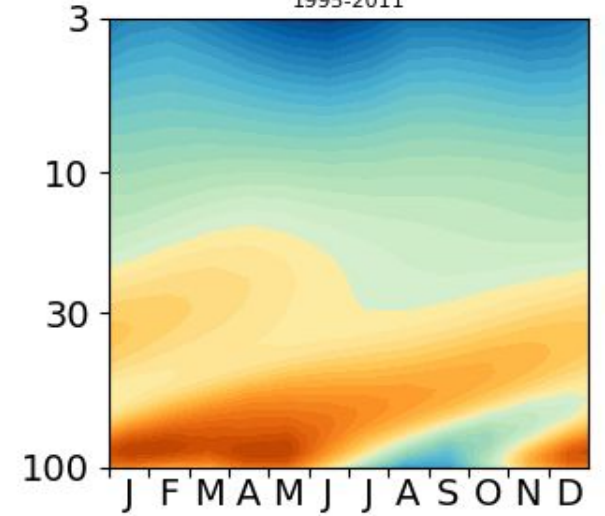
T4S

1995-2011



T1S

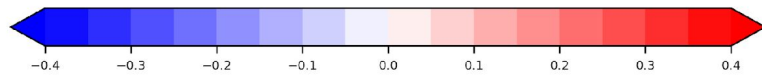
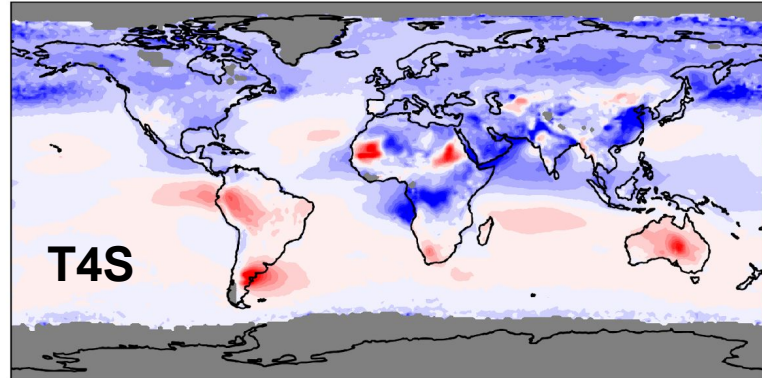
1995-2011



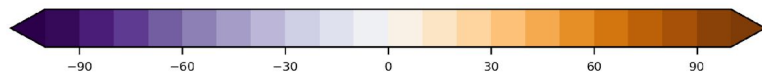
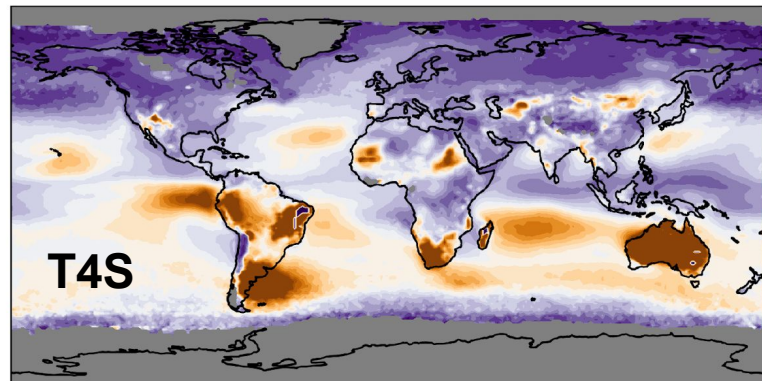
T4S & T1S No Major Differences

AOD – Compared to MODIS

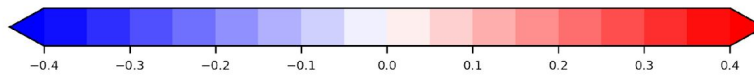
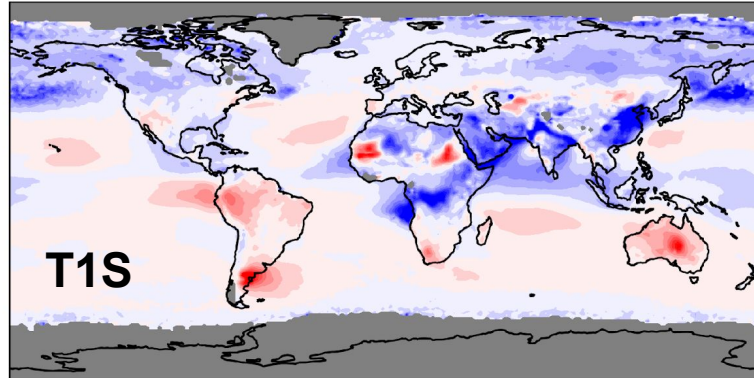
Model – MODIS, JJA



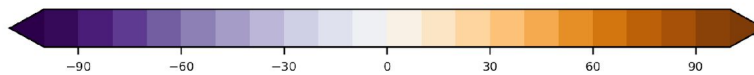
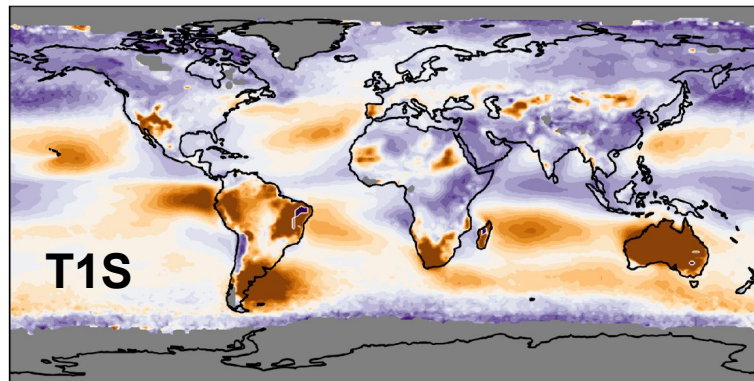
Percent Diff TS4 - TERRA MODIS
AOD 550 nm - Jun-Jul-Aug Mean -20



Model – MODIS, JJA



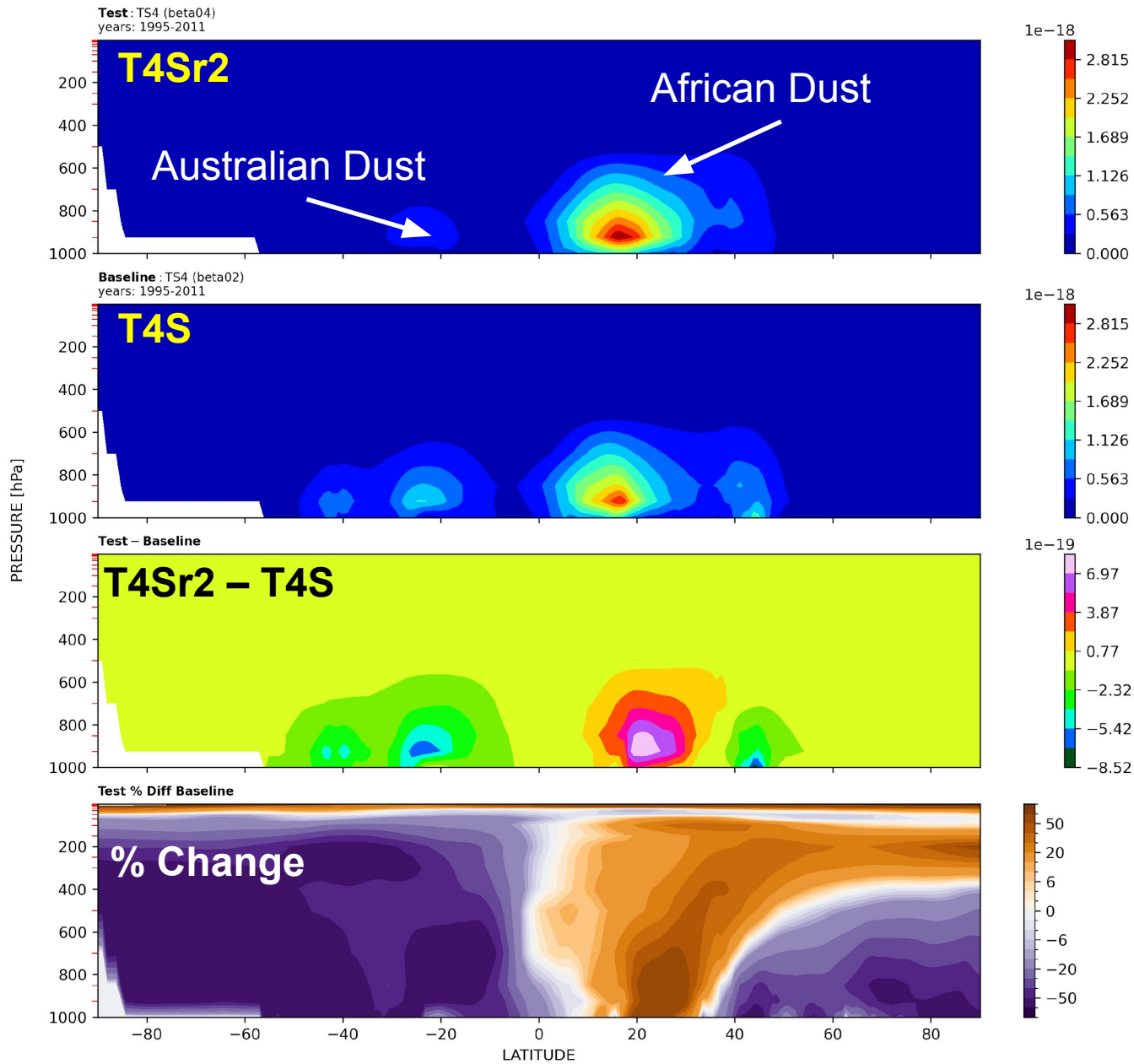
Percent Diff TS1 - TERRA MODIS
AOD 550 nm - Jun-Jul-Aug Mean -7.3



- No major difference between T4S and T1S.
- Low bias in NH
- High bias in SH

T4Sr2 – Dust (dst_a1)

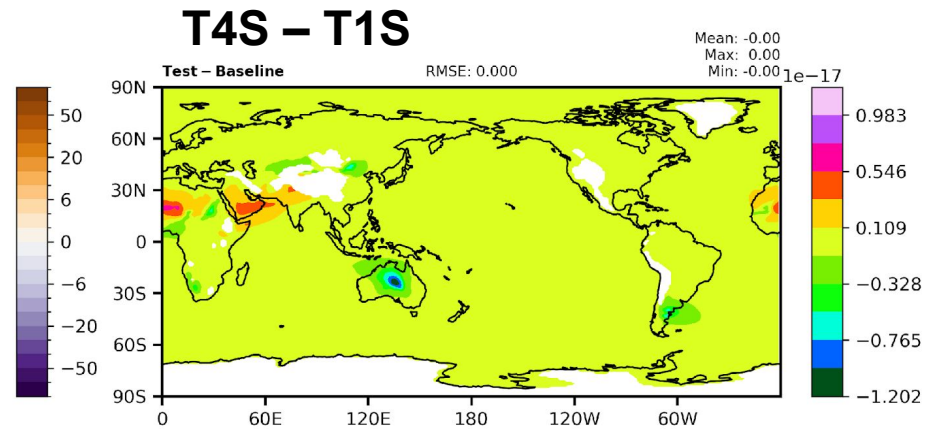
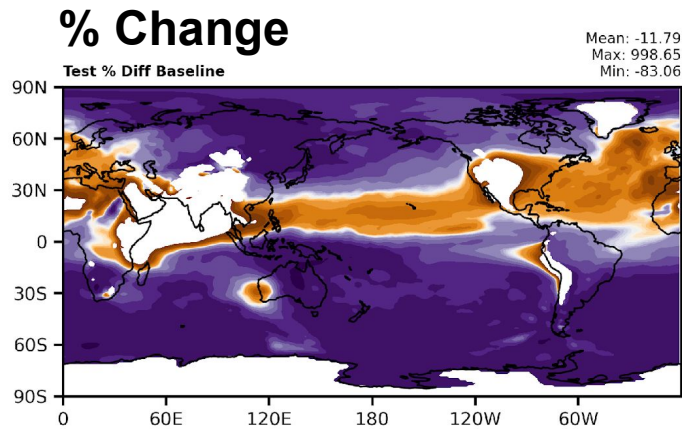
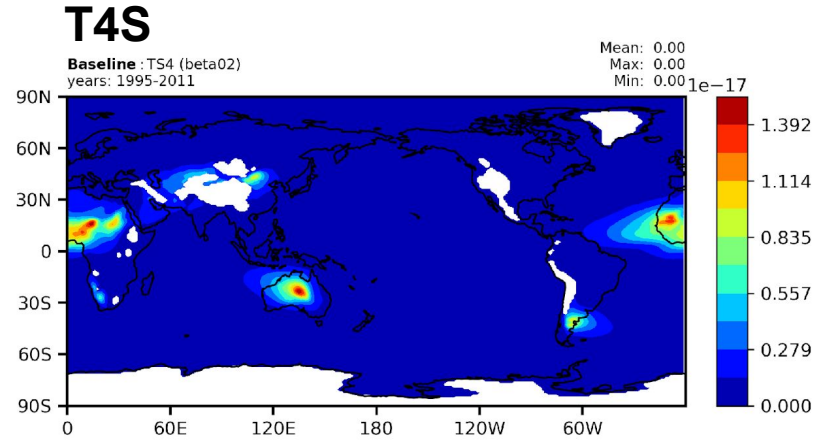
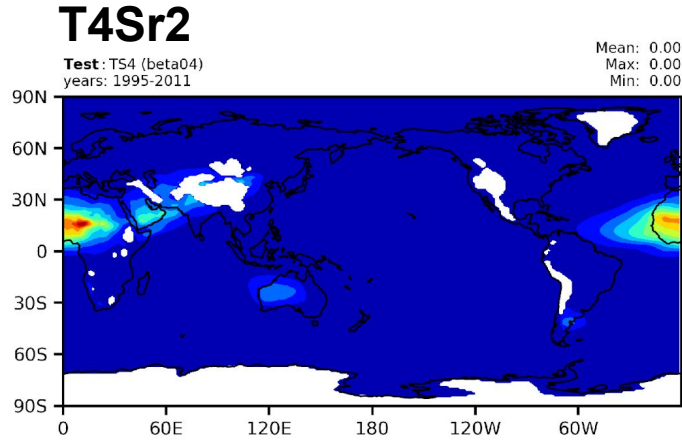
dst_a1 – ANN - Zonal



- Reminder: T4Sr2 contains updated dust tuning.
- A little more dust in NH around 20N lat
- Less elsewhere.

T4Sr2 – Dust (dst_a1)

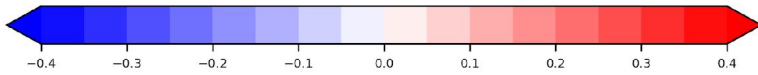
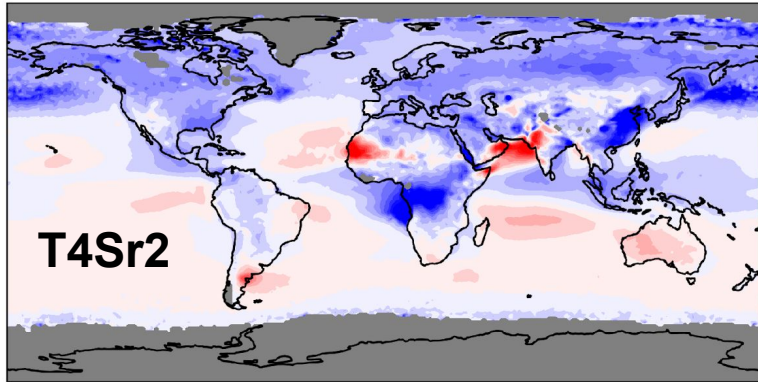
dst_a1 – 850 hPa - ANN - Map



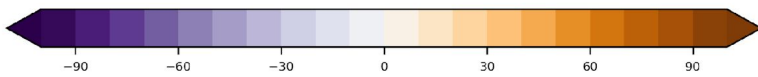
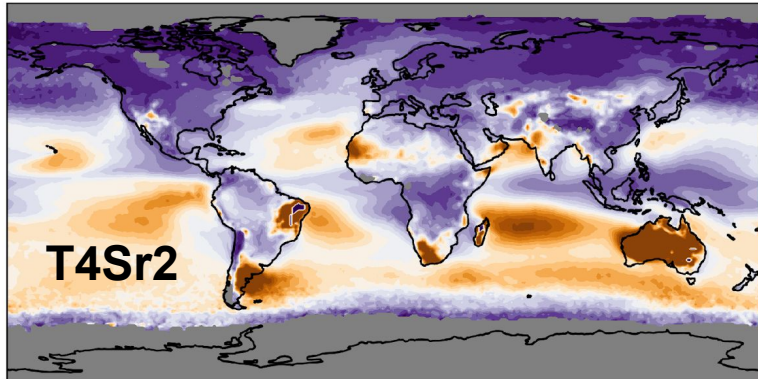
- More African Dust
- Less Australian Dust
- NH low/mid latitudes higher
- Elsewhere lower

T4Sr2 - AOD

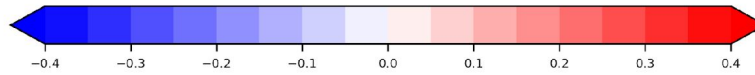
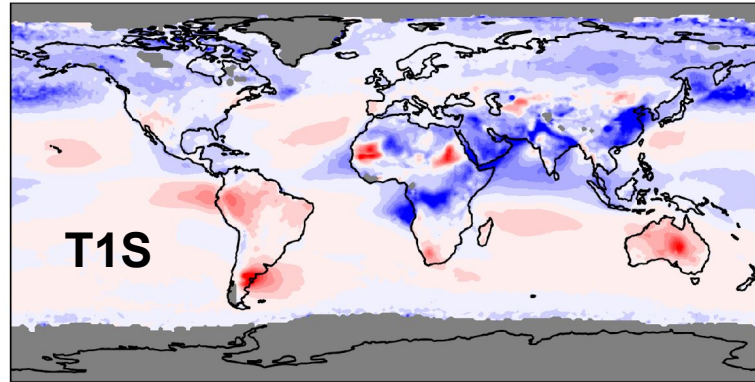
Model – MODIS, JJA



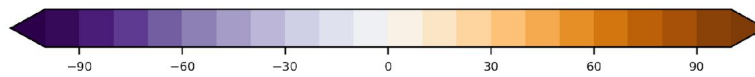
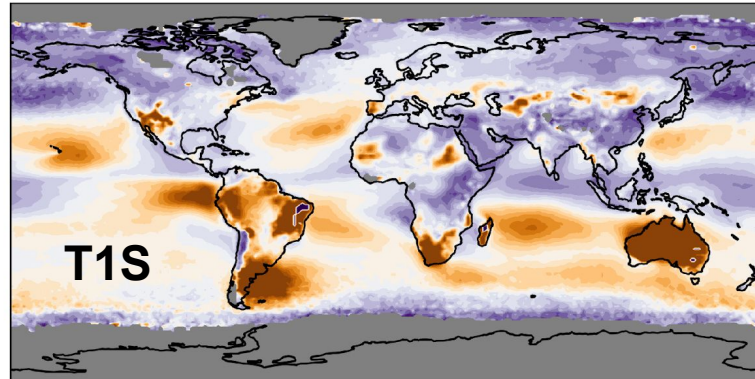
Percent Diff TS4 - TERRA MODIS
AOD 550 nm - Jun-Jul-Aug Mean -22



Model – MODIS, JJA



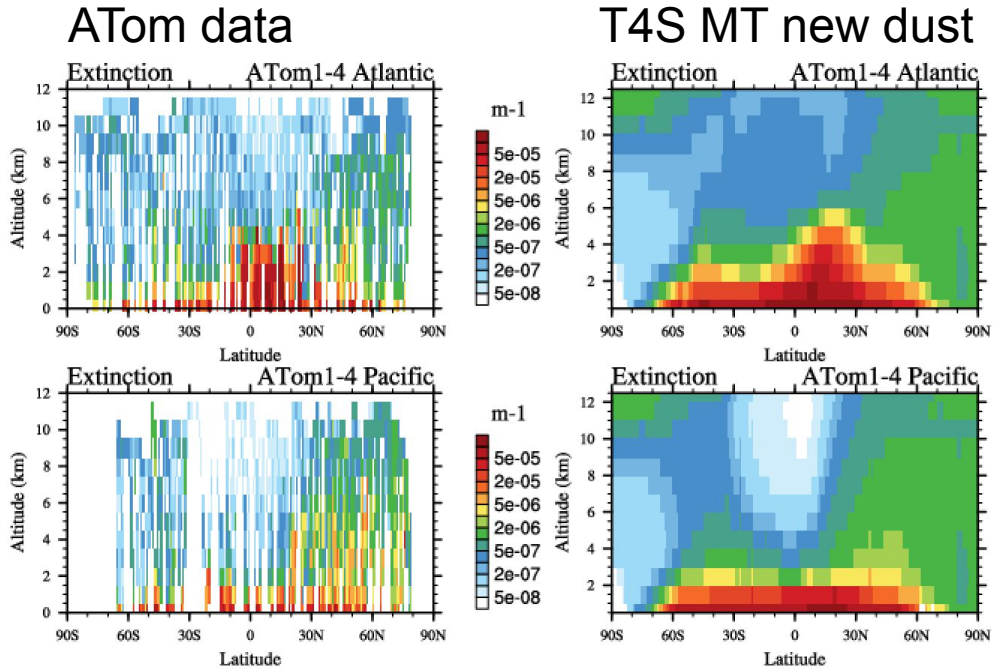
Percent Diff TS1 - TERRA MODIS
AOD 550 nm - Jun-Jul-Aug Mean -7.3



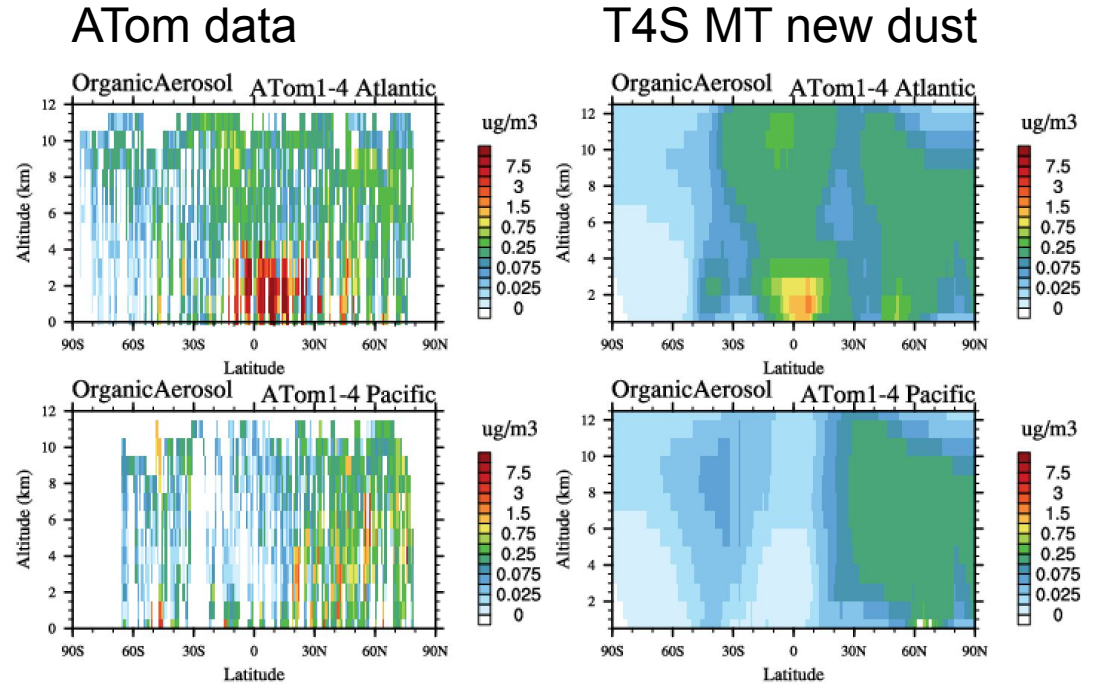
- T4Sr2 more significant low bias in NH.
- T4Sr2 SH high bias reduced

T4S MT performance: Comparisons to Aircraft Data

Extinction



Organic Aerosol

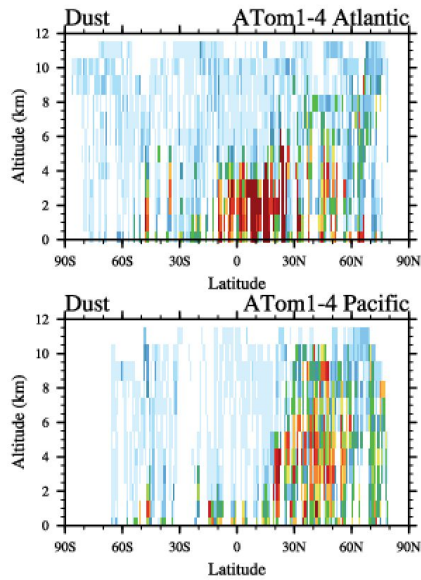


- Extinction is reasonable, some underestimation over the Pacific mid- to high latitudes
- Underestimation of Organic Aerosol (possible due to reduced biogenetic precursor emissions)

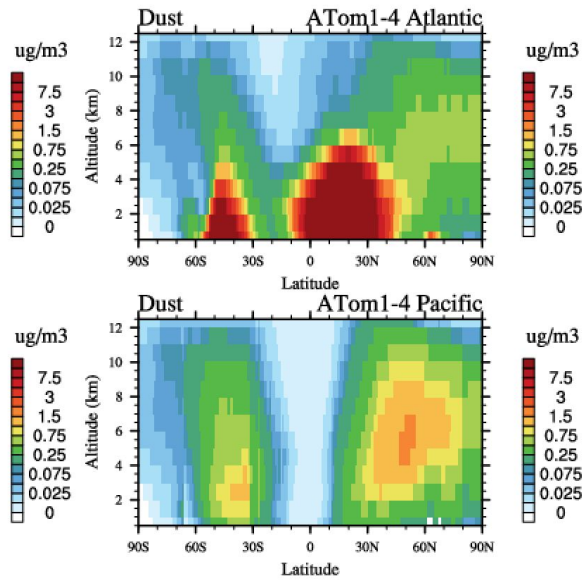
T4S MT performance: Comparisons to Aircraft Data

Dust

ATom data

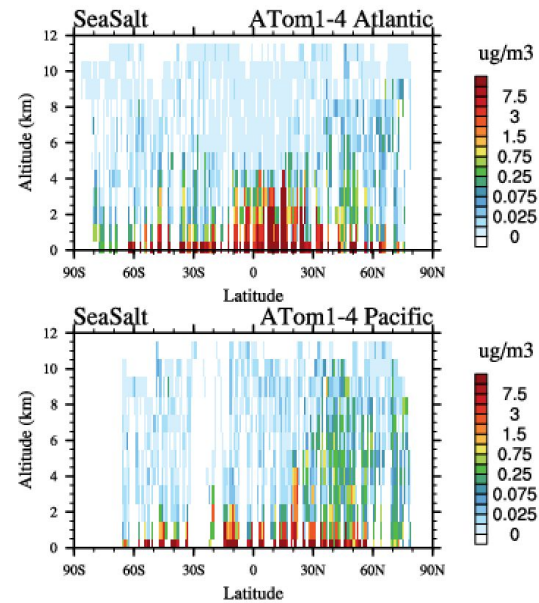


T4S MT new dust

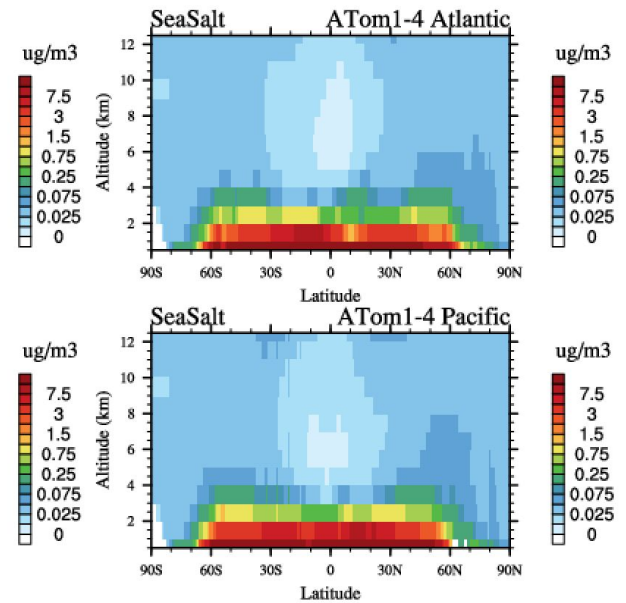


SeaSalt (factor 1.0)

ATom data



T4S MT new dust



- Dust has improved, but still a bit high compared to observations
- SeaSalt (using tuning factor 1.0) is reasonable

Budget Tables

| Variable | T1S | T4S (% diff) | T4Sr2 (% diff) |
|------------------------|--------------|---------------------|-----------------------|
| O3_BURDEN (Tg) | 301.927 | 298.665 (-1%) | 294.549 (-2.4%) |
| O3_CHEM_LOSS (Tg/yr) | 3253.96 | 3190.16 (-2%) | 3066.2 (-6%) |
| O3_CHEM_PROD (Tg/yr) | 3786.55 | 3624.24 (-4%) | 3503.55 (-8%) |
| O3_LIFETIME (days) | 28.196 | 28.347 (0.5%) | 28.95 (2.6%) |
| O3_TEND (Tg/yr) | 395.981 | 377.67 (-4.7%) | 373.244 (-6%) |
| O3_STE (Tg/yr) | 260.995 | 280.272 (7%) | 276.641 (6%) |
| CO_EMIS (Tg/yr) | 766.079 | 765.452 (-0.1%) | 748.275 (-2.3%) |
| DUST_EMIS (Tg/yr) | 4180.63 | 4174.27 (-0.14%) | 3573.95 (-16%) |
| DUST_BURDEN (Tg) | 22.277 | 22.381 (0.47%) | 21.722 (-2.5%) |
| DUST_LIFETIME (days) | 2.332 | 2.344 (0.5%) | 2.613 (11.4%) |
| SALT_BURDEN (Tg) | 4.13 | 4.12 (-0.25%) | 5.295 (25%) |
| SOA_BURDEN (Tg) | 0.564 | 0.433 (-26%) | 0.298 (-62%) |
| POM_BURDEN (Tg) | 0.455 | 0.417 (8.7%) | 0.417 (8.7%) |
| BC_BURDEN (Tg) | 0.115 | 0.105 (-9%) | 0.105 (-9%) |
| SO4_BURDEN (Tg) | 0.411 | 0.414 (0.73%) | 0.408 (-0.73%) |
| CH4_LIFETIME (years) | 9.316 | 9.439 (1.3%) | 9.111 (2.25%) |
| ISOP_EMIS (Tg/yr) | 304.857 | 297.229 (-2.5%) | 173.33 (-55%) |

- T4S not significantly different from T1S with exception of SOA
- T4Sr2 shows more differences with T1S than T4S does.
- T4Sr2 dust variables show biggest difference

Takeaways

Evaluation of the differences between simulations using the MOZART-T1S and MOZART-T4S chemical mechanisms

- Findings (T4S & T1S)
 - T4S is approximately 40% cheaper and faster than T1S
 - Overall, species compare well
 - Share same biases
 - Largest differences: SH UTLS Ozone (10%) & SOA Burden (26%)
- T4S & T4Sr2
 - More African and less Australian dust in T4Sr2
 - AOD looked better in T4Sr2 with respect to Australia
 - Results in a bias shift – low bias in NH even lower, high bias in SH reduced.