NetCDF Diagnostic Validation in GEOS-Chem "Classic"

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Overview

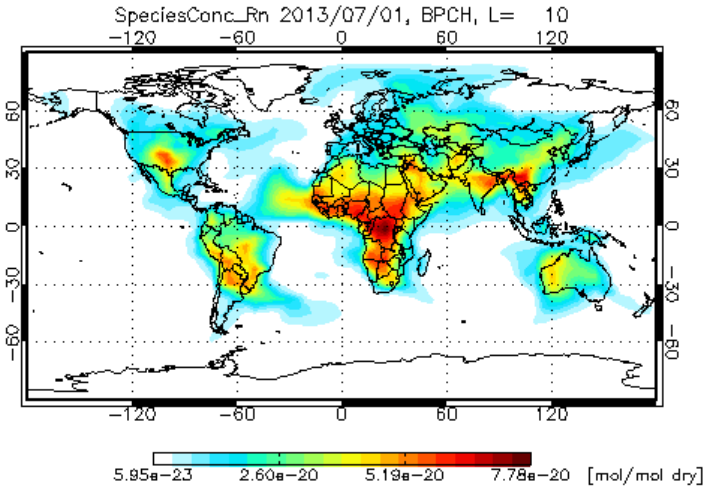
- Output taken from these GEOS-Chem “Classic” simulations:
  - geosfp_4x5_RnPbBe
  - geosfp_4x5_aerosol
  - geosfp_4x5_benchmark (ND43 only)
    - 24-hour time-averaged diagnostics (2013/07/01)
- For time-averaged collections, the “Update” interval is set to the “heartbeat” timestep
  - “Heartbeat” = dynamic timestep = 10 min

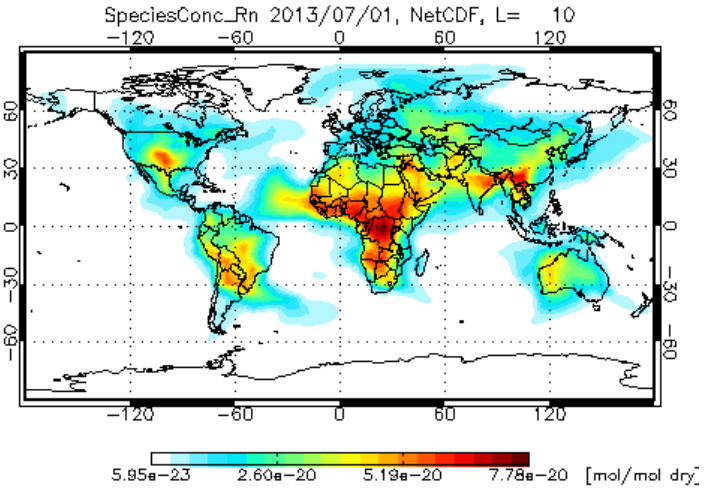
Species concentration (ND45)

- Species concentrations are converted to [mol/mol dry air] at the end of each “heartbeat” timestep (=10 min)
  - From Rn/Pb/Be simulation, these are plotted:
    - Rn222,
    - Pb210,
    - Be7
  - From aerosol-only simulation, these are plotted:
    - SO2,
    - DST1

Rn222 species concentration (ND45), Units: mol/mol dry, Level 10 (870 hPa)

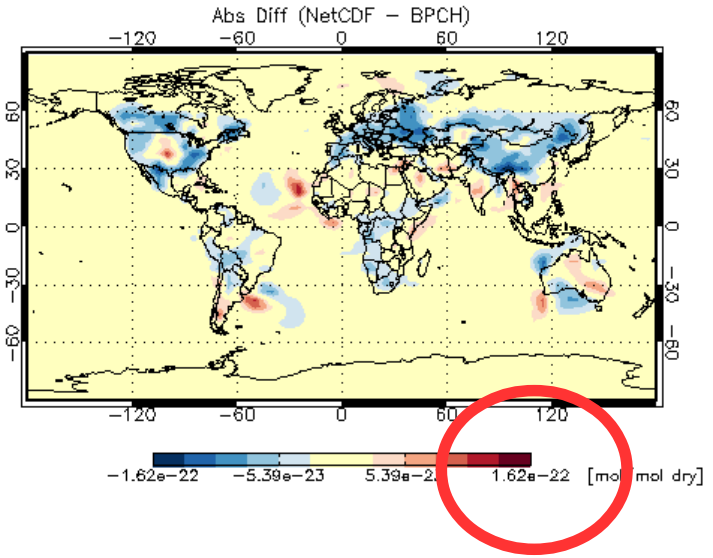
Data from bpch file

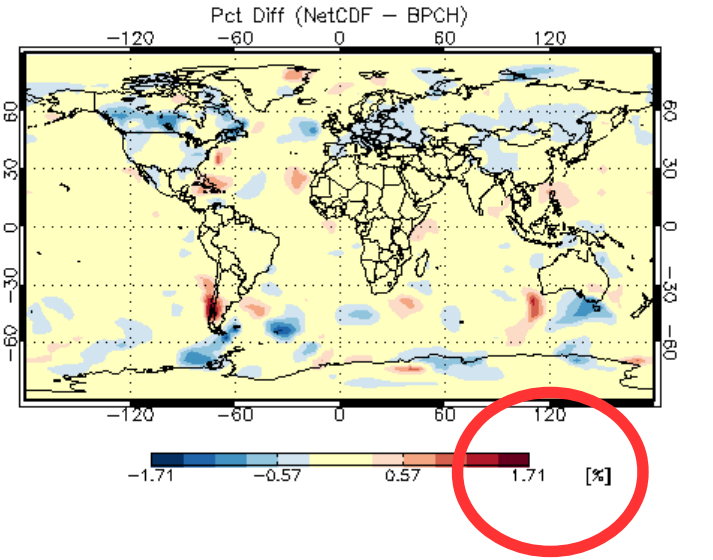




Data from netCDF file

Absolute difference



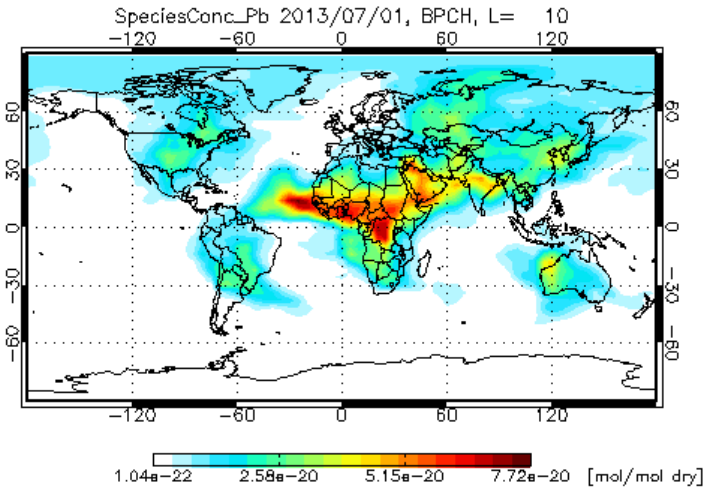


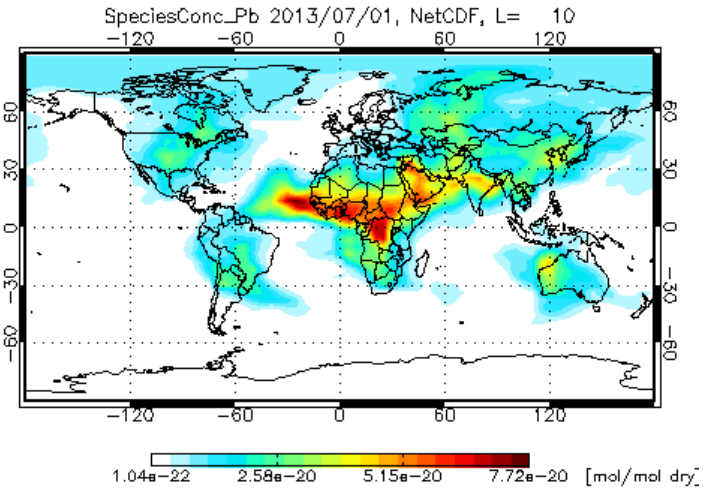
Percent difference

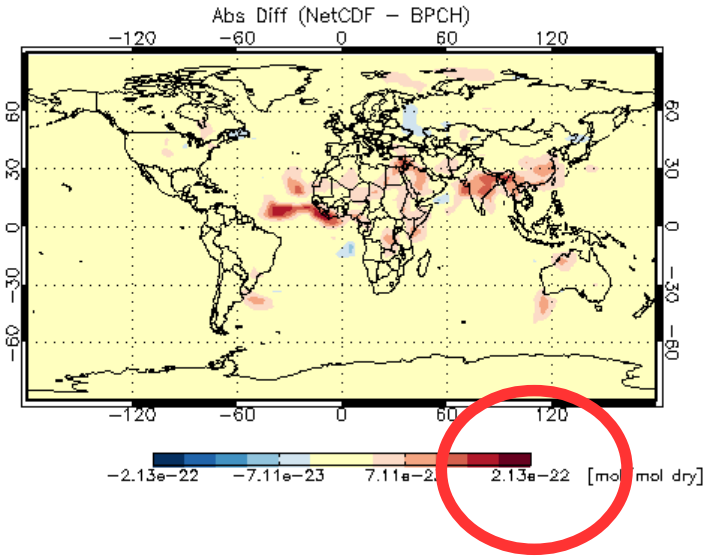
NOTE: we are looking for abs diff of approx 1e-6X or 1e-7 lower than the quantities being plotted. This reflects roundoff caused by REAL*4 vs. REAL*8.

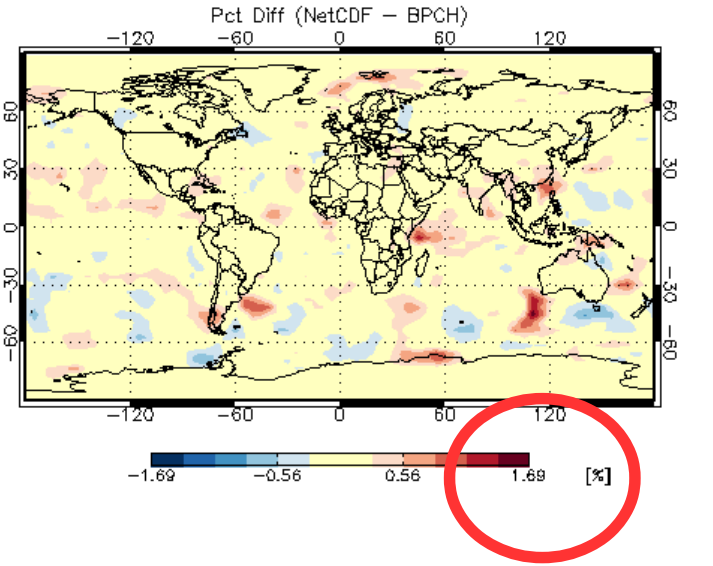
Why such big diffs?

Pb210 species concentration (ND45), Units: mol/mol dry, Level 10 (870 hPa)



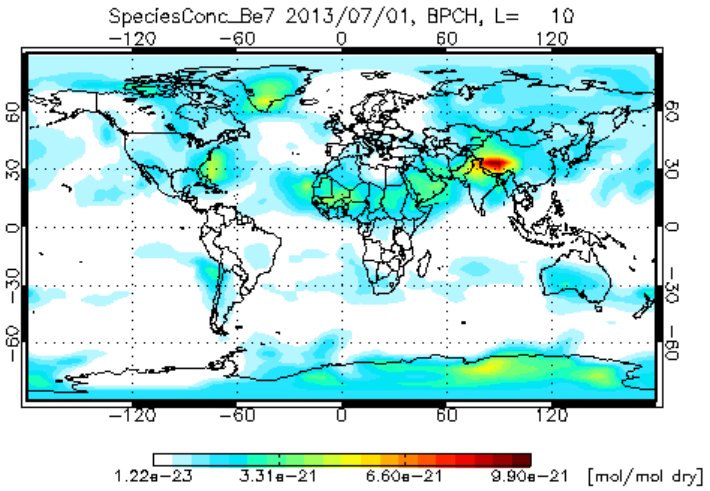


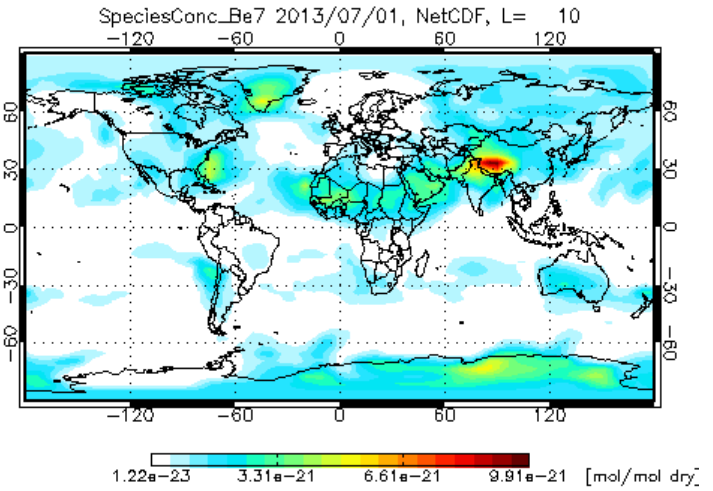


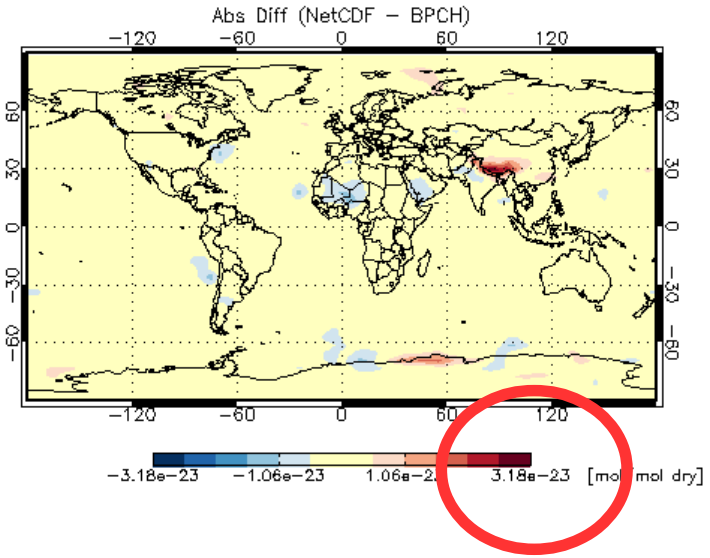


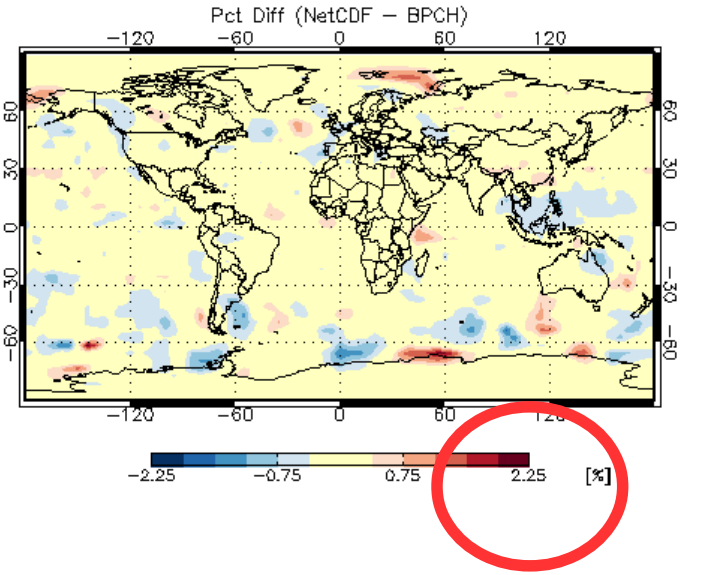
Why such big diffs?

Be7 species concentration (ND45), Units: mol/mol dry, Level 10 (870 hPa)



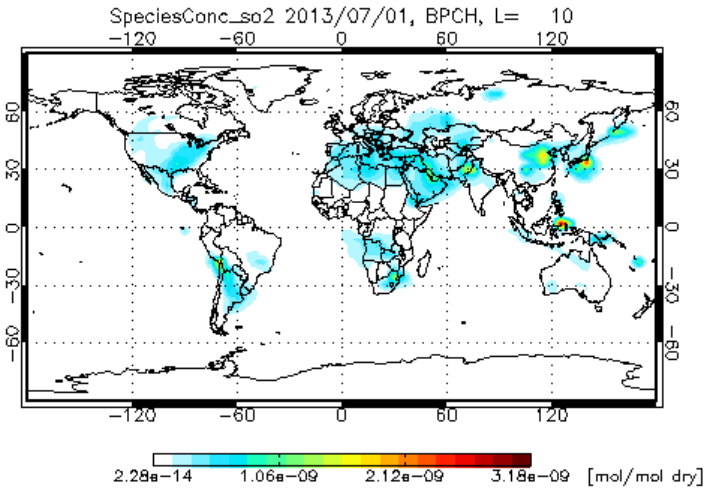


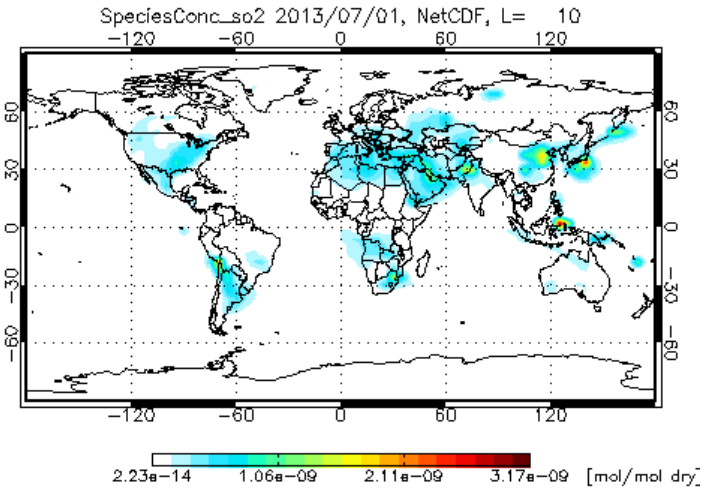


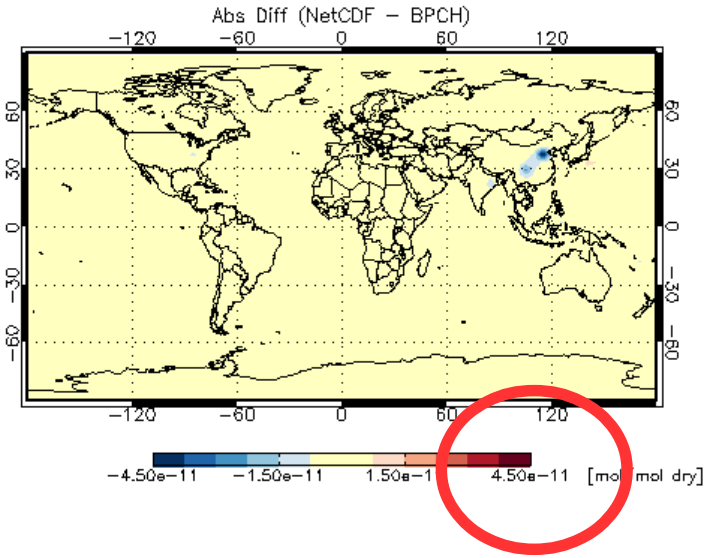


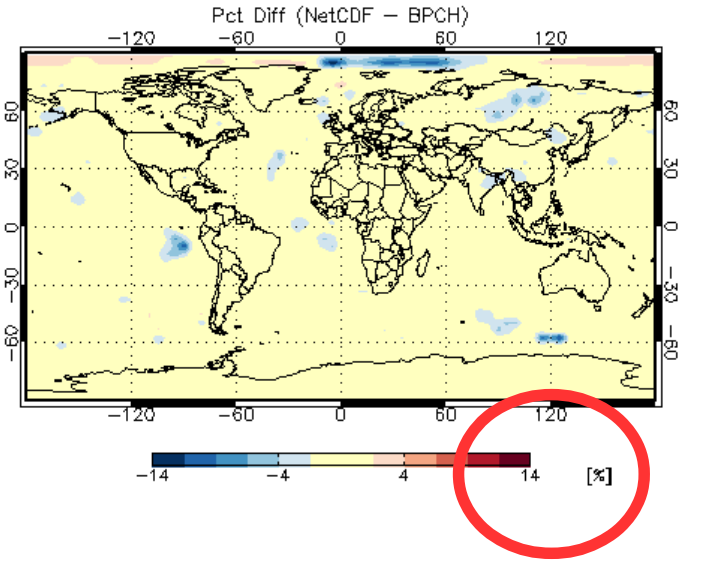
Why such big diffs?

SO2 species concentration (ND45), Units: mol/mol dry, Level 10 (870 hPa)



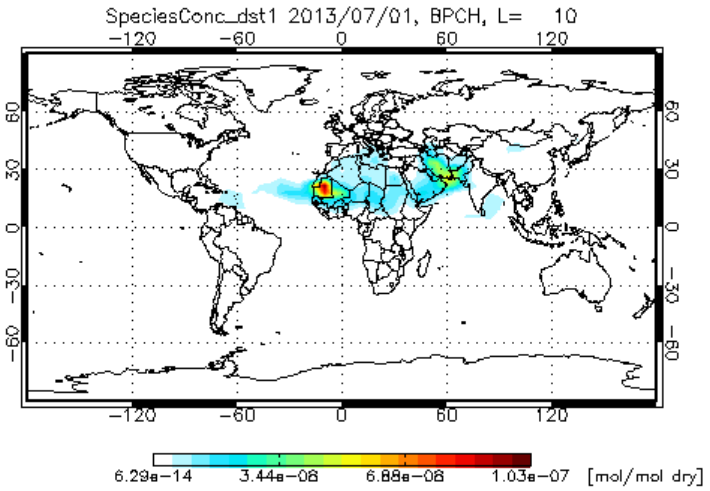


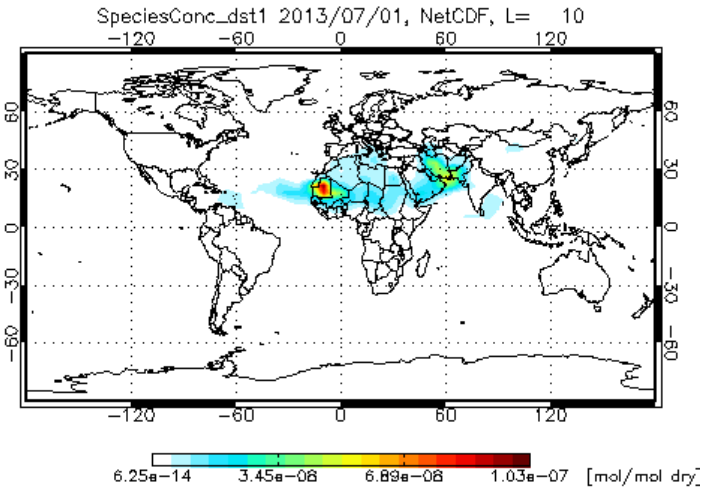


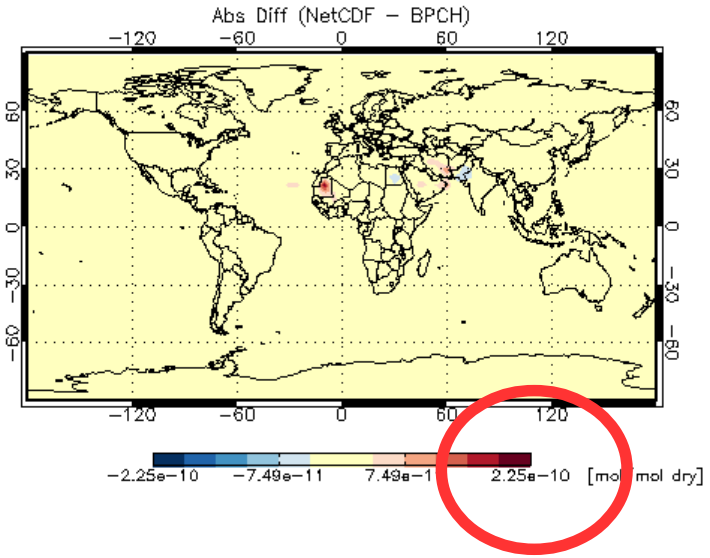


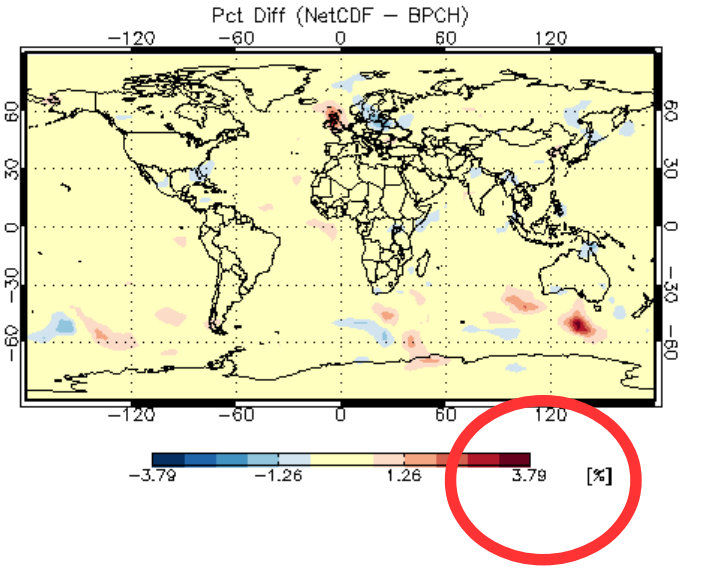
Why such big diffs?

DST1 species concentration (ND45), Units: mol/mol dry, Level 10 (870 hPa)



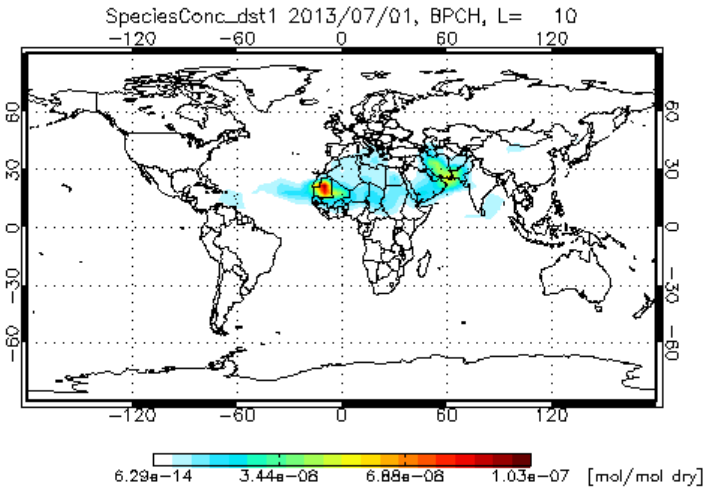


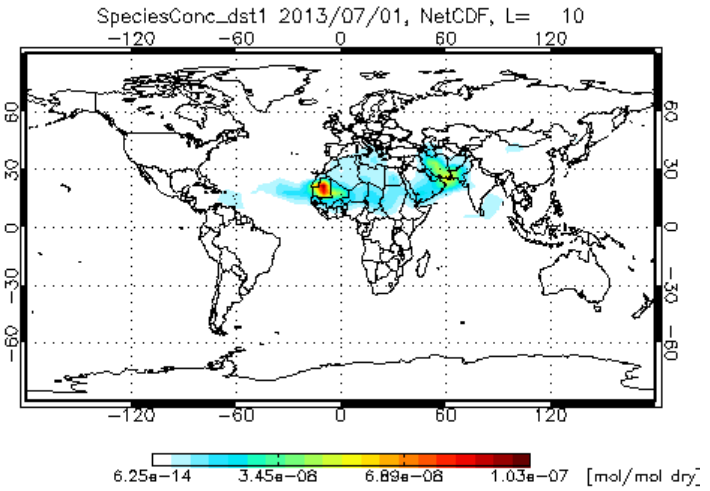


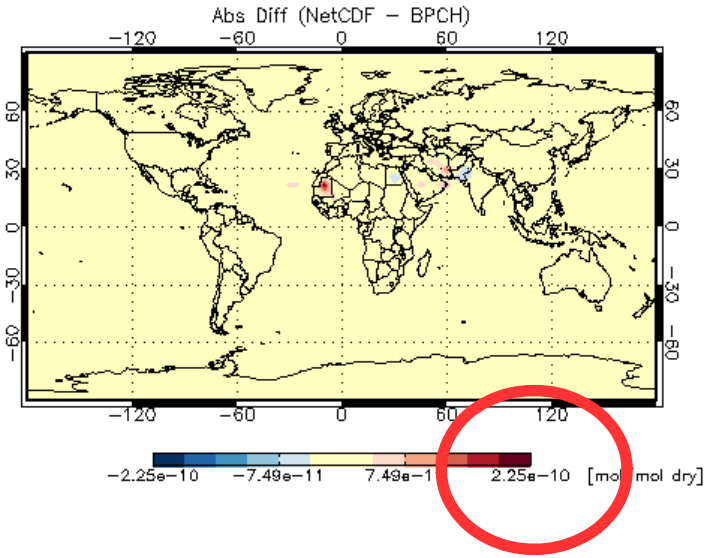


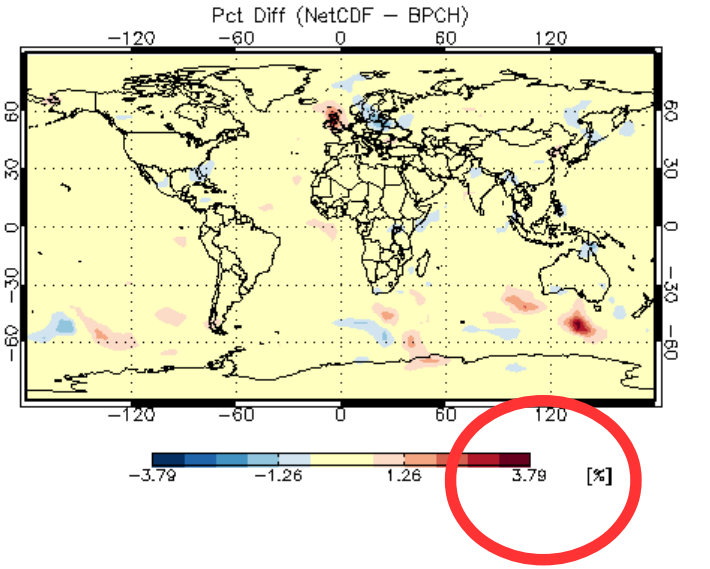
Why such big diffs?

DST1 species concentration (ND45), Units: mol/mol dry, Level 10 (870 hPa)









Why such big diffs?

Differences in species concentrations, explained

- Time-averaged collections update every "heartbeat" timestep (= 10 min) by default
- The following bpch diagnostics update every chemistry timestep (omitting obsolete diags):
  - ND30 (landmap)
  - ND31 (pressures)
  - ND42 (SOA diagnostic)
  - ND44 (drydep fluxes, in PBL mixing)
  - **ND45 (species concentrations)**

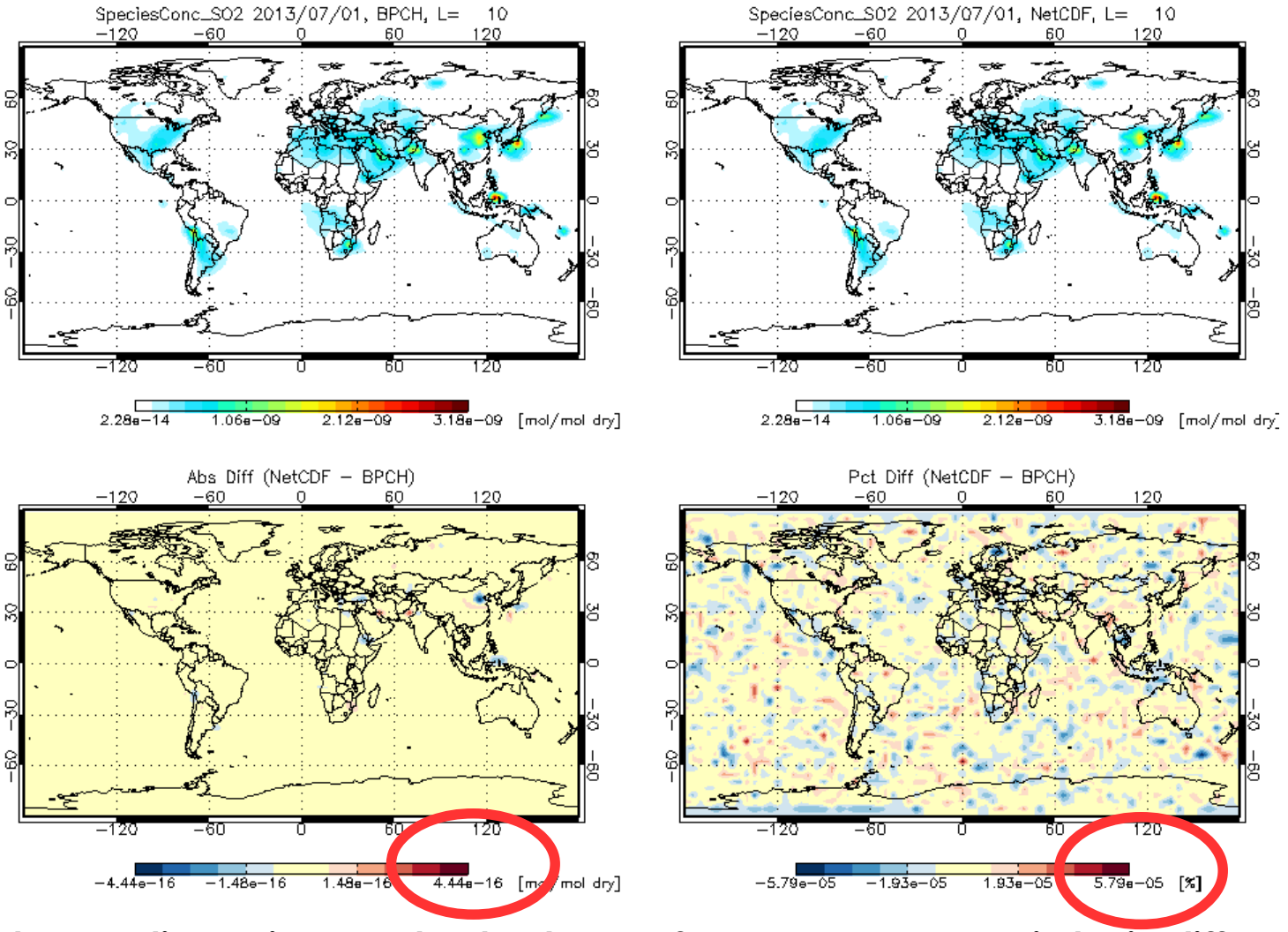
Differences in species concentrations, explained

- Diags updated at the chemistry timestep (cont'd)
  - ND44 (drydep velocity; drydep fluxes, in chemistry)
  - ND54 (# of times box was in troposphere)
  - ND57 (Potential temperature)
  - ND63 (PARANOx diagnostic)
  - ND67 (PBL top pressure)
  - ND68 (box height, airnumden, etc. fields)
  - ND71 (Maximum hourly sfc concentration)
  - And all of the timeseries (ND48, ND49, ND50, ND51)

Differences in species concentrations, explained

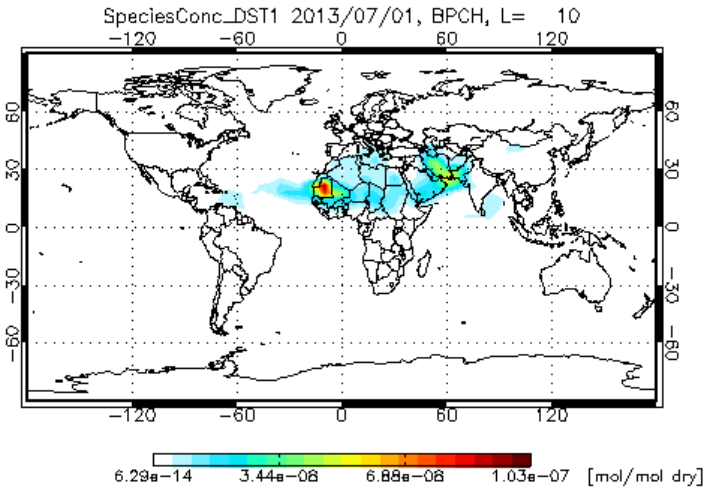
- When comparing bpch (updated every 20 min) vs. NetCDF (updated every 10 min), this discrepancy is enough to cause the differences we have been seeing in the species concentration output.
- To verify this, I submitted another simulation where the netCDF diagnostics were only updated every 20 mins (once per chemistry timestep).
- Results on next 2 slides …

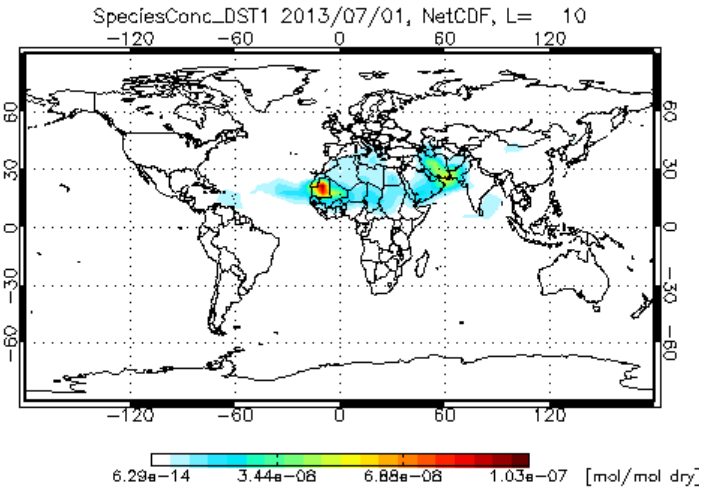
SO2 species concentration (ND45), Units: mol/mol dry, Level 10 (870 hPa), 20 min update

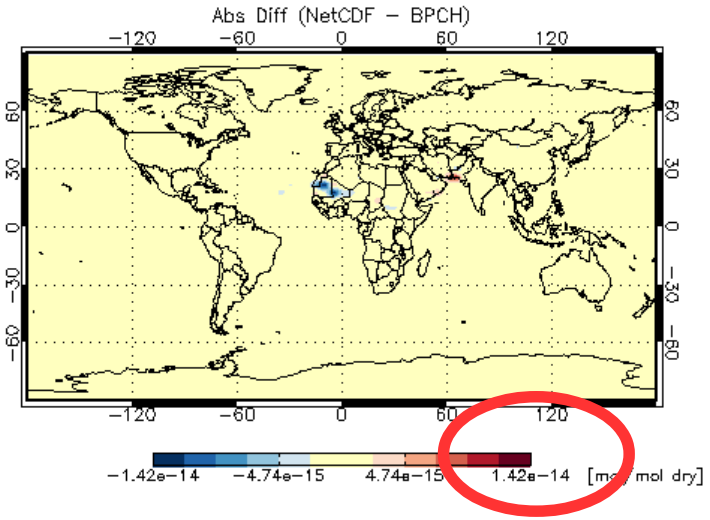


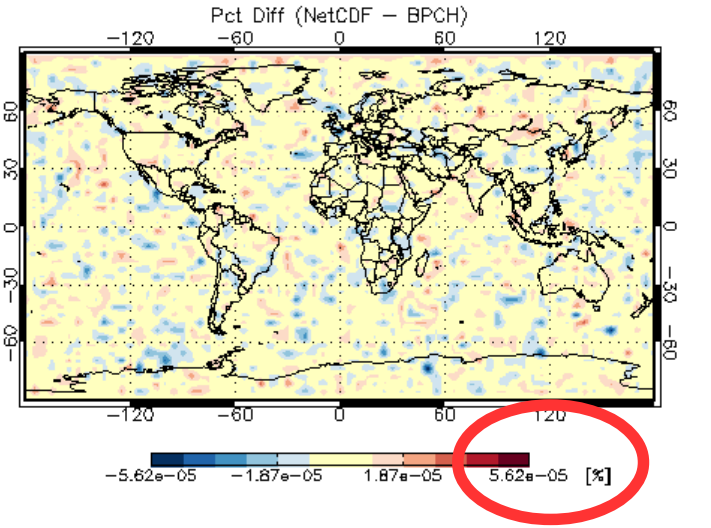
When bpch and netCDF diagnostics are updated at the same frequency, we get numerical noise differences (of order 1e-6 lower than the concentrations), which are caused by REAL*4 / REAL*8 differences in the computation.

DST1 species concentration (ND45), Units: mol/mol dry, Level 10 (870 hPa), 20 min update







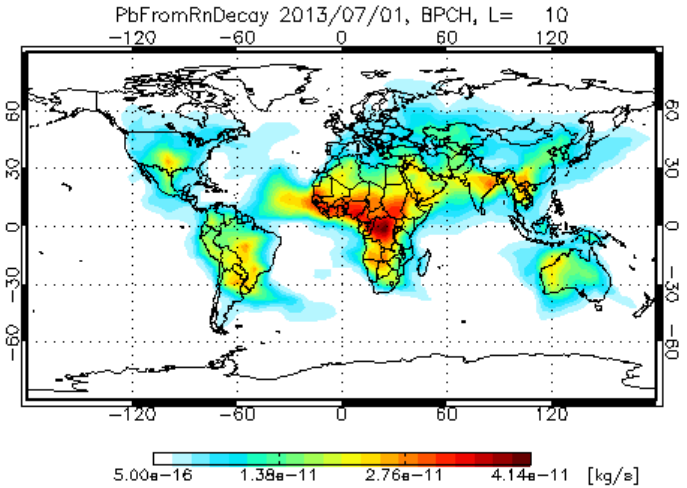


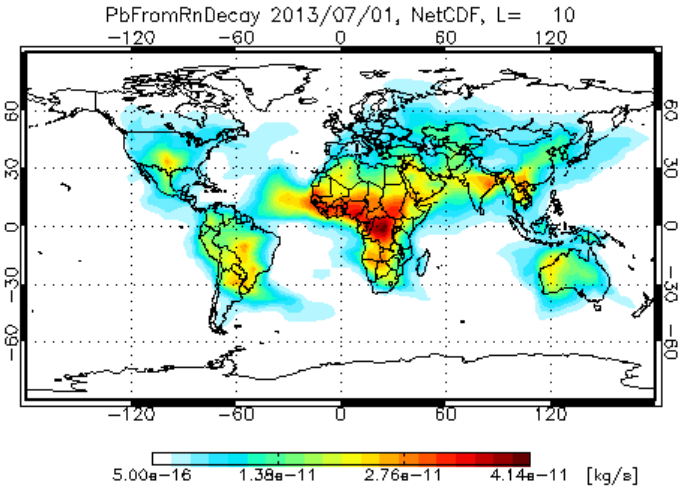
We get the same patttern regardless of the species.

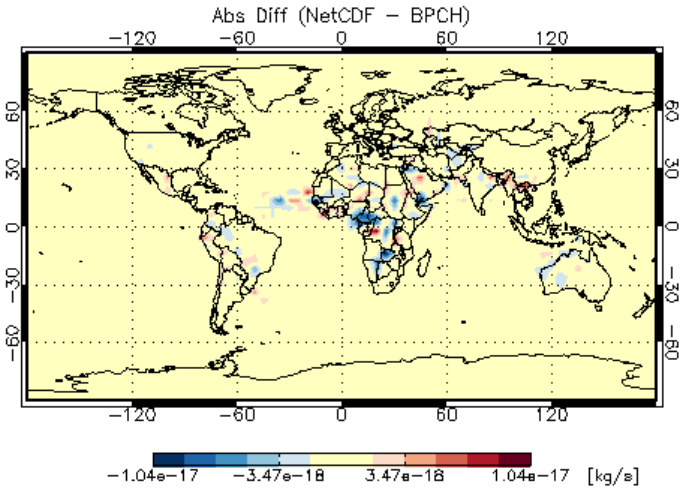
Rn-Pb-Be source and decay diagnostics

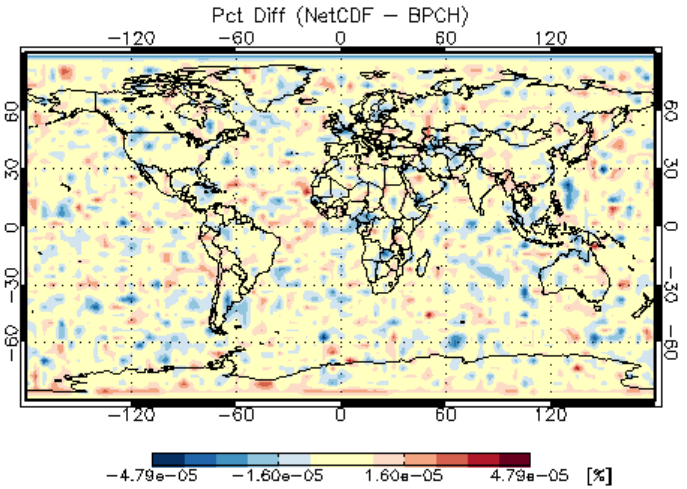
- The next set of diagnostics are all updated each “heartbeat” timestep (= 10 min)for both bpch and netCDF output:
  - ND01: Source of Pb^{210} from Rn^{222} decay (kg/s)
    - NOTE: Emissions of Rn and Be7 are handled via HEMCO and are not shown here.
  - ND02: Radioactive decay of Rn^{222}, Pb^{210}, Be^{7} (kg/s)

Pb from Rn decay (ND01, #2), Units: kg/s, Level 10 (870 hPa)

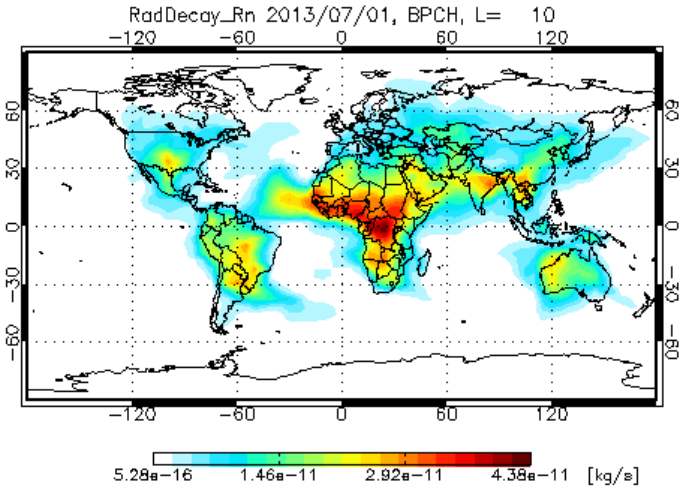


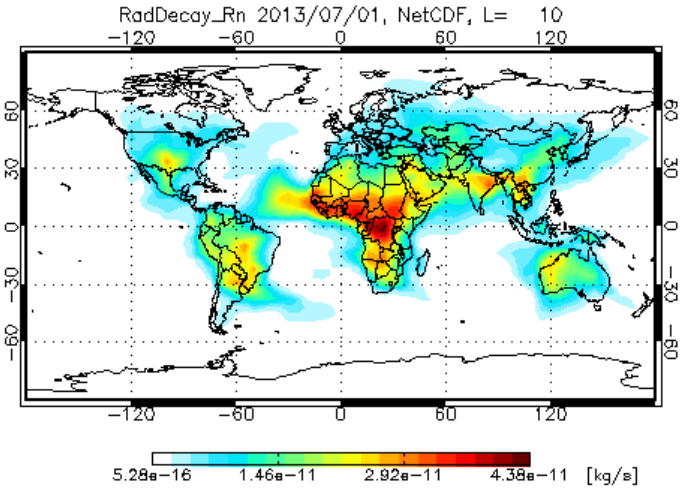


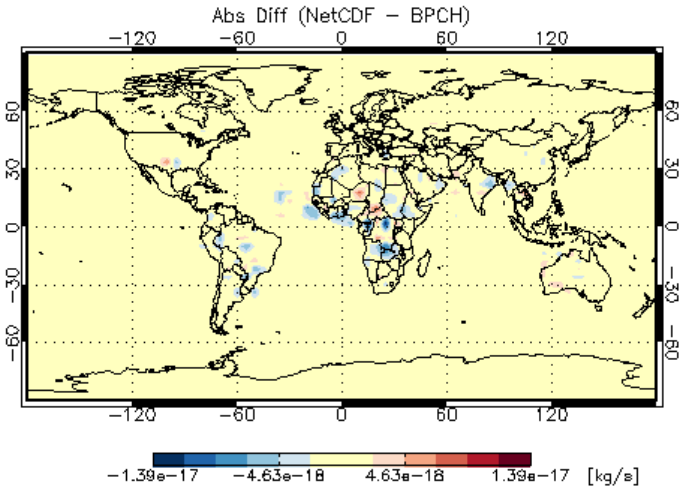


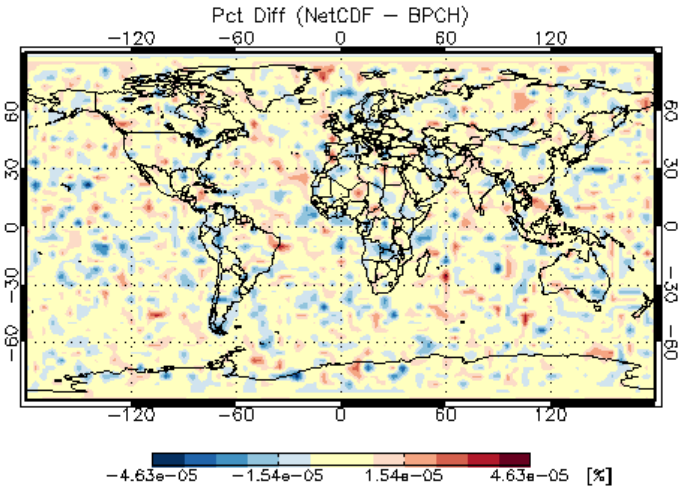


Decay of Rn (ND02, #1), Units: kg/s, Level 10 (870 hPa)

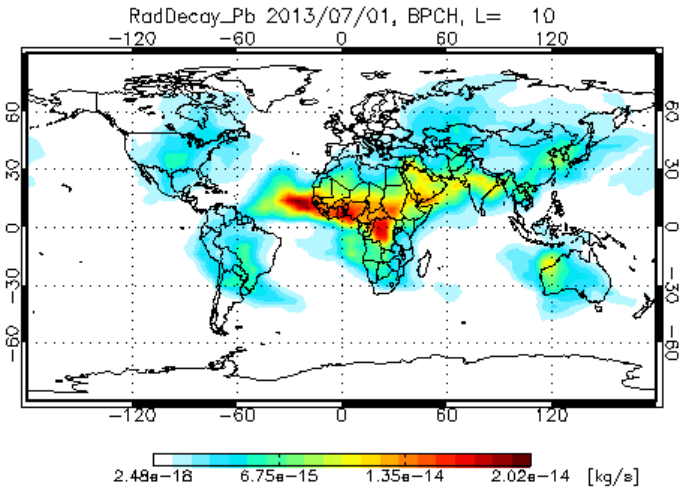


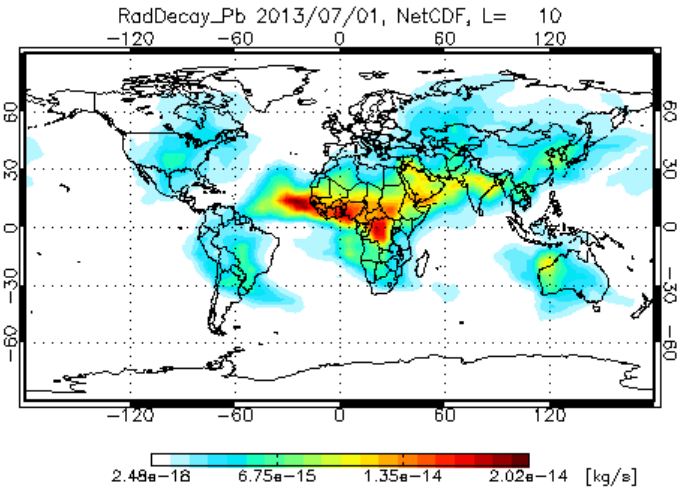


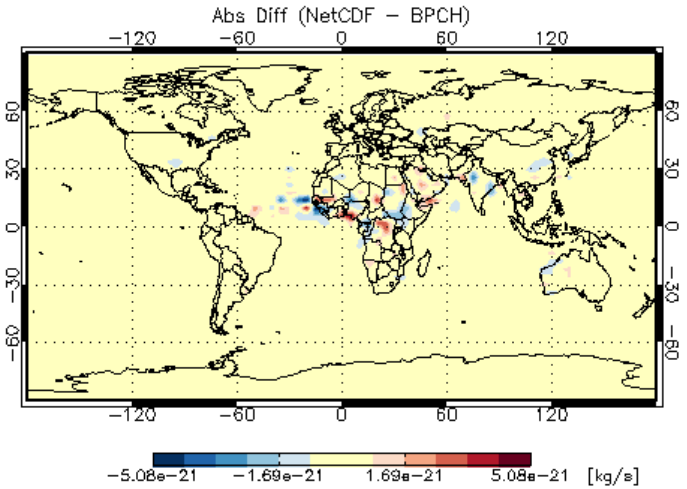


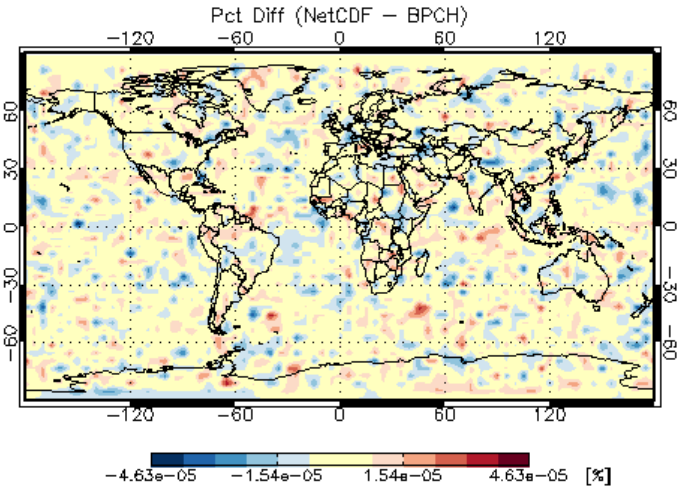


Decay of Pb (ND02, #2), Units: kg/s, Level 10 (870 hPa)

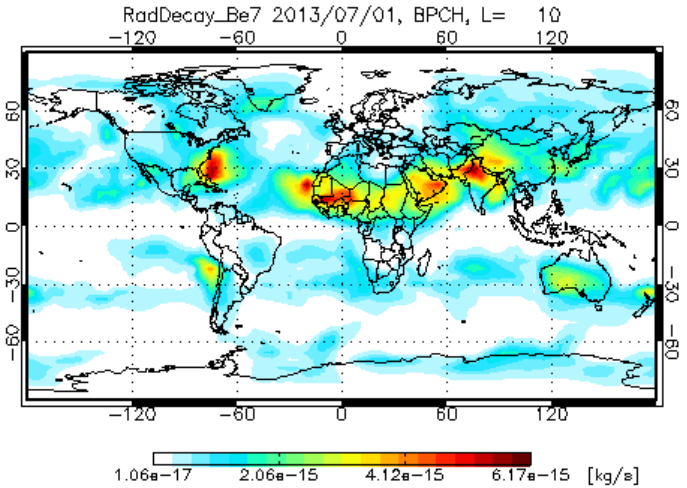


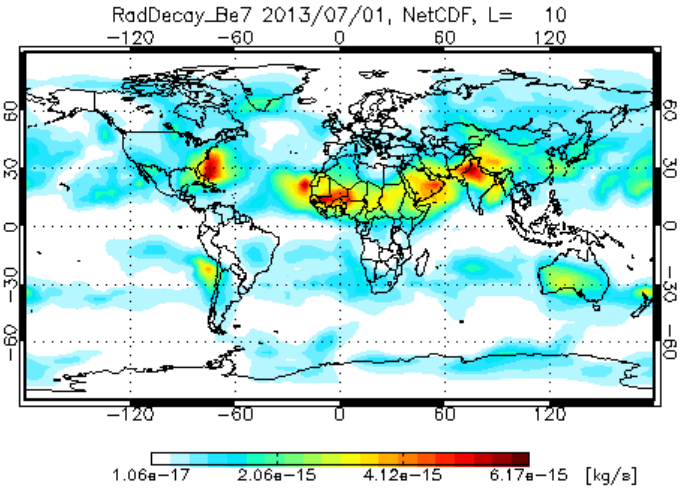


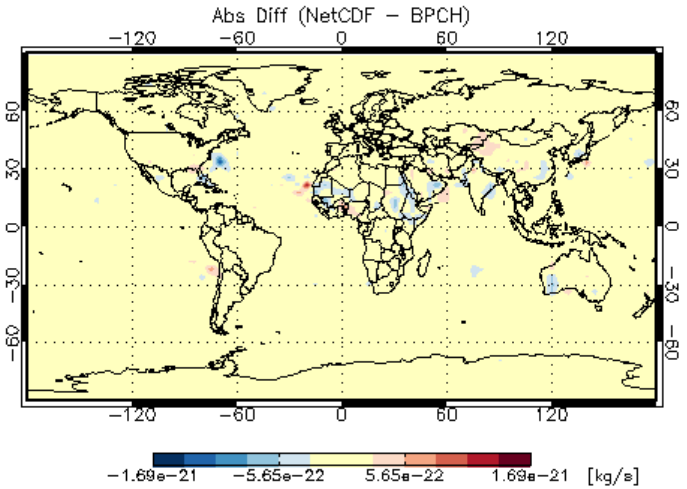


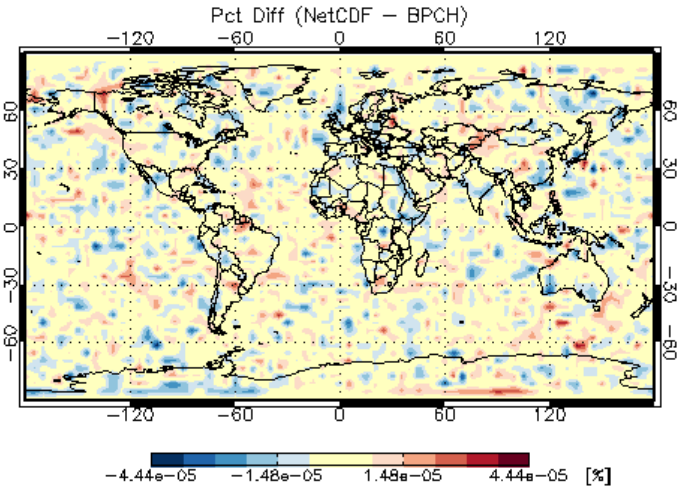


Decay of Be7 (ND02, #2), Units: kg/s, Level 10 (870 hPa)





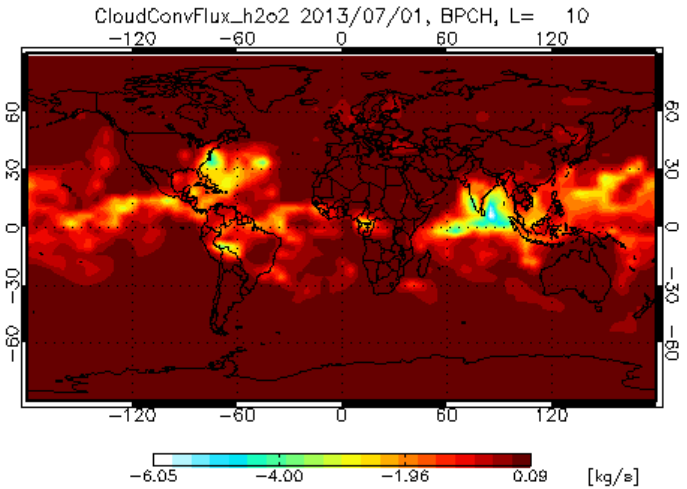


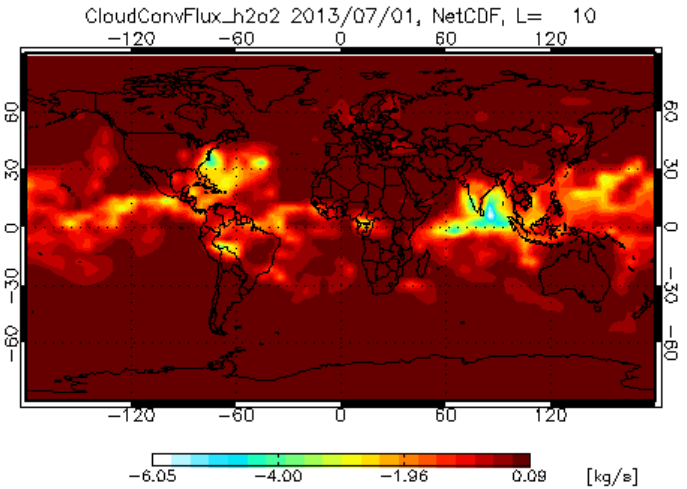


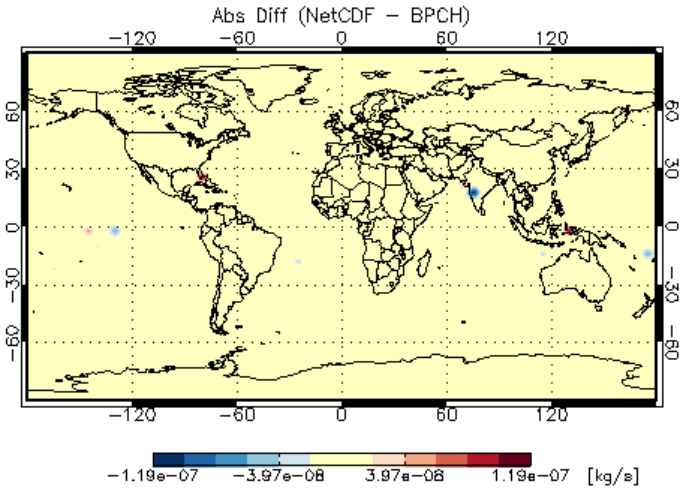
Wet deposition and convection diagnostics

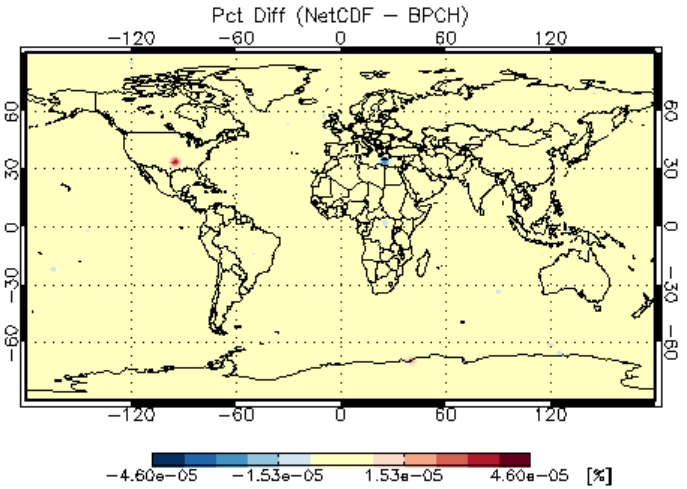
- The next set of diagnostics are all updated each “heartbeat” timestep for both bpch and netCDF output:
  - ND14: Mass flux in cloud convection (kg/s)
  - ND38: Loss of soluble species to convection (kg/s)
  - ND39: Loss of soluble species in wet deposition (kg/s)
  - Output taken from the geosfp_4x5_aerosol simulation

Cloud convection flux of H2O2 (ND14), Units: kg/s, Level 10 (870 hPa)



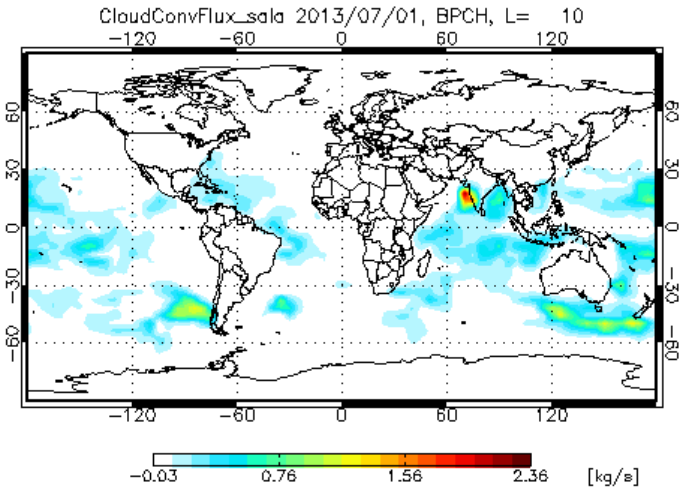


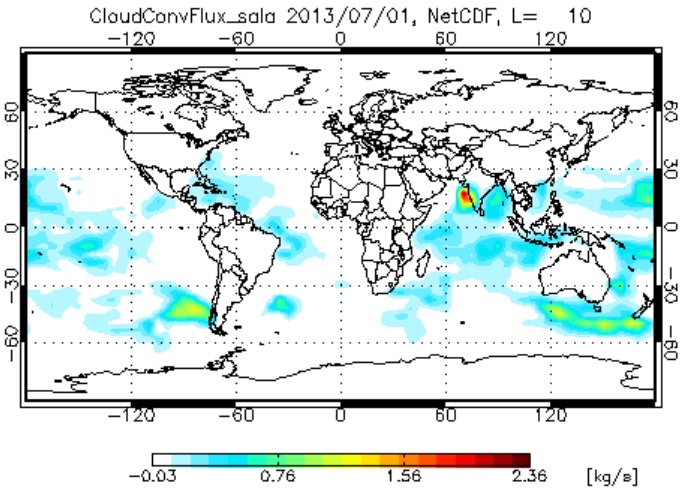


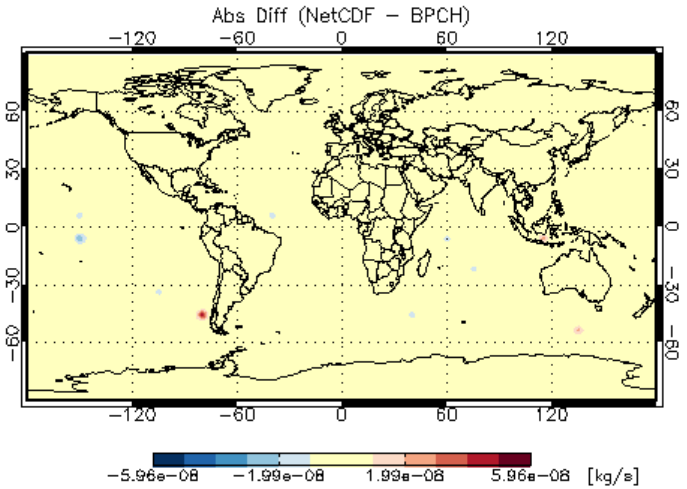


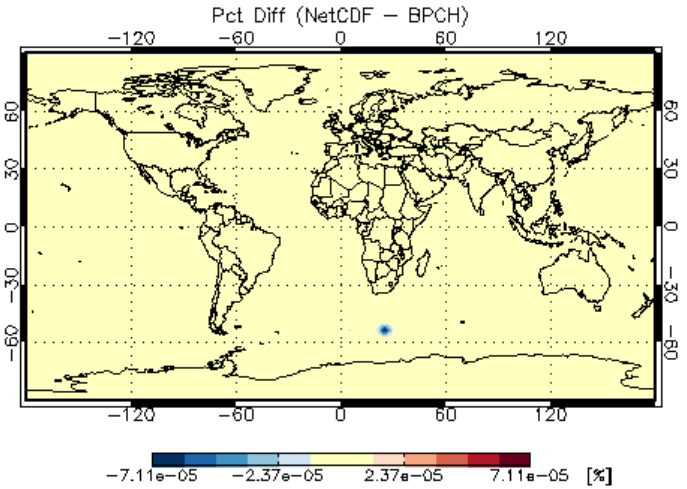
These differences are on the order of numerical noise. This is to be expected because the bpch and netCDF diagnostics are updated at the same frequency.

Cloud convection flux of SALA (ND14), Units: kg/s, Level 10 (870 hPa)



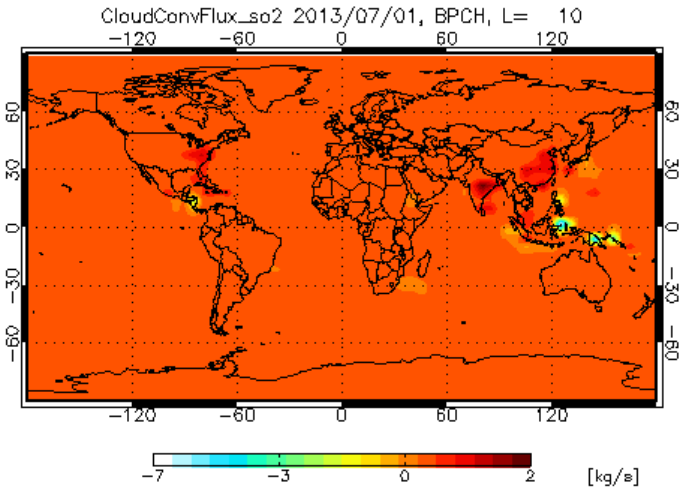


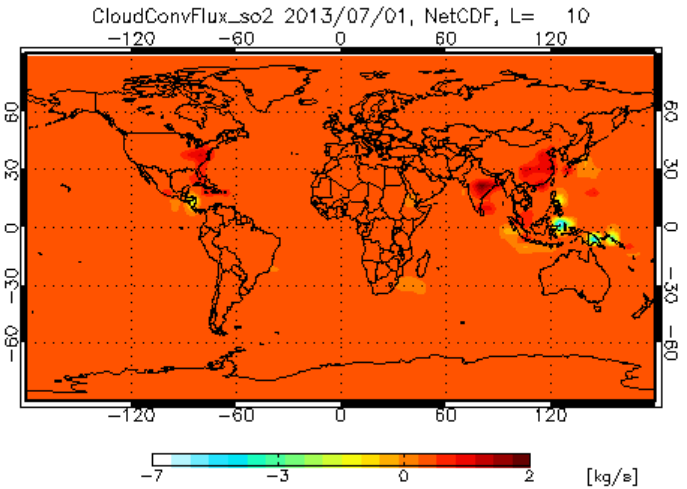


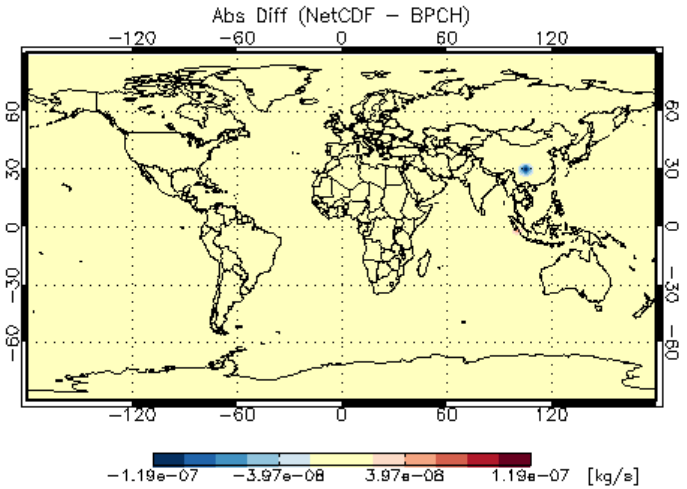


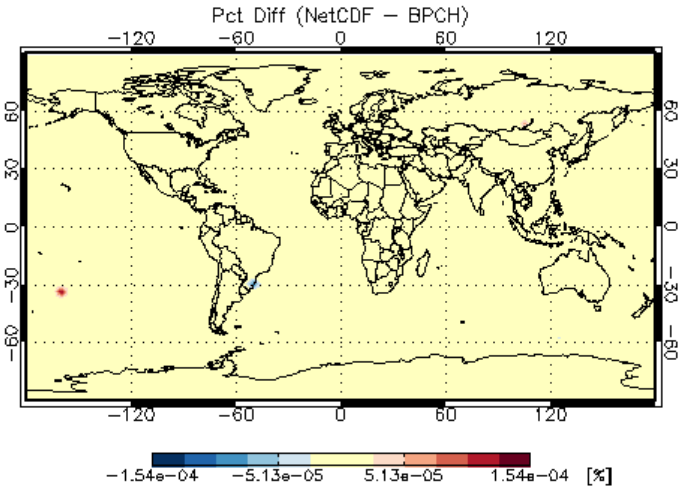
Etc. for all of these other plots …

Cloud convection flux of SO2 (ND14), Units: kg/s, Level 10 (870 hPa)

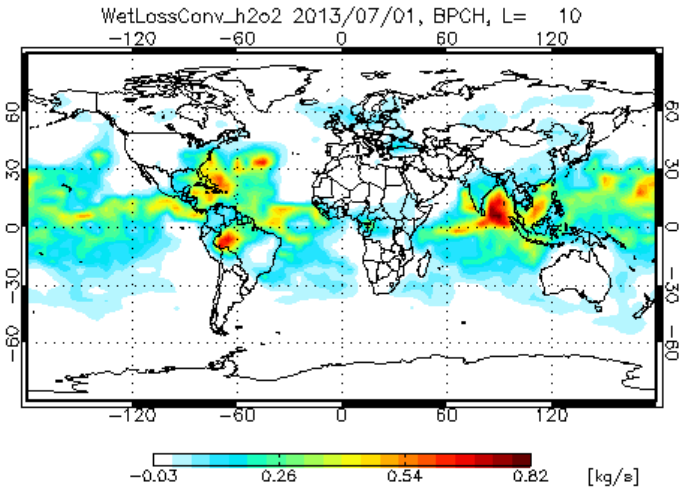


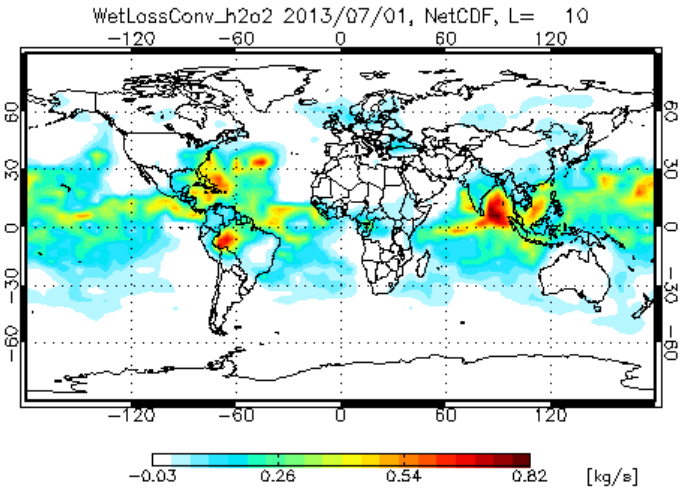


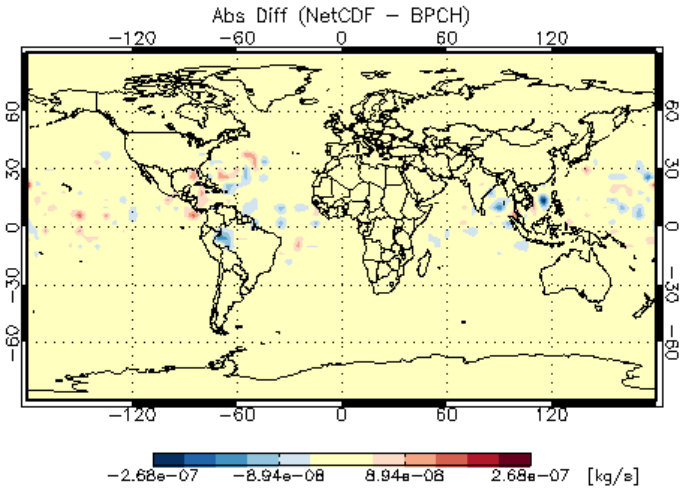


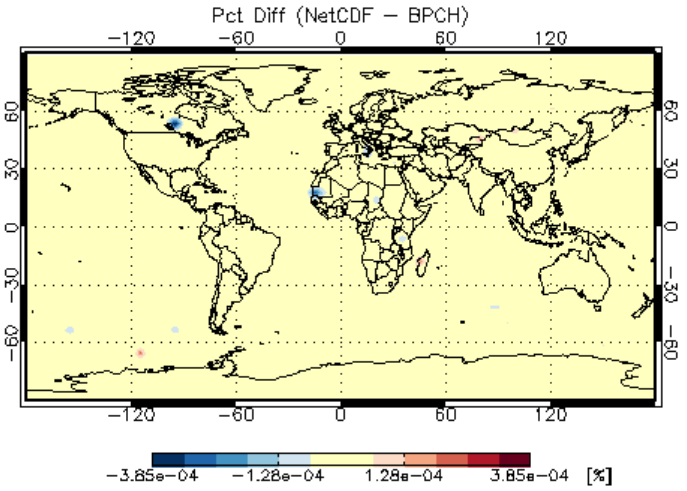


H2O2 lost in convective updraft (ND38), Units: kg/s, Level 10 (870 hPa)

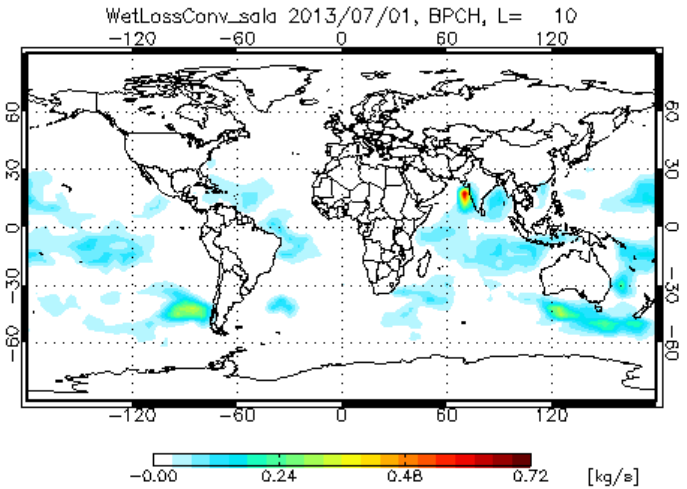


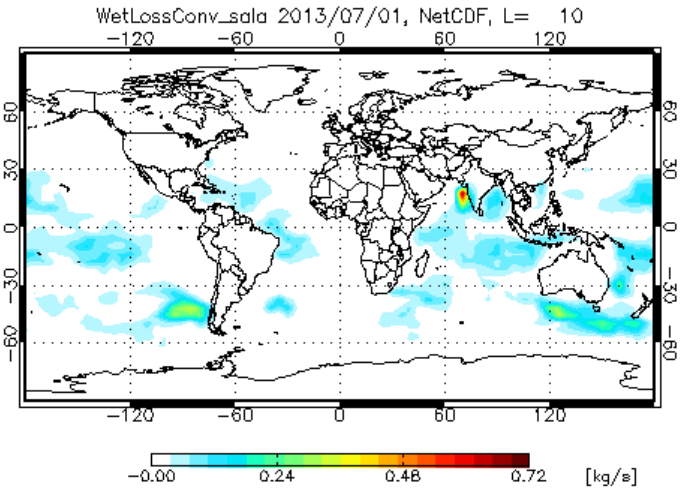


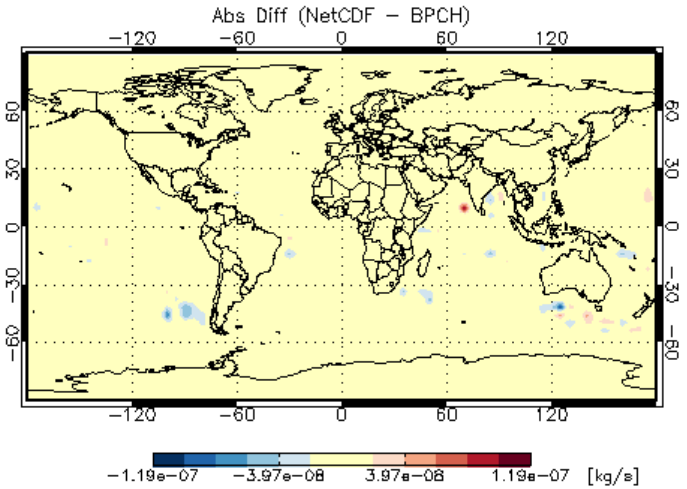


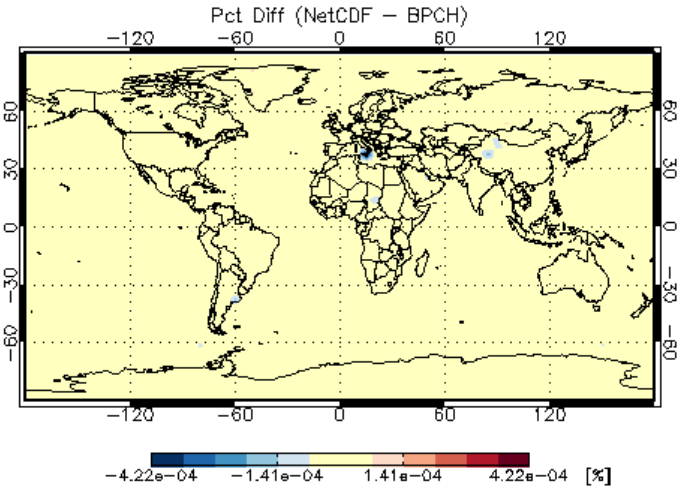


SALA lost in convective updraft (ND38), Units: kg/s, Level 10 (870 hPa)

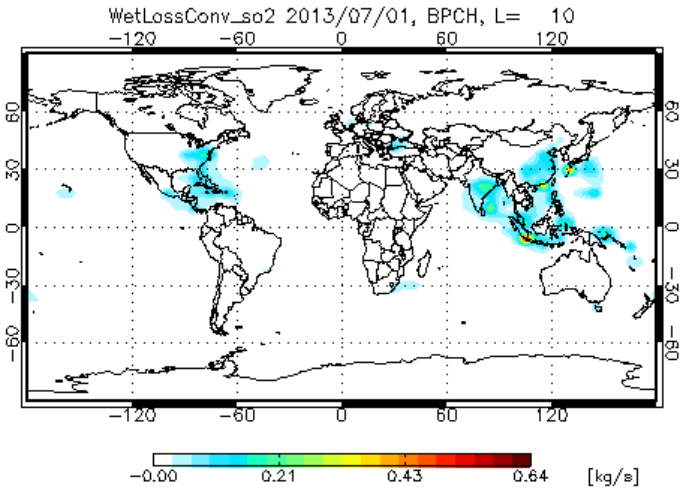


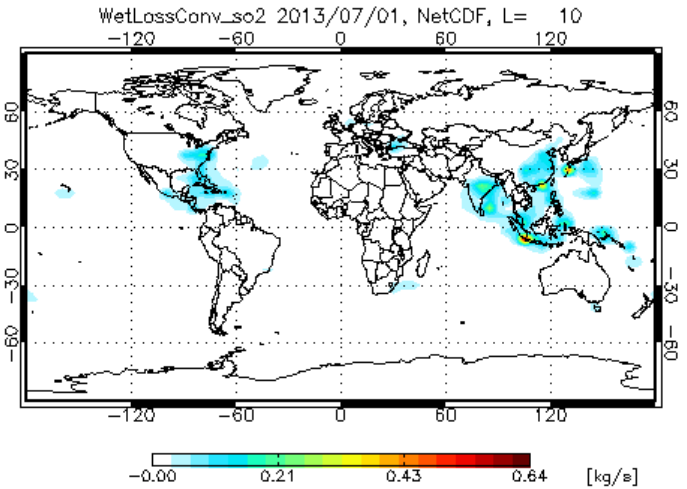


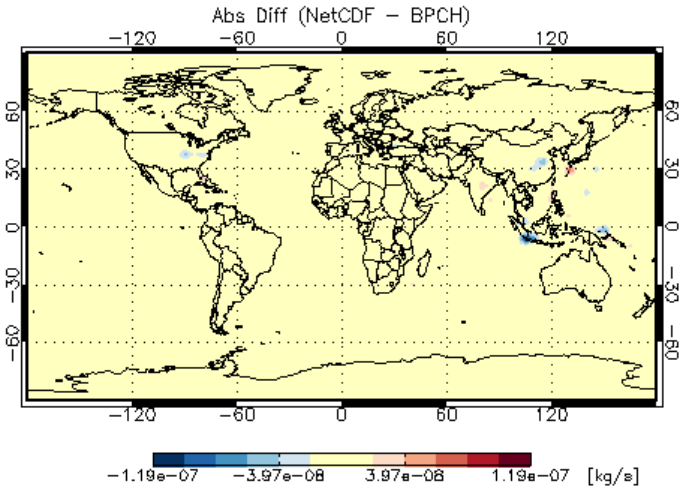


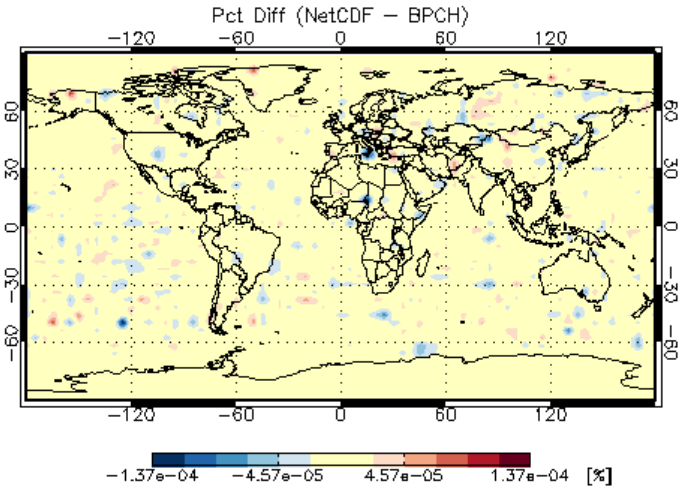


SO2 lost in convective updraft (ND38), Units: kg/s, Level 10 (870 hPa)

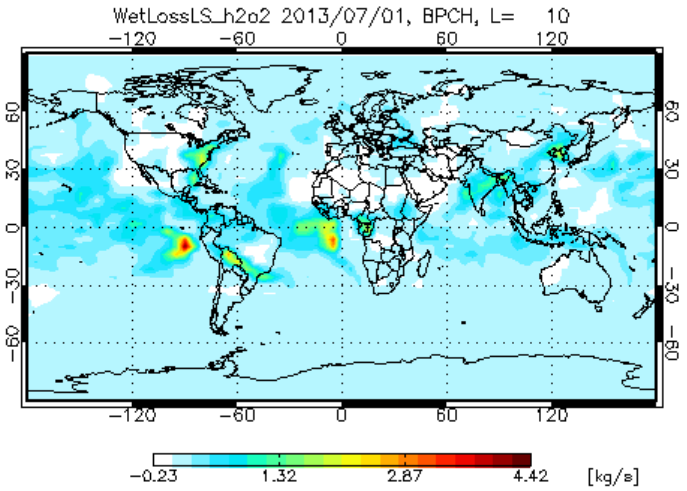


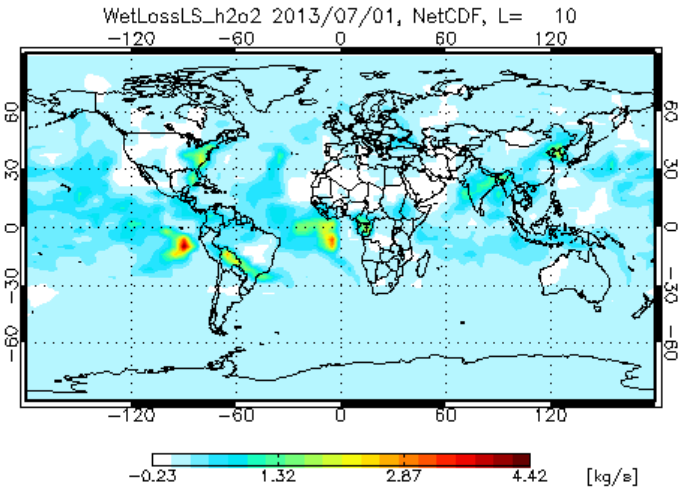


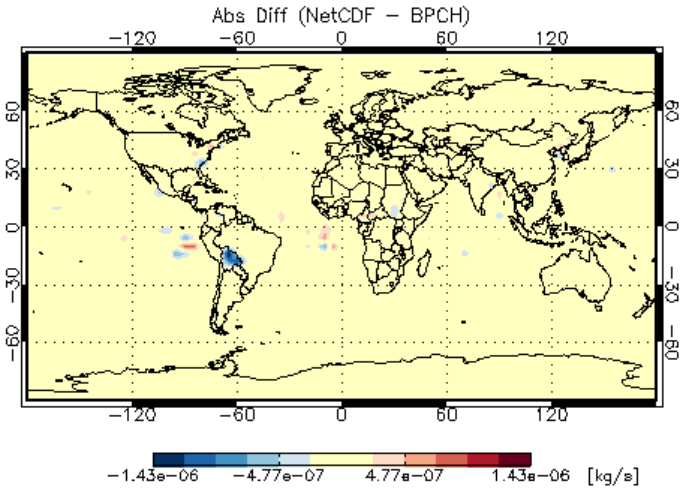


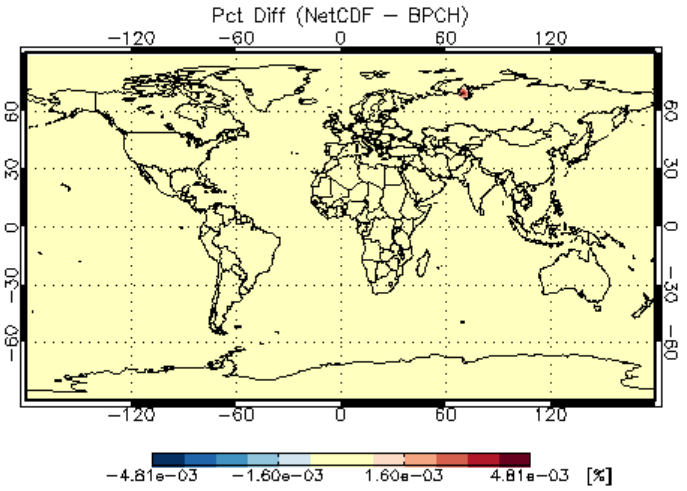


H2O2 lost in large-scale wetdep (ND39), Units: kg/s, Level 10 (870 hPa)

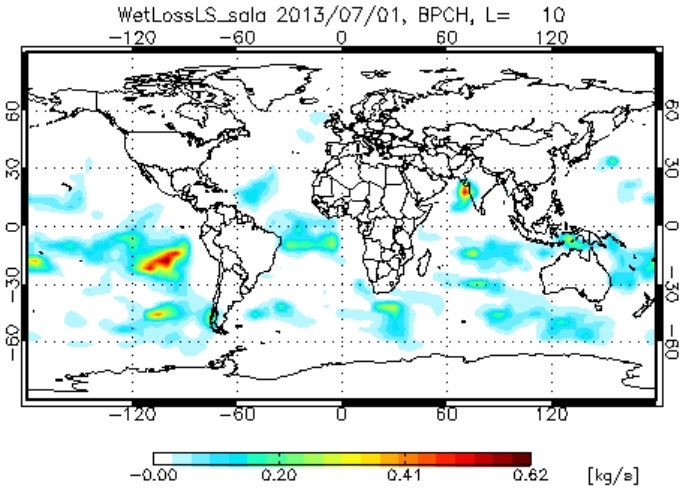


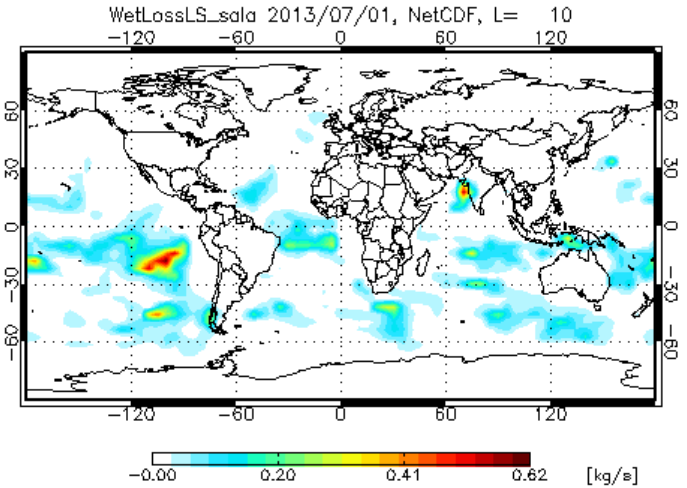


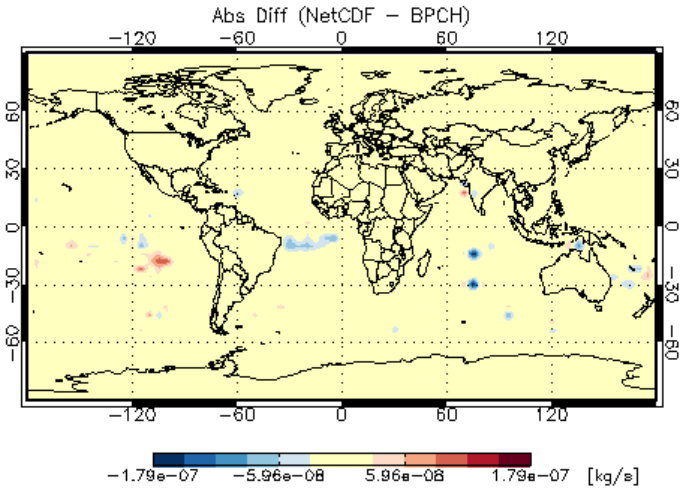


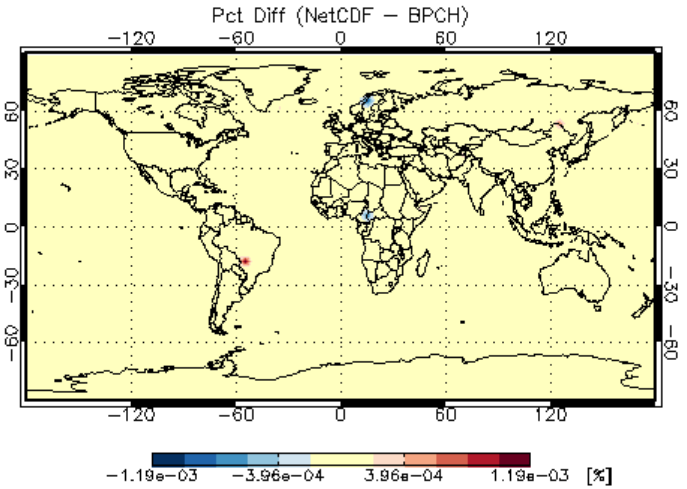


SALA lost in large-scale wetdep (ND39), Units: kg/s, Level 10 (870 hPa)

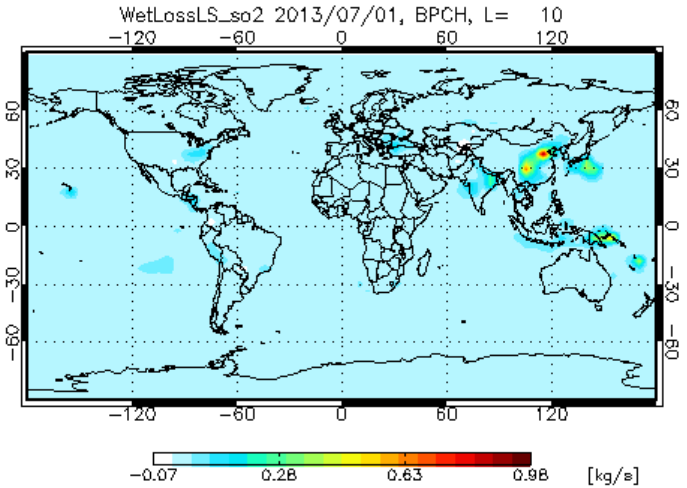


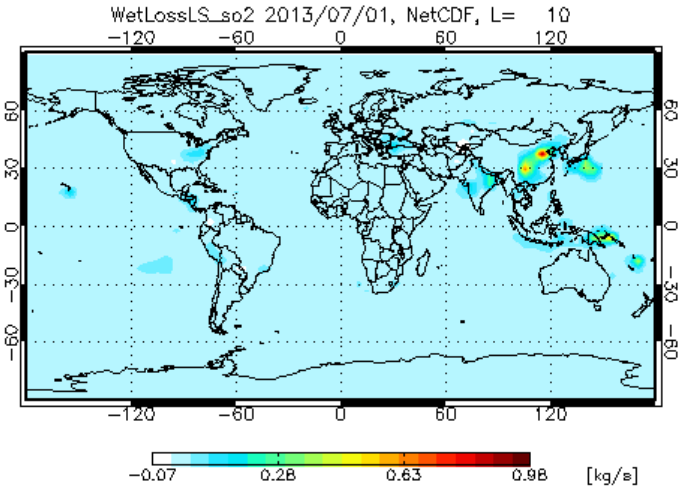


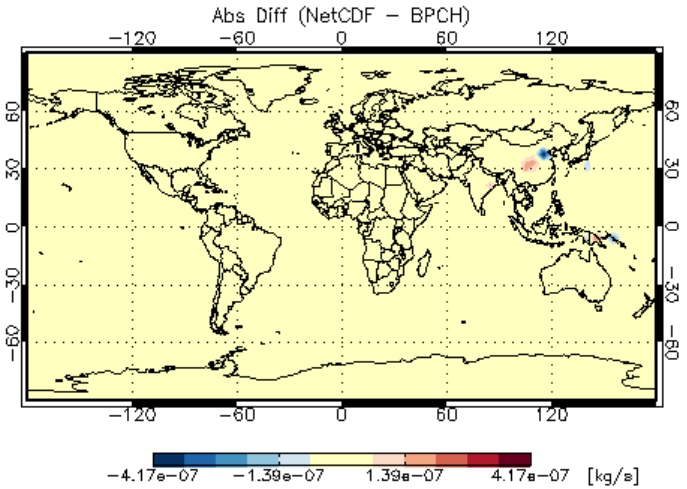


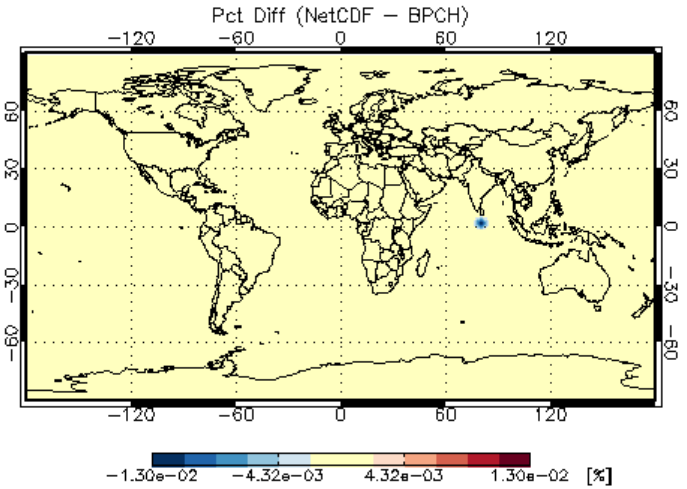


SO2 lost in large-scale wetdep (ND39), Units: kg/s, Level 10 (870 hPa)





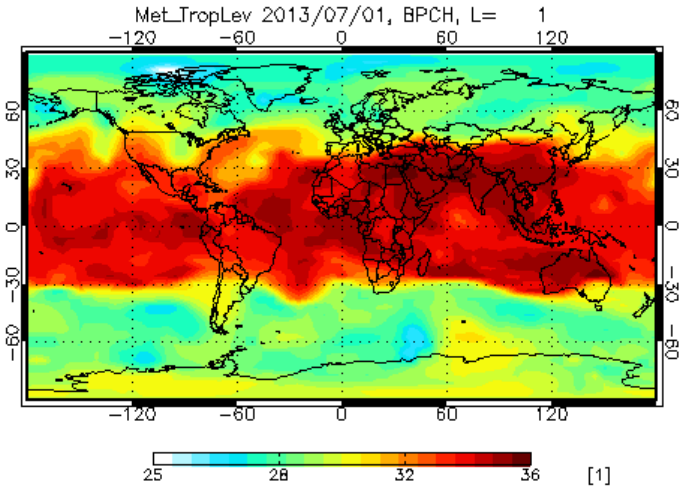


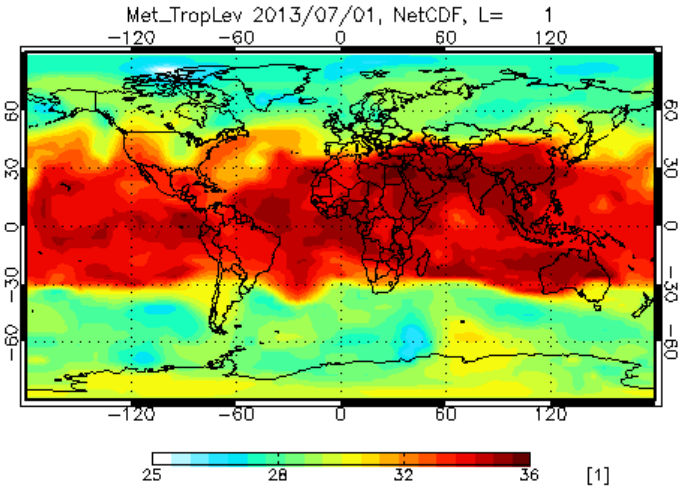


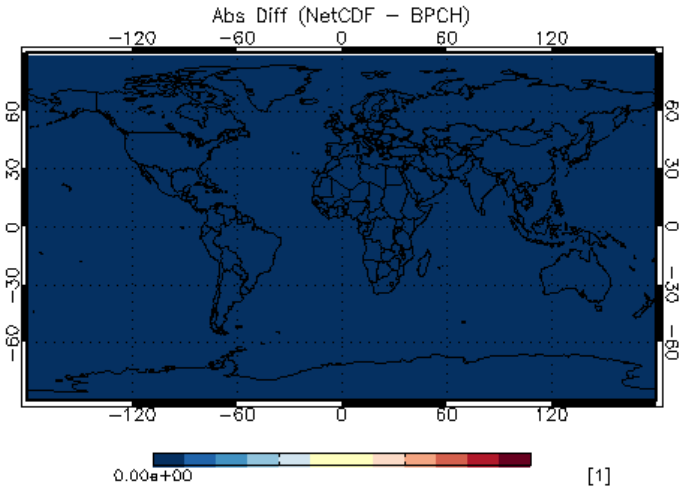
Tropopause diagnostics

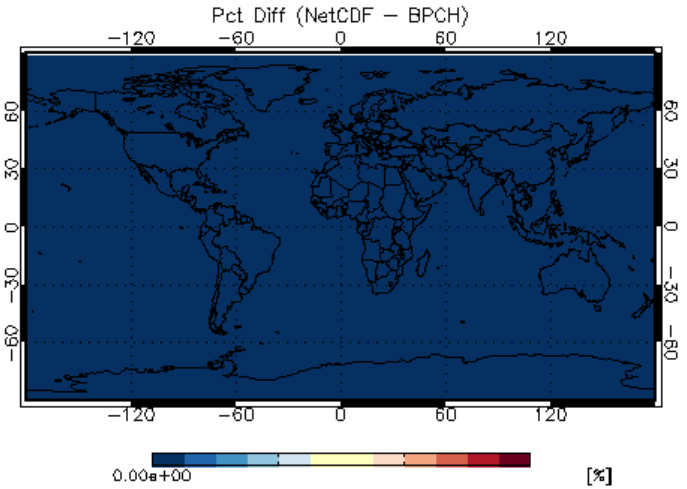
- Tropopause level
- Tropopause height [km]
- Tropopause pressure [hPa]

Tropopause level (ND55, #1)
Unit: [1]

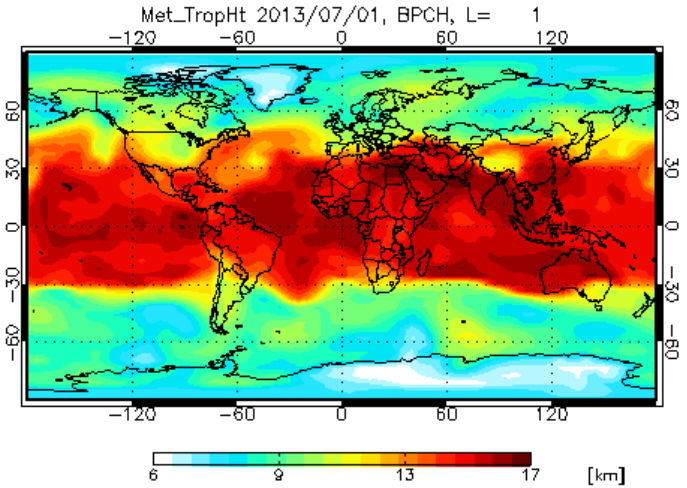


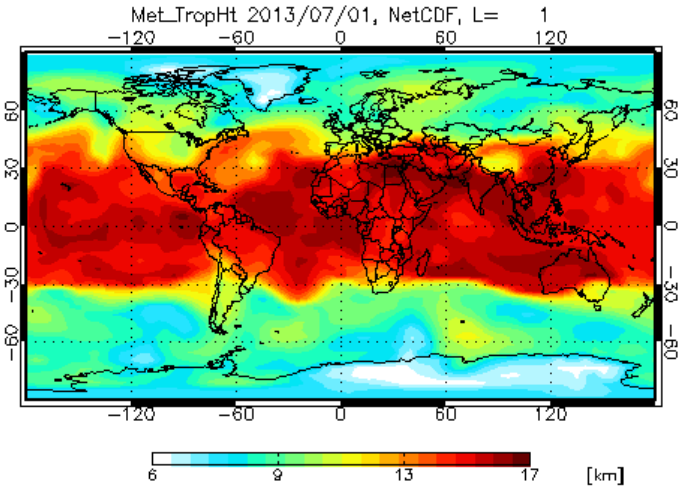


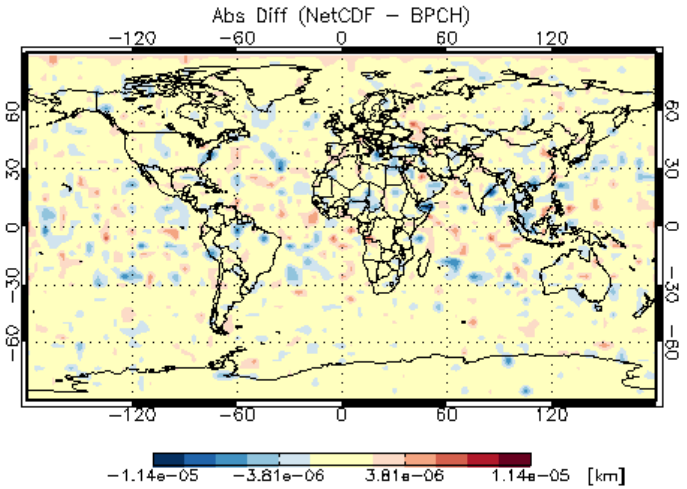


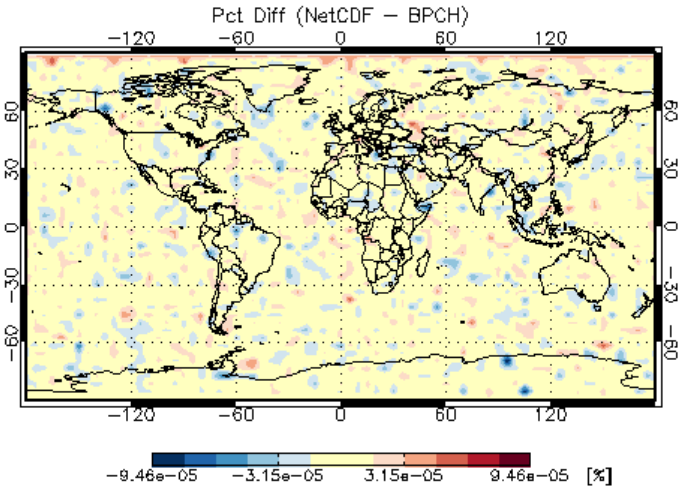


Tropopause height
Units: [km]

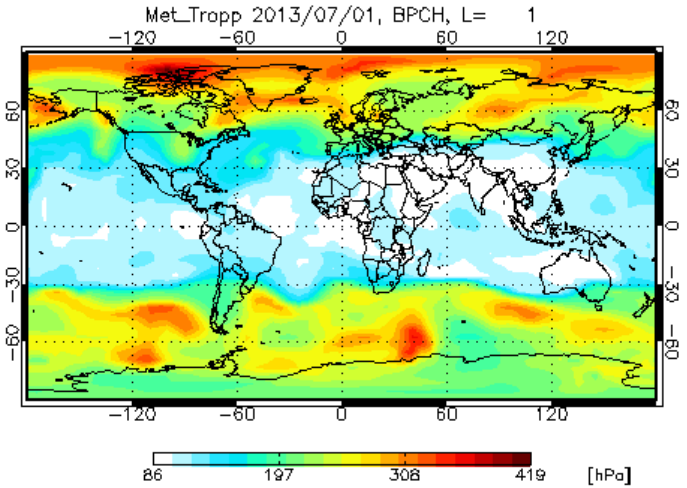


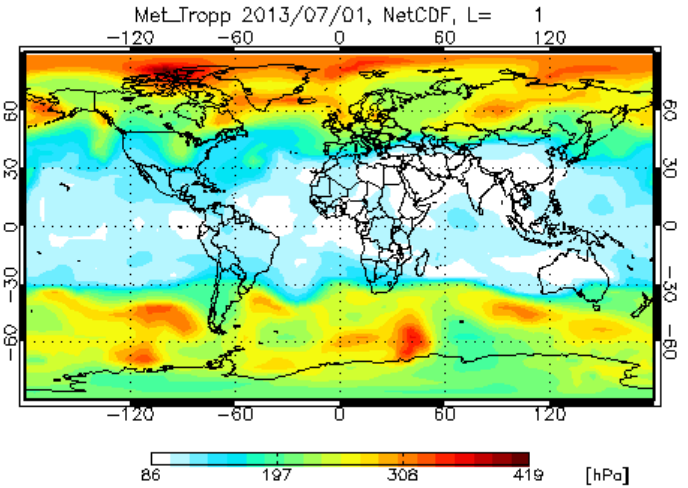


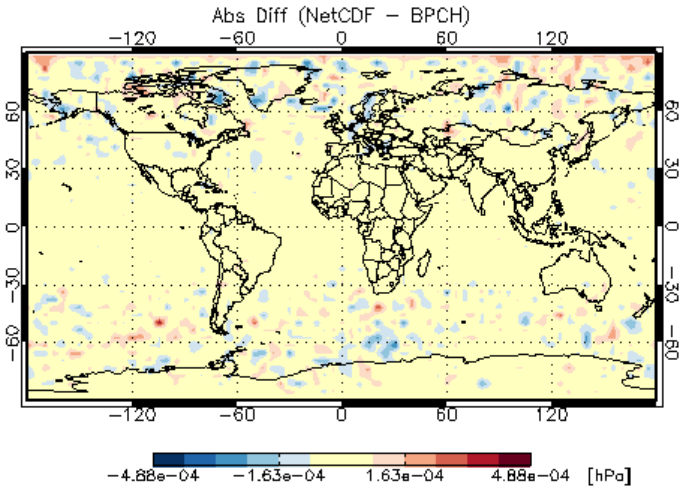


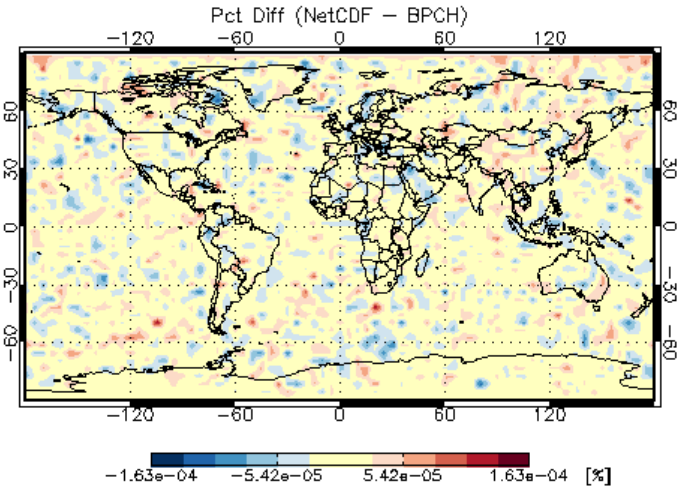


Tropopause Pressure
Units: [hPa]





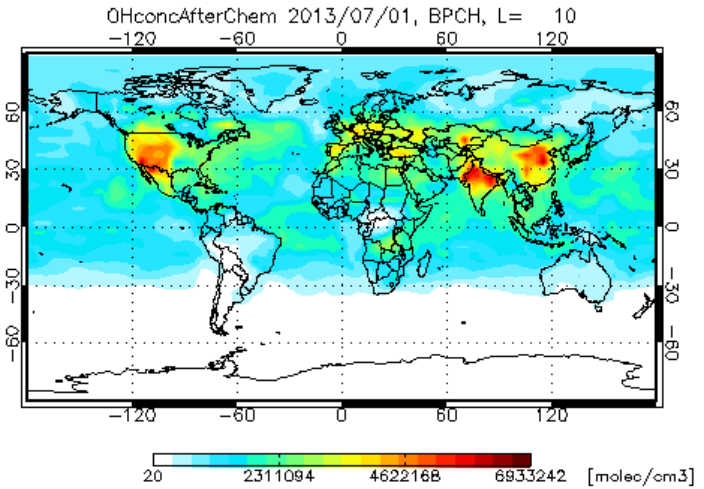


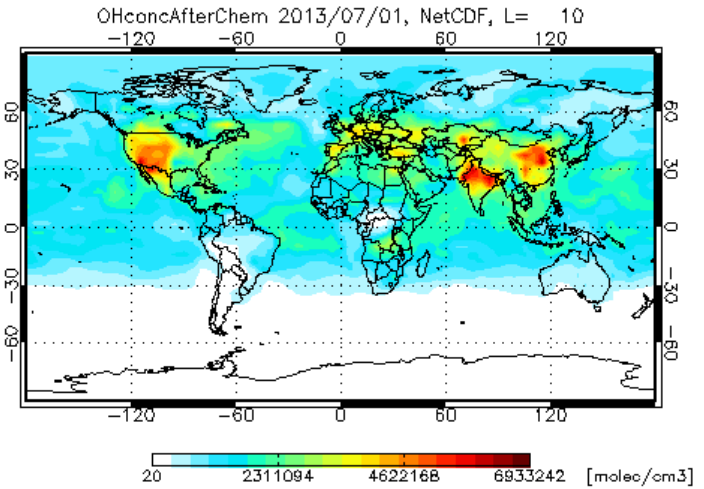


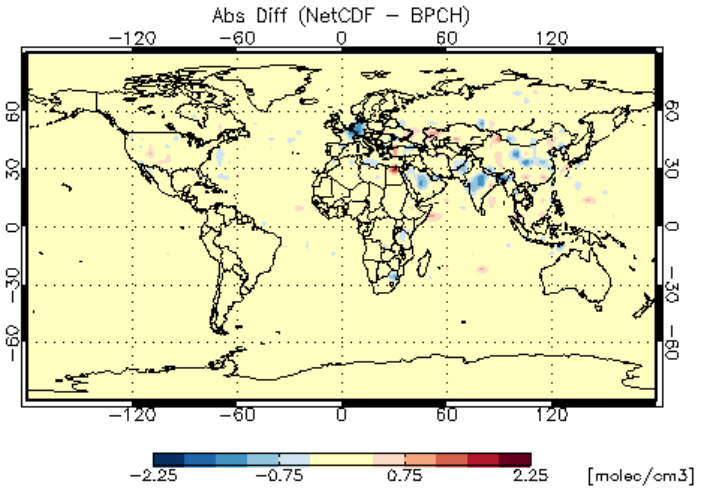
Chemical production diagnostics (ND43)

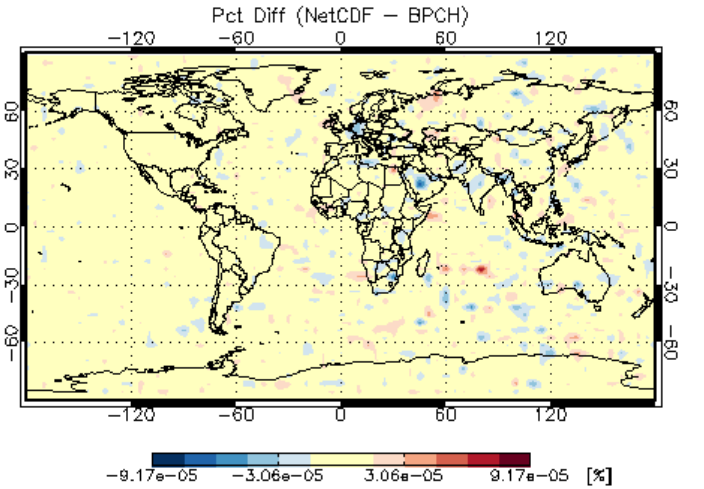
- OH after chemistry solver [molec/cm3]
- HO2 after chemistry solver [mol/mol]
- O1D after chemistry solver [molec/cm3]
- O3P after chemistry solver [molec/cm3]
  - These are used in the benchmark plots, especially the OH concentration.
  - Output plotted from geosfp_4x5_benchmark

OH concentration after KPP solver (ND43, #1), Units: molec/cm3, Level 10 (870 hPa)

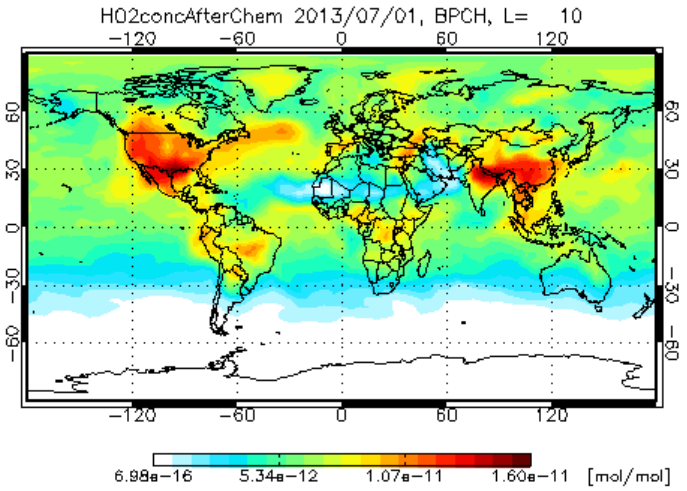


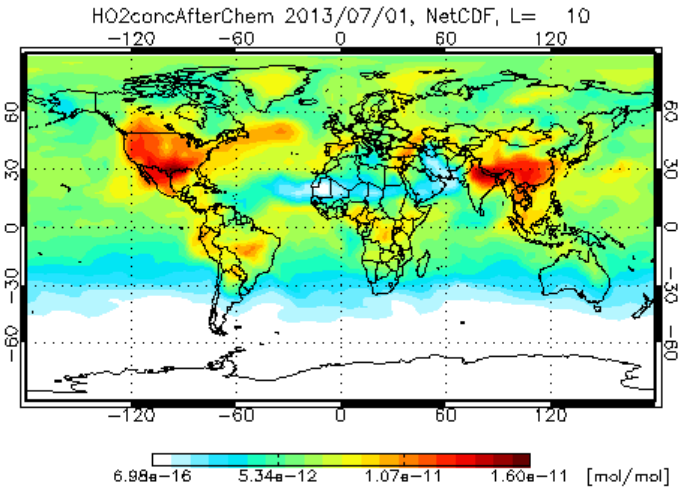


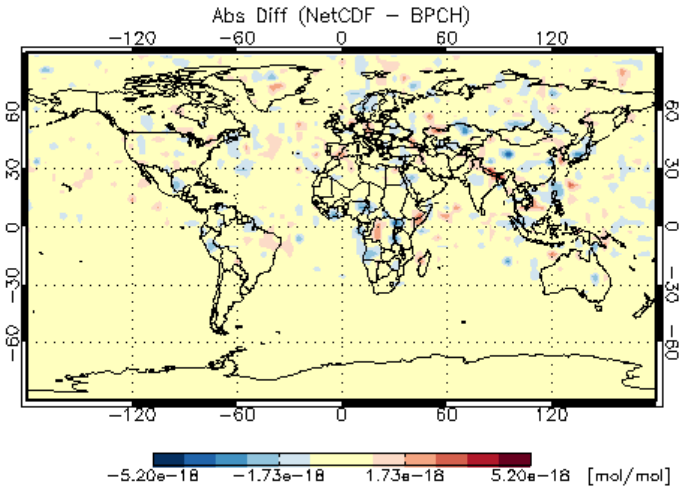


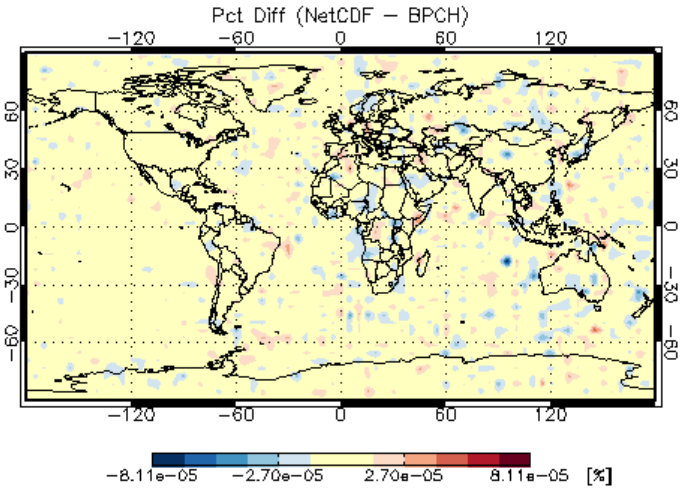


HO2 concentration after KPP solver (ND43, #2), Units: mol/mol, Level 10 (870 hPa)

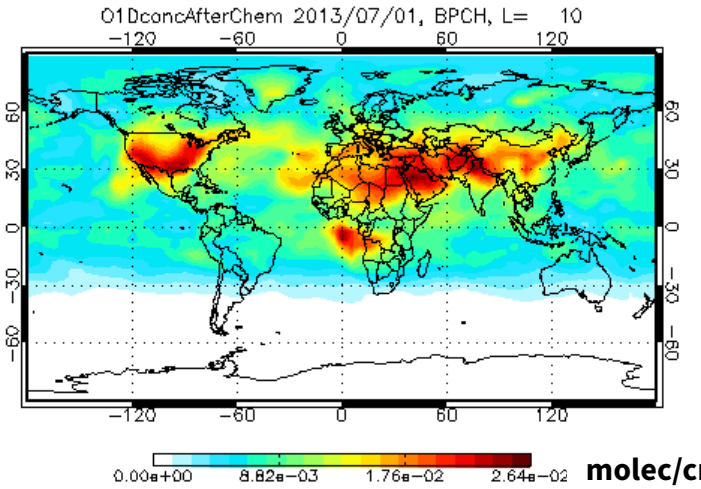




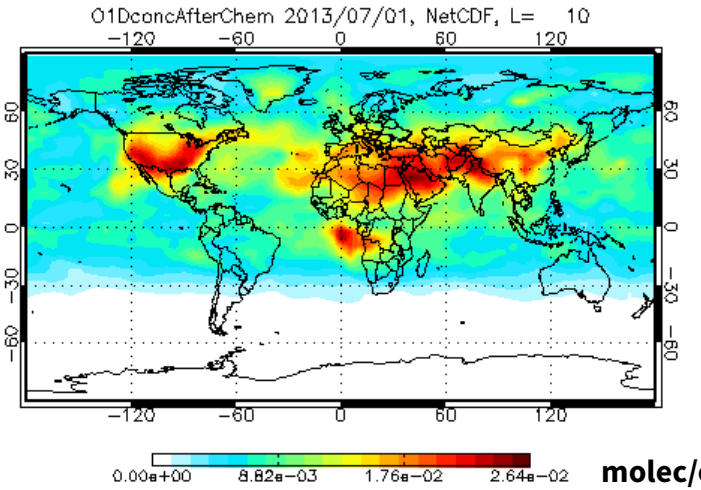




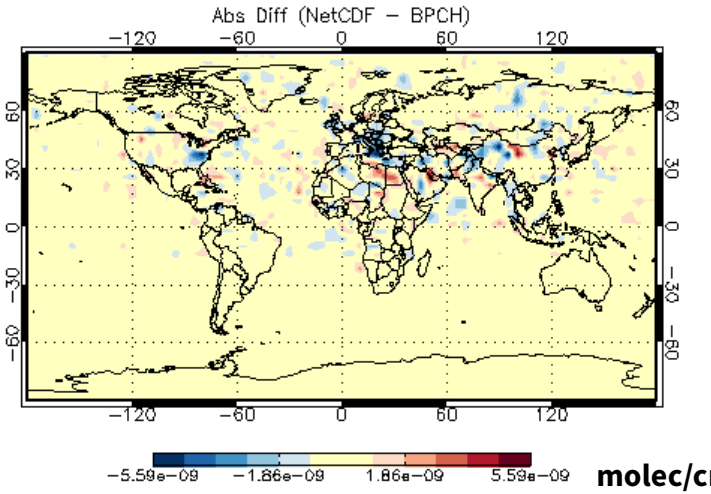
O1D concentration after KPP solver (ND43, #3), Units: molec/cm3, Level 10 (870 hPa)



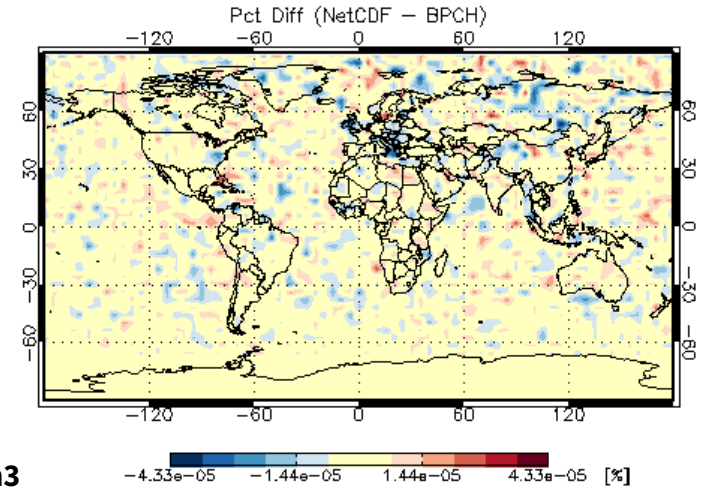
molec/cm3



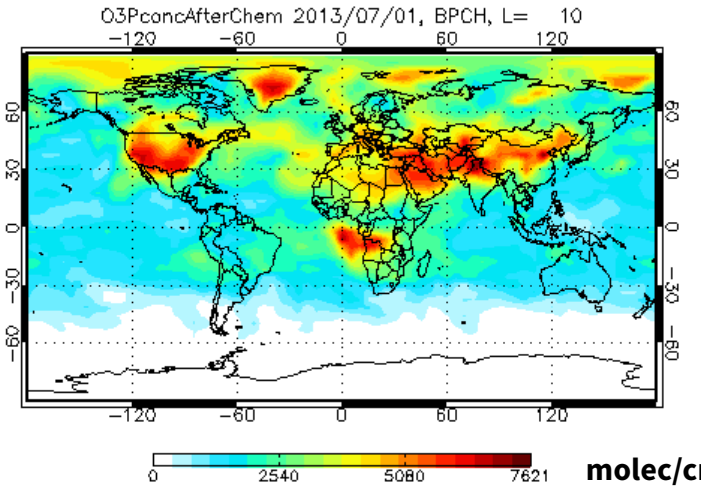
molec/cm3



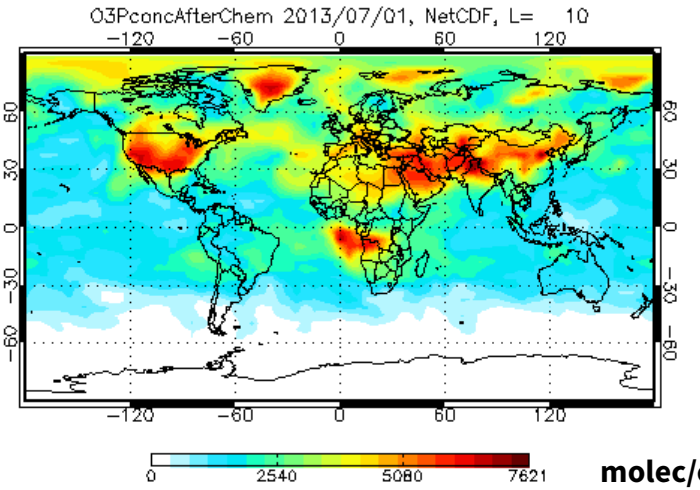
molec/cm3



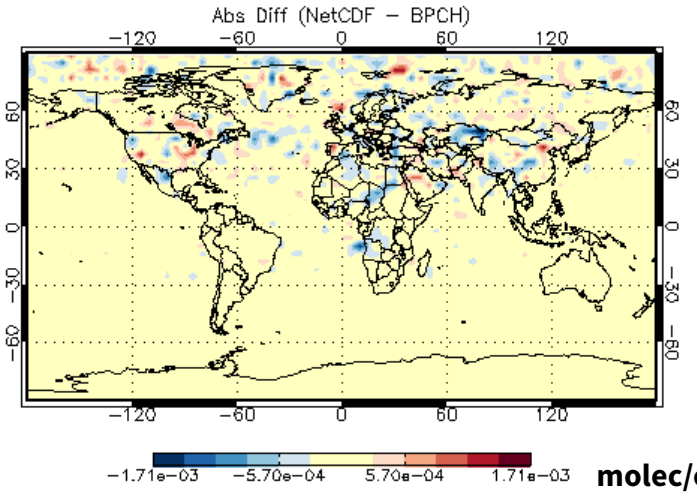
O3P concentration after KPP solver (ND43, #3), Units: molec/cm3, Level 10 (870 hPa)



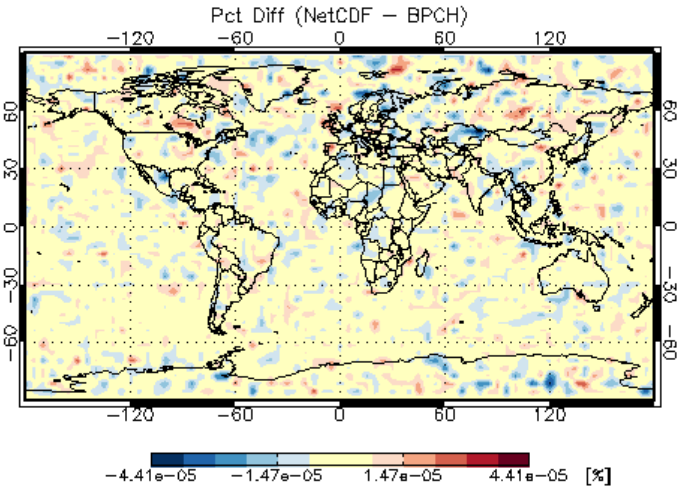
molec/cm3



molec/cm3



molec/cm3



Conclusions

- Rn/Pb/Be diagnostics (ND01, ND02): OK
- Convection diagnostics (ND14, ND38): OK
- Wetdep diagnostic (ND39): OK
  - But problems w/ precipitation fractions (ND16, ND17, ND18) still need to be addressed
  - These are optional diagnostics (not needed for benchmarks) so we will skip for now
- Concentrations after KPP (ND43): OK
- Tropopause diagnostics (ND55): OK

Conclusions

- Species concentrations (ND45): OK
  - Diffs between bpch/netCDF are on the level of numerical noise **as long as the update frequencies are the same**
  - Larger differences when netCDF is updated every 10 min and bpch every 20 min
  - Need to explain this to the GEOS-Chem users
  - GCST recommends updating diagnostics every "heartbeat" timestep, as this is what GCHP does.

Conclusions

- Drydep diagnostics (not shown here) have contributions that are updated on different timesteps:
  - Drydep flux in mixing: “heartbeat timestep” = 10 min
  - Drydep vel; Drydep fluxes in chemistry = 20 min
  - Need to deal with this at some point. Potential for double-counting is there.
  - This type of discrepancy may show up for other diagnostics as well

Conclusions

- Also, please see the wiki for the latest info on the diagnostic naming convention, etc:
- http://wiki.geos-chem.org/List_of_diagnostics_for_v11-02