Using superfast chemistry to emulate MOZART within the CESM CAM-Chem: Strengths, weaknesses, and possibilities

Benjamin Brown-Steiner

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Louisa Emmons, Simone Tilmes

Using superfast chemistry *instead of* MOZART within the CESM CAM-Chem: Strengths, weaknesses, and possibilities

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Outline

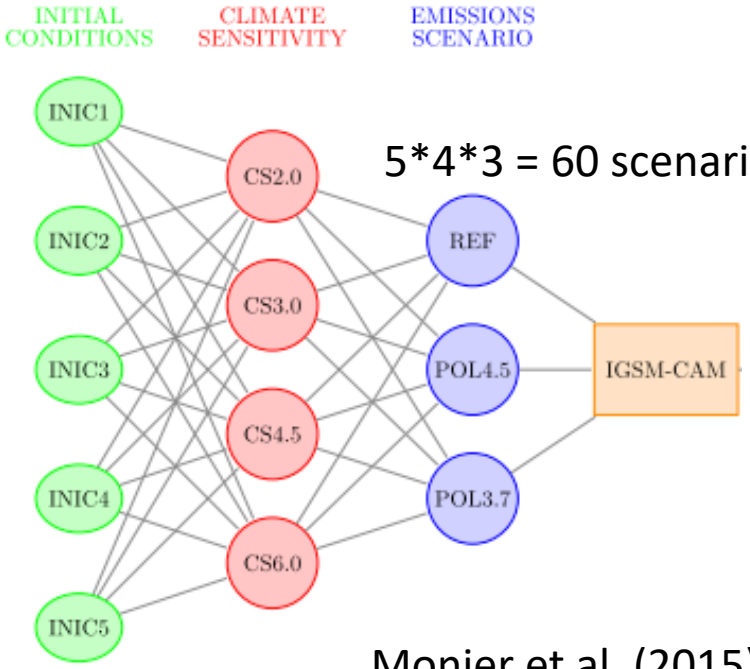
- Superfast is Super Simple
  - So it’s super fast
  - But it’s also sometimes not so great…
- What it does well
- What it does poorly
- “Emulation”
  - ”Calibrated” with MOZART
- Can it be fixed?

Superfast Chemistry

Cameron-Smith et al. (2006) + ACCMIP

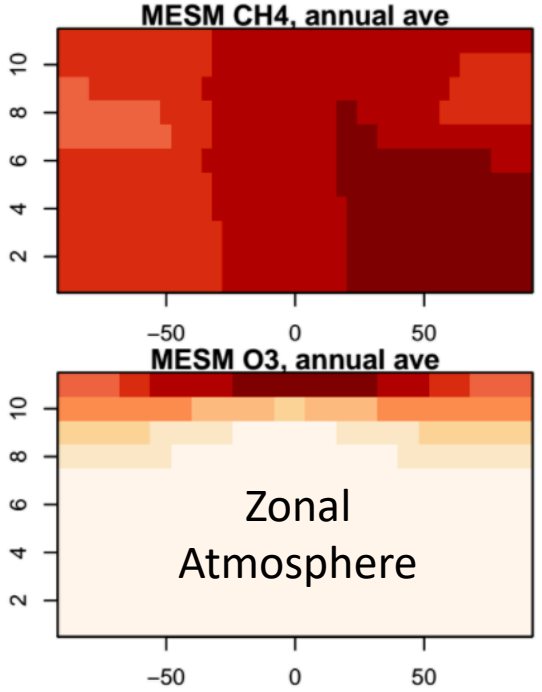
```
  CHEMISTRY
      Photolysis
[j2oh->,jo3_a] O3 + hv -> 2*OH
[jh2o2]        H2O2 + hv -> 2*OH
[jno2]         NO2 + hv -> NO + O3
[jch2o_a]      CH2O + hv -> CO + 2*HO2
[jch2o_b]      CH2O + hv -> CO
[jch3ooh]      CH3OOH + hv -> CH2O + HO2 + OH
      End Photolysis

      Reactions
               O3 + OH -> HO2 + O2                                  ;   1.700E-12, -940
[out6]         HO2 + O3 -> 2*O2 + OH                                ;   1.000E-14, -490
               HO2 + OH -> H2O + O2                                 ;   4.800E-11, 250
[usr_HO2_HO2]  HO2 + HO2 -> H2O2 + O2
               H2O2 + OH -> H2O + HO2                               ;   1.800E-12
               NO + O3 -> NO2 + O2                                  ;   3.000E-12, -1500
               HO2 + NO -> NO2 + OH                                 ;   3.500E-12, 250
               NO2 + OH + M -> HNO3                                 ;   1.800E-30, 3.00, 2.800E-11, 0.00, 0.6
               CH4 + OH -> CH3O2 + H2O                              ;   2.450E-12, -1775
[usr_oh_co]    CO + OH -> HO2
               CH2O + OH -> CO + H2O + HO2                          ;   5.500E-12, 125
               CH3O2 + HO2 -> CH3OOH + O2                           ;   4.100E-13, 750
               CH3OOH + OH -> CH3O2 + H2O                           ;   2.700E-12, 200
               CH3OOH + OH -> CH2O + H2O + OH                       ;   1.100E-12, 200
               CH3O2 + NO -> CH2O + HO2 + NO2                       ;   2.800E-12, 300
               CH3O2 + CH3O2 -> 2*CH2O +  0.80*HO2                  ;   9.500E-14, 390
[het_no2_h2o]  H2O + NO2 ->  0.50*HNO3
               DMS + OH -> SO2                                      ;   1.100E-11, -240
[usr_oh_dms]   DMS + OH ->  0.75*SO2
[tag_so2_oh_m] OH + SO2 + M -> SO4                                  ;   3.300E-31, 4.30, 1.600E-12, 0.00, 0.6
[aq_so2_h2o2]  H2O2 + SO2 -> SO4
[aq_so2_o3]    O3 + SO2 -> SO4
*[isop_oh]     ISOP + OH -> 2*CH3O2 -1.5*OH                         ;   2.700E-11, 390
[isop_oh]      ISOP + OH -> 2*CH3O2                                 ;   2.700E-11, 390
               ISOP + OH -> ISOP                                    ;   2.700E-11, 390
               ISOP + OH -> ISOP + 0.5*OH                           ;   2.700E-11, 390
[isop_o3]      ISOP + O3 -> 0.87*CH2O + 1.86*CH3O2 + 0.06*HO2 + 0.05*CO     ;   5.590E-15, -1814
```

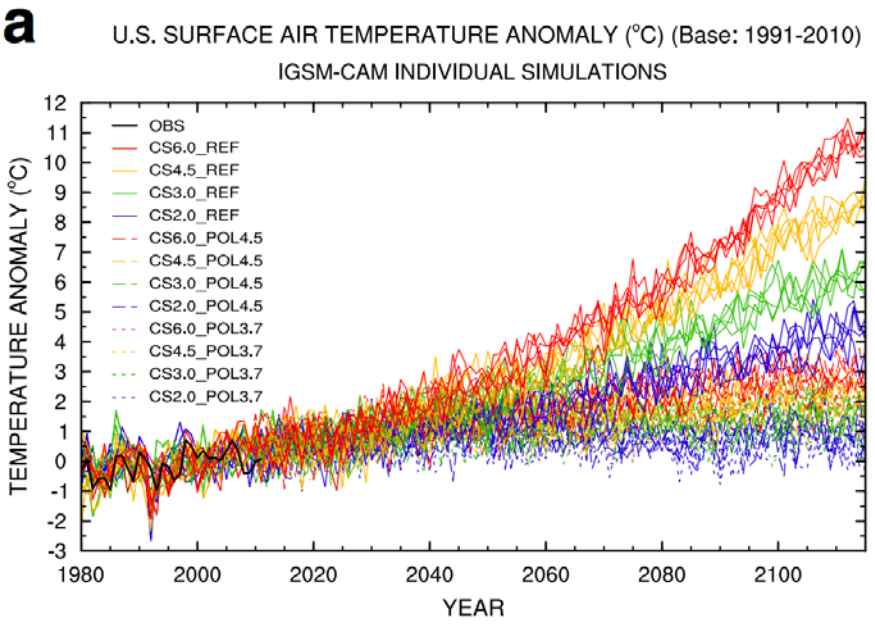
Why do we want fast chemistry?



5*4*3 = 60 scenarios

Monier et al. (2015)





Simulations

- MERRA meteorology (1990 – 2015)
- Year 2000 Cycled Emissions
- Mechanisms:
  - MOZART-4 / SOA
  - Superfast
    - Our Approach: Applying Superfast to MOZART Compset
  - (also Reduced Hydrocarbon, but not talked about here)

```
 Overall Metrics:
   Model Cost:                911.05   pe-hrs/simulated_year
   Model Throughput:            5.06   simulated_years/day

 Overall Metrics:
   Model Cost:                512.17   pe-hrs/simulated_year
   Model Throughput:            9.00   simulated_years/day

 Overall Metrics:
   Model Cost:                262.60   pe-hrs/simulated_year
   Model Throughput:           17.55   simulated_years/day
```

MOZART

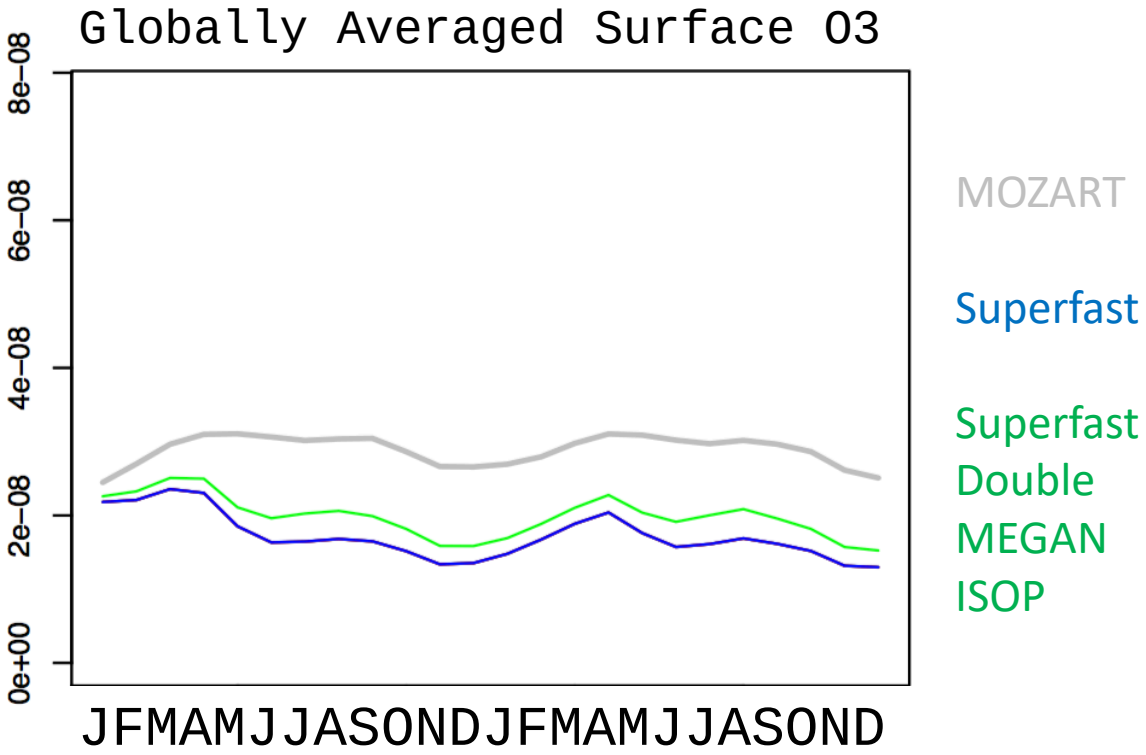
Reduced Hydrocarbon

Superfast

(Cheyenne: Fully Coupled B1850 case: 4,560 pe-hours/yr)

In person meetings are good…

- I had a chance to review the mechanism with Philip yesterday, and we walked through some of the problems he had originally, and we identified a major one:
  - MOZART specifies CH4 as a single value [[CHECK THIS]]]
  - Superfast requires reading in CH4 from a file

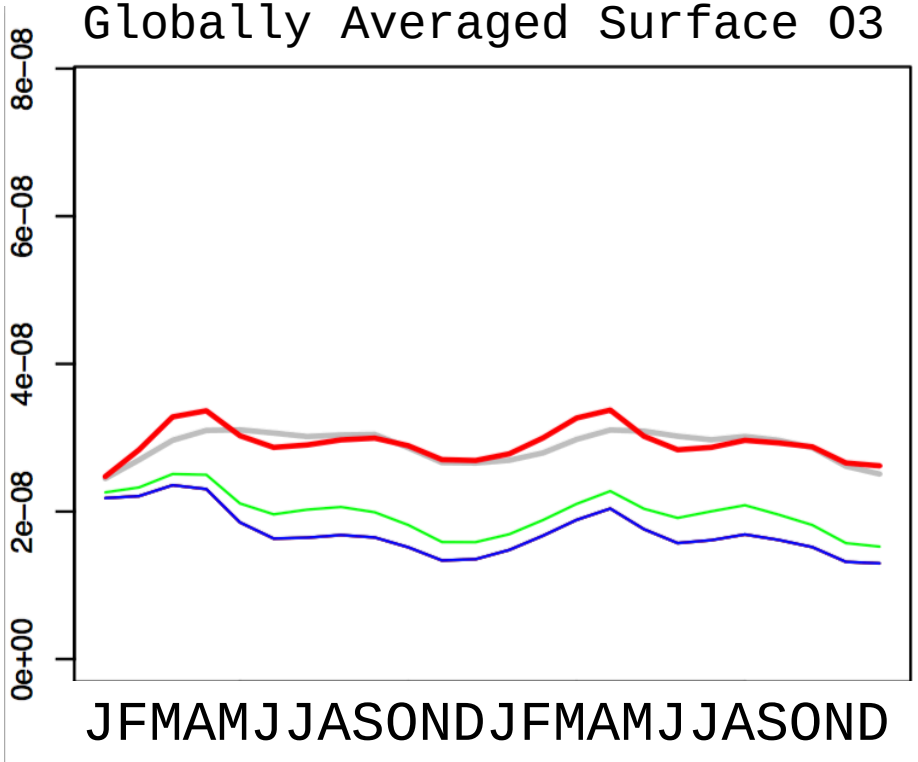


In person meetings are good…

- I had a chance to review the mechanism with Philip yesterday, and we walked through some of the problems he had originally, and we identified a major one:
  - MOZART specifies CH4 as a lower BC
  - Superfast requires reading in CH4 from a file

```
&chem_surfva
 co2vmr
 flbc_cycle_
 flbc_file
 flbc_list
 flbc_type
/
```

```
tracer_cnst_cycle_yr
tracer_cnst_datapath
tracer_cnst_file
tracer_cnst_filelist
tracer_cnst_specifier
tracer_cnst_type
```



MOZART

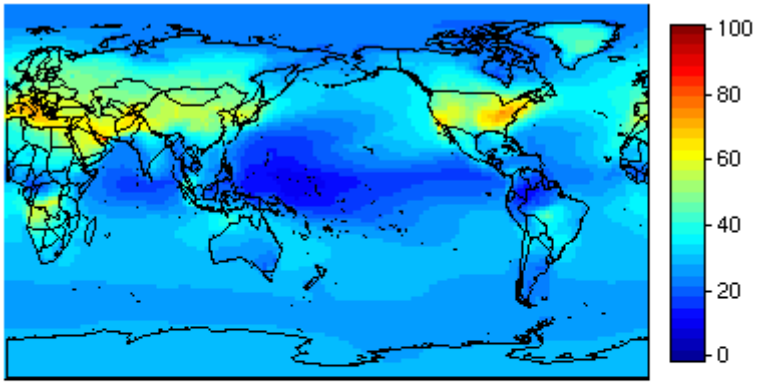
Superfast

Superfast Double MEGAN ISOP

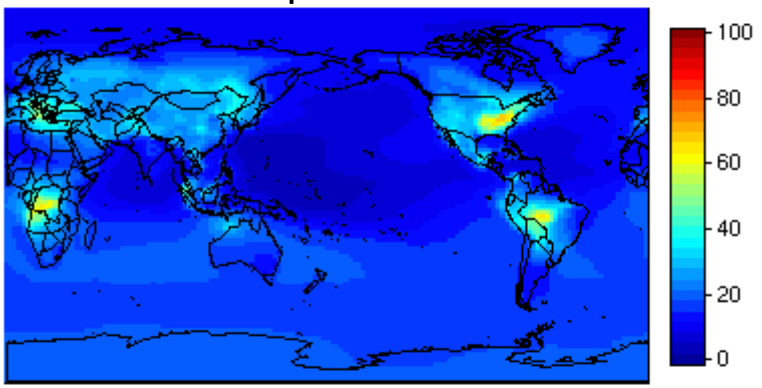
Superfast With CH4 File

update

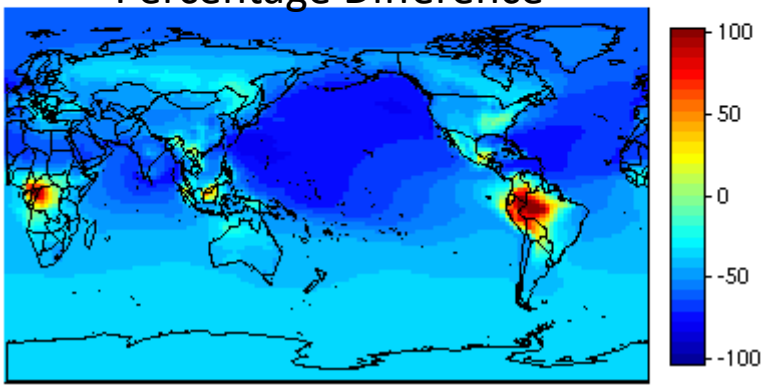
MOZART



Superfast



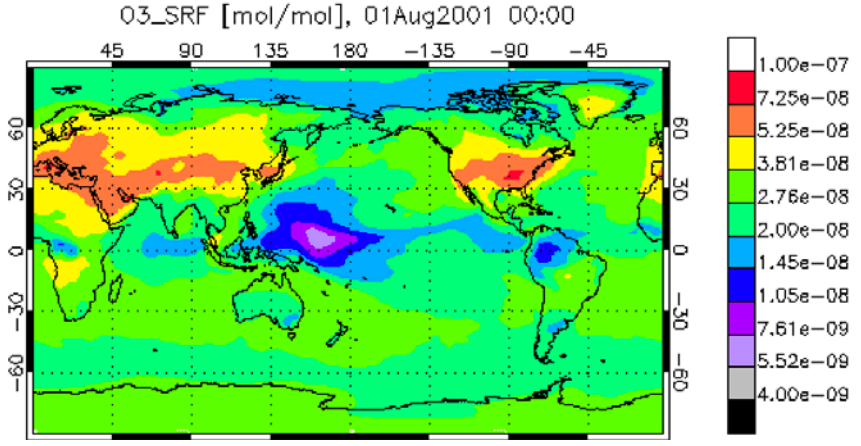
Percentage Difference



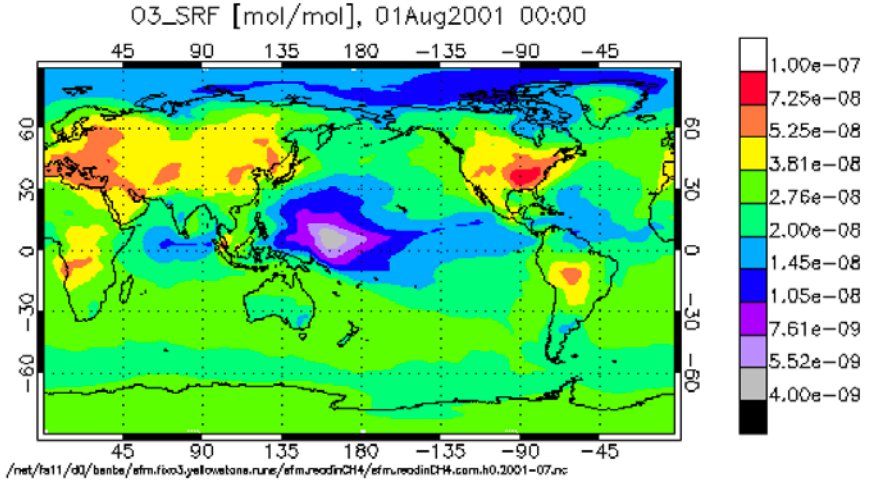
Results

- JJA Surface Ozone Average from 1990 – 2015
- The Good:
  - Superfast captures spatial pattern well
- The Bad:
  - Superfast has a much lower mean ozone almost everywhere
  - Too much ozone over regions of intense biogenic and biomass burning emissions

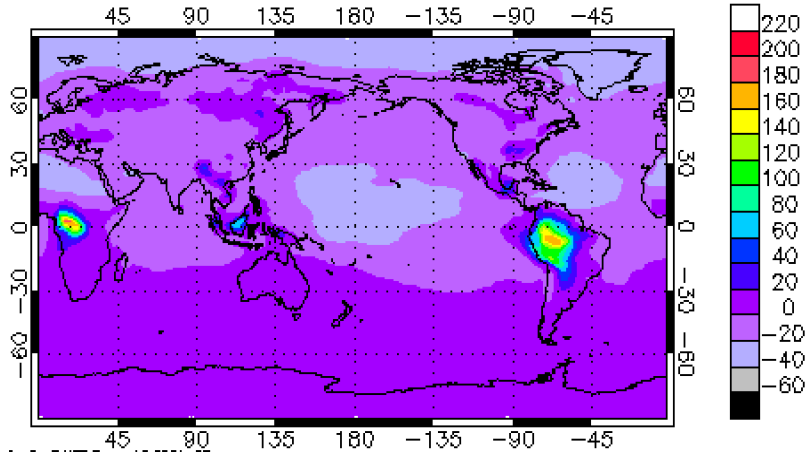
MOZART



Superfast



Percentage Difference



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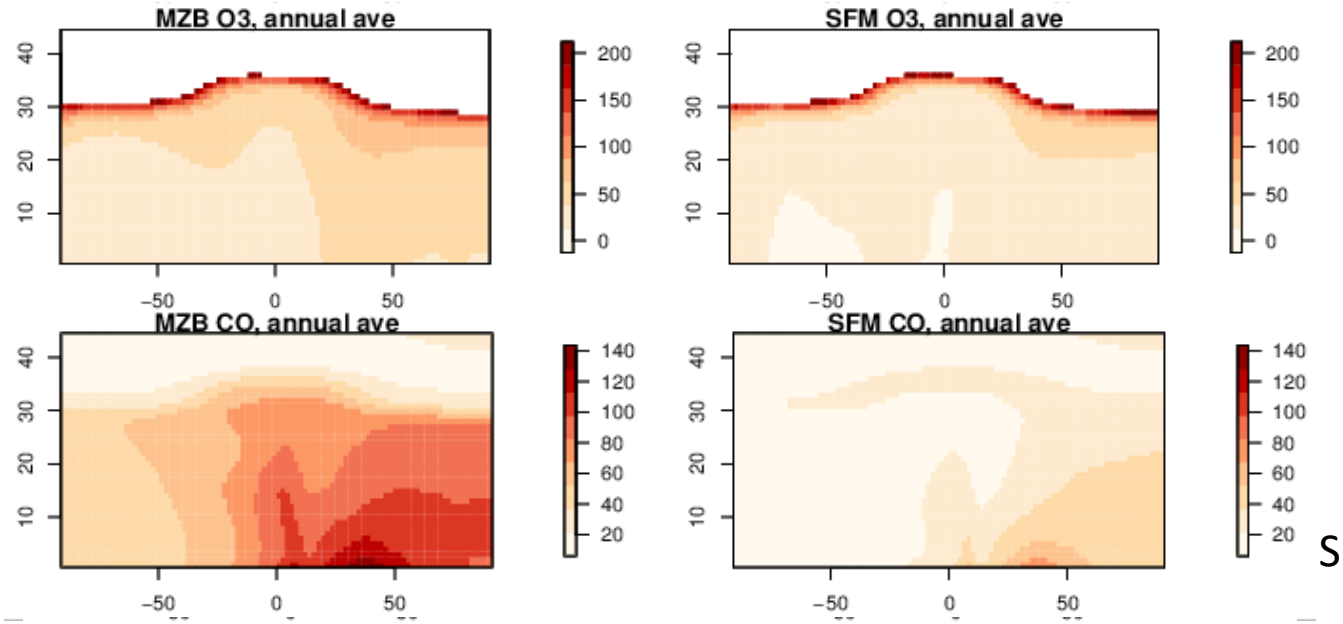
update

Results

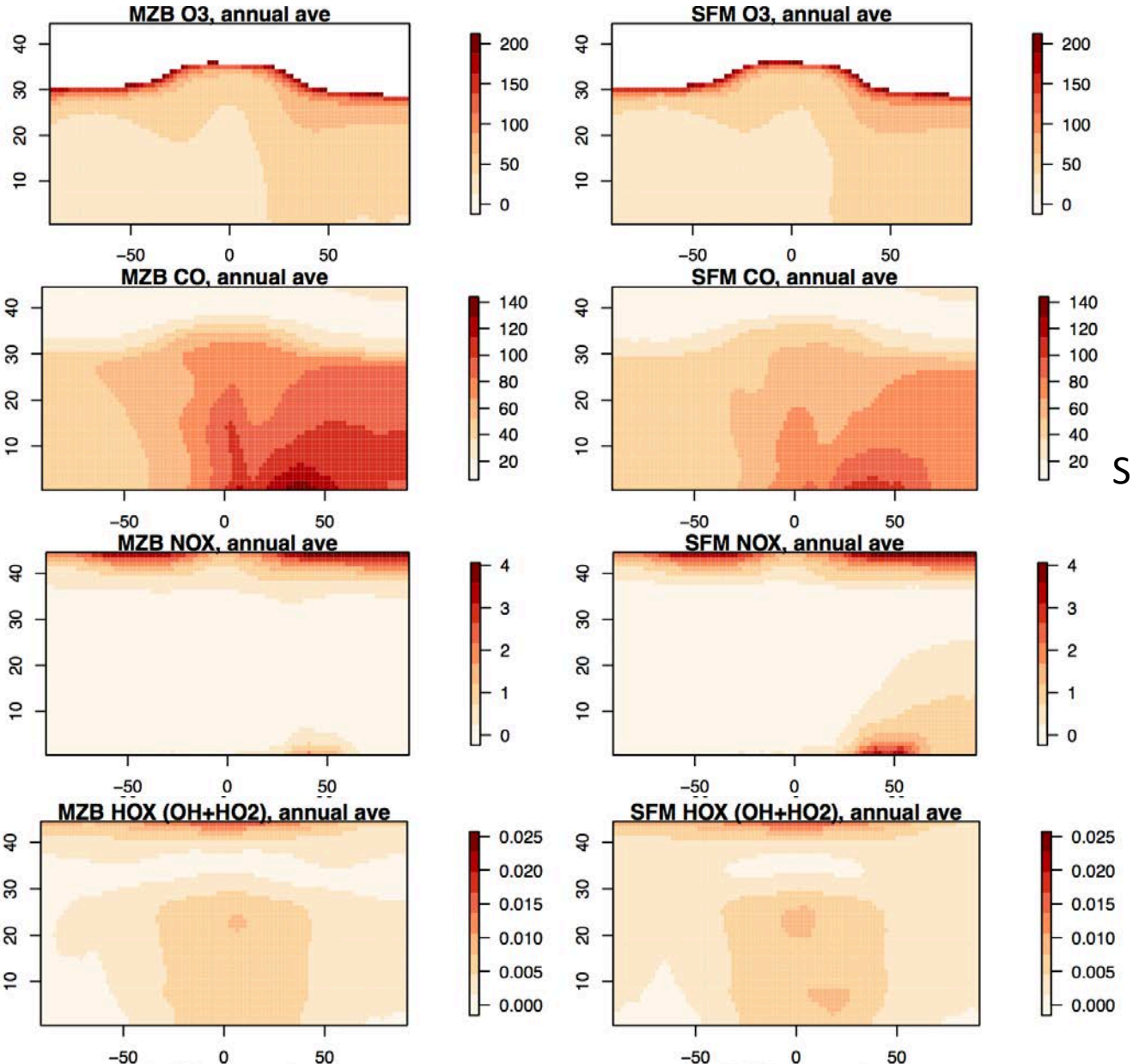
MOZART



Superfast

Results

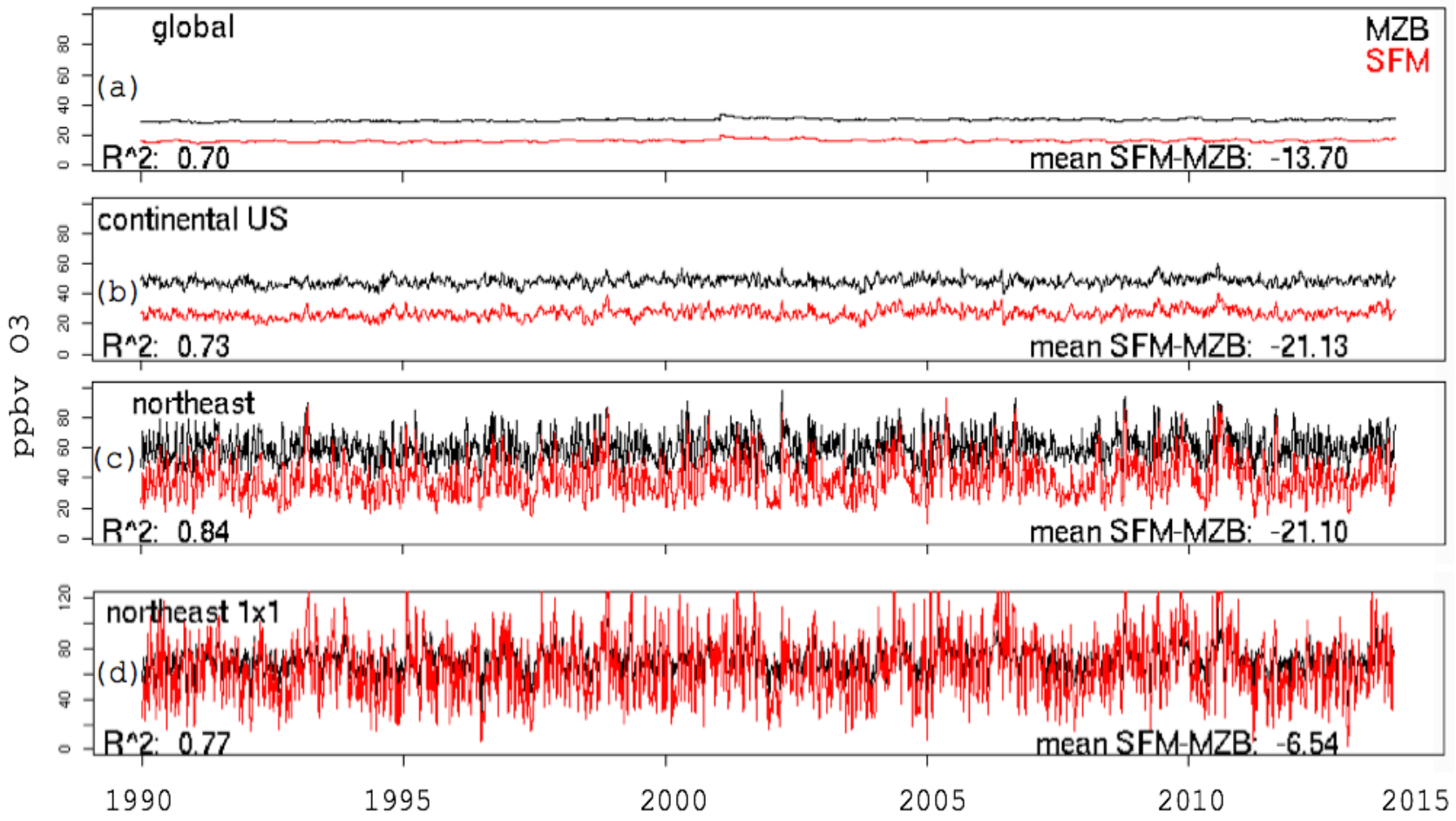
MOZART



Superfast

update

Results
JJA Daily Surface Ozone



Results

	R2
Global	0.7
Continental US	0.73
Western US	0.86
Eastern US	0.8
Midwestern US	0.83
Southeastern US	0.86
Northeastern US	0.84
Midwest 1x1	0.87
Southeast 1x1	0.89
Northeast 1x1	0.77

- Superfast has high correlation with MOZART at all spatial scales
- But also is ~50% too low for most of the globe
- Certain regions (e.g. Northeastern US) show smaller differences
- But maybe for the wrong reasons…

	Global				Continental US				Northeastern US				Northeast 1x1			
	MOZART	Superfast	Δ	Δ (%)	MOZART	Superfast	Δ	Δ (%)	MOZART	Superfast	Δ	Δ (%)	MOZART	Superfast	Δ	Δ (%)
mean	30.0	16.3	-13.7	-46%	48.1	26.9	-21.1	-44%	61.0	39.9	-21.1	-35%	71.9	65.3	-6.5	-9%

Now What?

- Two ways to go:
  - Take Superfast as a given and use MOZART to “calibrate” its results
    - (next few slides)
  - Fix Superfast
    - Can it be fixed?
    - Fixed for what? It’s never going to be perfect, but it might be malleable…
      - …based on your question…
        - …
          - …
            - …
              - …
                - …

Now What?

- Two ways to go:
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      - …based on your question…
        - …
          - …
            - …
              - …
                - …

“Calibration” Route

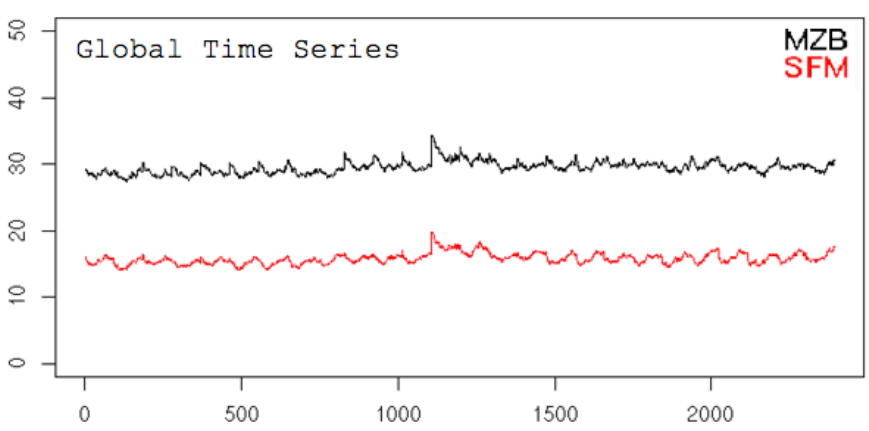
Standardized Anomalies normalize data such that the mean = 0 and the standard deviation = 1 while the shape of the distribution is maintained (Wilks, 2006):

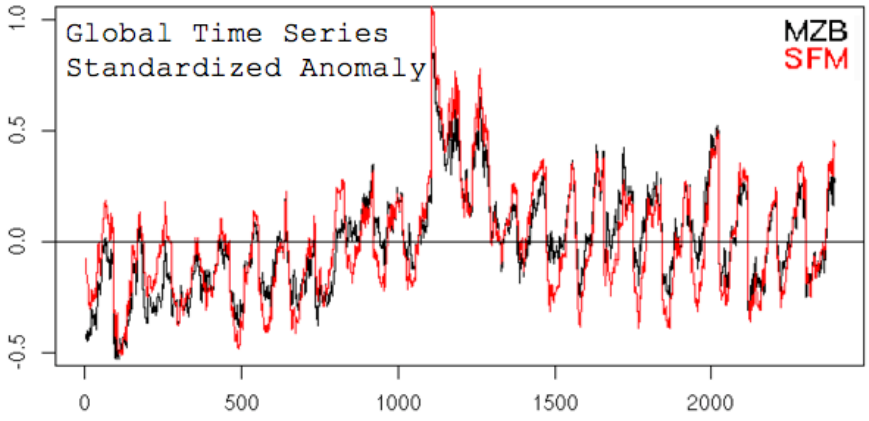
$$A(t) = \frac{x(t) - \bar{x}}{s} \tag{1}$$

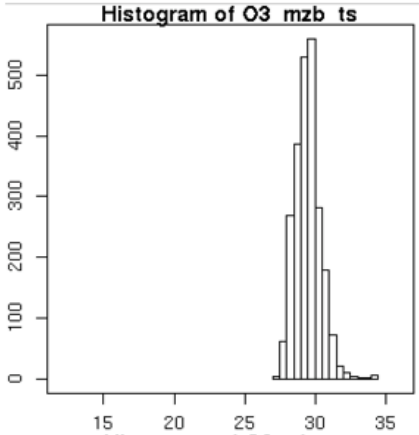
$$A_{MO}(t) = \frac{x_{MO}(t) - \bar{x}_{MO}}{s_{MO}} \qquad A_{SF}(t) = \frac{x_{SF}(t) - \bar{x}_{SF}}{s_{SF}} \tag{2}$$

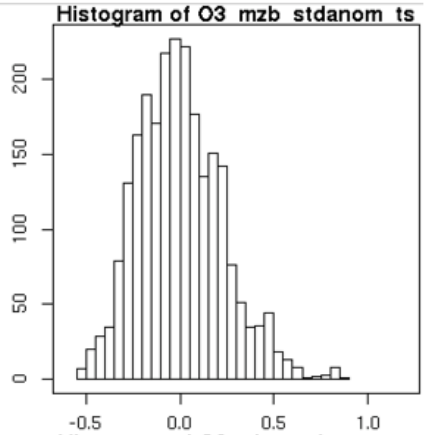
$$x_{MO/SF}(t) = A_{SF}(t) * s_{MO} + \bar{x}_{MO} \tag{3}$$

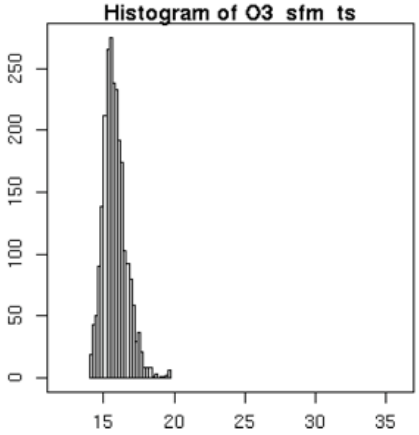
“Calibration” Route

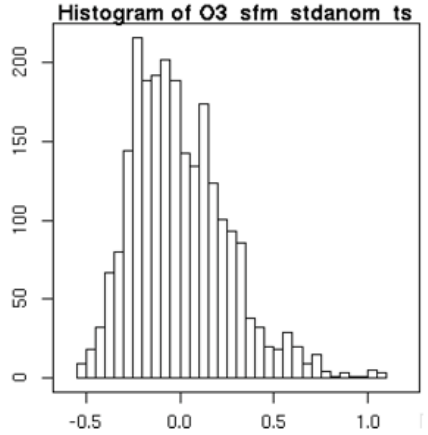




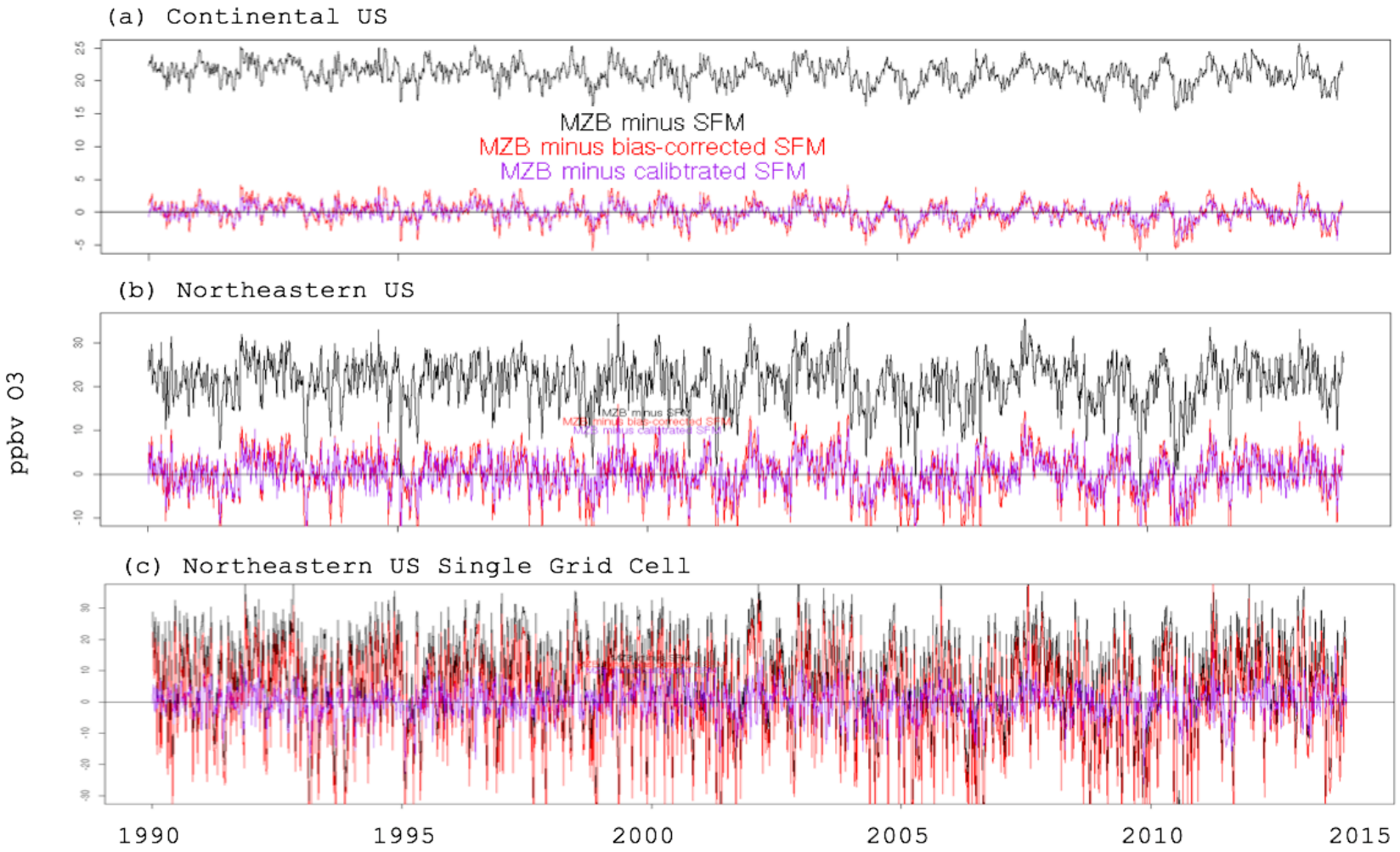






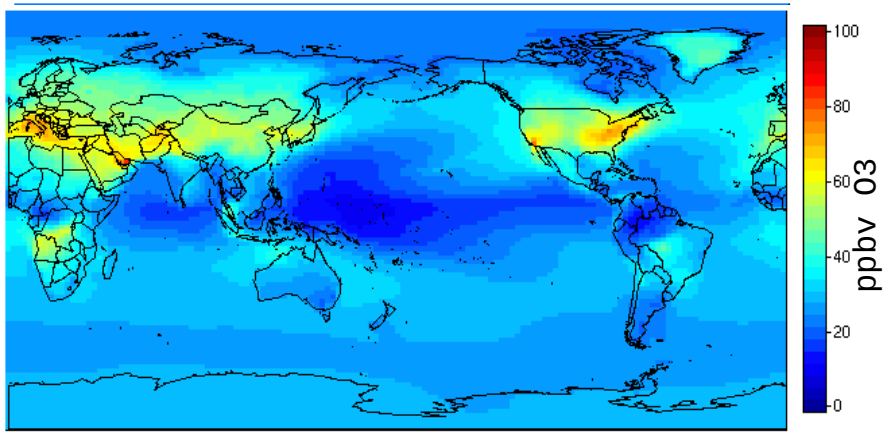


“Calibration” Route

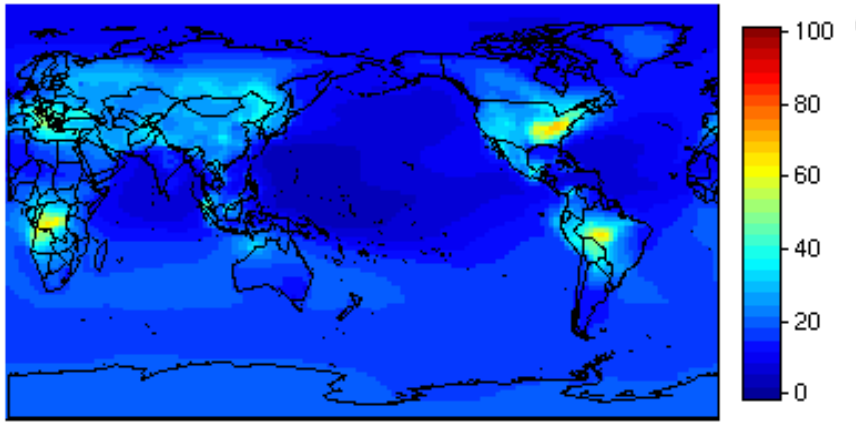


“Calibration” Route

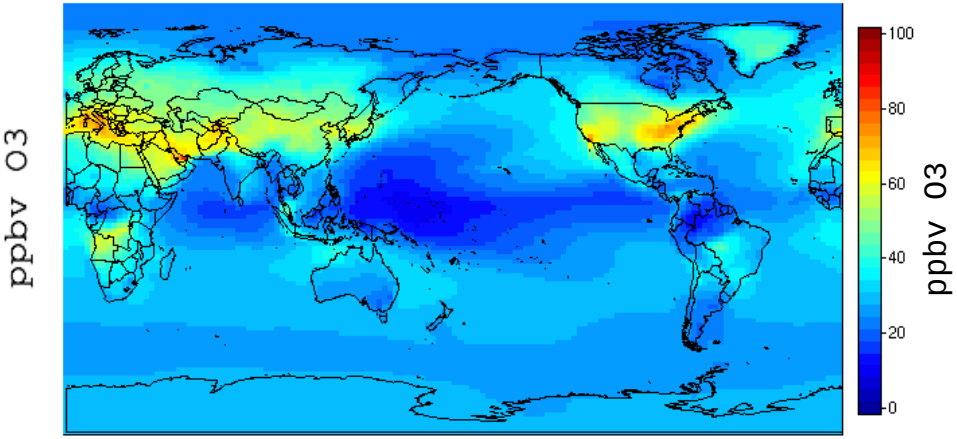
(a) MOZART



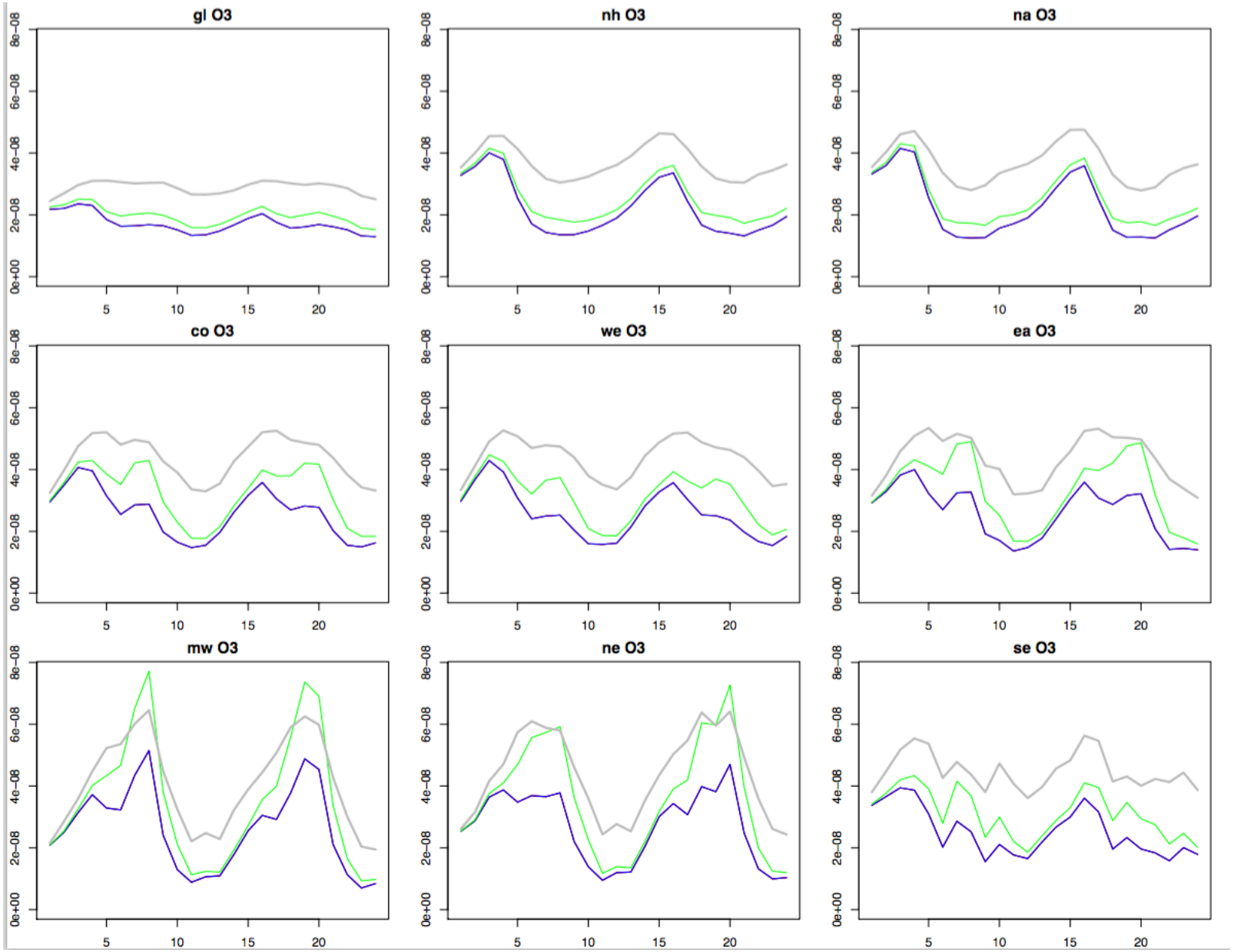
(b) Superfast



(b) MOZART Emulation Using Superfast

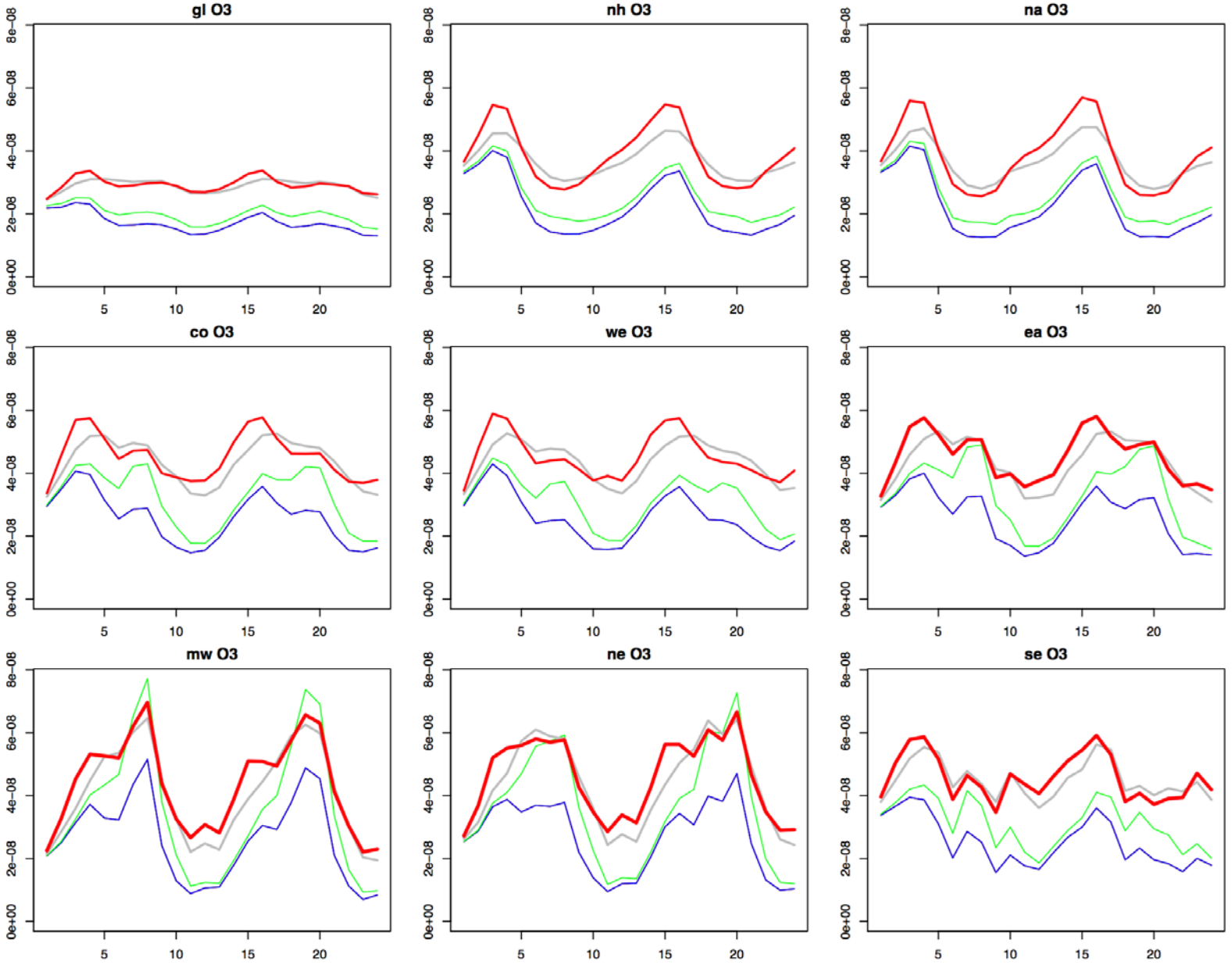


“Can I fix it?” Route



MOZART Superfast Superfast Double MEGAN ISOP

“Can I fix it?” Route

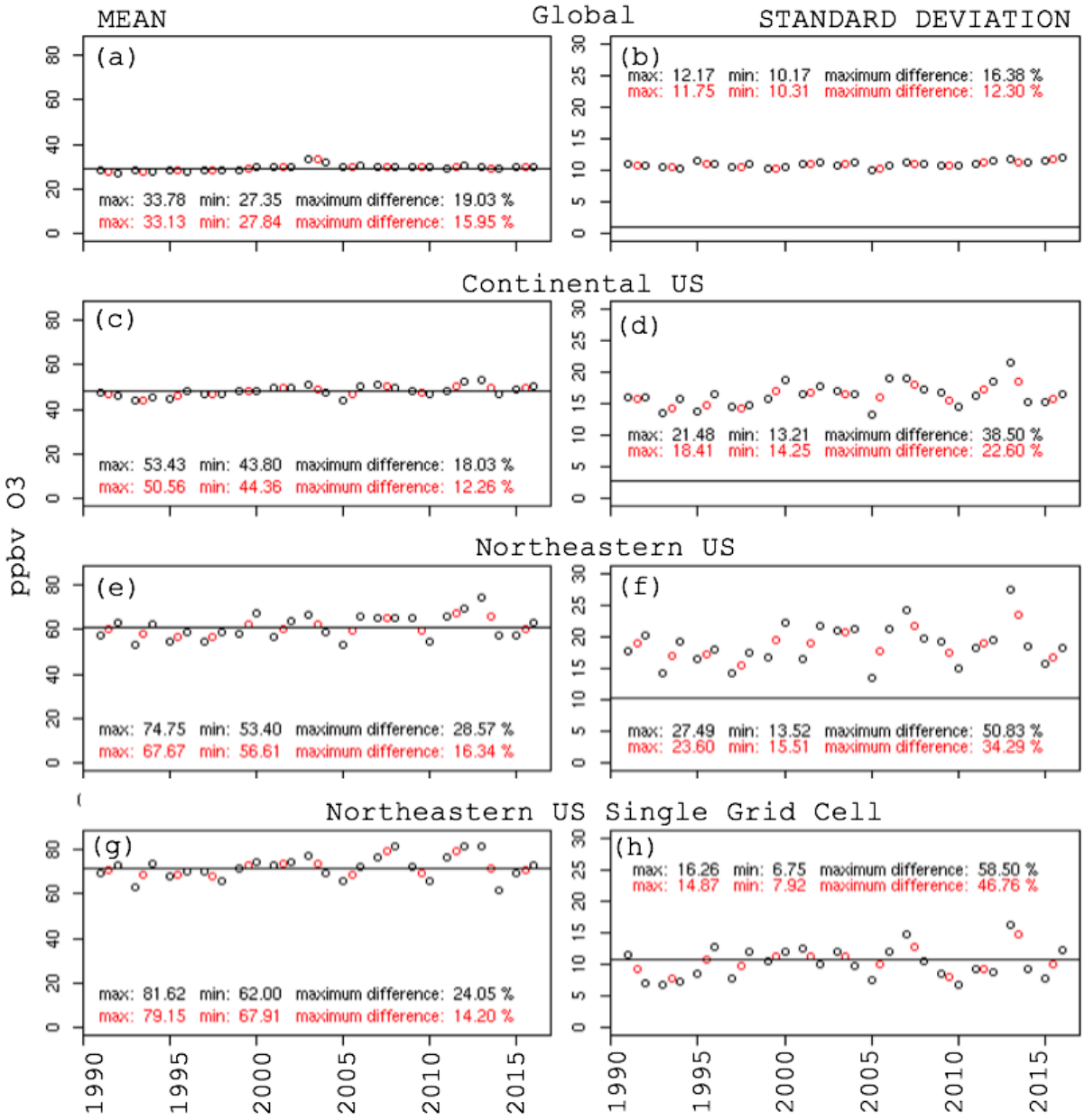


Superfast With CH4 File

MOZART Superfast Superfast Double MEGAN ISOP

“Can I fix it?” Route

Thank You!


MEAN
Global
STANDARD DEVIATION
(a)
max: 33.78 min: 27.35 maximum difference: 19.03 %
max: 33.13 min: 27.84 maximum difference: 15.95 %
(b)
max: 12.17 min: 10.17 maximum difference: 16.38 %
max: 11.75 min: 10.31 maximum difference: 12.30 %
Continental US
(c)
max: 53.43 min: 43.80 maximum difference: 18.03 %
max: 50.56 min: 44.36 maximum difference: 12.26 %
(d)
max: 21.48 min: 13.21 maximum difference: 38.50 %
max: 18.41 min: 14.25 maximum difference: 22.60 %
Northeastern US
(e)
max: 74.75 min: 53.40 maximum difference: 28.57 %
max: 67.67 min: 56.61 maximum difference: 16.34 %
(f)
max: 27.49 min: 13.52 maximum difference: 50.83 %
max: 23.60 min: 15.51 maximum difference: 34.29 %
Northeastern US Single Grid Cell
(g)
max: 81.62 min: 62.00 maximum difference: 24.05 %
max: 79.15 min: 67.91 maximum difference: 14.20 %
(h)
max: 16.26 min: 6.75 maximum difference: 58.50 %
max: 14.87 min: 7.92 maximum difference: 46.76 %
ppbv O3
0 20 40 60 80
0 5 10 15 20 25 30
1990 1995 2000 2005 2010 2015

- Are you reading in CH4 from a file, or just the specified value from TROP MOZART
  - (check this → where would this be in namelist?)

- tracer_cnst_cycle_yr = 1855 tracer_cnst_datapath = '/glade/p/cesmdata/cseg/inputdata/atm/cam/chem/methane' 1859_clim_c090605.nc' tracer_cnst_filelist = 'filelist_c090 tracer_cnst_type = 'CYCLICAL'

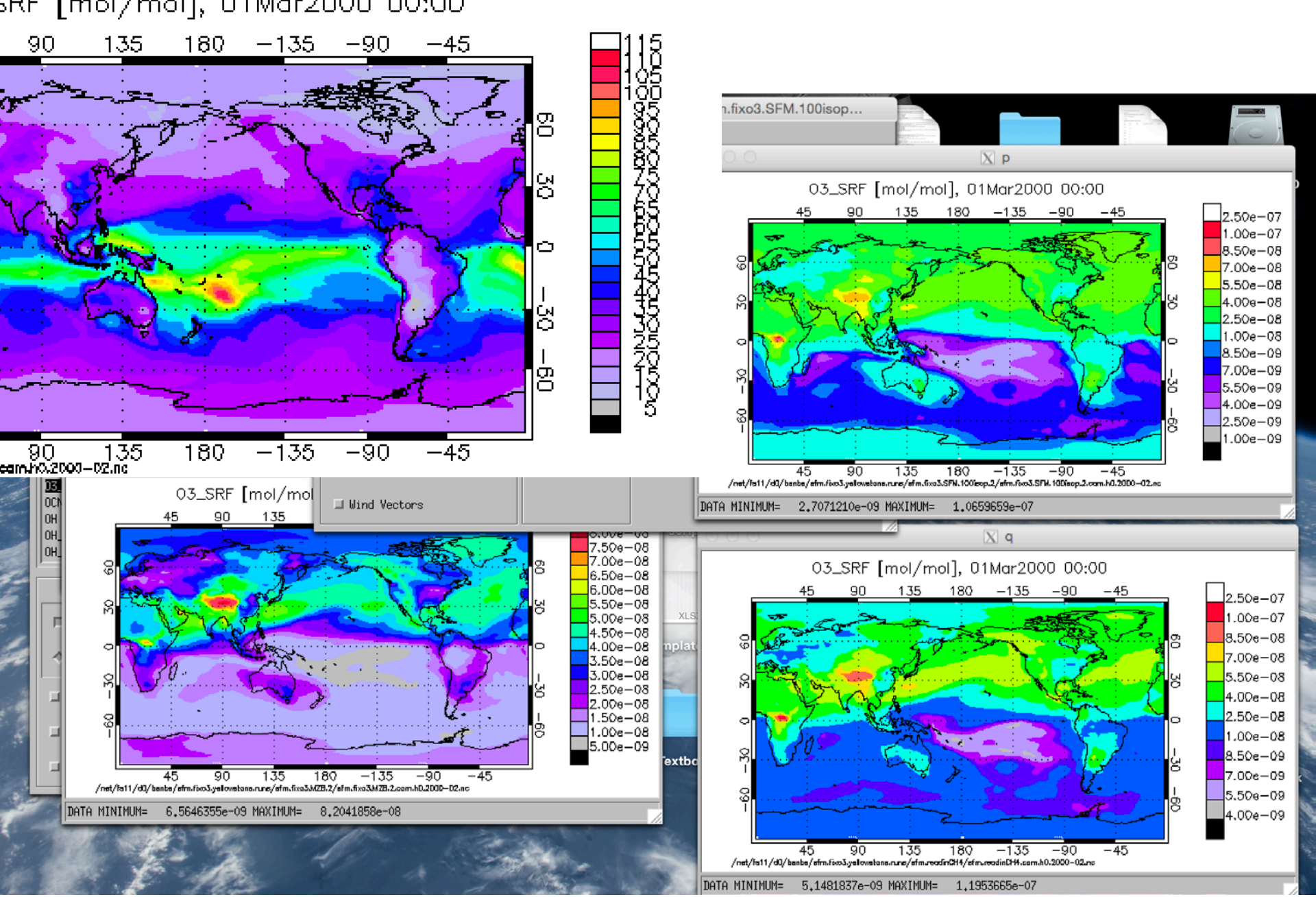
- you are not doing this in your MOZART simulation

- You'll have to look in the code too to make sure it's doing the ri ot have the final say if there are defaults written somewhere in the cod

- Am I double counting NOx
  - 2D emissions
  - 2 different 3D emissions, hardwired into code
    - aircraft (ext_frc)
    - built in mechanism description file

    - lightning (check this too)
    - also a 3D emissions coupled with aircraft CO

```
Ext Forcing
   NO
   NO2 <- dataset
   SO2 <- dataset
   so4_a1 <- dataset
   so4_a2 <- dataset
   pom_a1 <- dataset
   bc_a1 <- dataset
   num_a1 <- dataset
   num_a2 <- dataset
End Ext Forcing
```


03_SRF [mol/mol], 01Mar2000 00:00
90 135 180 −135 −90 −45
60 30 0 −30 −60
p
03_SRF [mol/mol], 01Mar2000 00:00
2.50e−07
1.00e−07
8.50e−08
7.00e−08
5.50e−08
4.00e−08
2.50e−08
1.00e−08
8.50e−09
7.00e−09
5.50e−09
4.00e−09
2.50e−09
1.00e−09
DATA MINIMUM= 2.7071210e-09 MAXIMUM= 1.0659659e-07
Wind Vectors
7.50e−08
7.00e−08
6.50e−08
6.00e−08
5.50e−08
5.00e−08
4.50e−08
4.00e−08
3.50e−08
3.00e−08
2.50e−08
2.00e−08
1.50e−08
1.00e−08
5.00e−09
DATA MINIMUM= 6.5646355e-09 MAXIMUM= 8.2041858e-08
q
03_SRF [mol/mol], 01Mar2000 00:00
2.50e−07
1.00e−07
8.50e−08
7.00e−08
5.50e−08
4.00e−08
2.50e−08
1.00e−08
8.50e−09
7.00e−09
5.50e−09
4.00e−09
DATA MINIMUM= 5.1481837e-09 MAXIMUM= 1.1953665e-07

To Do with Superfast (after meeting with PCS)

- Check O3 after CH4 input fix (reading in the Ch4 file instead of just specifying a value, like MOZ does)
- Are you double counting NOx? (it was disturbingly high) Emissions and/or Lightning/Airplane? Talk to Simone and check “Ext Forcing” in chem_mech.in file and compare with MOZART. Make sure this is being done correctly.
- Are the user specified reactions doing what they should be doing? Also Talk to Simone, should they go automatically our should I comb through them and double check?
- Why is CO so low? (or is it, does CH4 fix also fix CO?)
- Are you using superfast BAM or the superfast_llnl_mam3? Would we want to? when you bring things over from superfast and push them into FMOZSOA, what are the things that are likely to get left out? (See previous four bullet points)
- Later, email PCS to see if you can get their “best of superfast” from somewhere in their archives

To Do With Simone

- Show “leak” results
- Look at mechanism…where would it be leaking and why
- Are there ways to “plug” the leak. If I can get it stable we can have a nice sliding scale of complexity which I think would be good to have within CESM / MESM