TM5-chemistry : C-IFS, Benchmarks & Bottlenecks

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2014-05-12

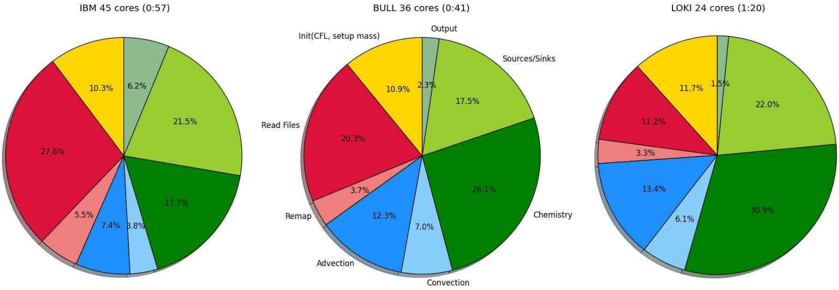
An investigation for TROPOMI

machine	BULL (KNMI)	IBM (ECMWF)	Loki (KNMI)
CPU model	Intel Xeon	Power7	
Compiler	ifort	IBM XLF	gfortran
MPI	Intel MPI	IBM POE	openMPI
max. cores	36	45/90	28

Setups

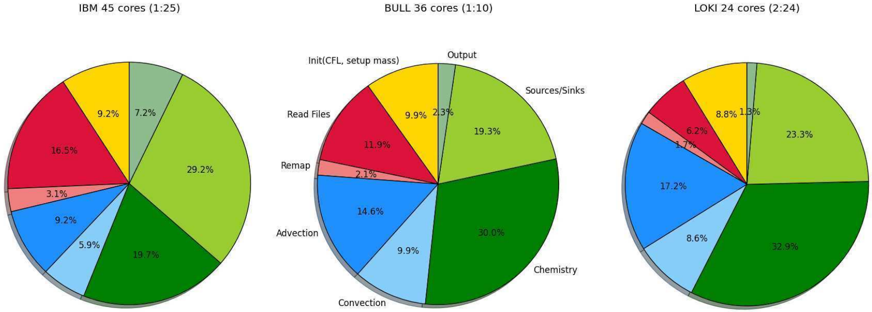
- 1 month run with r5107 (2014-04-08)
- EI-hdf, 34 and 60 levels, 3x2 and 1x1
- **no** M7
- Time-series output: 4 variables, 1h time step

3x2 - 34L



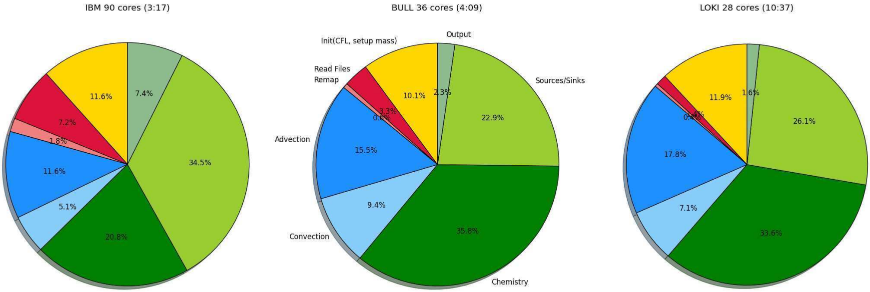
TM5 r5107 w/o M7 - 1 month run - 3x2, 34Lev

3x2 - 60L



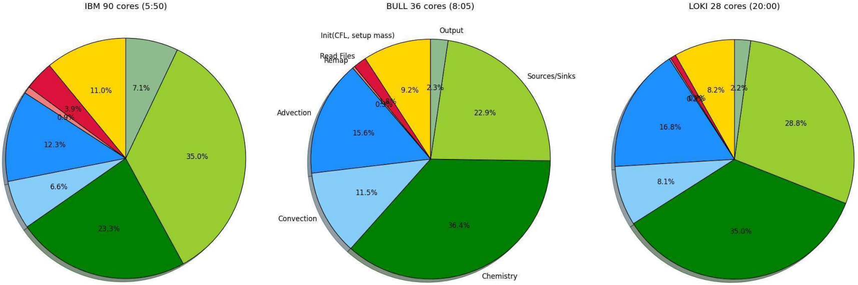
TM5 r5107 w/o M7 - 1 month run - 3x2, 60Lev

1x1 - 34L



TM5 r5107 w/o M7 - 1 month run - 1x1, 34Lev

1x1 - 60L



TM5 r5107 w/o M7 - 1 month run - 1x1, 60Lev

Conclusion for CBM4 w/o M7

bottleneck	rtime	what may help
reading meteo (low res, lot of cores)	20%	parallel IO with netCDF4
chemistry	20-35%	Rosenbrock solver (optimize tolerances)
sources (boundary)	20-35%	review nudging in boundary

Parallelization

improvement	needs
increase max nb cores	MPI decomposition of reduce grid
openMP	new (simpler) implementation

Outline

Comparison w/ previous version & observations

(1 year + 6 months spinup, @3x2 and 34Lev)

What's new?

- NO2 comparison with OMI
- CO comparison with MOPITT-NIR
- handles comparison b/w different resolutions
- done **often** : ease feature attribution (and debug)
- proj management app (redmine) –> document changes
  - interface w/ repos
  - issue tracker
  - http://dev.knmi.nl/projects/tm5
- "What's new in next cycle" on http://tm.knmi.nl/

dev.knmi.nl/projects/tm5/boards/3

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TM5

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Chemistry Benchmarks

documentation of changes from new features or/and bug fixes

Subject	Author	Created	Replies	Last message
search topics	Michiel van Weele	02/07/2014 09:12 am	0	
version #5099: NO2+OH --> HNO3 rate update	Philippe Le Sager	04/09/2014 01:06 pm	0	
version #5088: ODIN climatology				
version #5084: MEGAN emissions				
version #5077: diurnal cycle applied to NOx biomass burning emissions				
version #5069: MACC-City vs. EDGAR				
version #5036: Effect of convective fluxes from ERA-I				
Version #5016: Comparisons against observations of CO (het chem update)				
Version #5016: New heterogeneous chemistry scheme				
Version #4993: Global 1x1 compared with global 3x2				

(1-10/10) | Per page: 25, 50, 100

TM5 - version #5084: MEGAN emissions

dev.knmi.nl/boards/3/topics/13

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version #5084: MEGAN emissions

Added by Philippe Le Sager about 1 month ago

This is a comparison between

- r5077
- r5084 = same as r5077, but with the following emissions updates:
  - option MEGAN on (biogenic for CO, ISOP, NMVOC)
  - update conversion nmvoc-to-cbm4

Both runs are 2006 runs at 3x2_34L w/ TM5-mp, started in 2005-07-01 for a half-year spinup, and use ERA-I convective fluxes and

- The MEGAN inventory **increases** emissions of CO by 14 Tg, and of isoprene by 55 Tg (see budget file).
- The main differences are found in CO, PAN and CH2O. They are localized close to the sources in Africa, Australia, and S.-E. As
- Comparisons with observations show:
  - a drastic improvement in the J(O1D) vs OH at Hohenpeissenberg
  - CO is overestimated in the South Hemisphere, and unchanged in the North Hemisphere
    - MOZAIC: better CO, but this is limited to [20S-50N]
    - CMDL: over estimation of CO in Antartica and a couple of stations at mid-latitude in southern hemisphere
    - MOPITT: increase in the tropics and in the south hemisphere, the latter being too high.
  - better (worst) CH2O in central (north) Africa from SCIAMACHY comparisons.

budget_comparison_2006.txt (17.4 kB)
WINTER_2006.pdf (4.5 MB)
SUMMER_2006.pdf (4.5 MB)
comp_with_observations_overall.pdf (362.2 kB)

Latest benchmarks since v4

Revision	What's it about
4993	Hi-Res
5036	EI convective fluxes
5016	Heterogeneous chemistry
5069	MACC-City anth. emis.
5077	BMB-NOx diurnal cycle
5084	MEGAN biogenic emis.
5088	ODIN climatology [CO, HNO3]
5099	OH+NO2->HNO3 rates (Mollner et al, *Science*, 2010)
5114	Martin (JAS '94) cloud part. radius parametrization

Heteregeneous Chemistry

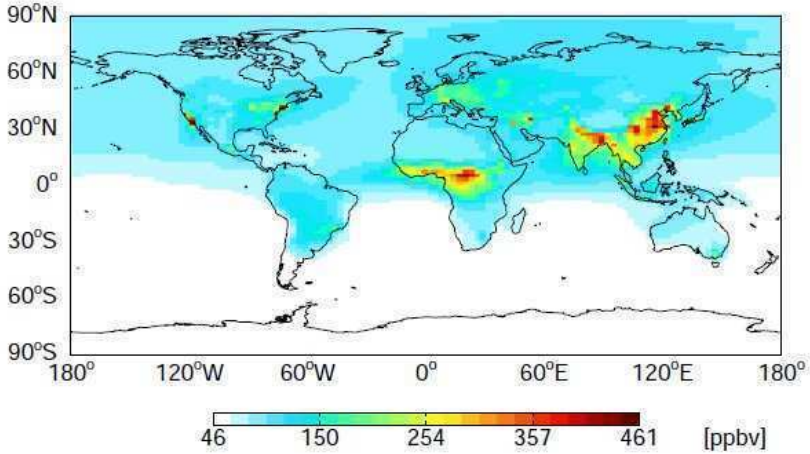
	v4	Het Chem	diff
Total pO3 tropo (Tg)	4500	4203	-297
Total lO3 tropo (Tg)	1737	1478	-259
O3 drydep (Tg)	799	762	-36
trop **O3 burden** (Tg)	310	304	**-7**
CO + OH tropo (Tg)	2142	2088	-54
trop **CO burden** (Tg)	295	306	**12**
Total pOH tropo(Tg)	1462	1273	-189

Surface CO

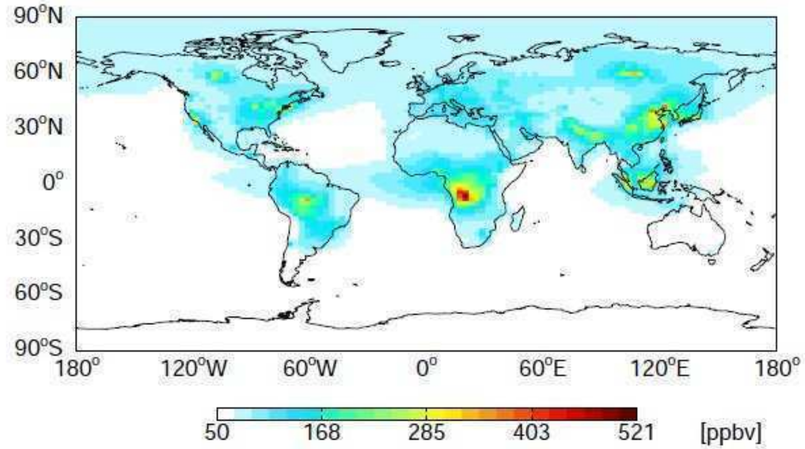
Winter

Summer

HETEROGENEOUS CHEM

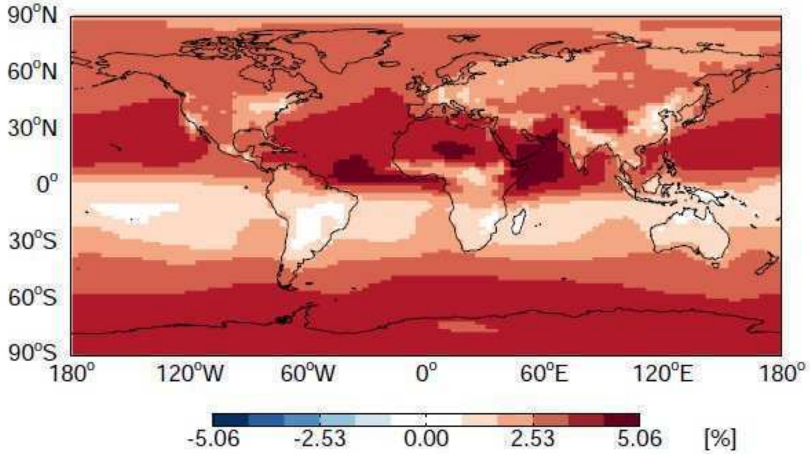


HETEROGENEOUS CHEM

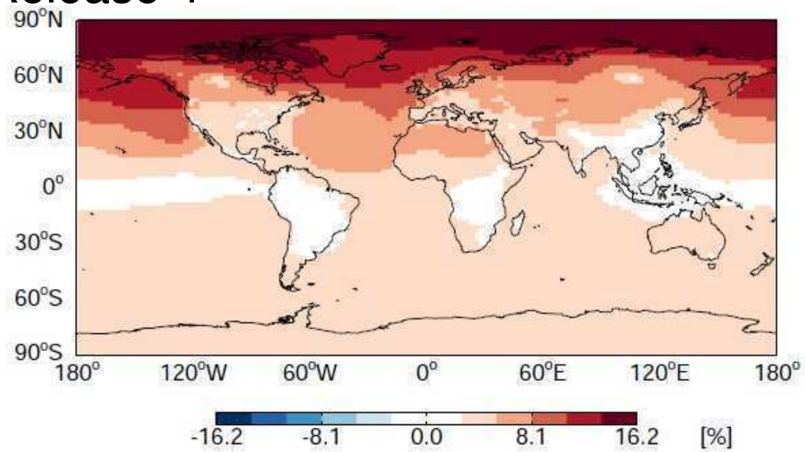


Relative to Release 4

Rel. Diff. [%]



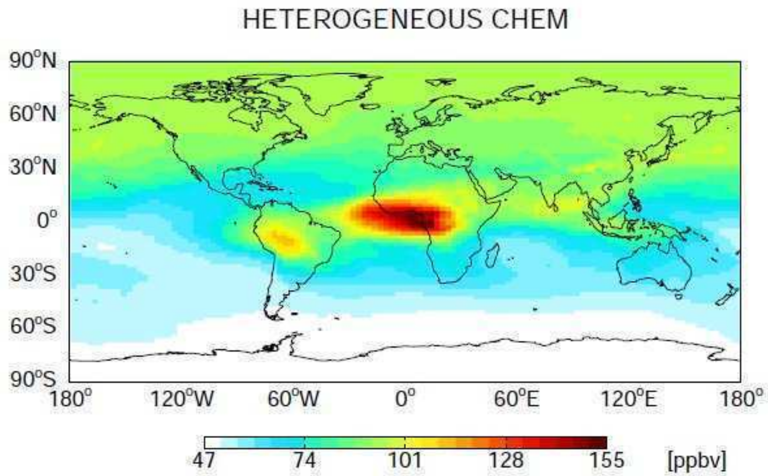
Rel. Diff. [%]

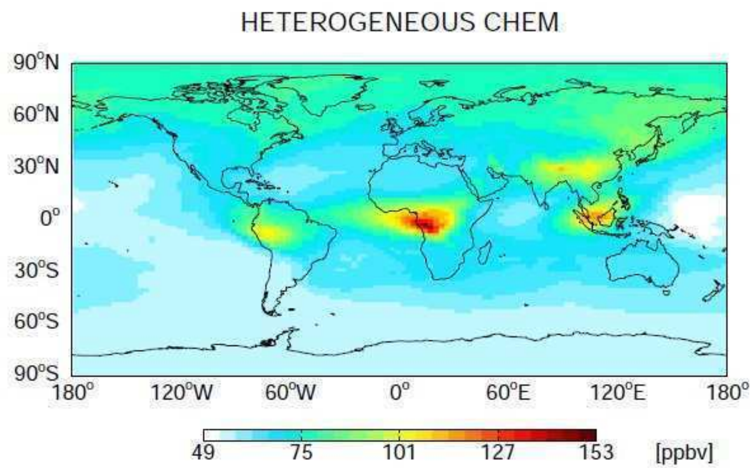


500 hPa CO

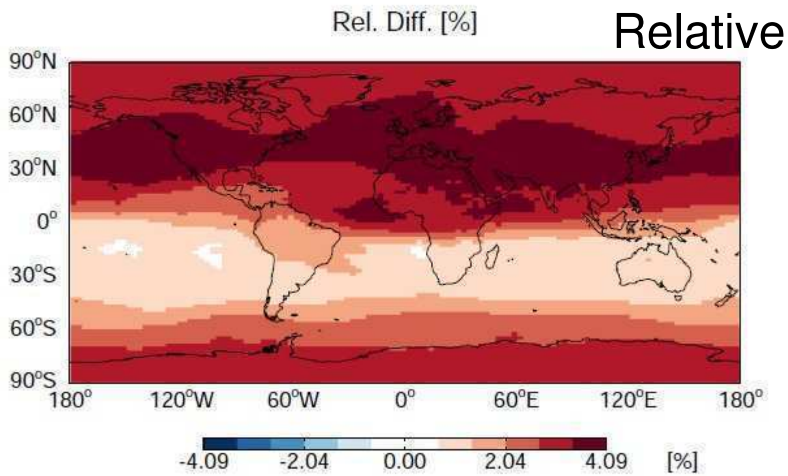
Winter

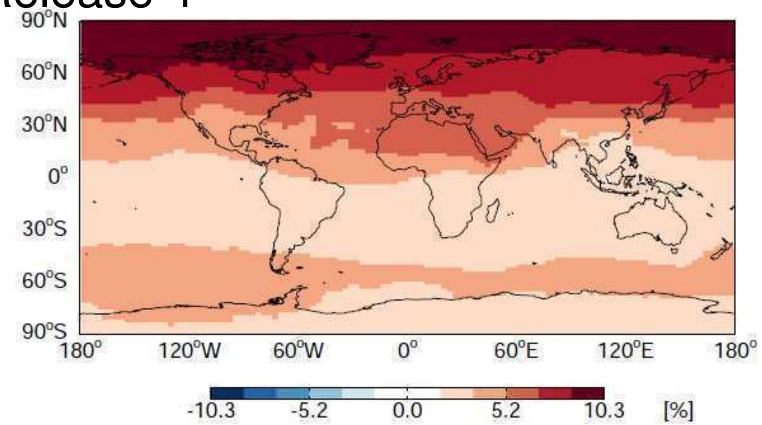
Summer

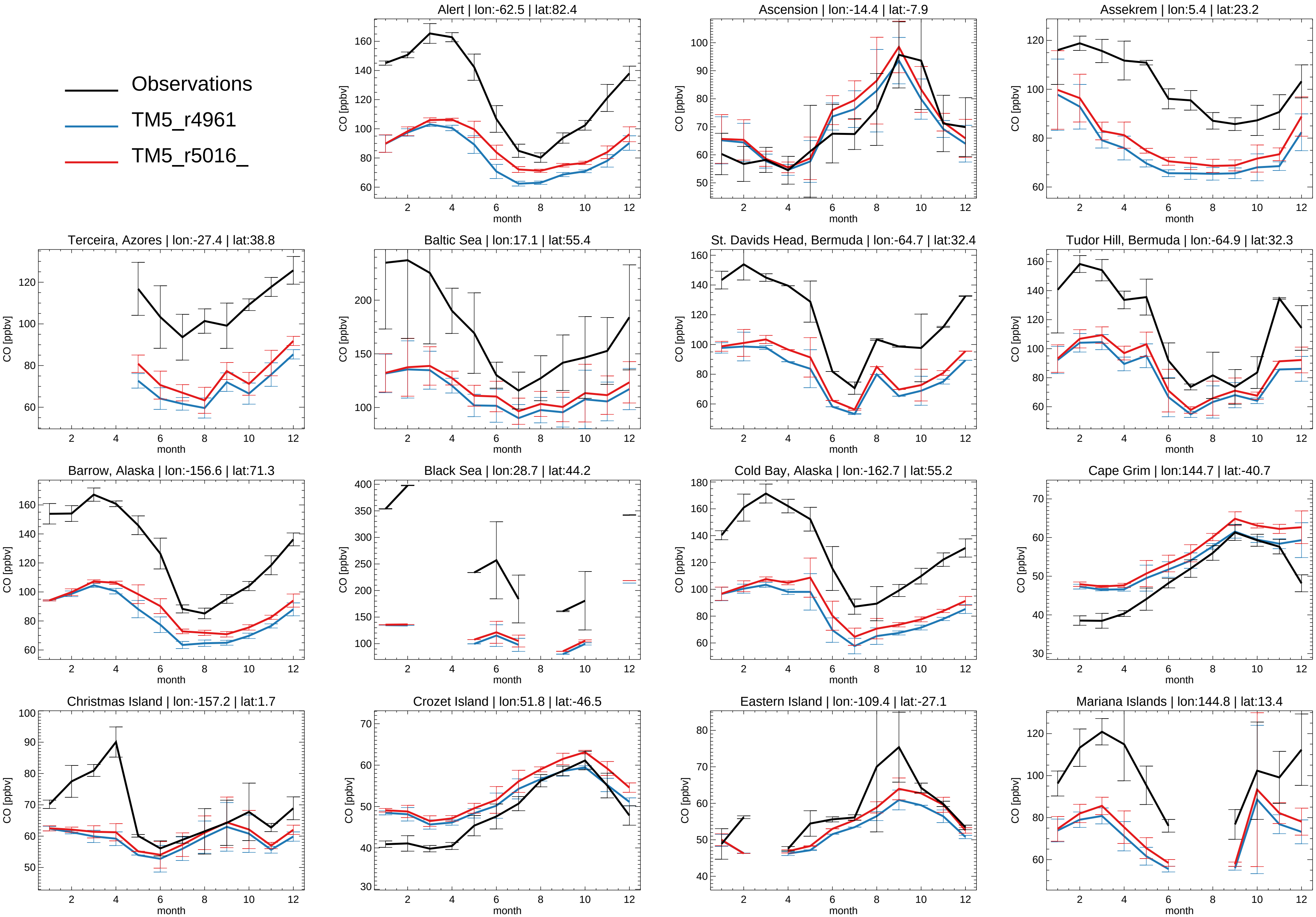


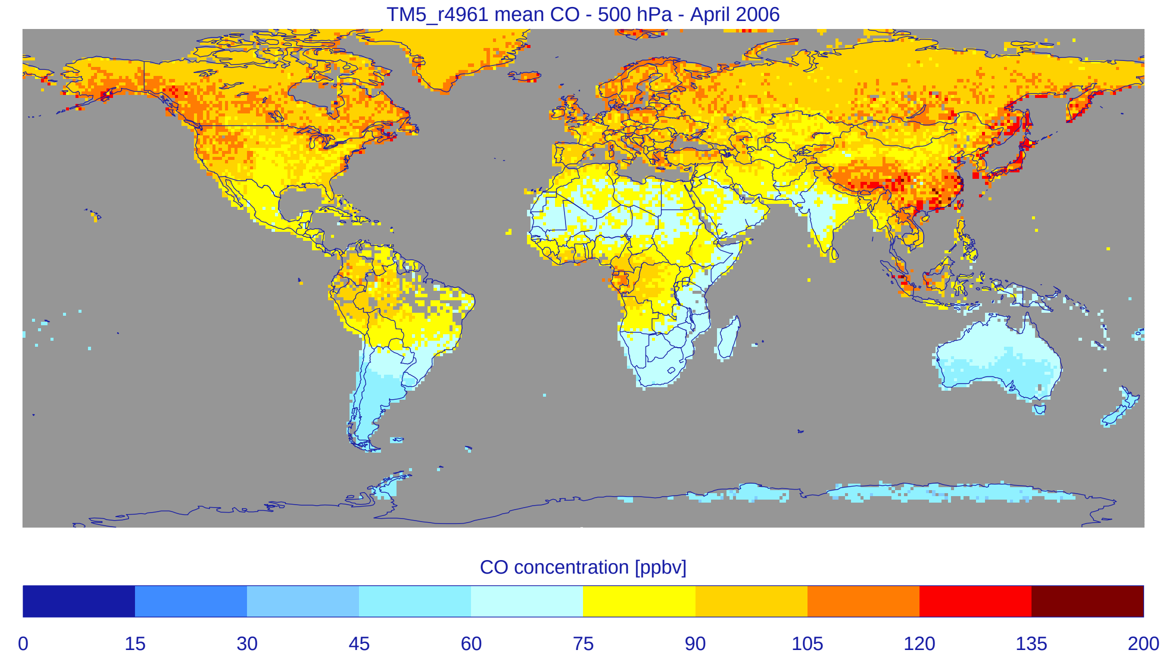


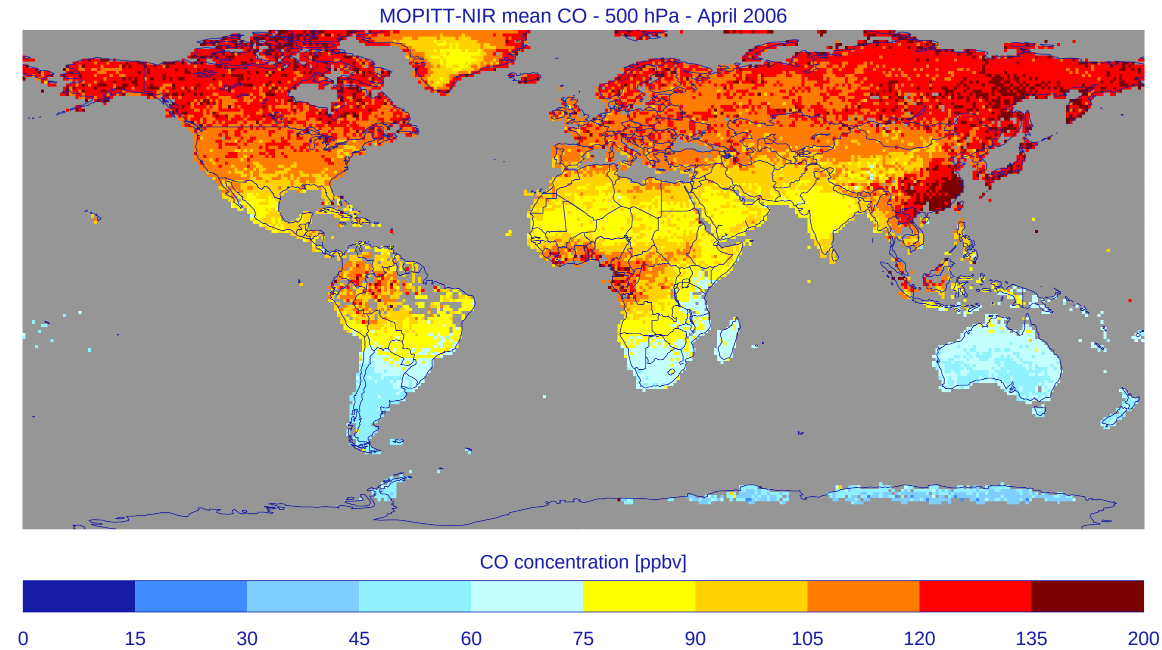
Relative to Release 4

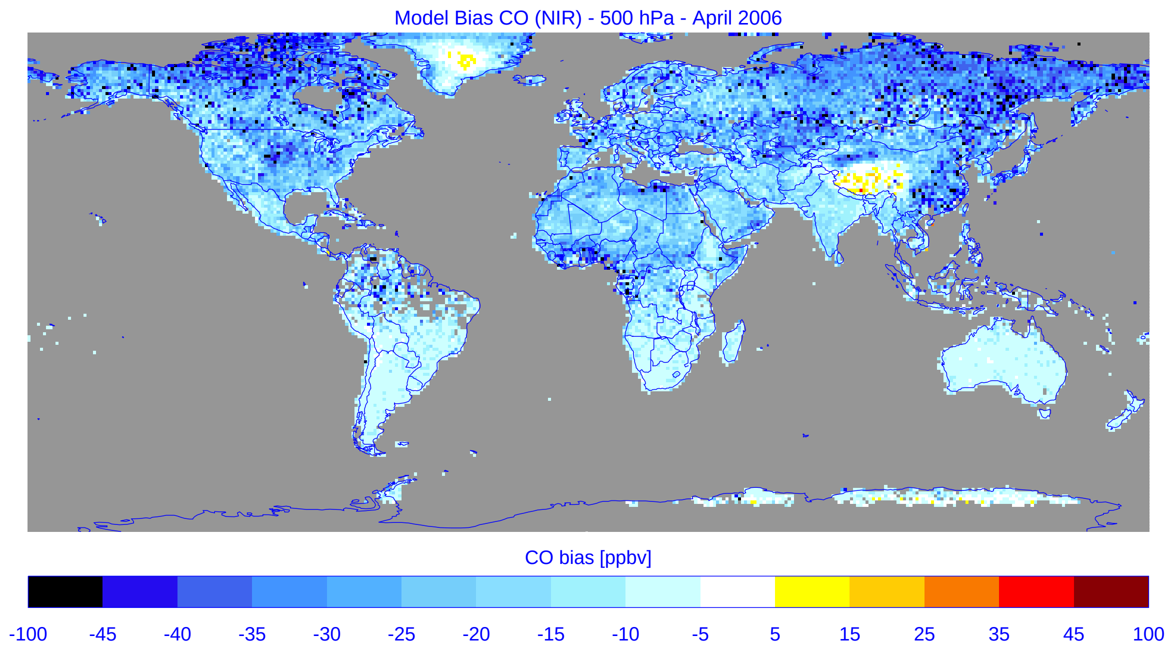




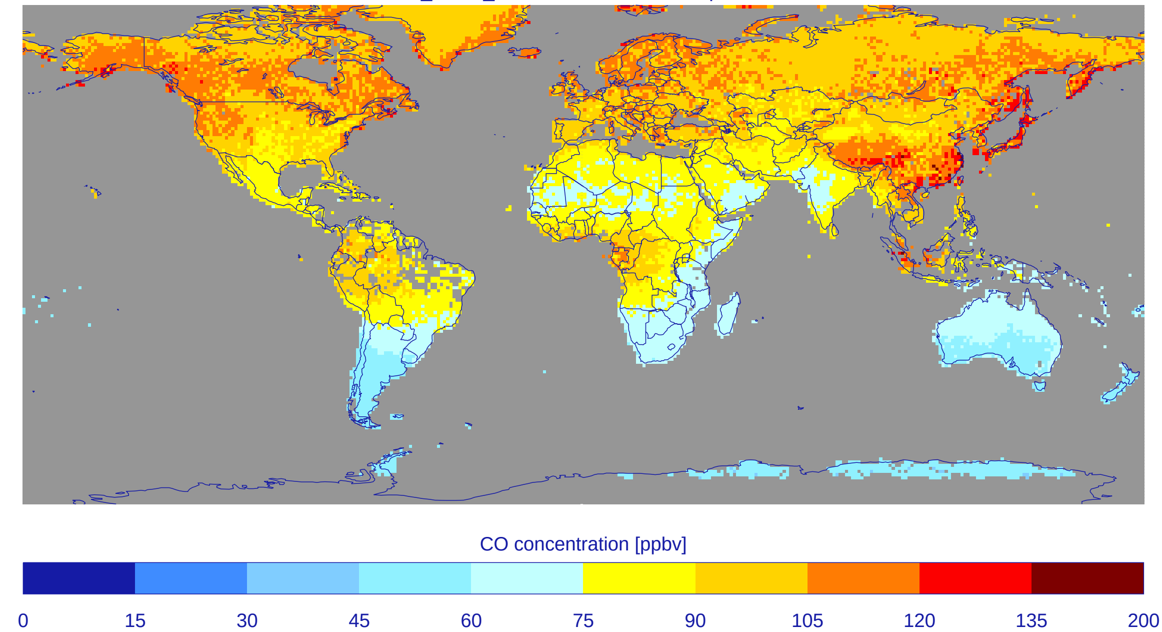

Observations
TM5_r4961
TM5_r5016_
Alert | lon:-62.5 | lat:82.4
Ascension | lon:-14.4 | lat:-7.9
Assekrem | lon:5.4 | lat:23.2
Terceira, Azores | lon:-27.4 | lat:38.8
Baltic Sea | lon:17.1 | lat:55.4
St. Davids Head, Bermuda | lon:-64.7 | lat:32.4
Tudor Hill, Bermuda | lon:-64.9 | lat:32.3
Barrow, Alaska | lon:-156.6 | lat:71.3
Black Sea | lon:28.7 | lat:44.2
Cold Bay, Alaska | lon:-162.7 | lat:55.2
Cape Grim | lon:144.7 | lat:-40.7
Christmas Island | lon:-157.2 | lat:1.7
Crozet Island | lon:51.8 | lat:-46.5
Eastern Island | lon:-109.4 | lat:-27.1
Mariana Islands | lon:144.8 | lat:13.4
CO [ppbv]
month


TM5_r4961 mean CO - 500 hPa - April 2006
CO concentration [ppbv]
0 15 30 45 60 75 90 105 120 135 200

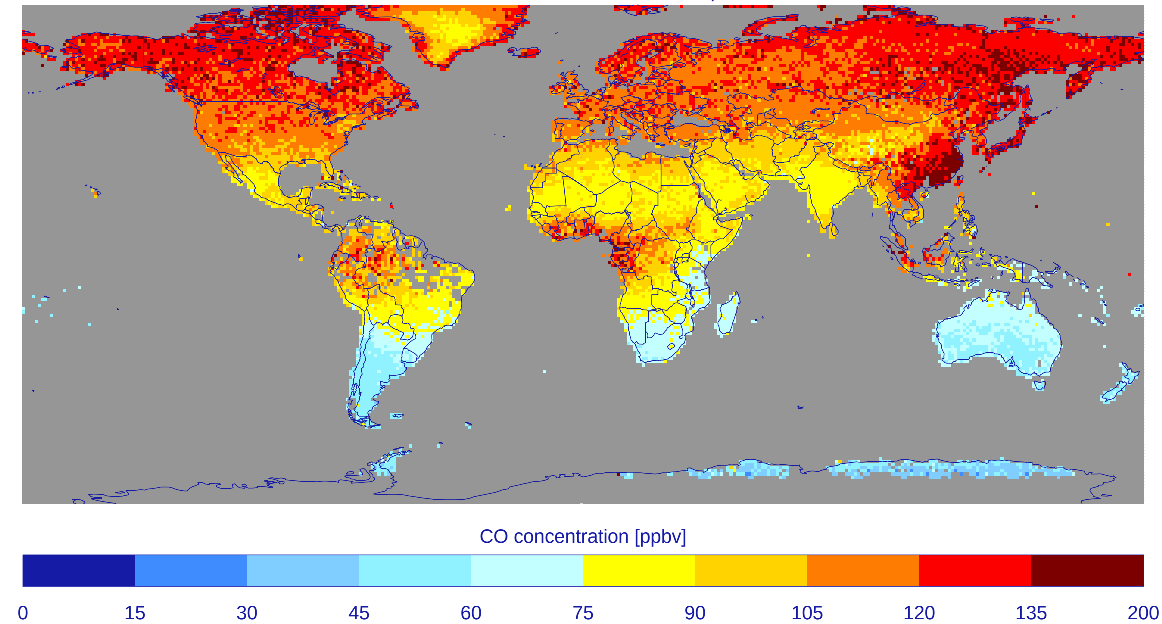

MOPITT-NIR mean CO - 500 hPa - April 2006
CO concentration [ppbv]
0 15 30 45 60 75 90 105 120 135 200


Model Bias CO (NIR) - 500 hPa - April 2006
CO bias [ppbv]
-100 -45 -40 -35 -30 -25 -20 -15 -10 -5 5 15 25 35 45 100

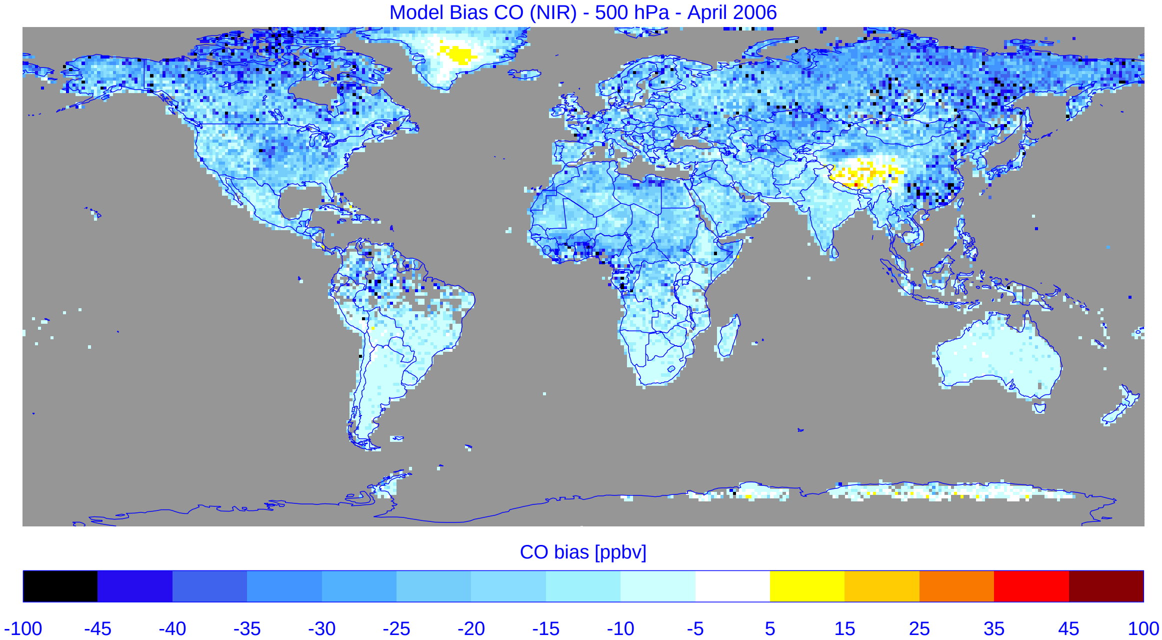
TM5_r5016_ mean CO - 500 hPa - April 2006



MOPITT-NIR mean CO - 500 hPa - April 2006



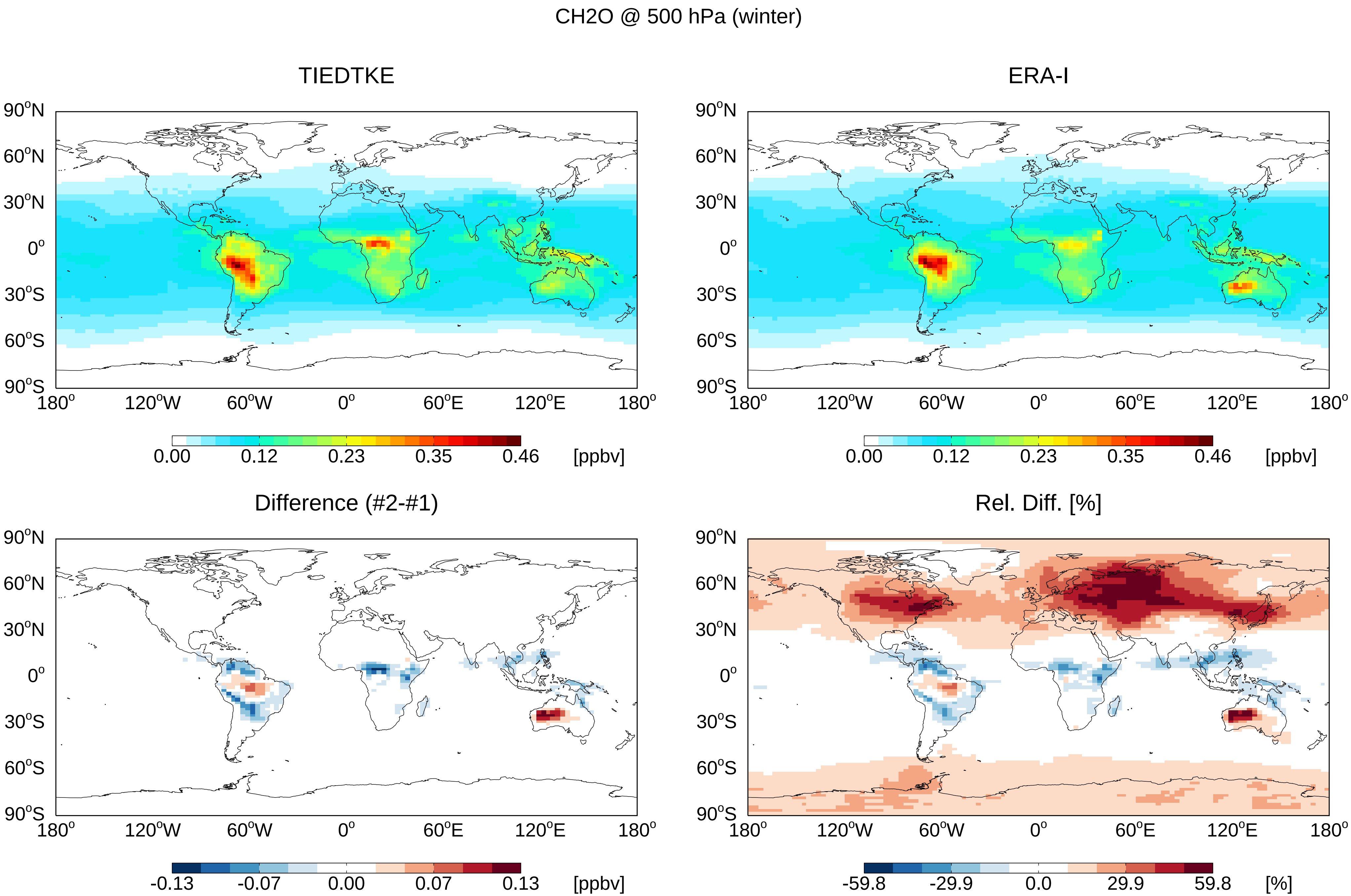
Model Bias CO (NIR) - 500 hPa - April 2006



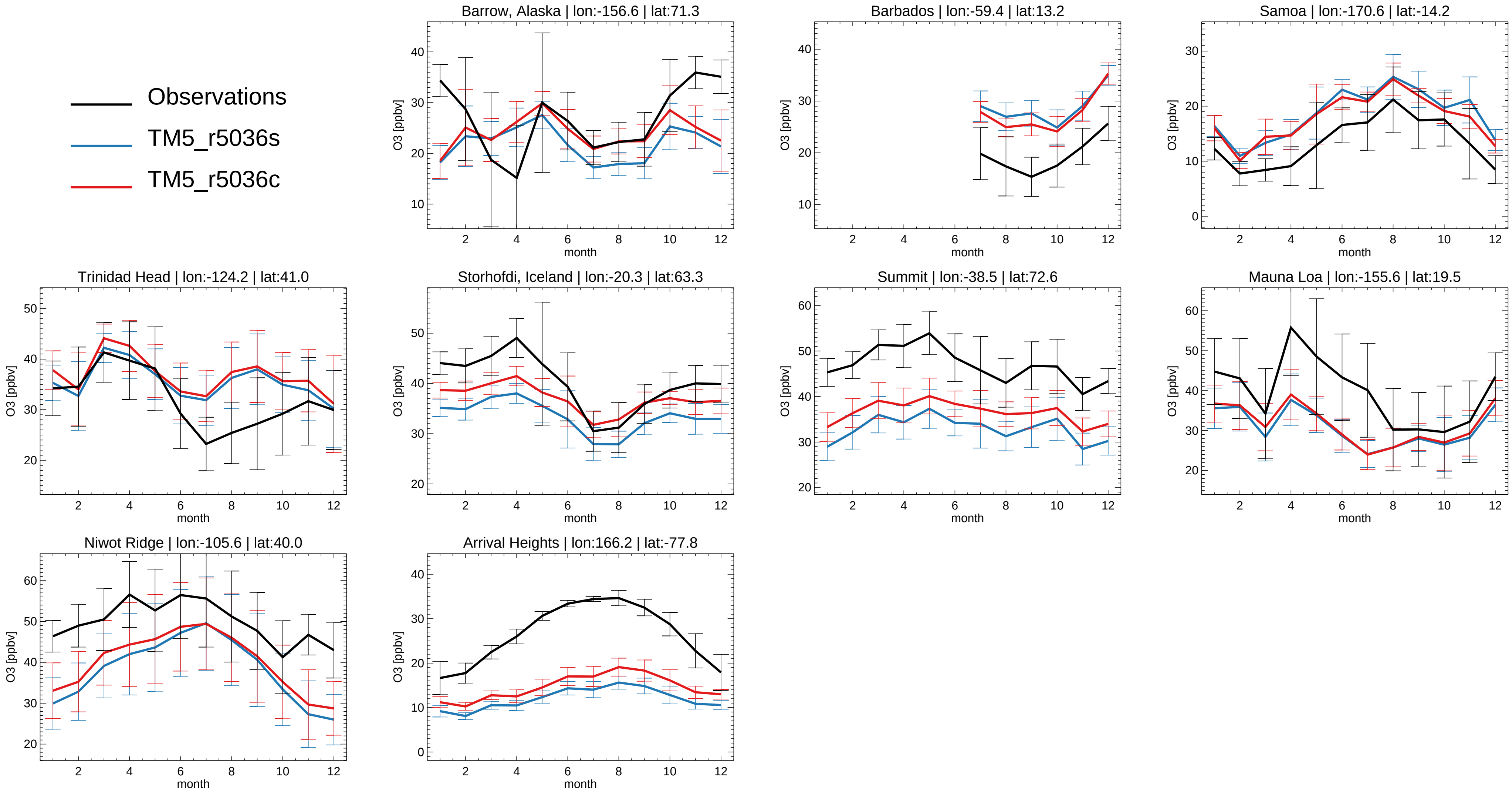
Convective fluxes

- increase LiNOx production => new scale factor
- significant changes in CH_2O @500 hPa above sources (Australia, Brazil)

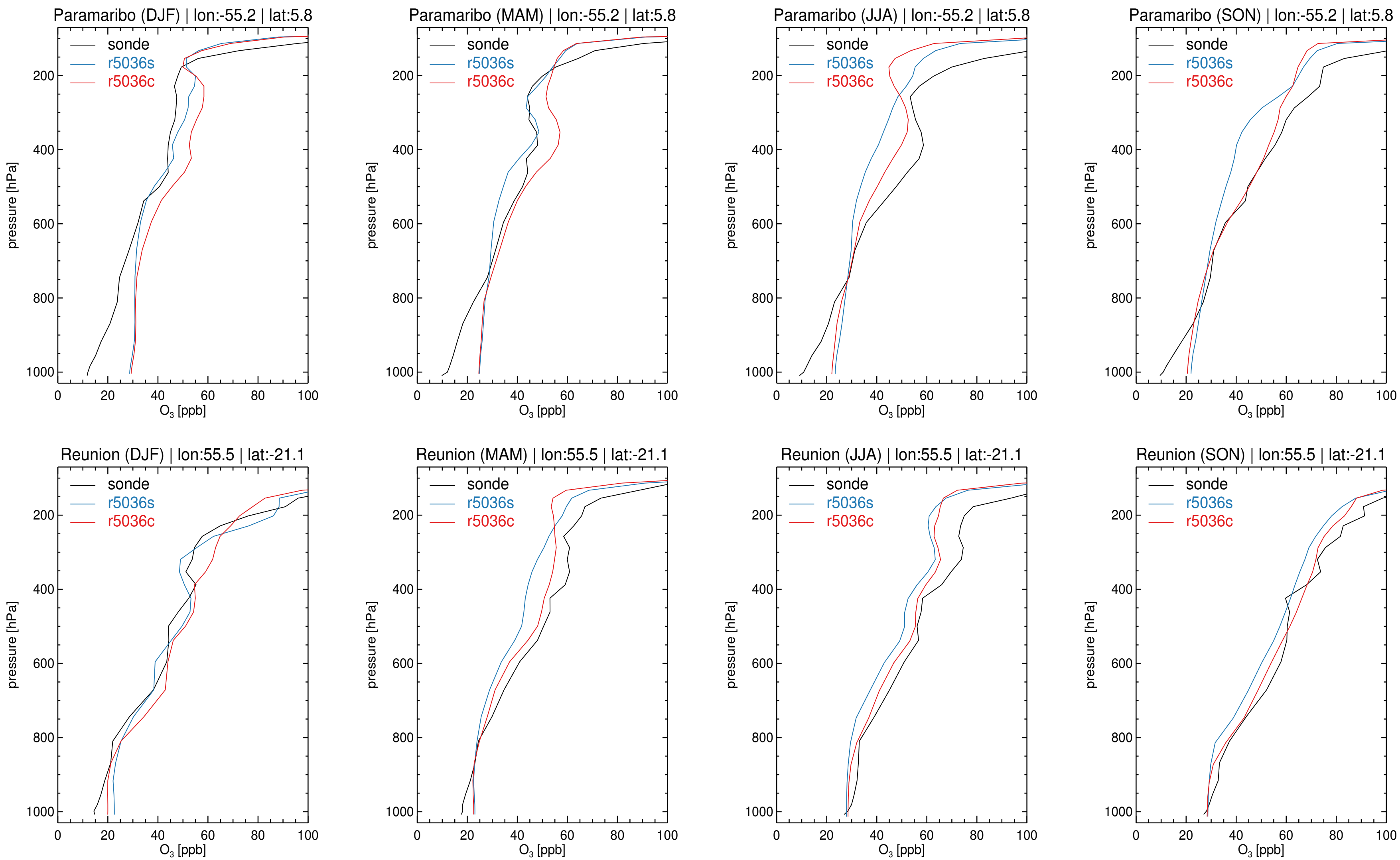
	Tiedkte	**EI fluxes**	diff.
Total pOH tropo(Tg)	1458	1512	54
Total pO3 tropo (Tg)	4492	4614	+121
Total lO3 tropo (Tg)	1735	1822	+87
tropO3 burden (Tg)	311	326	**+15**
CO burden (Tg)	313	302	**-10**



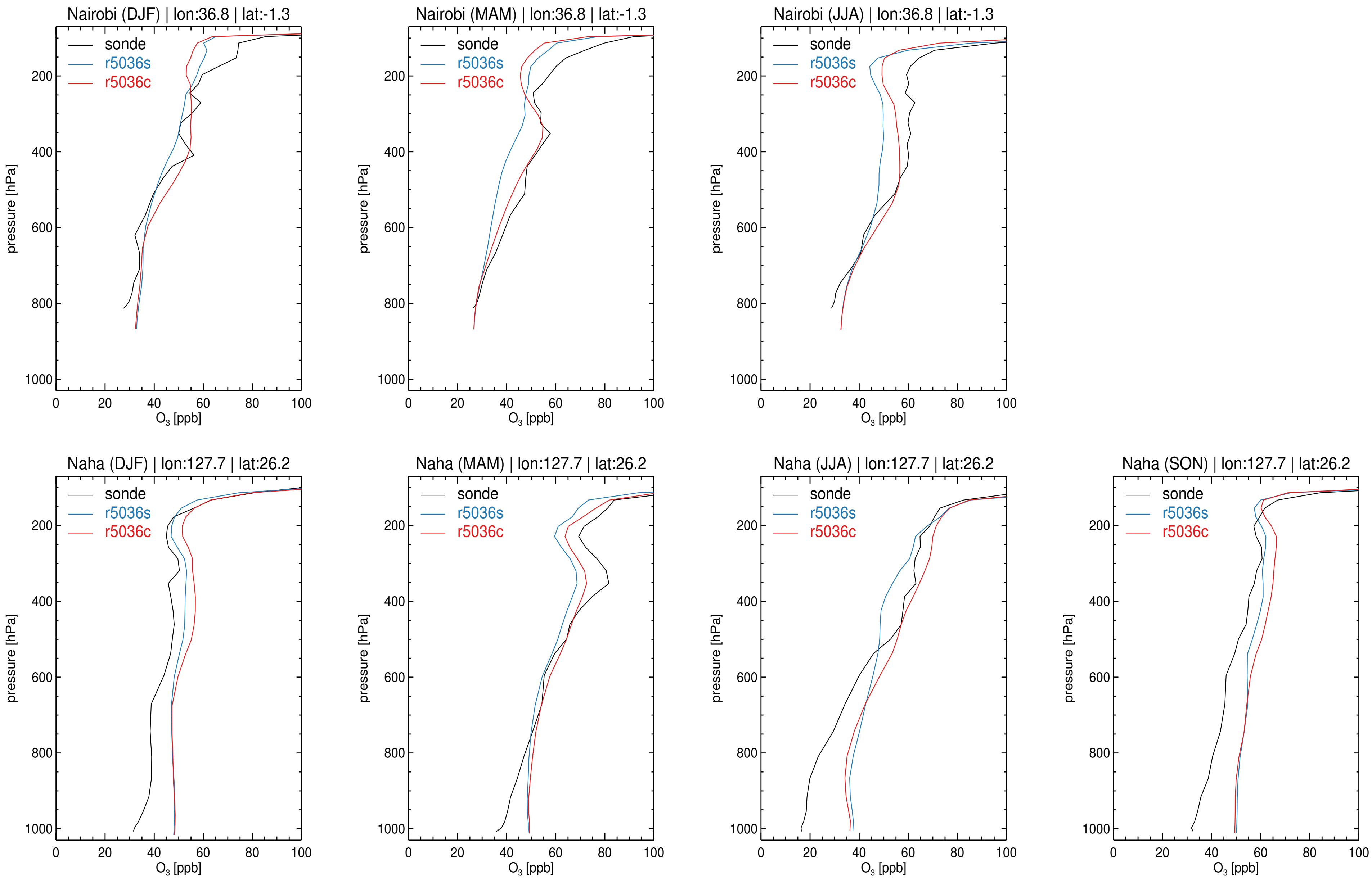
CH2O @ 500 hPa (winter)
TIEDTKE
ERA-I
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
0.00
0.12
0.23
0.35
0.46
[ppbv]
-0.13
-0.07
0.00
0.07
0.13
[ppbv]
-59.8
-29.9
0.0
29.9
59.8
[%]

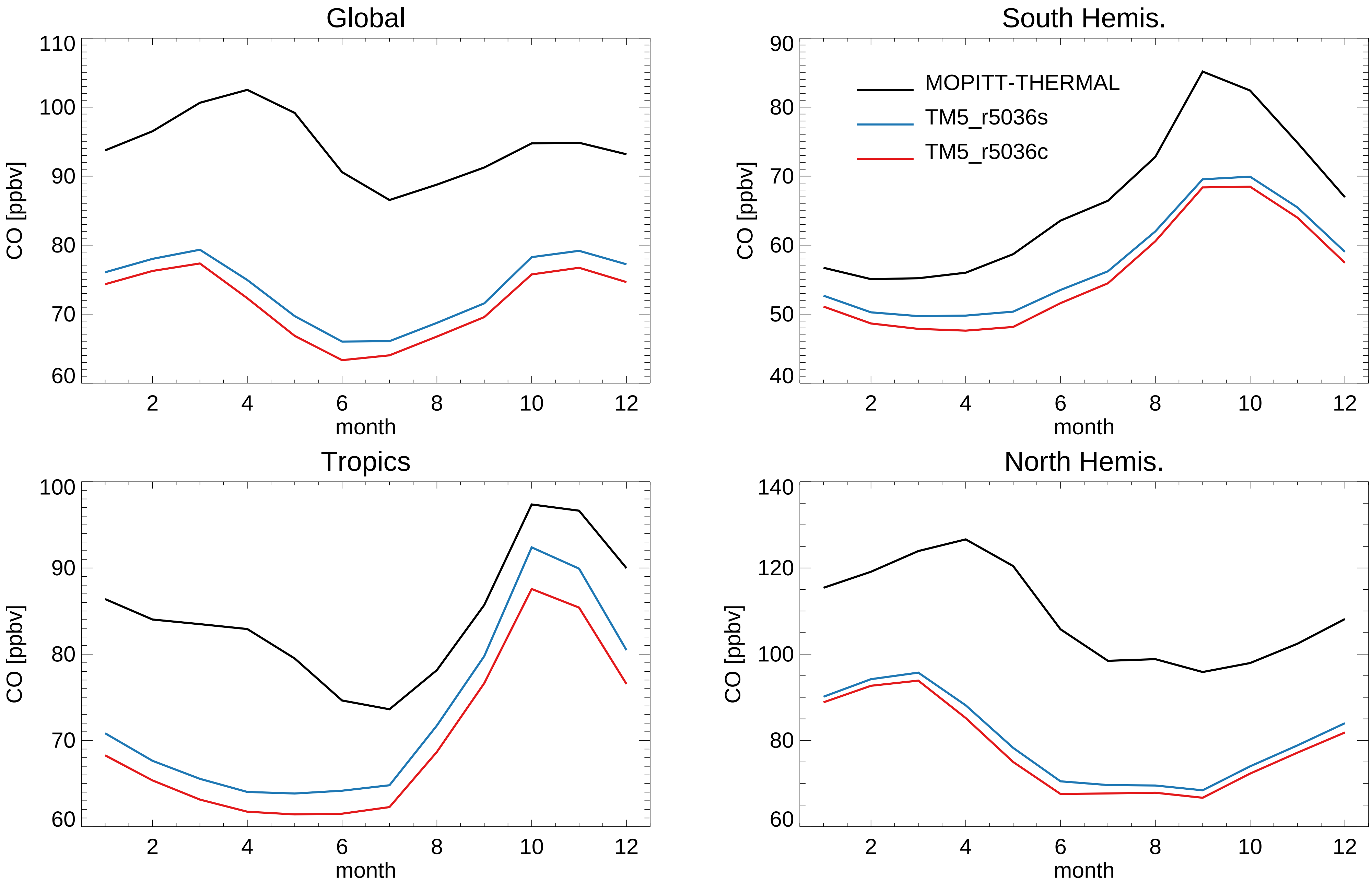


Monthly mean comparison of TM5 surface O3 against GMD(CMDL) surface observations
using co-located model output for 2006, sampled at the measurement times.
Error bars indicate the standard deviation in the monthly means.



Paramaribo (DJF) | lon:-55.2 | lat:5.8
Paramaribo (MAM) | lon:-55.2 | lat:5.8
Paramaribo (JJA) | lon:-55.2 | lat:5.8
Paramaribo (SON) | lon:-55.2 | lat:5.8
Reunion (DJF) | lon:55.5 | lat:-21.1
Reunion (MAM) | lon:55.5 | lat:-21.1
Reunion (JJA) | lon:55.5 | lat:-21.1
Reunion (SON) | lon:55.5 | lat:-21.1
sonde
r5036s
r5036c
pressure [hPa]
O_3 [ppb]
200
400
600
800
1000
0
20
40
60
80
100

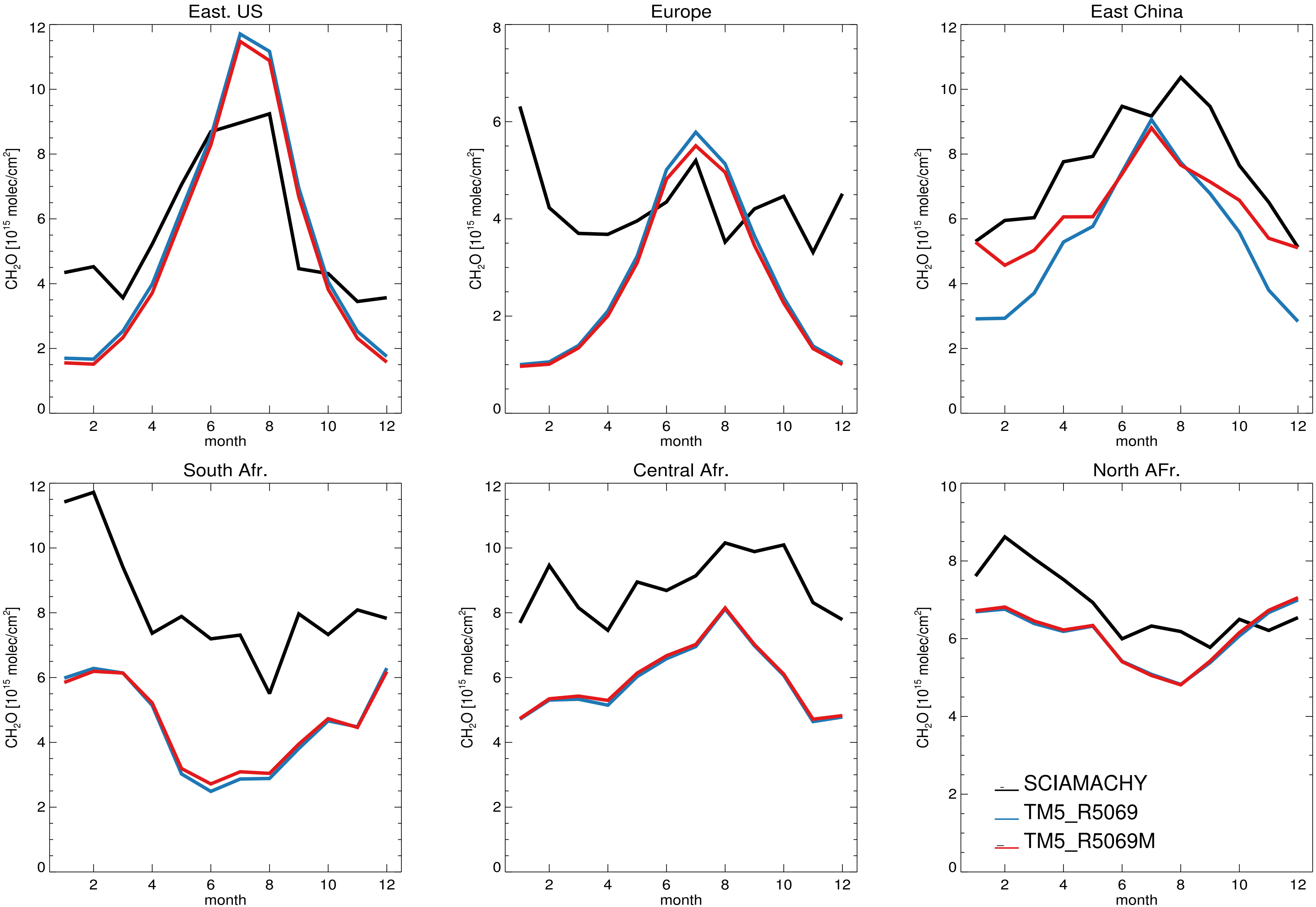

Nairobi (DJF) | lon:36.8 | lat:-1.3
Nairobi (MAM) | lon:36.8 | lat:-1.3
Nairobi (JJA) | lon:36.8 | lat:-1.3
Naha (DJF) | lon:127.7 | lat:26.2
Naha (MAM) | lon:127.7 | lat:26.2
Naha (JJA) | lon:127.7 | lat:26.2
Naha (SON) | lon:127.7 | lat:26.2
sonde
r5036s
r5036c
pressure [hPa]
200
400
600
800
1000
0
20
40
60
80
100
O3 [ppb]



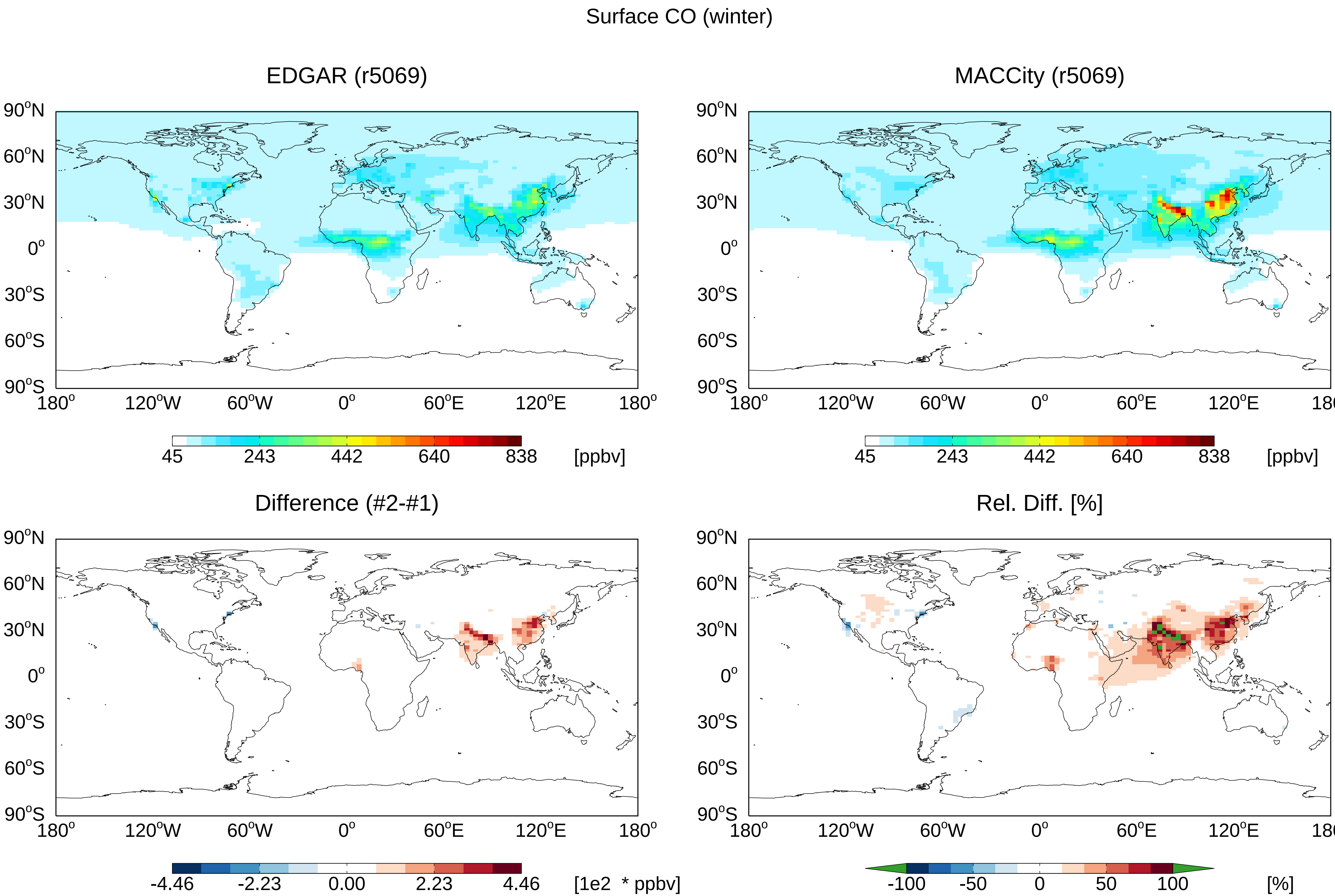
Annual cycle of mean, mass weighted CO in observations (black) and in TM5 for the MOPITT-THERMAL 500-hPa retrieval level.

MACC-City anthropogenic emissions

	EDGAR	MACC-City	Diff.
CO emission (Tg)	977	1067	**+90**
surf CO emission(Tg)	452	439	-13
trop CO burden (Tg)	292	297	5
Total pOH tropo(Tg)	1327	1360	33

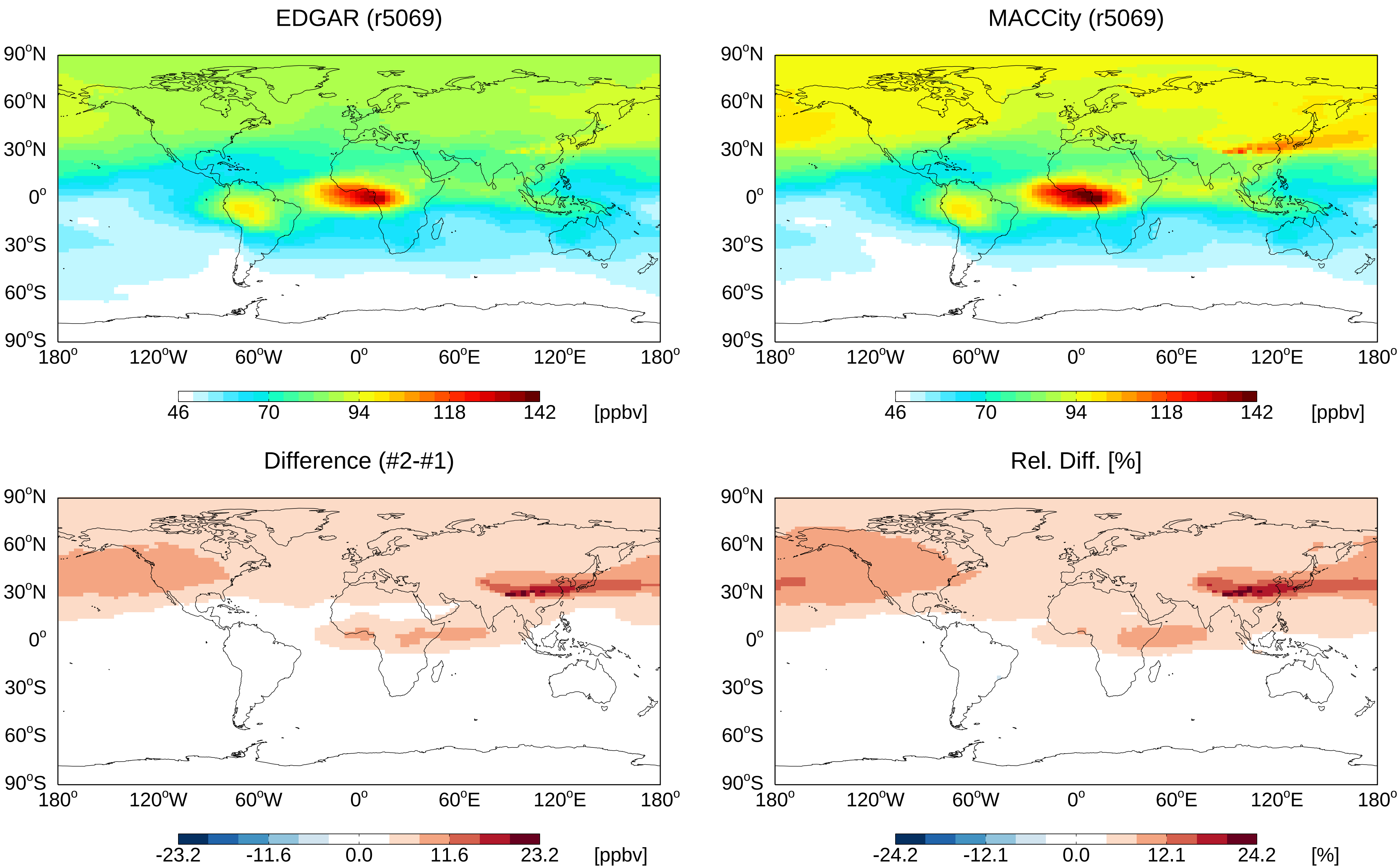


Annual cycle of CH2O columns integrated over different regions.



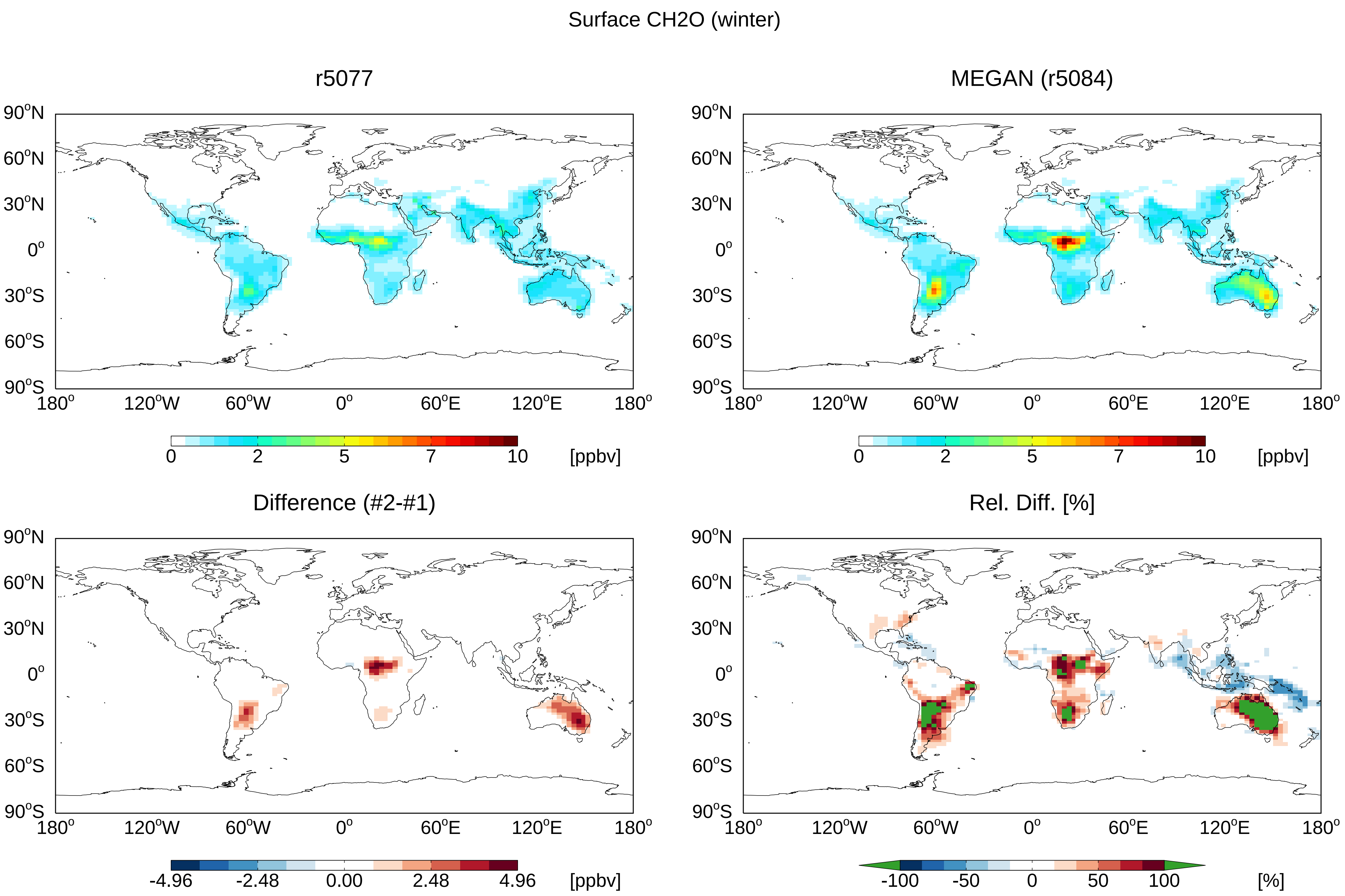
Surface CO (winter)
EDGAR (r5069)
MACCity (r5069)
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
45 243 442 640 838
[ppbv]
-4.46 -2.23 0.00 2.23 4.46
[1e2 * ppbv]
-100 -50 0 50 100
[%]

CO @ 500 hPa (winter)

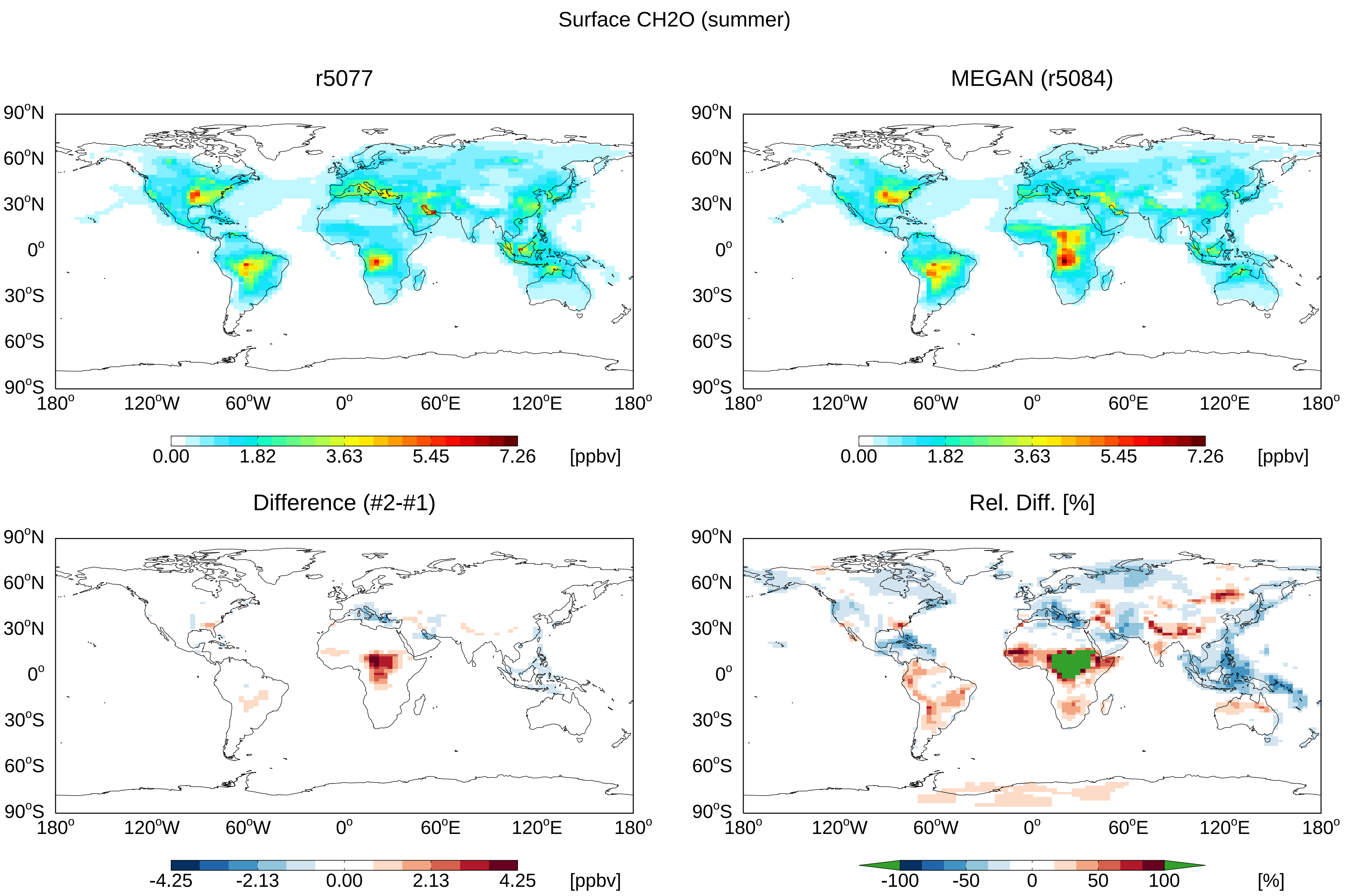


MEGAN biogenic emissions

	MACC	**MEGAN**	Diff.
ISOP emission (Tg)	523	579	**+55**
CO emission (Tg)	1067	1081	+14
CO burden (Tg)	321	344	23
Total pOH tropo(Tg)	1358	1405	46

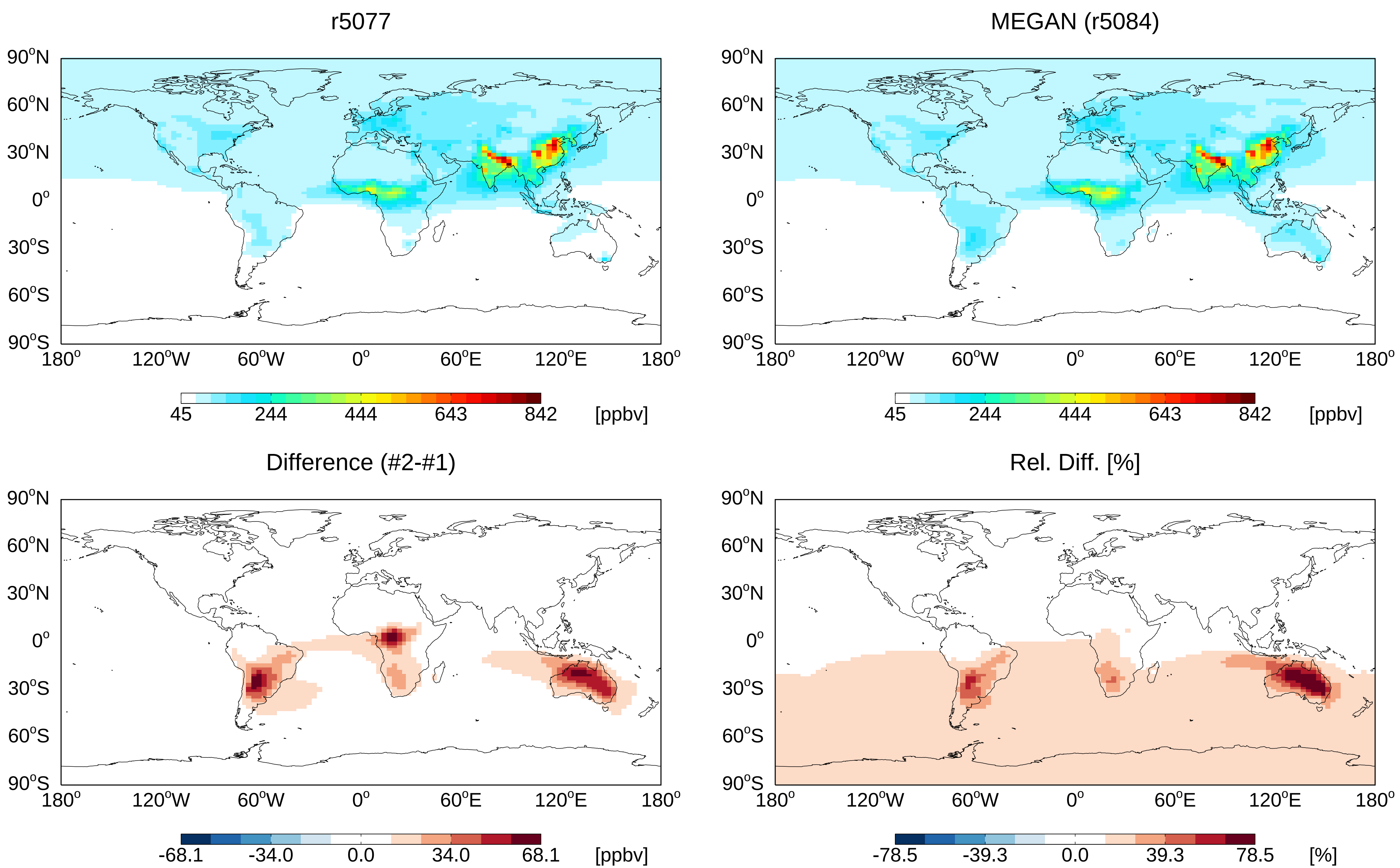


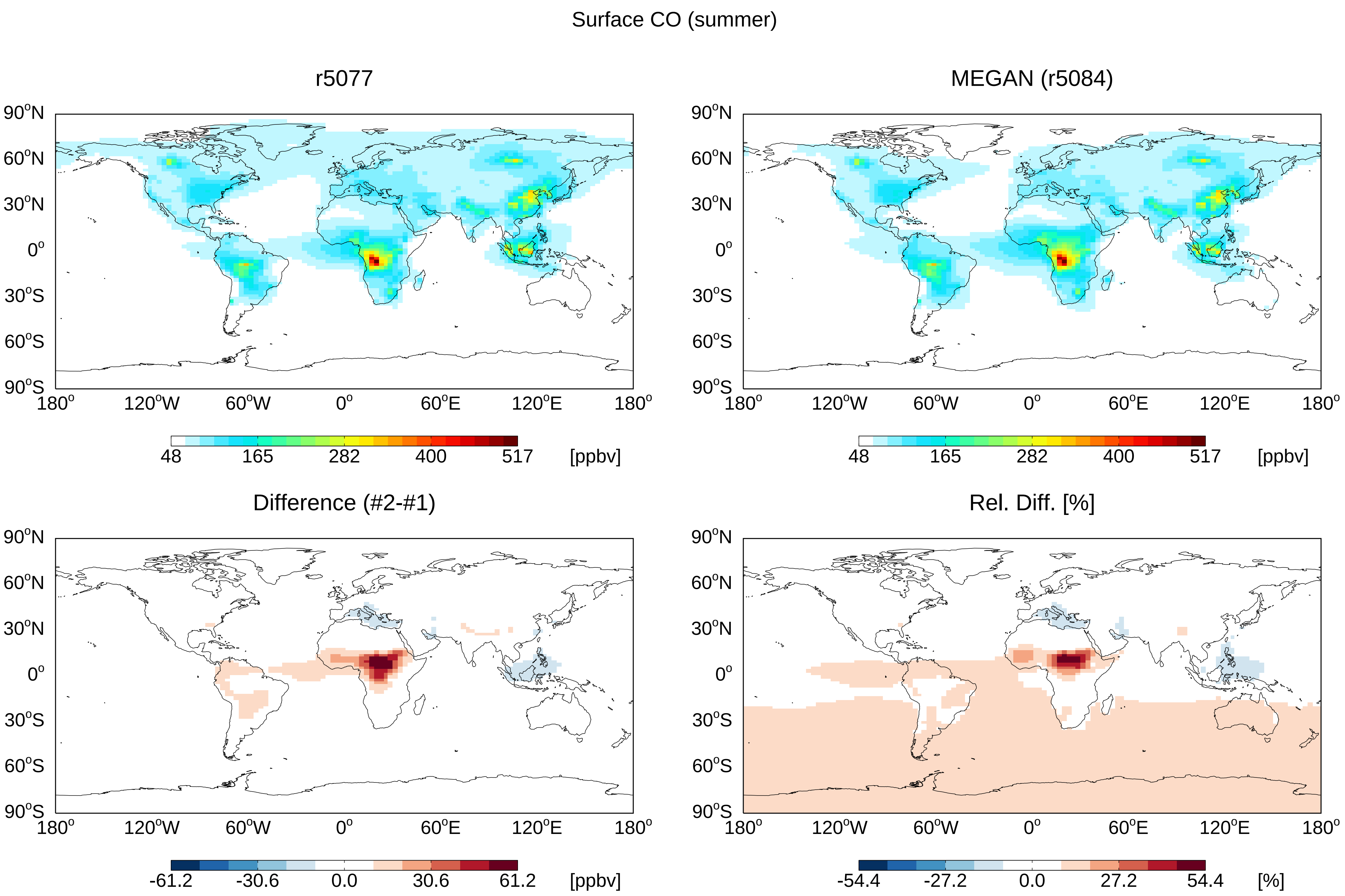
Surface CH2O (winter)
r5077
MEGAN (r5084)
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
0
2
5
7
10
[ppbv]
-4.96
-2.48
0.00
2.48
4.96
[ppbv]
-100
-50
0
50
100
[%]



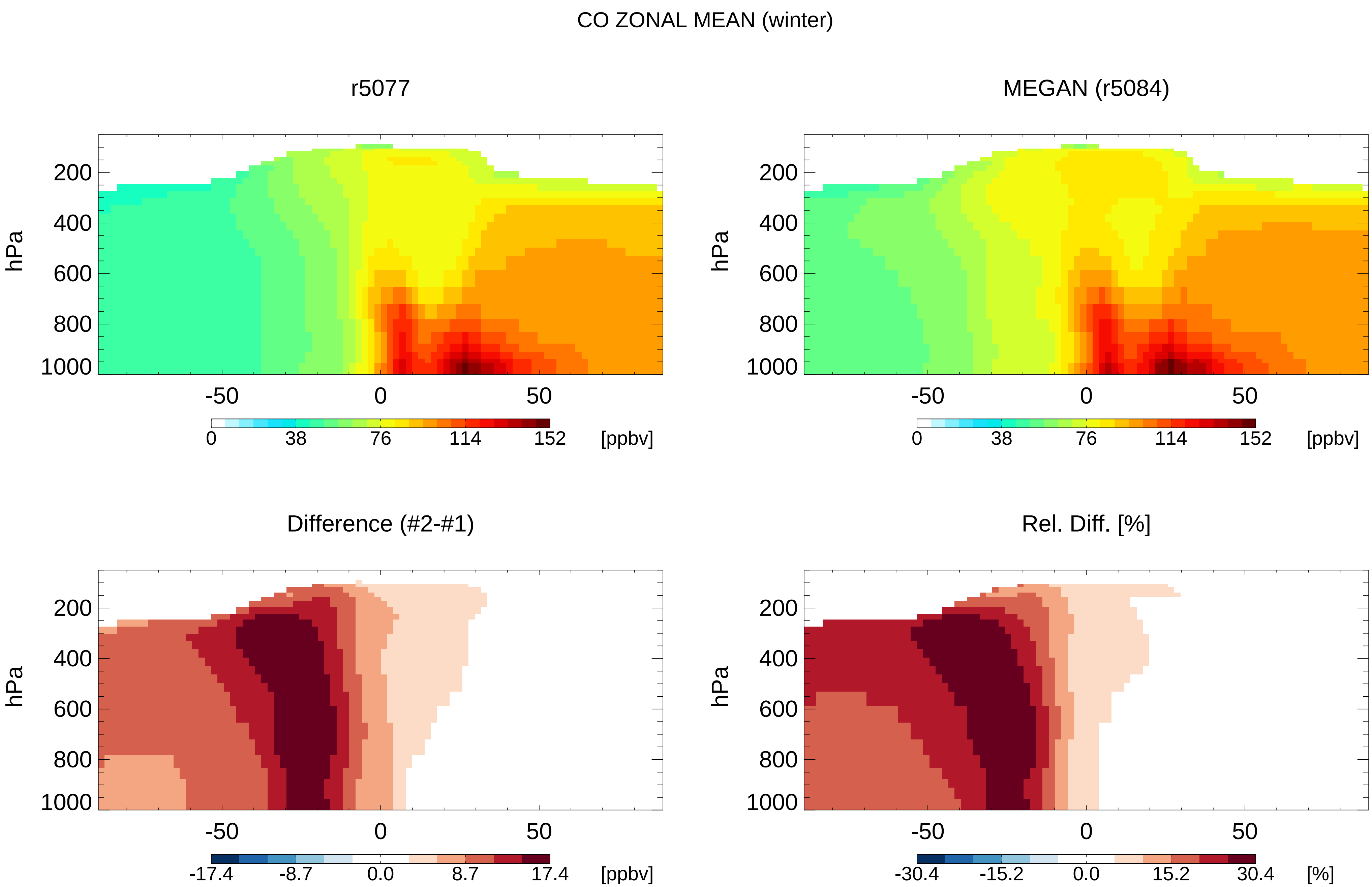
Surface CH2O (summer)
r5077
MEGAN (r5084)
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
0.00
1.82
3.63
5.45
7.26
[ppbv]
-4.25
-2.13
0.00
2.13
4.25
[ppbv]
-100
-50
0
50
100
[%]

Surface CO (winter)



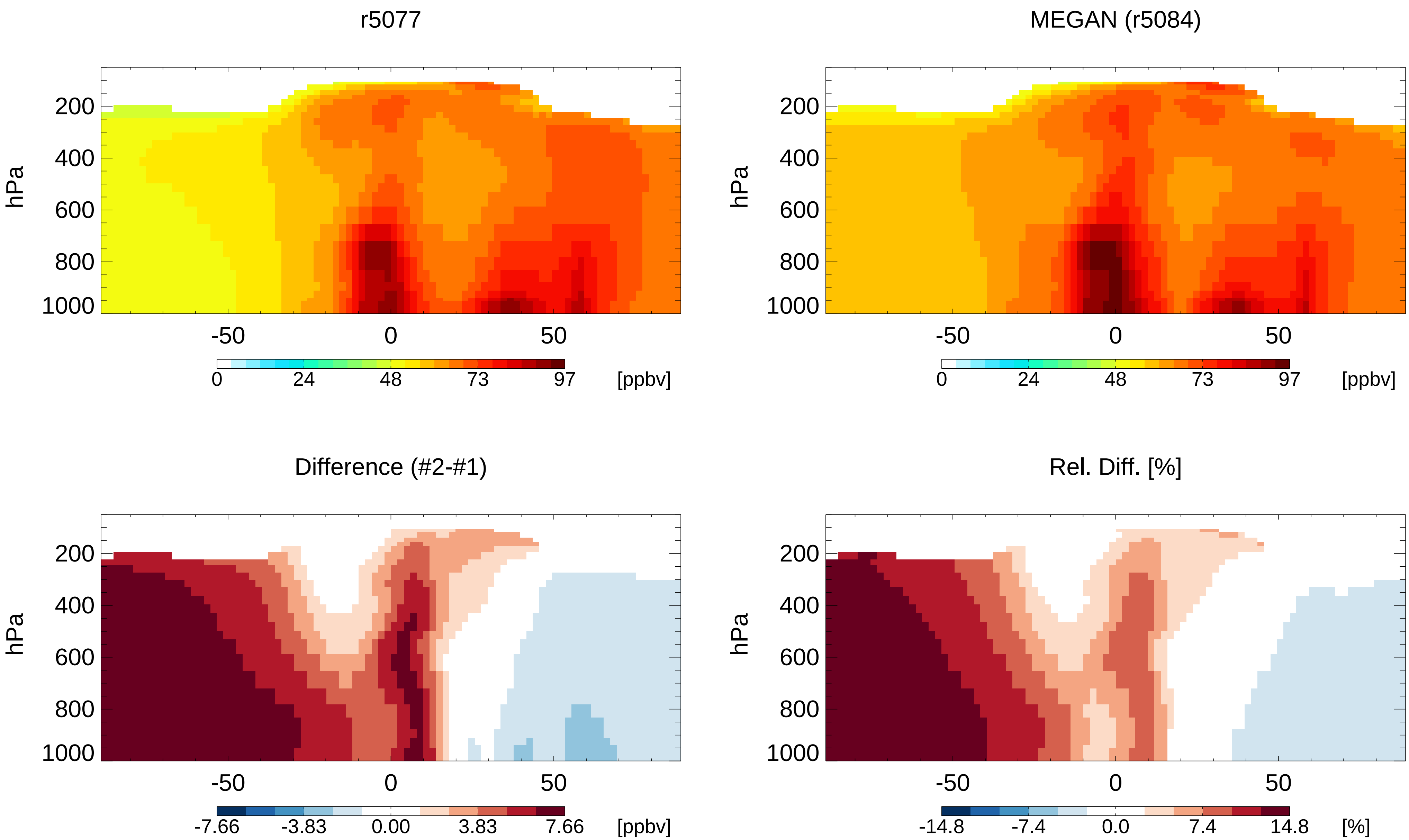


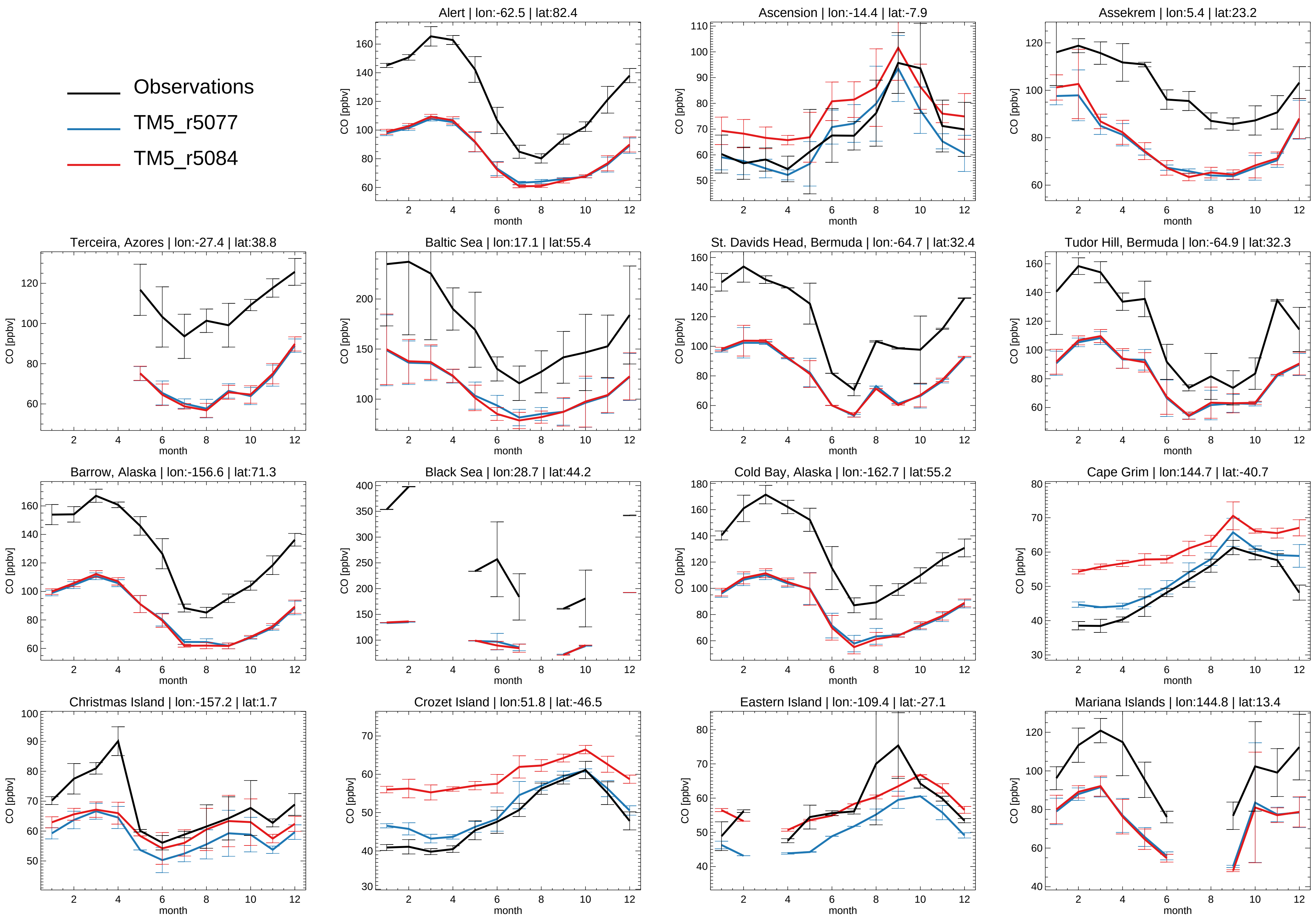
Surface CO (summer)
r5077
MEGAN (r5084)
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
48
165
282
400
517
[ppbv]
-61.2
-30.6
0.0
30.6
61.2
[ppbv]
-54.4
-27.2
0.0
27.2
54.4
[%]

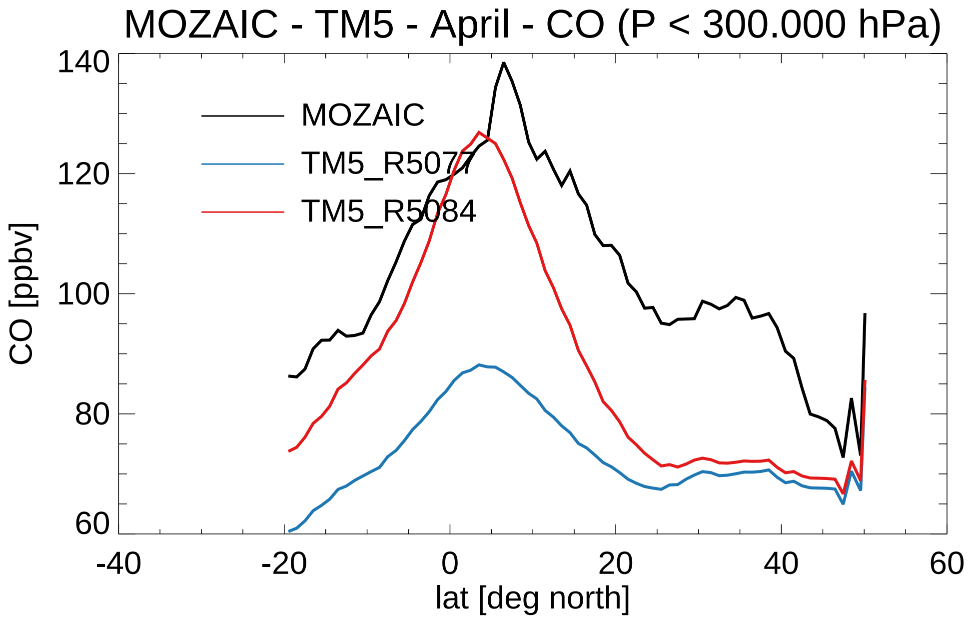


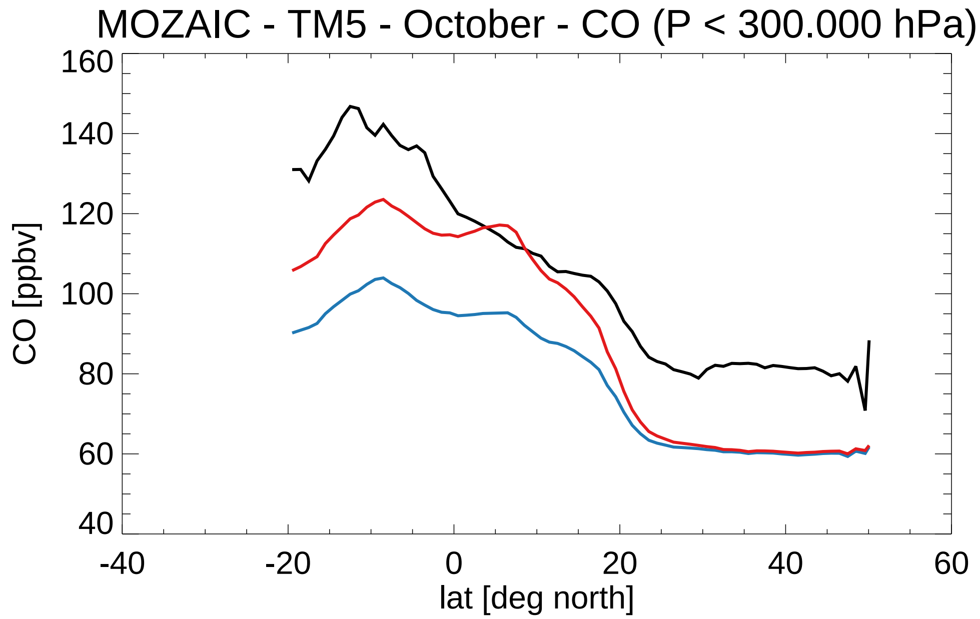
CO ZONAL MEAN (winter)
r5077
MEGAN (r5084)
Difference (#2-#1)
Rel. Diff. [%]
hPa
200
400
600
800
1000
-50
0
50
0
38
76
114
152
[ppbv]
-17.4
-8.7
0.0
8.7
17.4
[ppbv]
-30.4
-15.2
0.0
15.2
30.4
[%]

CO ZONAL MEAN (summer)

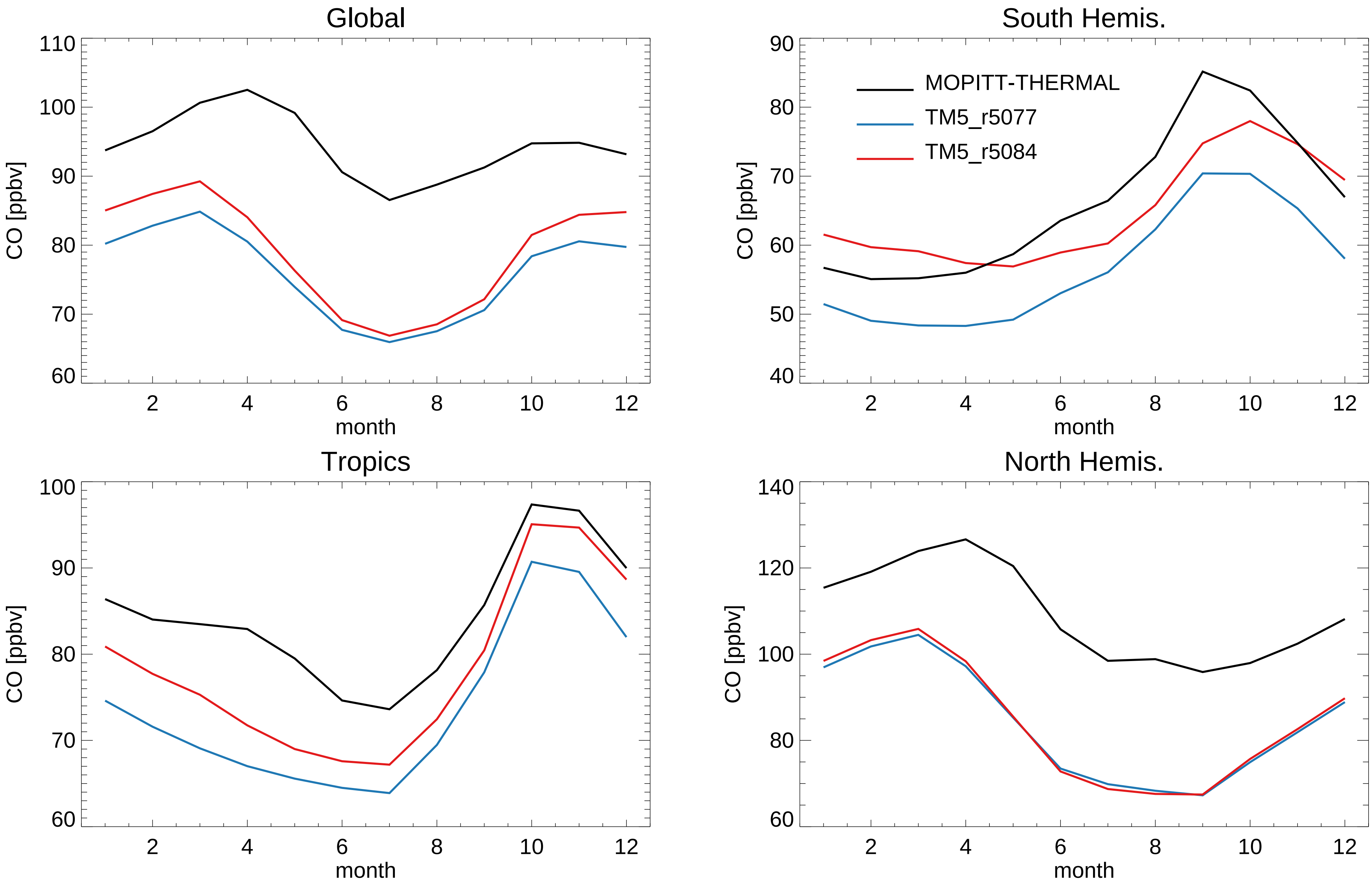



Observations
TM5_r5077
TM5_r5084
Alert | lon:-62.5 | lat:82.4
Ascension | lon:-14.4 | lat:-7.9
Assekrem | lon:5.4 | lat:23.2
Terceira, Azores | lon:-27.4 | lat:38.8
Baltic Sea | lon:17.1 | lat:55.4
St. Davids Head, Bermuda | lon:-64.7 | lat:32.4
Tudor Hill, Bermuda | lon:-64.9 | lat:32.3
Barrow, Alaska | lon:-156.6 | lat:71.3
Black Sea | lon:28.7 | lat:44.2
Cold Bay, Alaska | lon:-162.7 | lat:55.2
Cape Grim | lon:144.7 | lat:-40.7
Christmas Island | lon:-157.2 | lat:1.7
Crozet Island | lon:51.8 | lat:-46.5
Eastern Island | lon:-109.4 | lat:-27.1
Mariana Islands | lon:144.8 | lat:13.4
CO [ppbv]
month

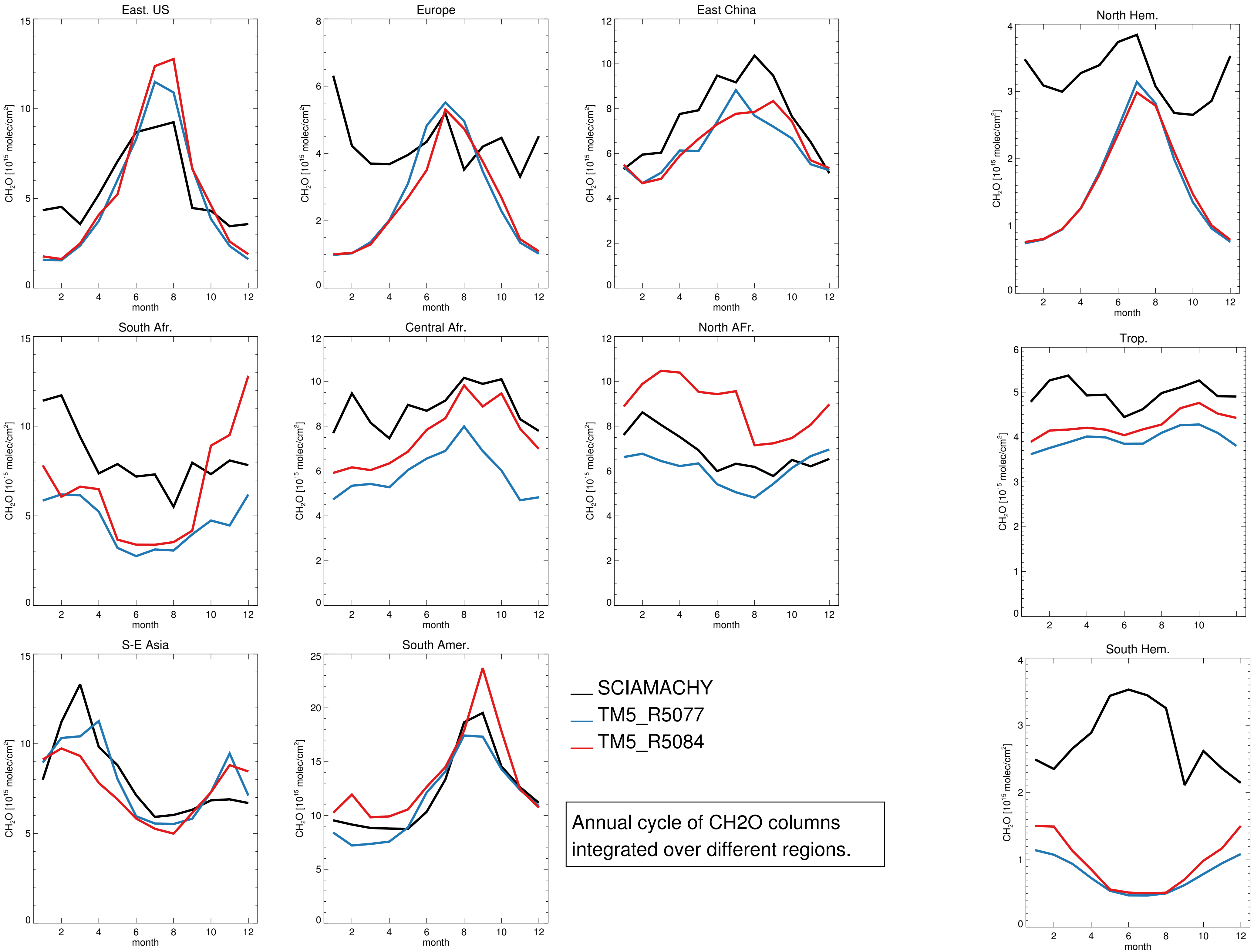




Monthly mean comparisons of TM5 UTLS CO concentrations sampled at the measurement place and time against MOZAIC flight data between Frankfurt (N50.0, E8.6) and Windhoek (E17.7, S22.5) for April (left column) and October 2006 (right). Data at pressures higher than 300 hPa has been filtered out.



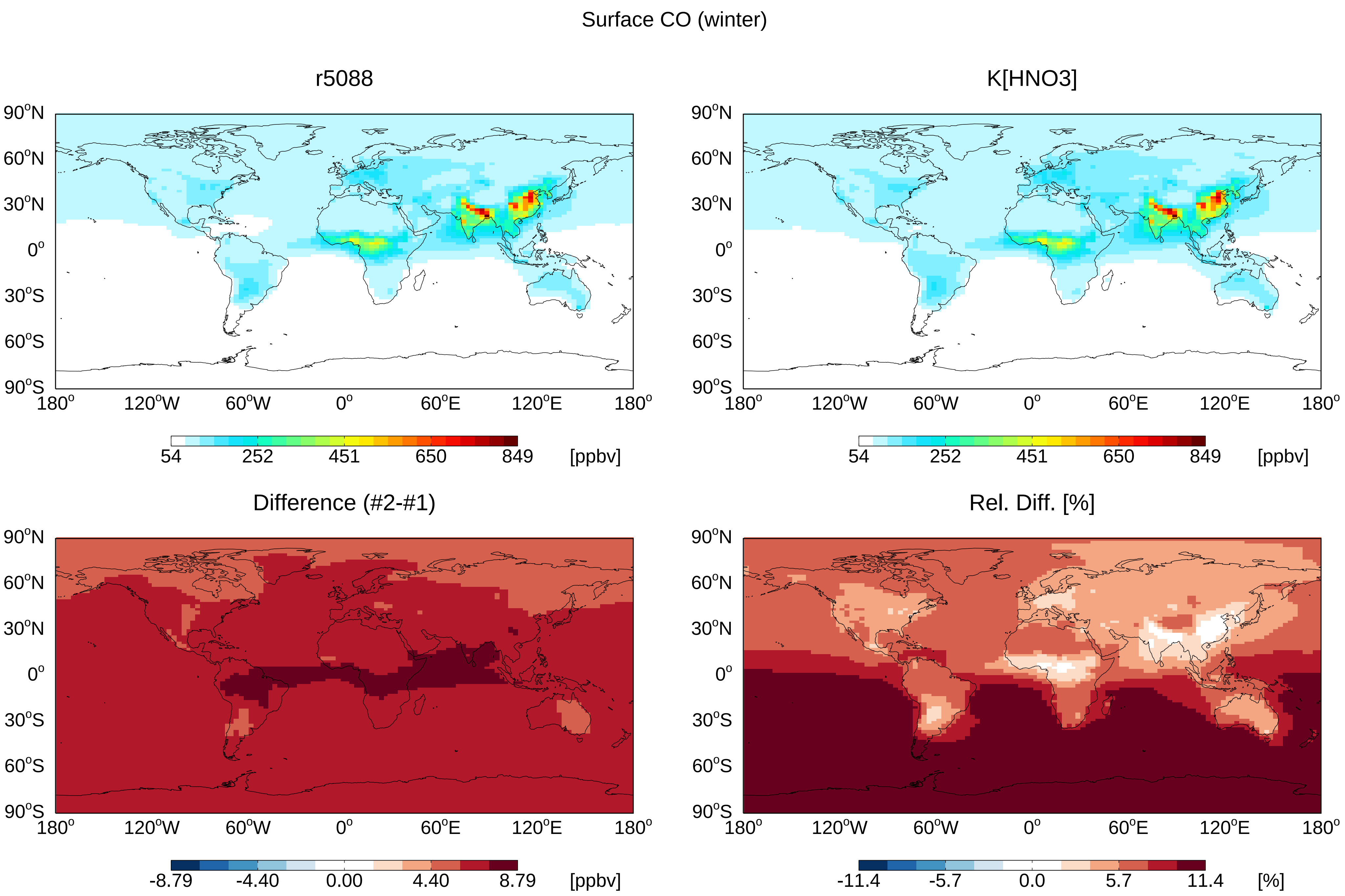
Annual cycle of mean, mass weighted CO in observations (black) and in TM5 for the MOPITT-THERMAL 500-hPa retrieval level.

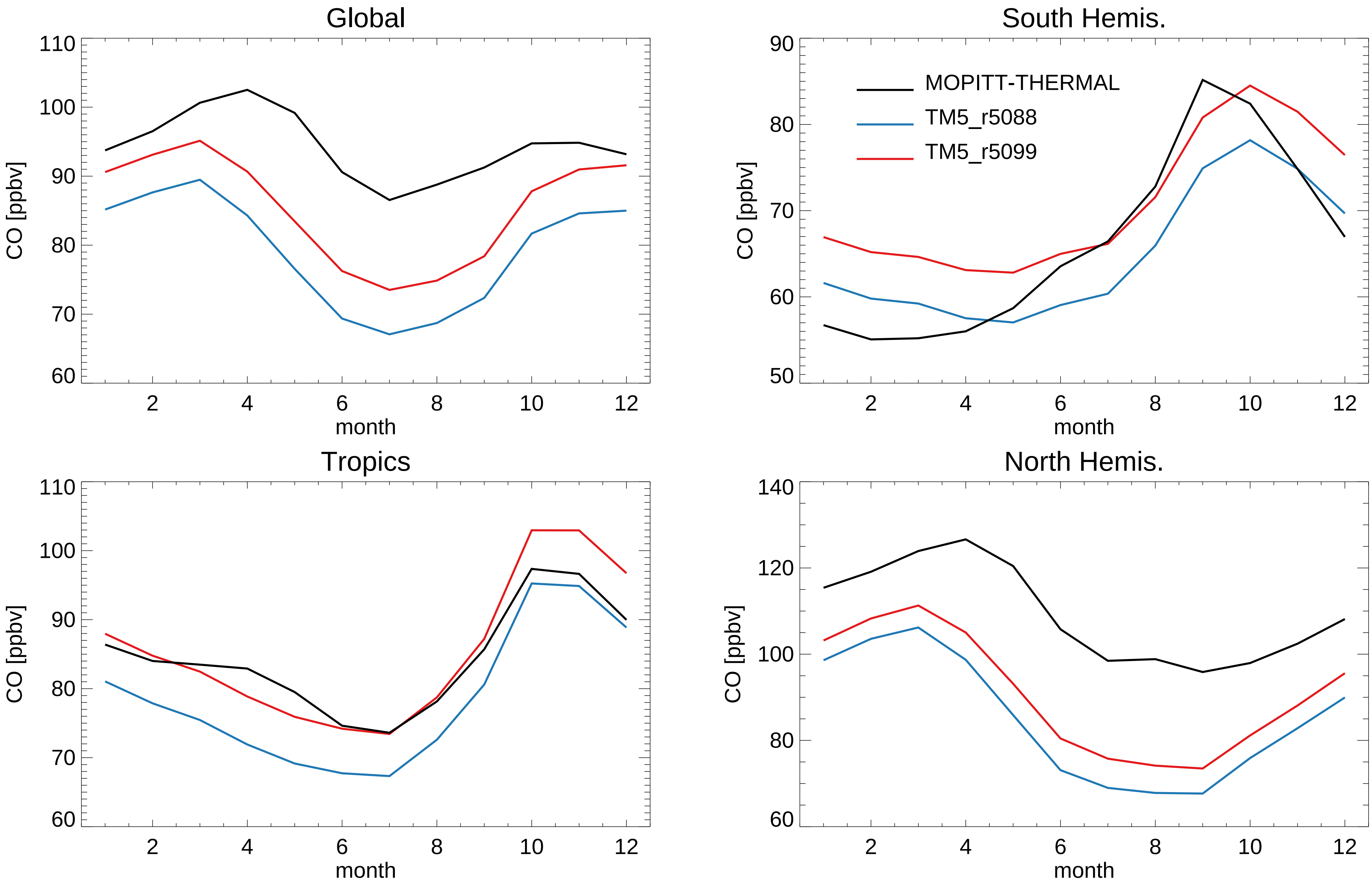


Annual cycle of CH2O columns integrated over different regions.

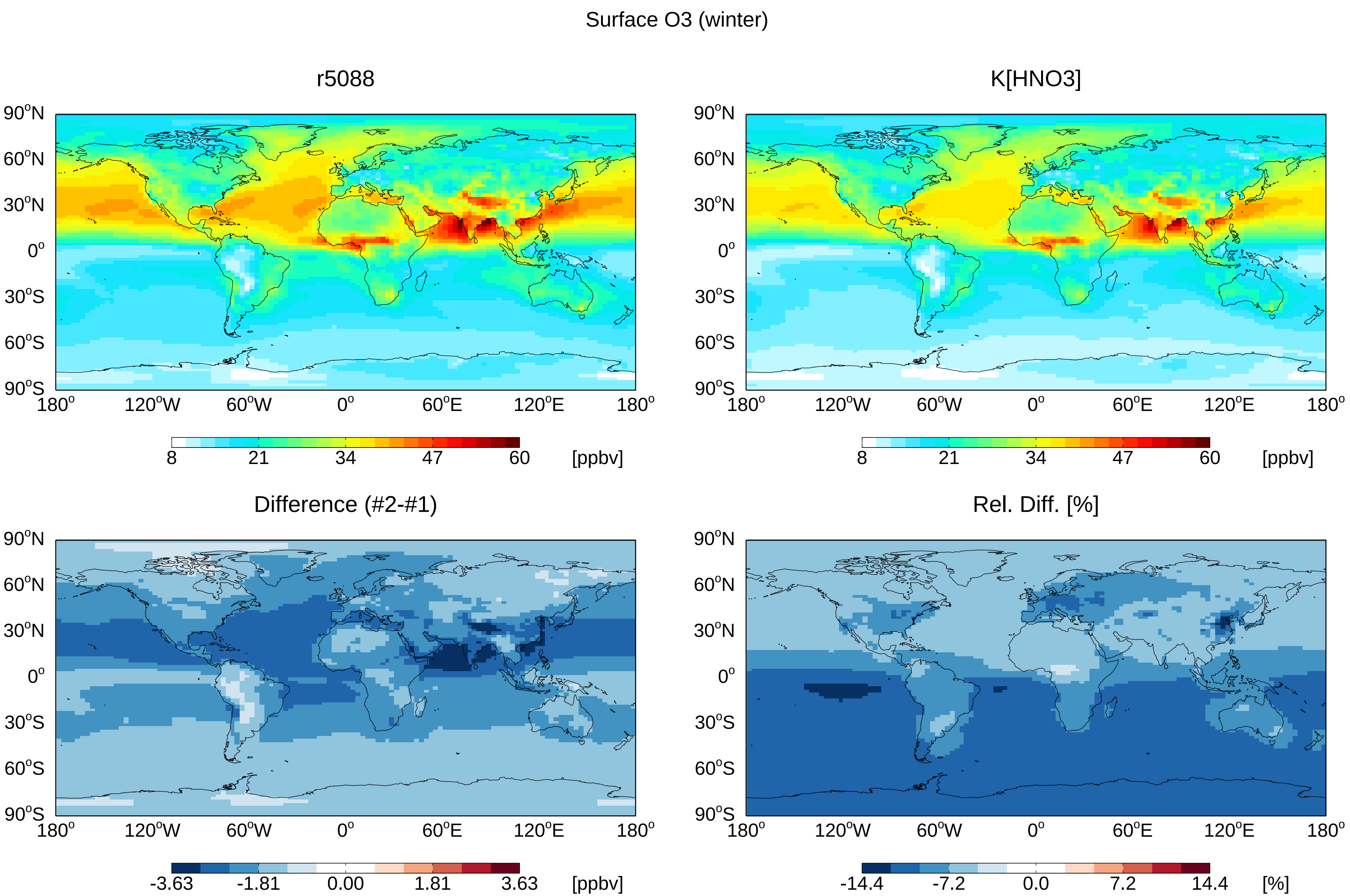
OH+NO2->HNO3 new rates

K[HNO3]	old	new	Diff.
O3 + hv tropo(Tg)	2340	2171	-170
O3 drydep (Tg)	812	749	-63
trop O3 chng (Tg)	3	3	0
tropO3 burden (Tg)	327	305	**-23**
Total pO3 tropo (Tg)	4490	4064	**-426**
Total lO3 tropo (Tg)	1648	1447	**-201**
CO + OH tropo (Tg)	2279	2186	-92
CO burden (Tg)	349	379	**+30**
Total pOH tropo(Tg)	1403	1269	**-133**

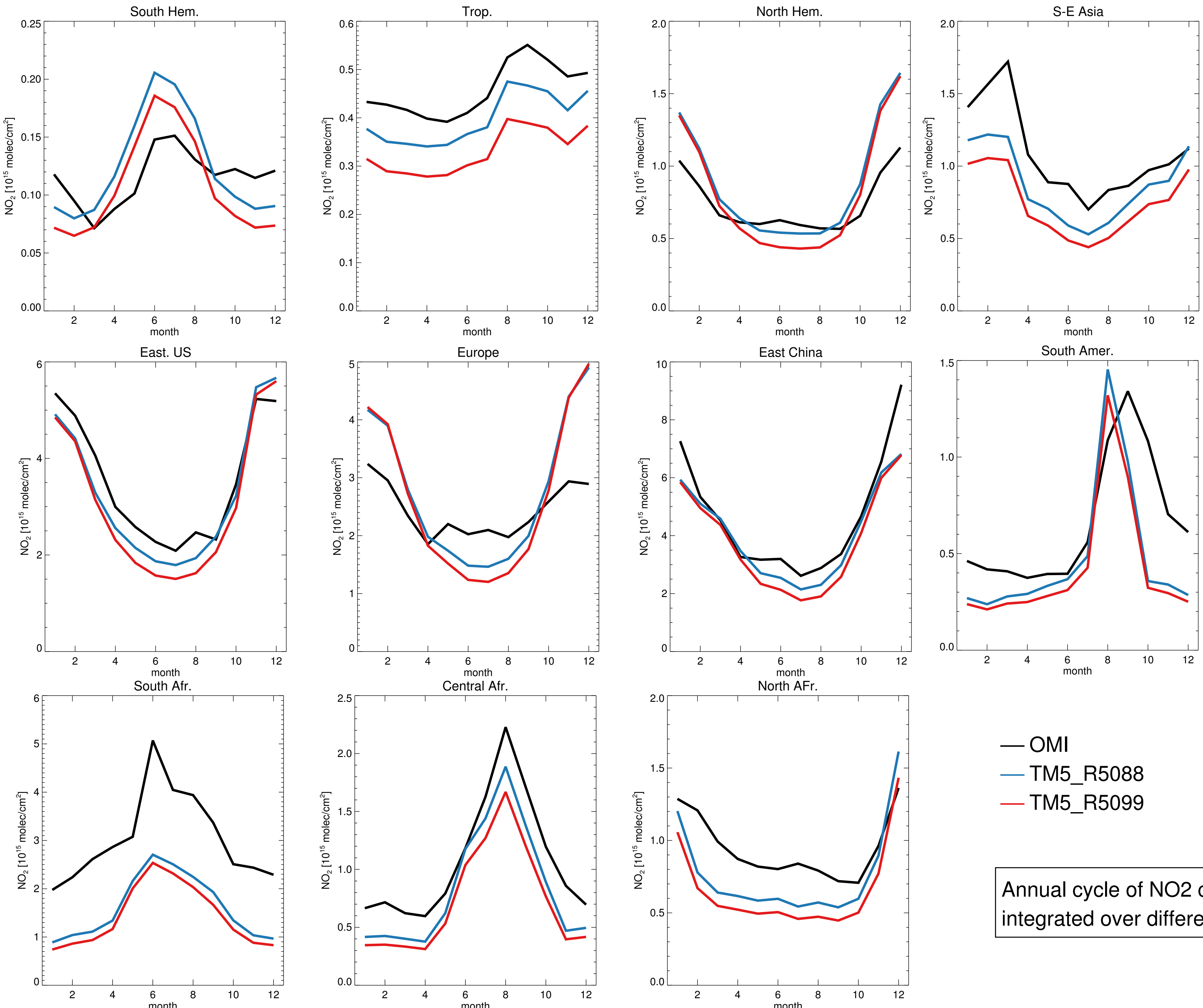

Surface CO (winter)
r5088
K[HNO3]
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
54
252
451
650
849
[ppbv]
-8.79
-4.40
0.00
4.40
8.79
[ppbv]
-11.4
-5.7
0.0
5.7
11.4
[%]



Annual cycle of mean, mass weighted CO in observations (black) and in TM5 for the MOPITT-THERMAL 500-hPa retrieval level.



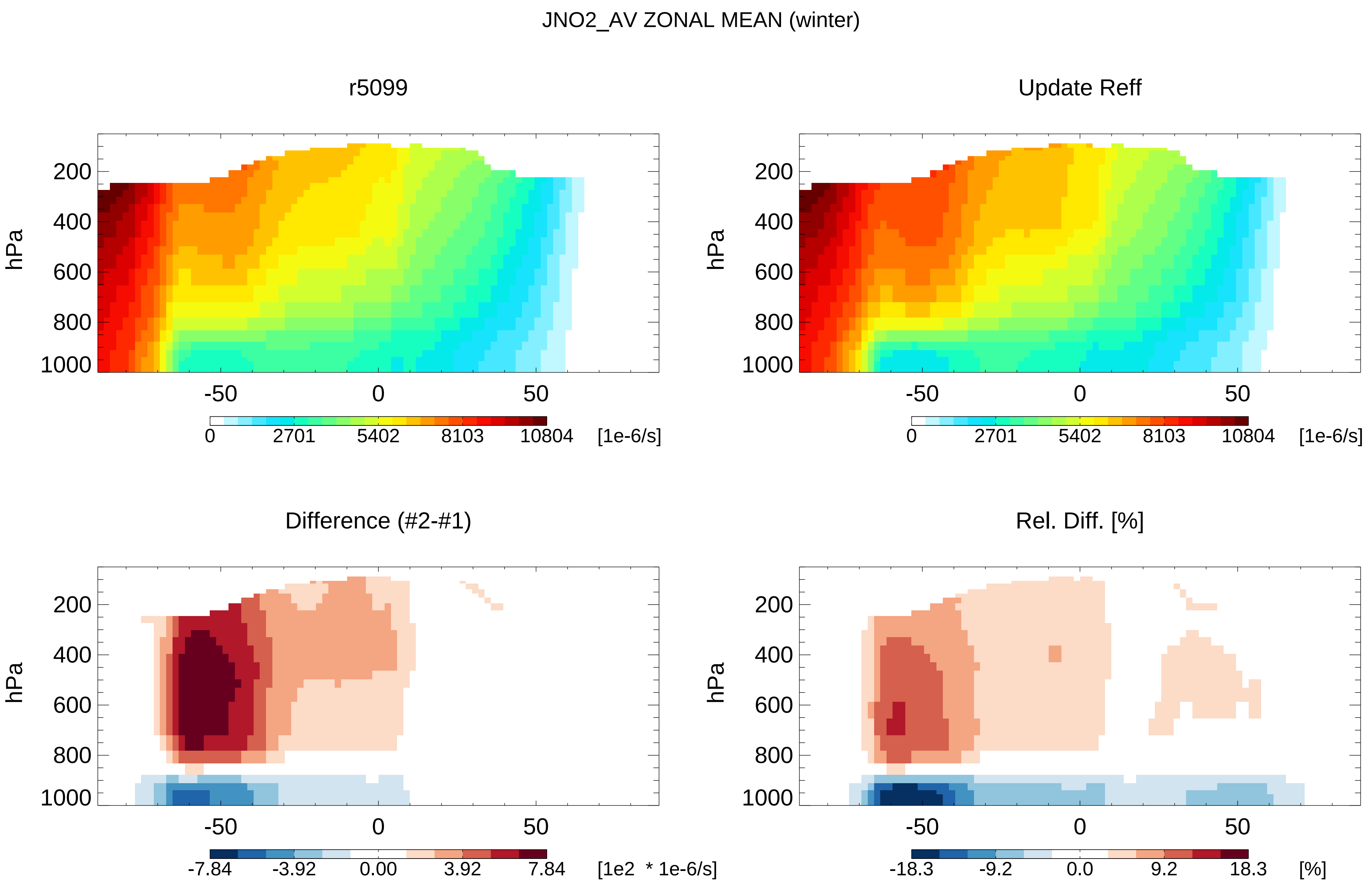
Surface O3 (winter)
r5088
K[HNO3]
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
8
21
34
47
60
[ppbv]
-3.63
-1.81
0.00
1.81
3.63
[ppbv]
-14.4
-7.2
0.0
7.2
14.4
[%]

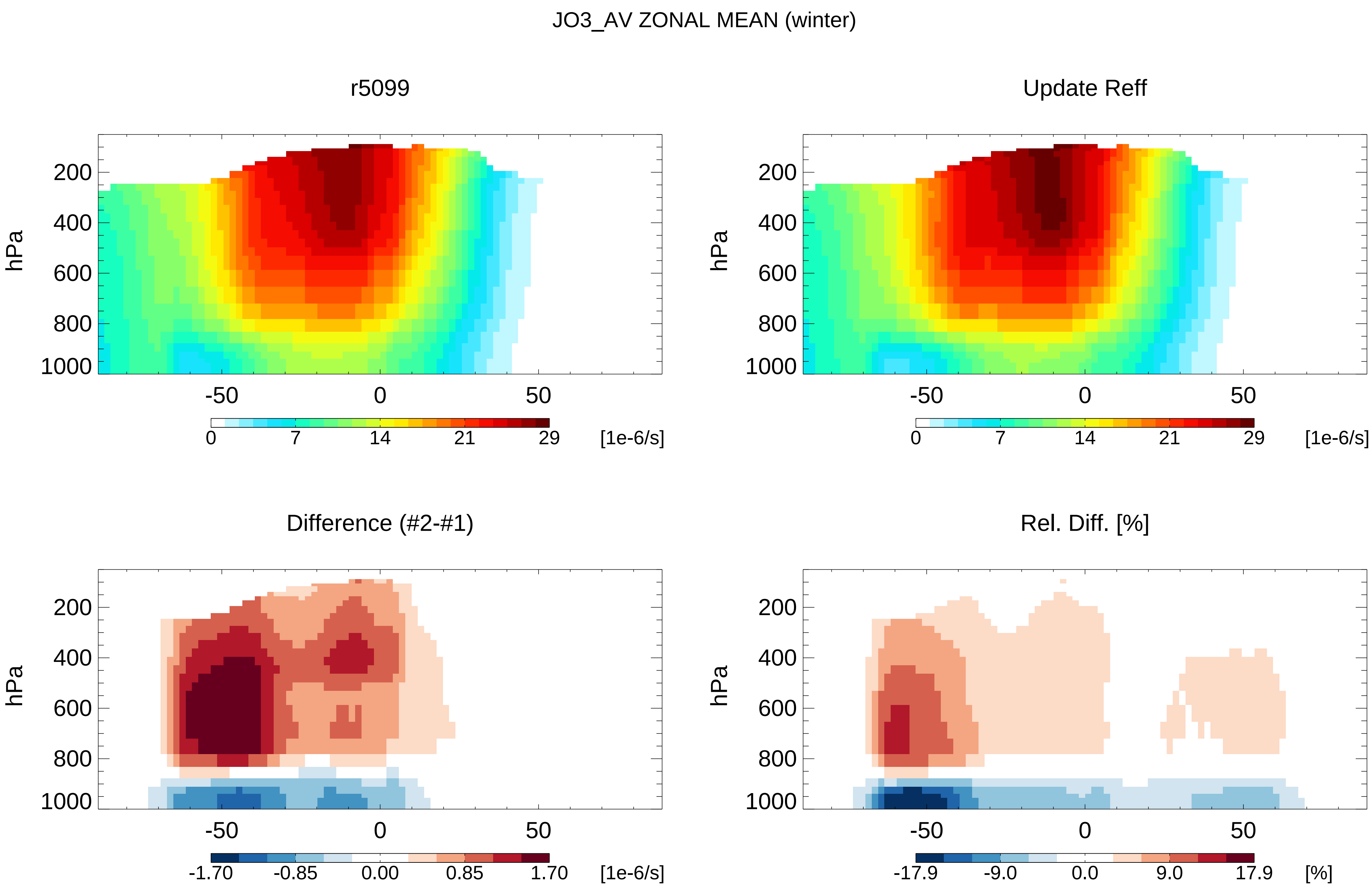


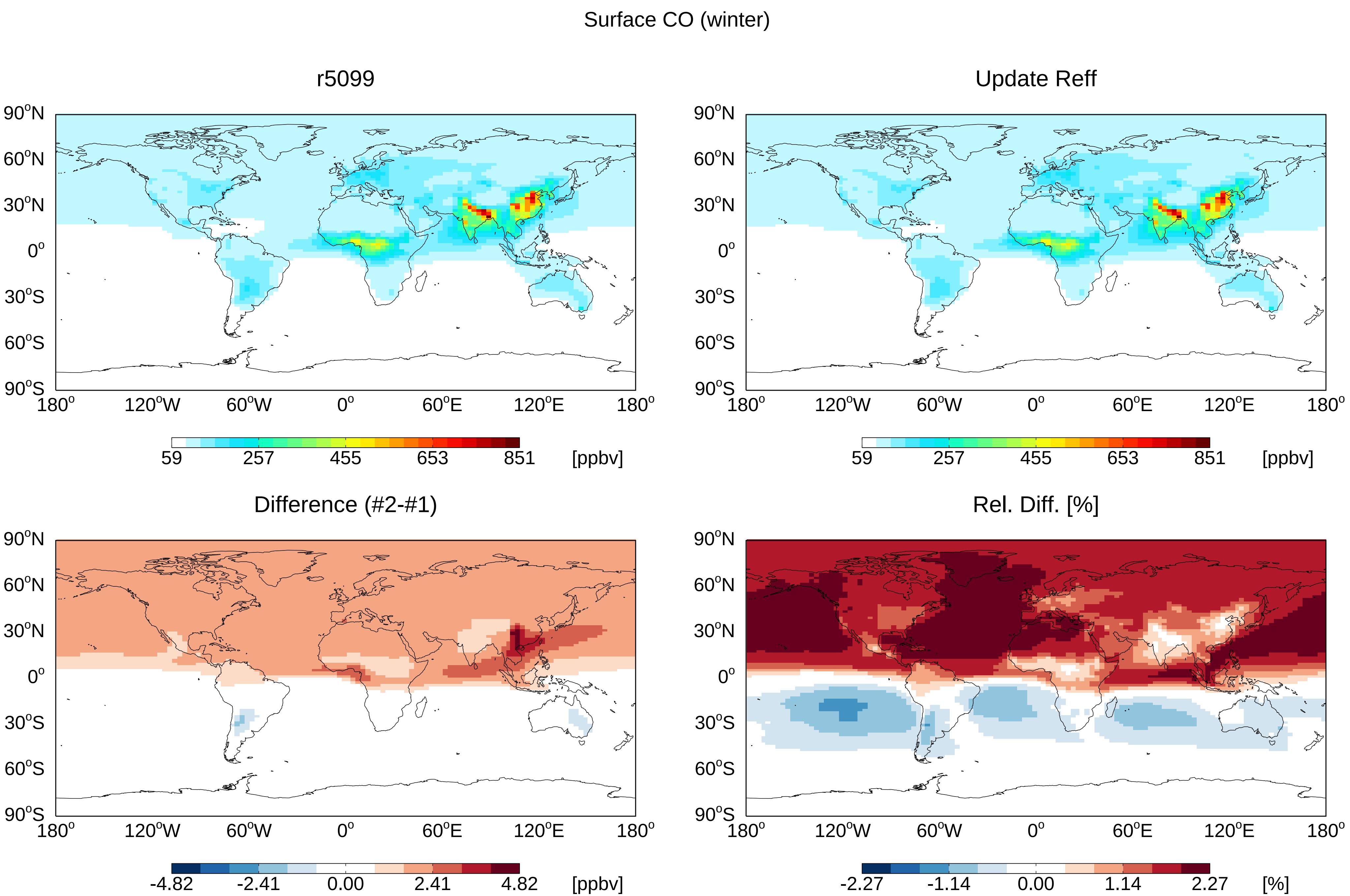
Annual cycle of NO2 columns integrated over different regions.

New cloud particles radius parametrization

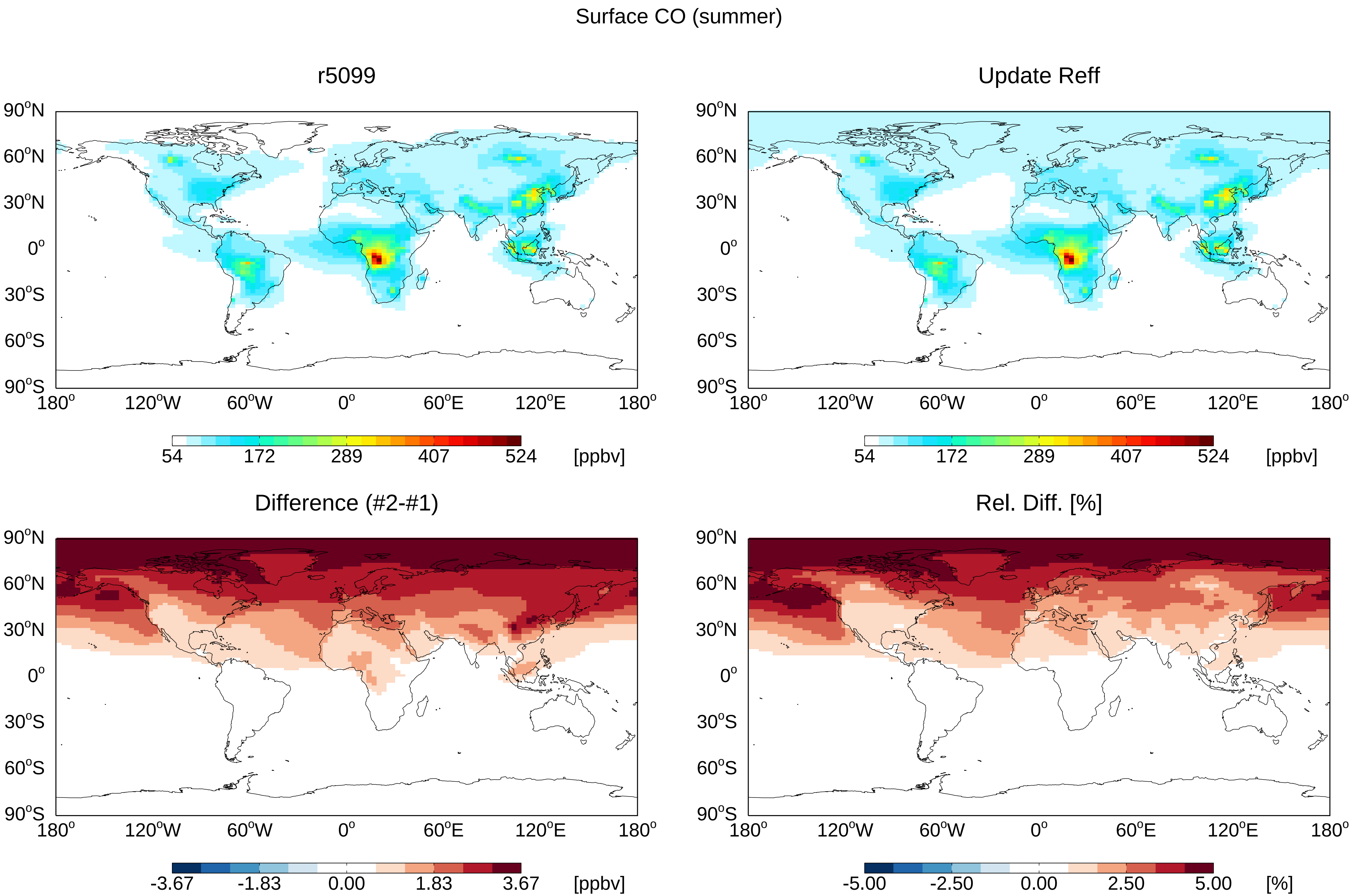
	LWP	Martin	Diff.
O3 drydep (Tg)	749	740	-9
Total pO3 tropo (Tg)	4064	3986	-78
Total lO3 tropo (Tg)	1447	1348	-99
O3 + hv tropo (Tg)	2170	2203	31
tropO3 burden (Tg)	305	305	**0**
Total pOH tropo(Tg)	1269	1189	**-80**


JNO2_AV ZONAL MEAN (winter)
r5099
Update Reff
hPa
200
400
600
800
1000
-50
0
50
0
2701
5402
8103
10804
[1e-6/s]
Difference (#2-#1)
Rel. Diff. [%]
-7.84
-3.92
0.00
3.92
7.84
[1e2 * 1e-6/s]
-18.3
-9.2
0.0
9.2
18.3
[%]


JO3_AV ZONAL MEAN (winter)
r5099
Update Reff
Difference (#2-#1)
Rel. Diff. [%]
hPa
200
400
600
800
1000
-50
0
50
0
7
14
21
29
[1e-6/s]
-1.70
-0.85
0.00
0.85
1.70
-17.9
-9.0
0.0
9.0
17.9
[%]



Surface CO (winter)
r5099
Update Reff
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
59
257
455
653
851
[ppbv]
-4.82
-2.41
0.00
2.41
4.82
[ppbv]
-2.27
-1.14
0.00
1.14
2.27
[%]


Surface CO (summer)
r5099
Update Reff
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
54
172
289
407
524
[ppbv]
-3.67
-1.83
0.00
1.83
3.67
[ppbv]
-5.00
-2.50
0.00
2.50
5.00
[%]

Outline

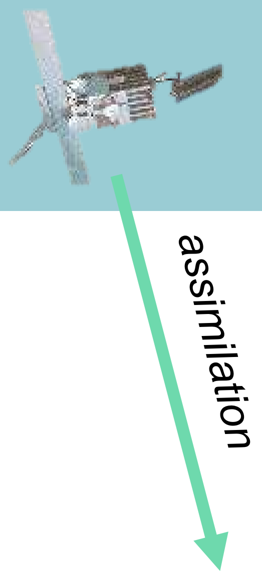
Where are the bottlenecks?

Benchmarks

C-IFS

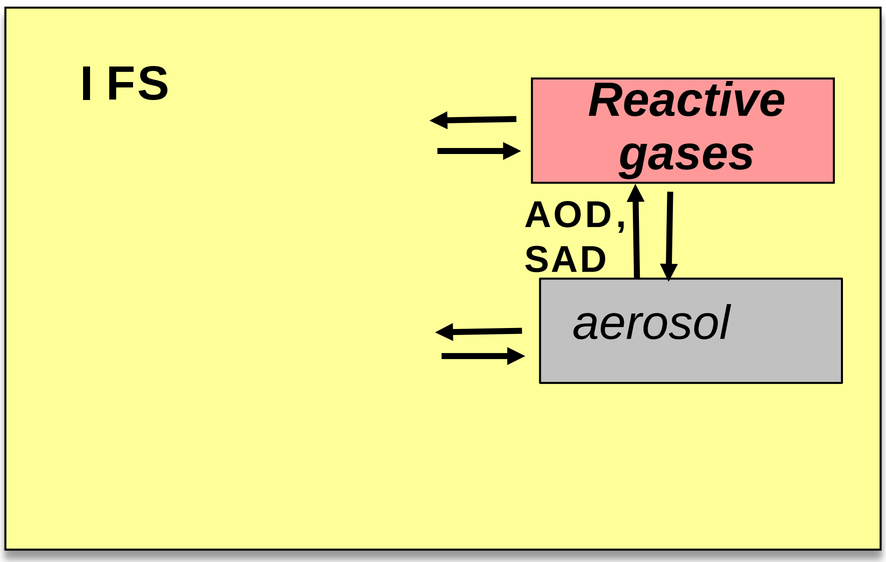
Extra

C-IFS-TM5:



Tropospheric chemistry in ECMWF's Integrated Forecasting System

Vincent Huijnen



-modified CB05 tropospheric chemistry (Williams et al., 2013)
- strat. O_3 constrained by analyses
-GEOS-Chem wet deposition
-MOCAGE dry deposition velocities

MACC aerosol model:
-Incl. sea salt (3x), dust (3x), BC(2x), OC(2x), SO_4
-Constrained by assimilation of MODIS

Emissions:
-MACCity anthropogenic emissions
-GFASv1.0 biomass burning emissions

Status of C-IFS

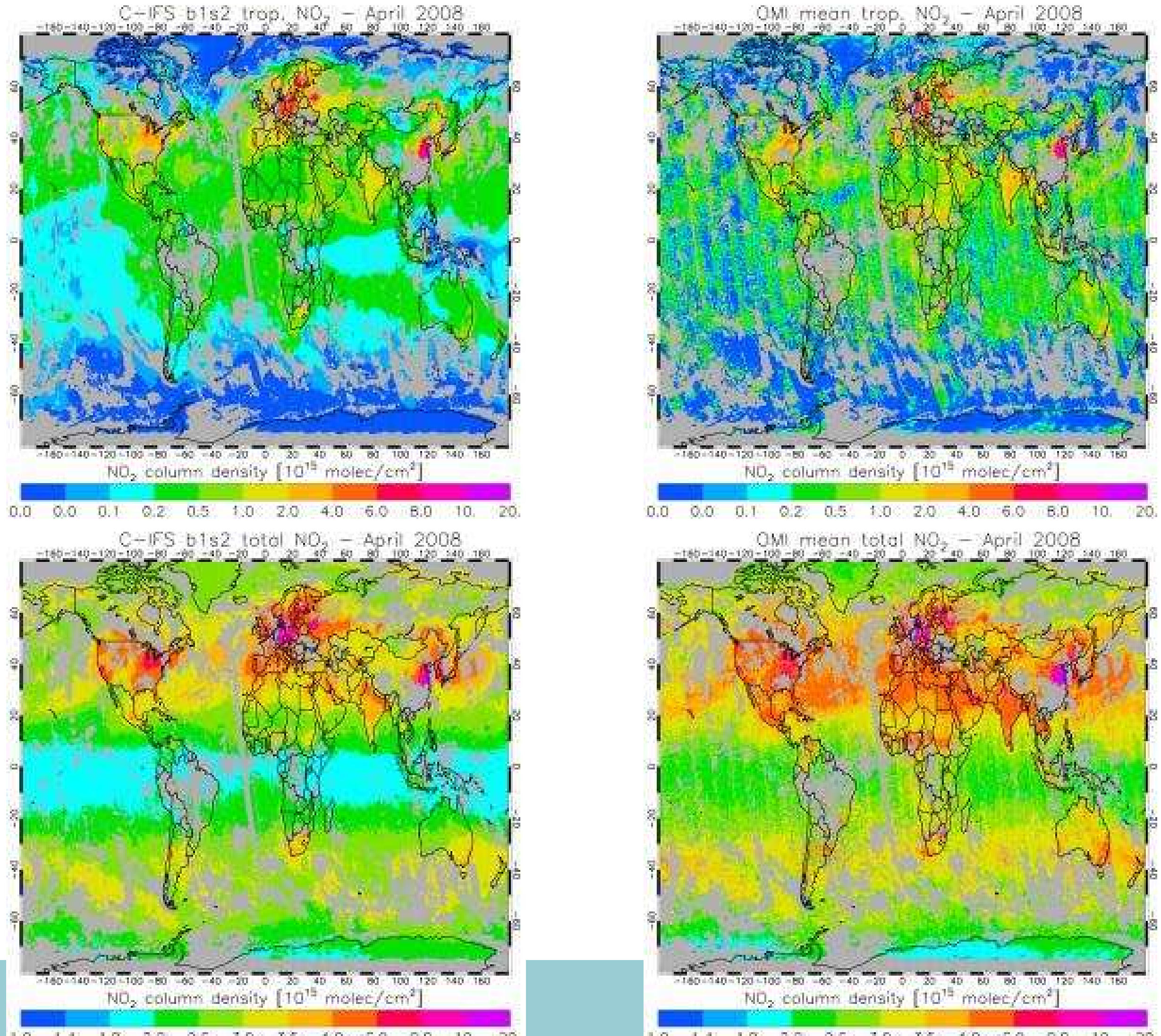
- Evaluation of C-IFS shows equal or better performance wrt chemistry versions of TM5. Essential differences to TM5 are wet deposition and transport.
- C-IFS-TM5 will replace coupled IFS-MOZART soon, to provide MACC operational forecasts.
- HO_2 heterogeneous chemistry study is in discussion in ACPD – we likely over-estimate the contribution of HO_2 uptake on clouds.
- C-IFS-TM5 contributes in HTAP to provide BC.
- Stratospheric chemistry based on Belgian BASCOE system is currently under development, based on KPP solver.

Sneak Preview: NO_2 columns in C-IFS-BASCOE-TM5 (1-2 Apr 2008)

CI FS-TM5-BASCOE **OMI**

Trop

TC



Outline

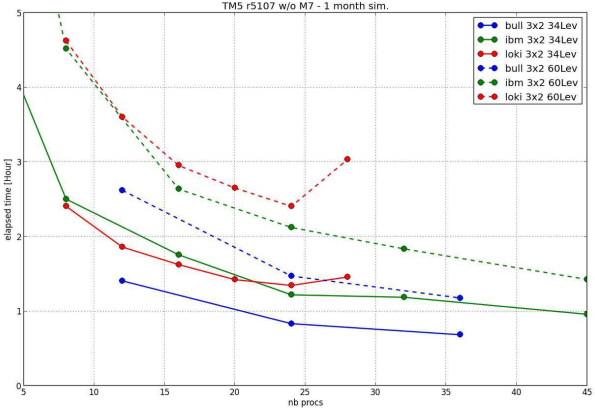
Where are the bottlenecks?

Benchmarks

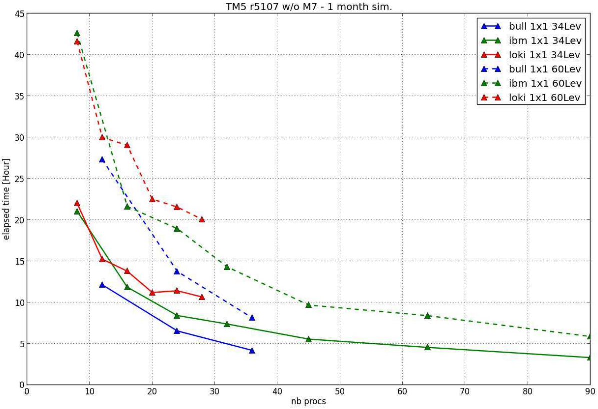
C-IFS

Extra

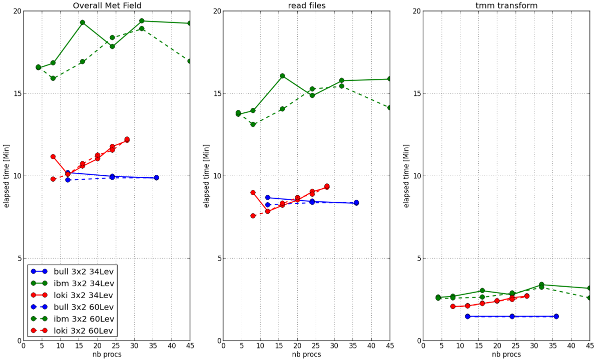
Overview @3x2



Overview @1x1

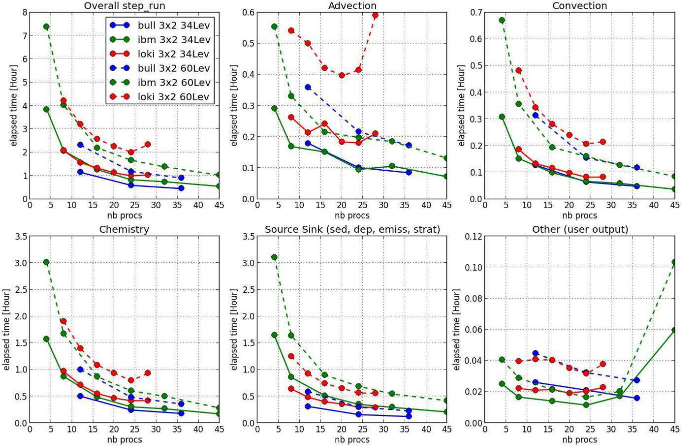


“Meteo” part



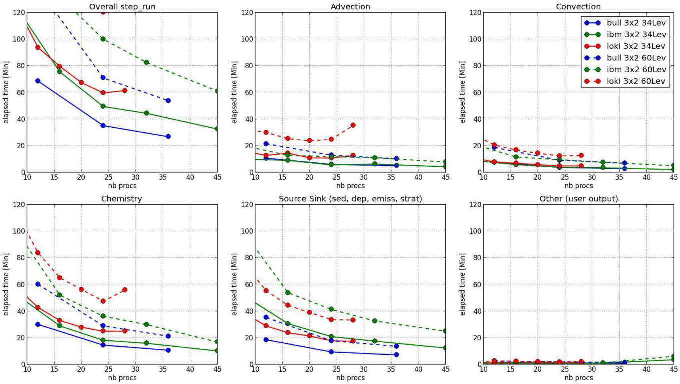
- reading meteo files: up to 20% (bull) and 25% (ibm)
- serial reading

"Run step" part 3x2



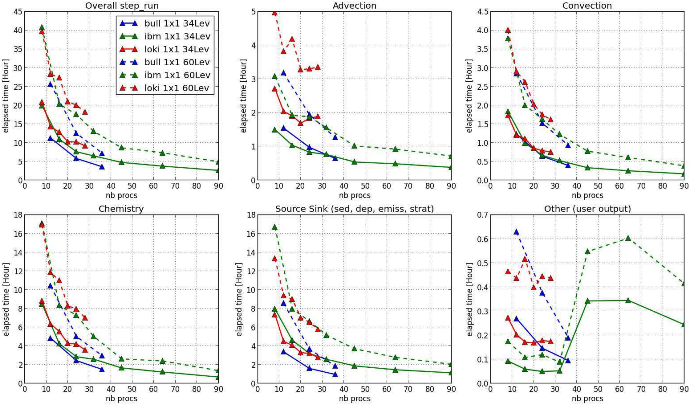
- **output**: parallel IO works on the Bull

Run step: Chem + Sources/Sinks = 40% of runtime



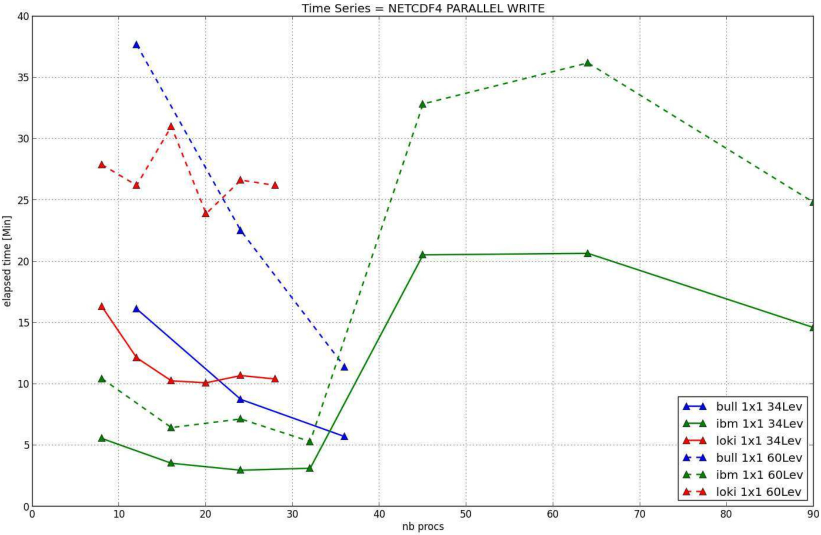
- MPI issue in source/sinks = nudging?

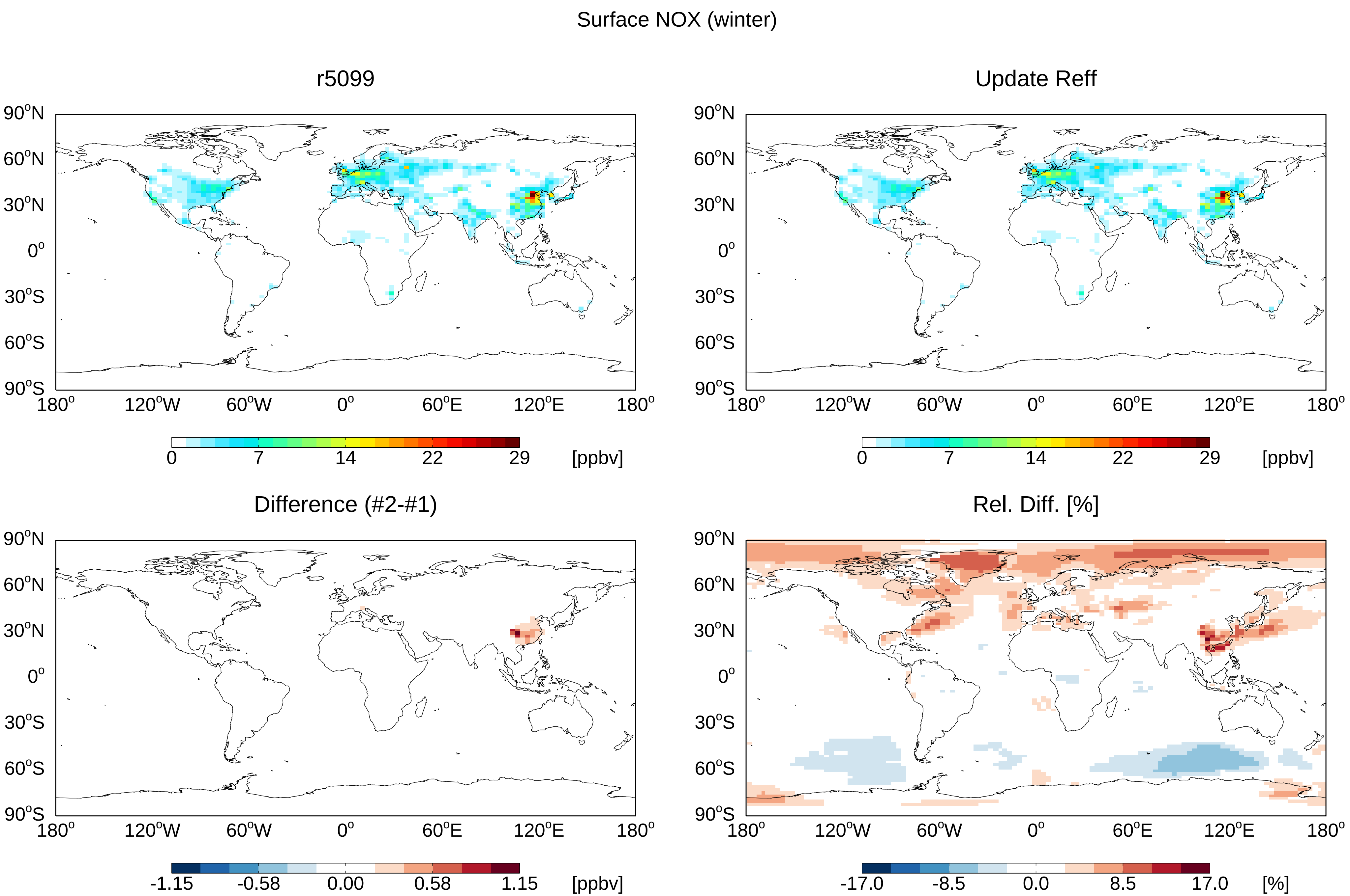
“Run step” part 1x1



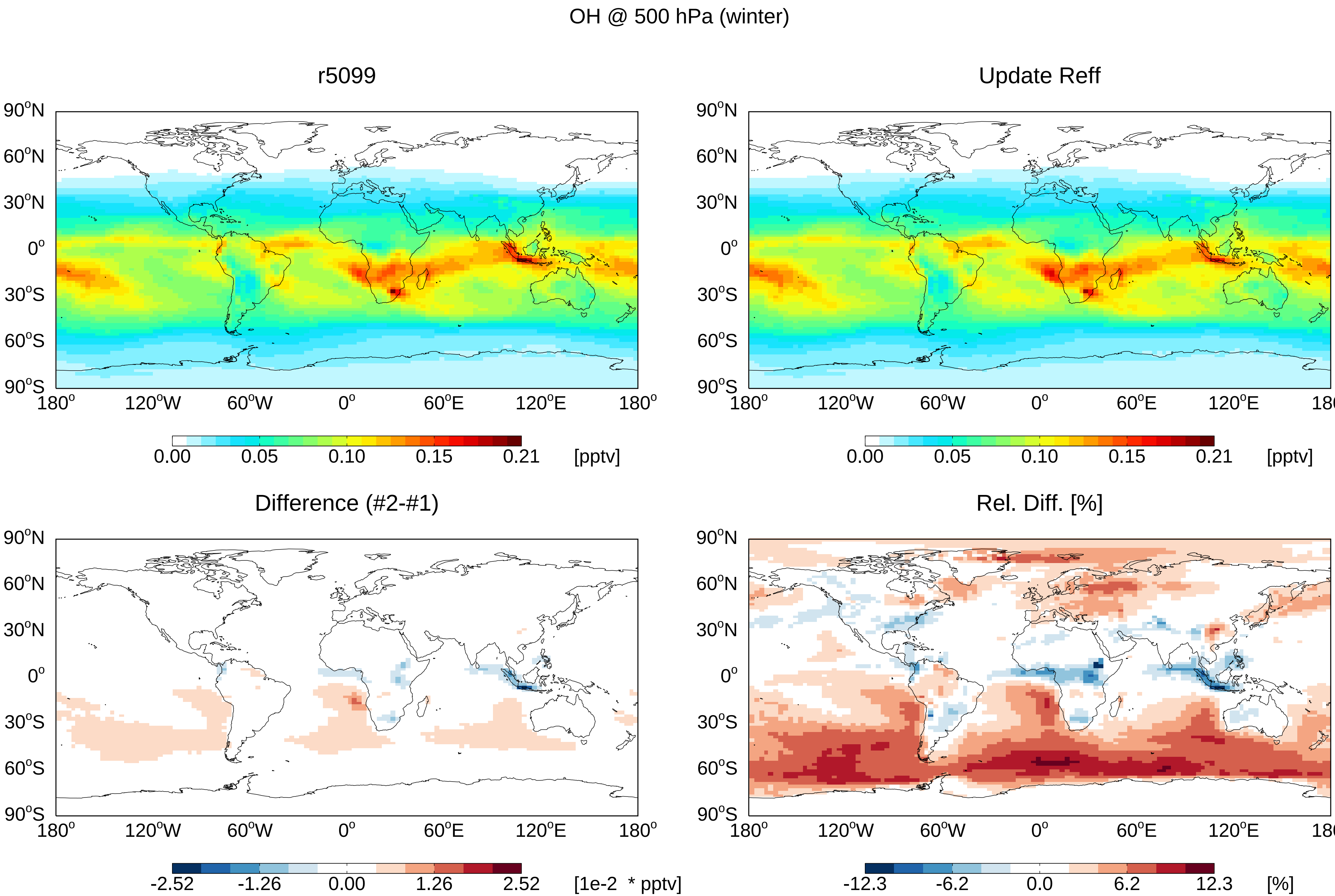
- **output**: parallel IO really works on the Bull!

Parallel IO can scale!





Surface NOX (winter)
r5099
Update Reff
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
0
7
14
22
29
[ppbv]
-1.15
-0.58
0.00
0.58
1.15
[ppbv]
-17.0
-8.5
0.0
8.5
17.0
[%]


OH @ 500 hPa (winter)
r5099
Update Reff
Difference (#2-#1)
Rel. Diff. [%]
90°N
60°N
30°N
0°
30°S
60°S
90°S
180°
120°W
60°W
0°
60°E
120°E
180°
0.00
0.05
0.10
0.15
0.21
[pptv]
-2.52
-1.26
0.00
1.26
2.52
[1e-2 * pptv]
-12.3
-6.2
0.0
6.2
12.3
[%]