Supplemental information about the EMAC model setup for the ESCiMo simulations
and
Supplemental information about results from a first evaluation

This document is part of the electronic supplement to our article
"Earth System Chemistry Integrated Modelling (ESCiMo) with the Modular Earth Submodel System (MESSy, version 2.51)"
in Geosci. Model Dev. Discuss. (2015), available at:
`http://www.geosci-model-dev-discuss.net`

Date: September 25, 2015

Contents

1 MECCA configuration files

```
# -*- Shell-script -*-

# - used for CCMI RC1/2-base
# - create SCAV-L-mechanism with: (Sc && !I && !Hg)
# The shell variables defined here will be used by xmecca
# when it is run in batch mode (i.e. not interactively).

 set apn          = 0                # number of aerosol phases [0...99, default=0]
 set gaseqnfile   = gas_mim1.eqn
 set rplfile      = CCMI-base-02     #
 set wanted       = "(((Tr && (G || Het) && \!I) || St) && \!Hg)"
 set enthalpy     = n                # activate enthalpy in kJ/mol?
 set mcfct        = n                # Monte-Carlo factor?
 set diagtracfile = CCMI             # diagnostic tracers?
 set rxnrates     = n                # calculate accumulated reaction rates?
 set tagdbl       = n                # tagging, doubling, both, none ??
 set kppoption    = 4                # k=kpp, 4=kp4
 set integr       = rosenbrock_mz    # integrator
 set vlen         = 256              # only for kp4 and integr=rosenbrock_vec
 set decomp       = 1                # remove indirect indexing
                                     # kp4: 0/1/2/3; kpp: y/n
 set deltmpkp4    = y                # delete temporary kp4 files
 set latex        = y                # latex list of reactions
 set graphviz     = y                # graphviz plots
 set deltmp       = y                # delete temporary xmecca files?
```

Figure S1: CCMI-base-02.bat configuration file of MECCA used for all simulations without interactive tropospheric aerosol. For simulations RC1-aero-06/07 and RC1-aecl-01/02 CCMI-aero-02.bat has been used, which differs only in one line: `set rplfile = CCMI-aero-02`. The corresponding replacement files (rplfile) are displayed in Figures S2 and S3, respectively.

```
// -*- kpp -*- kpp mode for emacs

#REPLACE <J8401>
<a>  CH3I    + hv = CH3O2                 : {%TrGJ}     JX(ip_CH3I); {&&}
#ENDREPLACE

// replace by original MIM:
#REPLACE <G4504>
<a> ISO2 + NO = .956 NO2 + .956 MVK + .956 HCHO + .956 HO2 + .044 ISON : {%TrGNC} 2.54E-12*EXP(360./temp); {&&1614}
#ENDREPLACE

// exclude C2H2 reactions (no source available !)
#REPLACE <G4222>
#ENDREPLACE

#REPLACE <G6411>
#ENDREPLACE

#REPLACE <G7406>
#ENDREPLACE

// exclude C2H6 + Cl reaction for backward compatibility
#REPLACE <G6412>
#ENDREPLACE

// O3s diagnostic
#REPLACE <>
<G01Diag> O3s            = LO3s        : {%StTrG} k_O3s; {&&1714}
#ENDREPLACE

// Hg chemistry without Ox and HOx oxidation
#REPLACE <G10100>
#ENDREPLACE

#REPLACE <G10200>
#ENDREPLACE

#REPLACE <G10201>
#ENDREPLACE

// additional diagnostic tracers
#REPLACE <>
<G10G6501>  CFCl3_c   + O1D  = O1D   : {%StGFCl}   2.3E-10{1.2}; {&2626}
<J11J6500>  CFCl3_c   + hv   = Dummy : {%StGFClJ}  jx(ip_CFCl3){}; {&&}
<G12G6500>  CF2Cl2_c  + O1D  = O1D   : {%StGFCl}   1.4E-10{1.25}; {&2626}
<J13J6501>  CF2Cl2_c  + hv   = Dummy : {%StGFClJ}  jx(ip_CF2Cl2){}; {&&}
<G14G3102a> N2O_c     + O1D  = O1D   : {%UpStGN}   7.25E-11{1.1}*EXP(20./temp); {&2626}
<G15G3102b> N2O_c     + O1D  = O1D + Dummy : {%StGN}     4.63E-11{1.1}*EXP(20./temp); {&2626}
<J16J3100>  N2O_c     + hv   = Dummy : {%UpStGNJ}  jx(ip_N2O){}; {&&}
<G17G6407>  CH3CCl3_c + O1D  = O1D   : {%StGCCl}   3.E-10{}; {&&}
<G18G6408>  CH3CCl3_c + OH   = OH    : {%StTrGCCl} 1.64E-12{1.15}*EXP(-1520./temp); {&2626}
<J19J6402>  CH3CCl3_c + hv   = Dummy : {%StGCClJ}    jx(ip_CH3CCl3){}; {&&}
<J20J7601>  CF2ClBr_c + hv   = Dummy : {%StGFBrJ}    jx(ip_CF2ClBr){}; {&&}
<J21J7500>  CF3Br_c   + hv   = Dummy : {%StGFBrJ}    jx(ip_CF3Br){}; {&&}
#ENDREPLACE
```

Figure S2: CCMI-base-02.rpl configuration file of MECCA used for all simulations without interactive tropospheric aerosol.

```
...

#REPLACE <G9200>
<a>  SO2    + OH    = SO3 + HO2 : {%StTrGS}   k_3rd(temp,cair,3.3E-31,4.3,1.6E-12,0.,0.6){1.1}; {&2626}
#ENDREPLACE

...

#REPLACE <>
<G9100>  SO + O2   = SO2 + O3P   : {%TrStGS} 1.25e-13*exp(-2190/temp); {&2626}
<G9101>  SO + O3   = SO2 + O2    : {%TrStGS} 3.4e-12*exp(-1100/temp); {&2626}
<G9102>  S  + O2   = SO  + O3P   : {%TrStGS} 2.3e-12; {&2626}
<G9201>  SH + O2   = OH  + SO    : {%TrStGS} 4.e-19; {&2626}
<G9202>  SO3 + H2O = H2SO4       : {%TrStGS} 8.5e-41*exp(6540./temp)*C(ind_H2O); {&&1555}
<G9406>  OCS + OH  = SH  + CO2   : {%TrStGS} 1.1e-13*exp(-1200./temp); {&2626}
<G9407>  OCS + O3P = CO  + SO    : {%TrStGS} 2.1e-11*exp(-2200./temp); {&2626}
<J9000>  OCS + hv  = CO  + S     : {%TrStGSJ} JX(ip_OCS); {&&}
<J9001>  SO2 + hv  = SO  + O3P   : {%TrStGSJ} 60.*JX(ip_OCS); {&&}
<J9002>  SO3 + hv   = SO2 + O3P  : {%TrStGSJ} JX(ip_SO3); {&&}
<J9003>  H2SO4 + hv = SO3 + H2O  : {%TrStGSJ} JX(ip_H2SO4); {&&}
#ENDREPLACE
```

Figure S3: Additional entries (compared to CCMI-base-02.rpl of Figure S2) in CCMI-aero-02.rpl configuration file of MECCA used for additional sulphur chemistry in simulations with interactive tropospheric aerosol (RC1-aero-06/07 and RC1-aecl-01/02).

2 Supplemental tables

Table S1: The initialisation of trace gas mixing ratios for January 1950 has been set up differently for two different groups: Short lived species were initialised with results for end of December 2000 of a previous EMAC simulation (Jöckel et al., 2010), as atmospheric mixing ratios adjust in the order of months. These short lived species comprise HNO_3, NO, NO_2, O_3, N_2O_5, and also C_3H_6, H_2O_2, CH_2O, ISOP, MEK, MVK, and ACET. Longer lived species were initialised by scaling the end of December 2000 mixing rations with individual scaling factors as listed here.

tracer	scaling factor
CO_2	0.843
N_2O	0.900
H_2	0.893
CH_3Cl	0.889
C_2H_6	0.733
CO	0.733
CH_3Br	0.677
CH_4	0.621
C_4H_{10}	0.520
PAN	0.333
$BrNO_3$	0.333
BrO	0.333
CCl_4	0.295
Cl_2	0.140
$ClNO_3$	0.140
HCl	0.140
CF_2Cl_2	0.038
$CFCl_3$	0.026
CH_3CCl_3	0.010

Table S2: Parameter settings used for the different model setups. Default values are listed in parentheses. Without coupled ocean model, *zinhoml* is calculated from the liquid water path.

	variable name	unit	submodel	T42L90MA	T42L47MA	T42L47MA coupled ocean
relative convective cloud mass–flux above level of non–buoyancy	cmfctop		CONVECT	(0.30)	0.35 (0.30)	0.21 (0.30)
entrainment rate for deep convection	entrpen	m^{-1}	CONVECT	$(1.0 \cdot 10^{-4})$	$0.5 \cdot 10^{-4}$ $(1.0 \cdot 10^{-4})$	$(1.0 \cdot 10^{-4})$
root–mean–square of the gravity wave induced horizontal wind speed at the launch level	rmscon	$m\ s^{-1}$	GWAVE	0.92 (1.0)	0.92 (1.0)	0.92 (1.0)
asymmetry factor of ice clouds	zasic		CLOUDOPT	(0.85)	(0.85)	0.91 (0.89)
cloud inhomogeneity factor (ice)	zinhomi		CLOUDOPT	(0.85)	(0.85)	(0.80)
cloud inhomogeneity factor (liquid)	zinhoml		CLOUDOPT			(0.70)

21 # 3 Supplemental figures

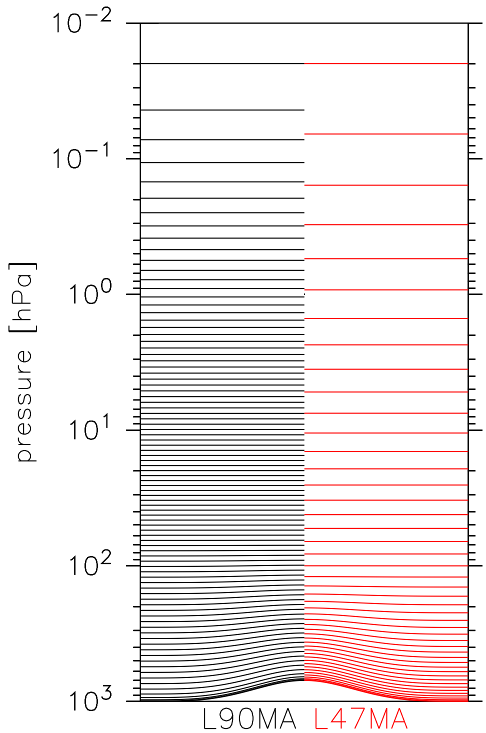

Figure S4: Hybrid pressure levels of vertical resolutions L90MA (left, black) and L47MA (right, red).

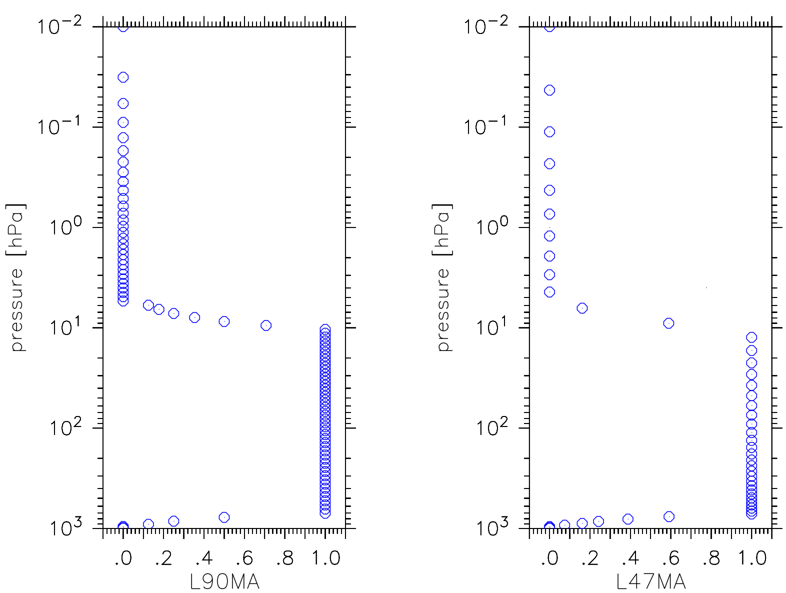

Figure S5: Vertical profile of relative (to the maximum) nudging strength as applied in L90MA (left) and L47MA (right) vertical resolution.

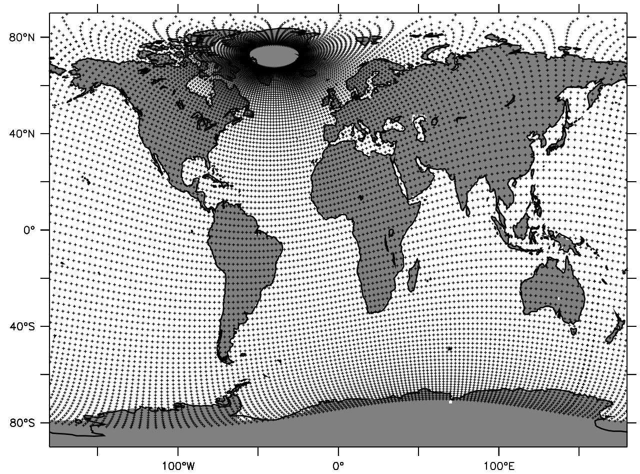

Figure S6: Rotated grid (GR30L40) of the ocean submodel MPIOM as used for simulation *RC2-oce-01*.

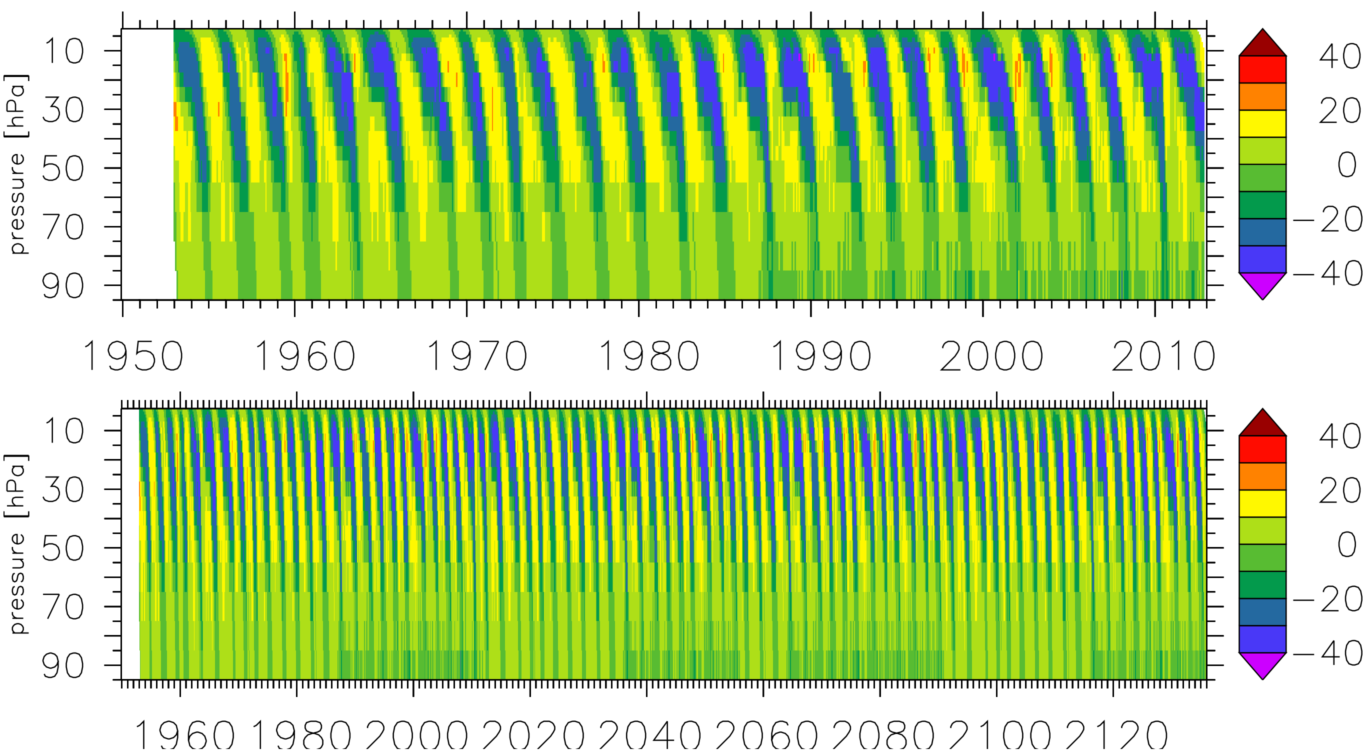

Figure S7: Equatorial zonal wind (in m/s) as nudged with submodel QBO. Upper panel: data from file FUB_01_hist_X_QBO_195001_201212.txt as used for *RC1* simulations; lower panel: data from file FUB_03_X_X_QBO_195001_213512.txt as used for *RC2* simulations.

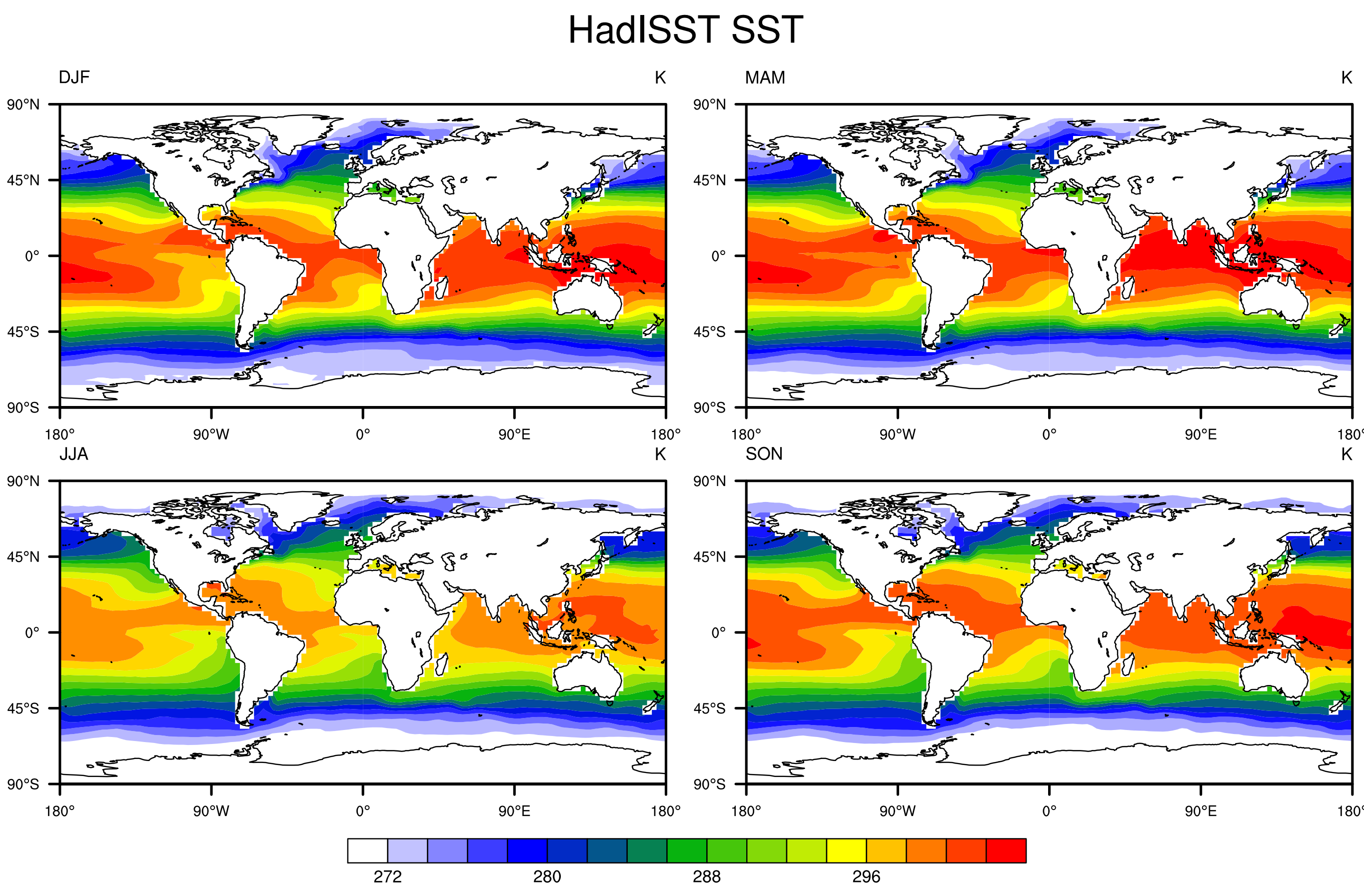

Figure S8: Mean sea surface temperatures (SSTs, in K) from HadISST averaged over years 2000 to 2009 in different seasons: December–January–February (DJF, upper left), March–April–May (MAM, upper right), June–July–August (JJA, lower left), September–October–November (SON, lower right).

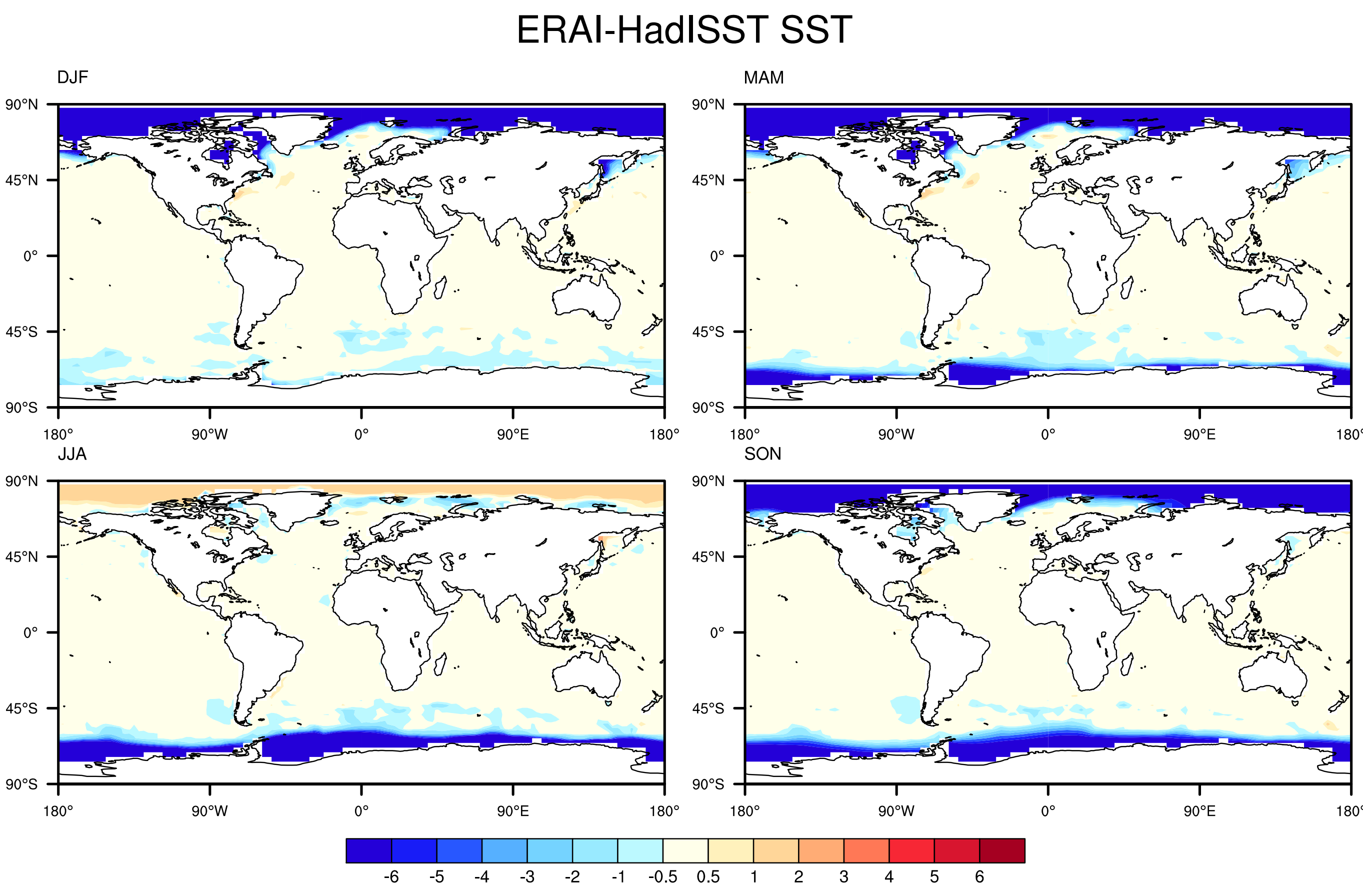

Figure S9: Difference (in K) in mean SSTs from ERAI minus HadISST averaged over years 2000 to 2009. Note the different definition of SSTs that causes the deviations at high latitude (HadISST: temperature of the sea below ice; ERAI: temperature of surface, i.e. on ice). The panels show the different seasons as in Figure S8.

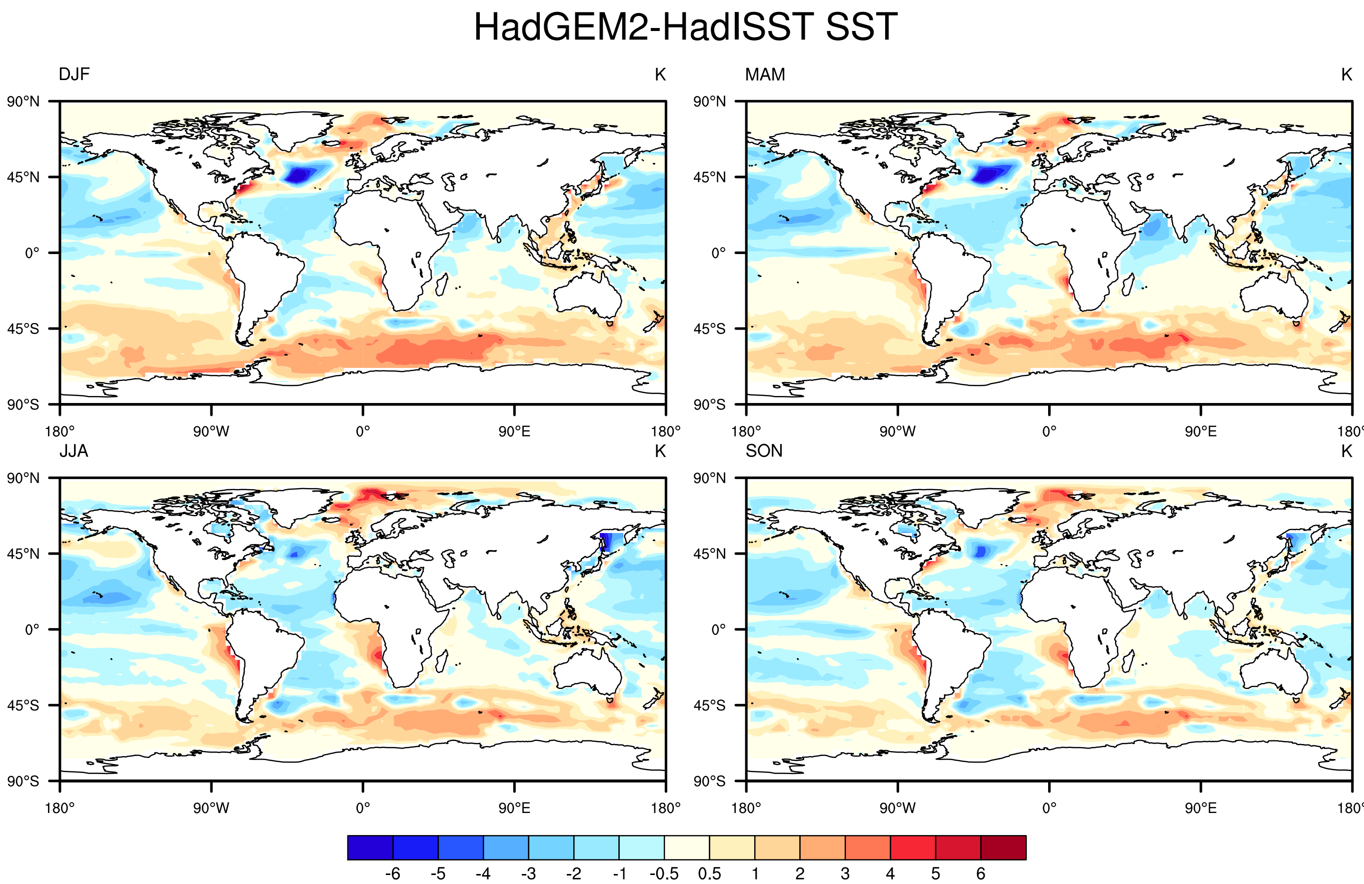

Figure S10: Difference (in K) in mean SSTs from HadGEM2 minus HadISST averaged over years 2000 to 2009. The panels show the different seasons as in Figure S8.

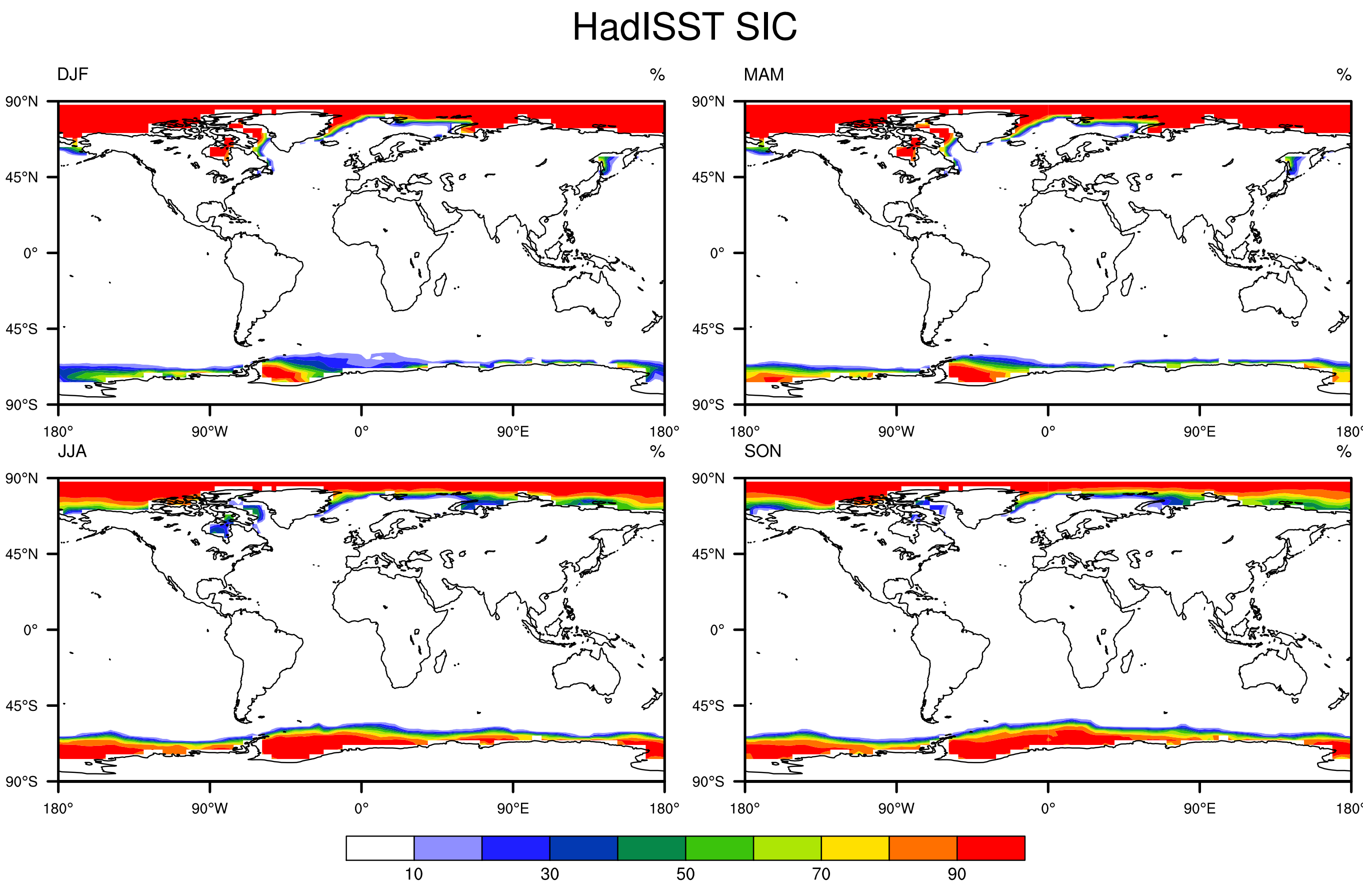

Figure S11: Mean sea ice concentration (SIC, in % of grid-box) from HadISST averaged over years 2000 to 2009. The panels show the different seasons as in Figure S8.

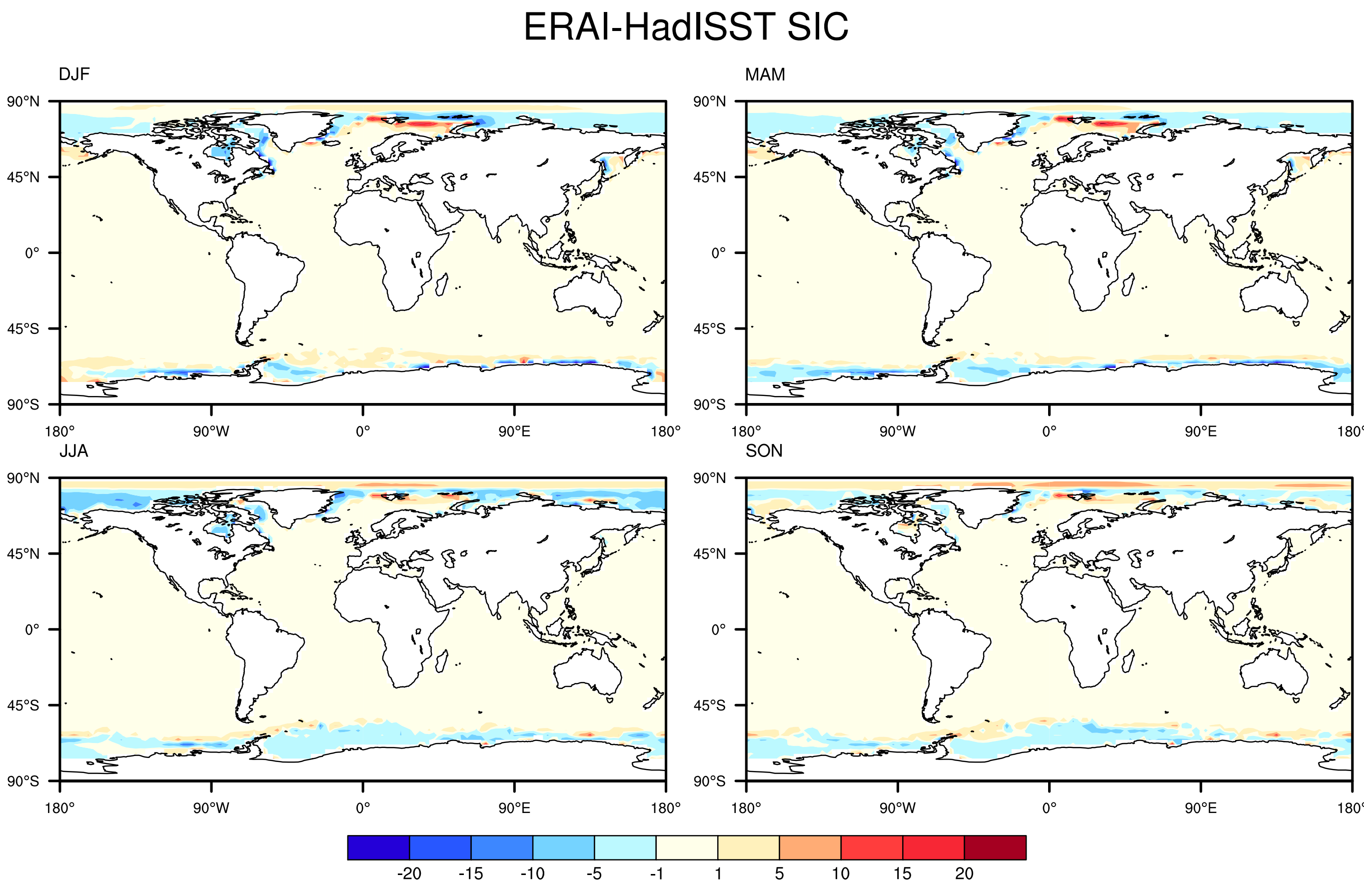

Figure S12: Absolute difference (in % of grid-box) in mean SIC from ERAI minus HadISST averaged over years 2000 to 2009. The panels show the different seasons as in Figure S8.

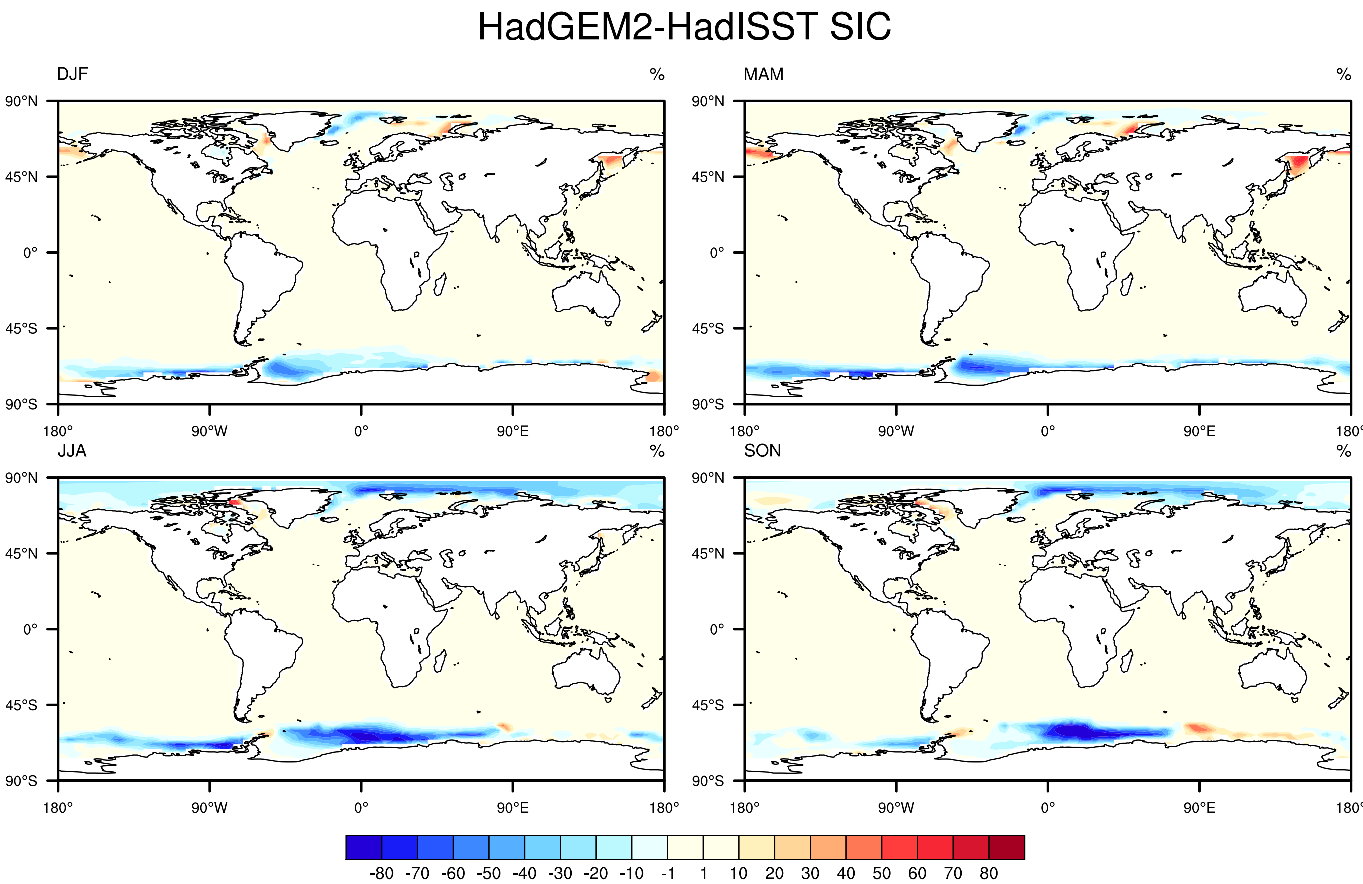

Figure S13: Absolute difference (in % of grid-box) in mean SIC from HadGEM2 minus HadISST averaged over years 2000 to 2009. The panels show the different seasons as in Figure S8.

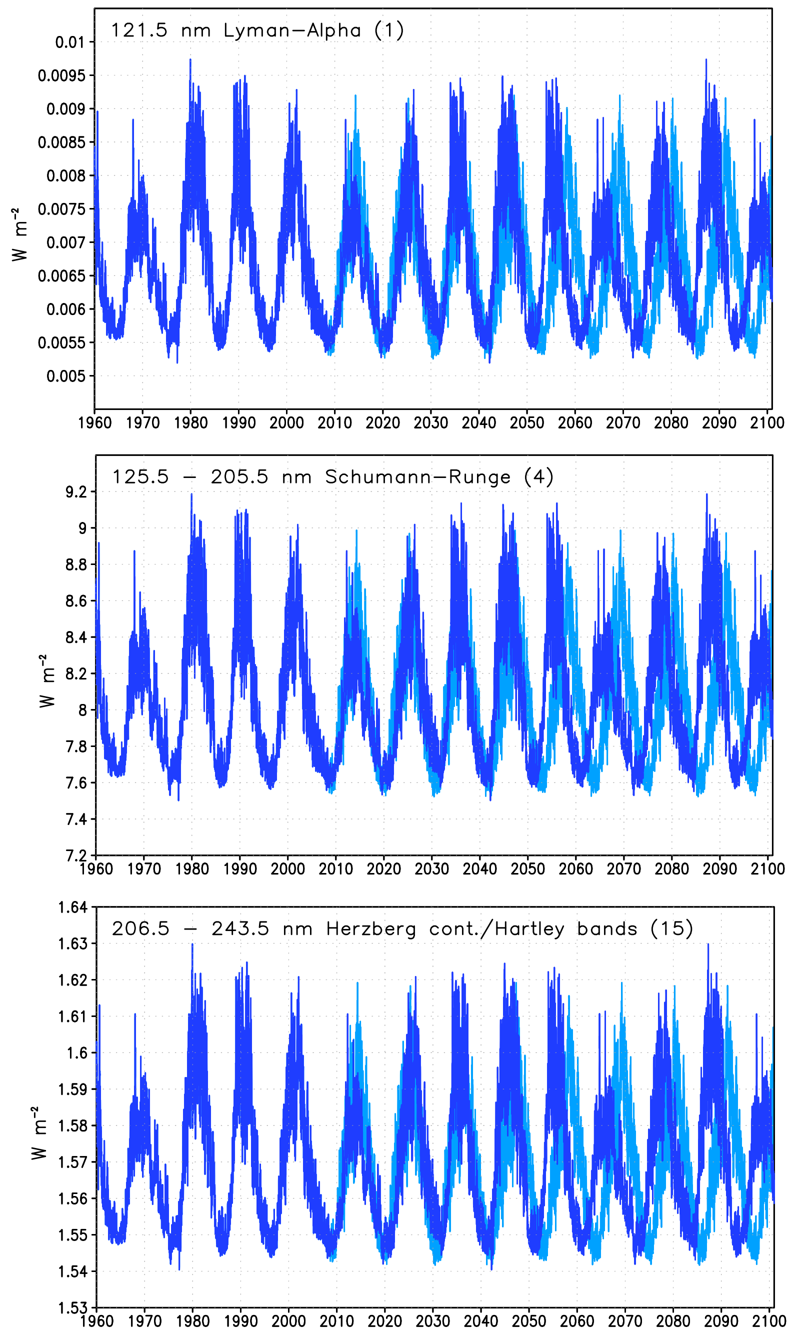

Figure S14: Time series of the daily spectral irradiances from the NRLSSI dataset (Lean et al., 2005) provided as input for FUBRAD at the Lyman-α line, the Schumann–Runge bands and continuum (4), and the Herzberg continuum / Hartley bands (15). The numbers in parentheses indicate the number of spectral intervals in the respective spectral region. The time series according to CCMI recommendations are displayed in dark blue (corresponding data file NRLSSI_FUB1.0_CCMI_X_spec055_19500101_21001231.txt), time series according to the CMIP5 realisation of HadGEM2-ES (Jones et al., 2011) are displayed in light blue (corresponding data file NRLSSI_FUB1.0_HadGEM_X_spec055_19500101_21001231.txt). The historical time series (NRLSSI_FUB1.0_hist_X_spec055_19500101_20111231.txt) used for the *RC1* simulations overlap between 1960 and 2008 with the shown data and are therefore not visualised separately. Note that only the light blue data has been used for consistency in all simulations. Corresponding files with solar data for the submodel JVAL are NRLSSI_FUB1.0_hist_X_solar1AU_19500101_20111231.txt (*RC1*) and NRLSSI_FUB1.0_HadGEM_X_solar1AU_19500101_21001231.txt (*RC2*), respectively.

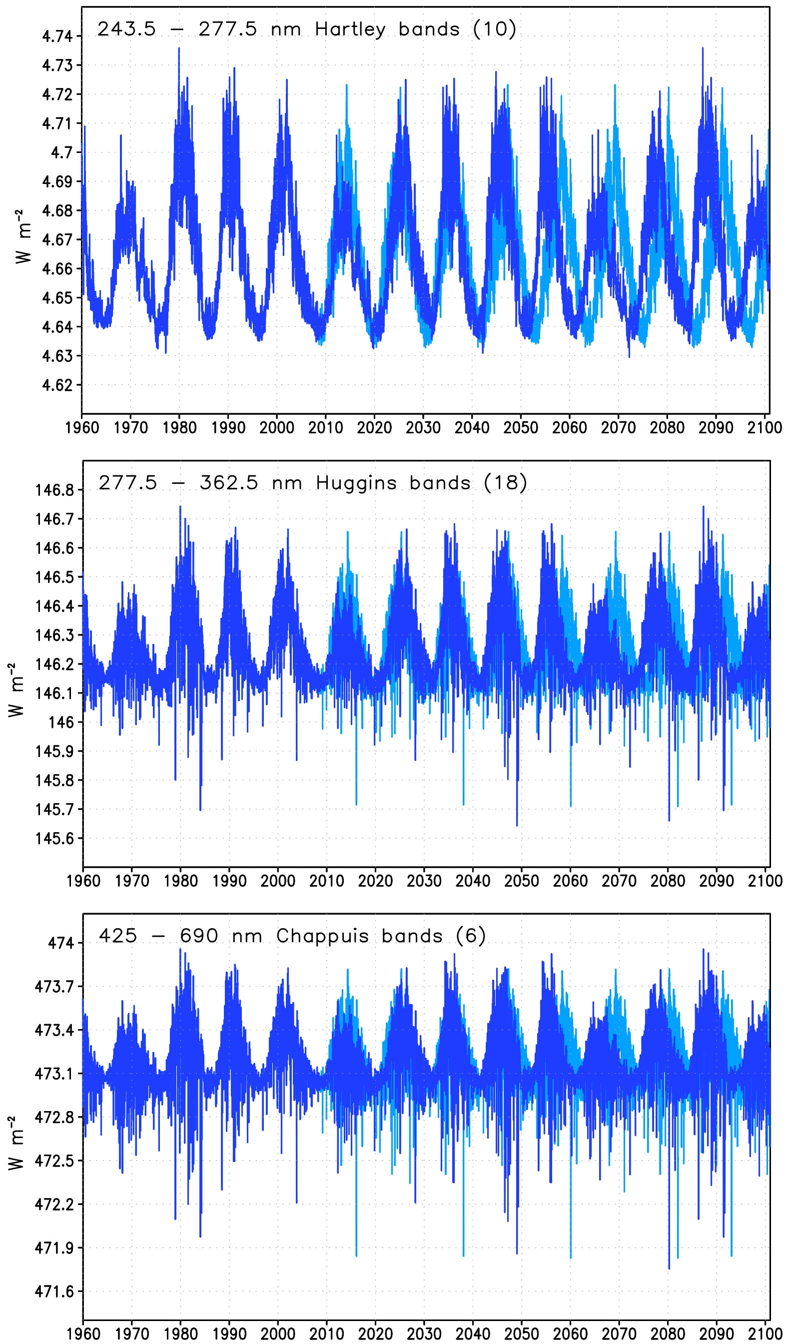

Figure S15: As Figure S14, but for the Hartley bands (10), the Huggins bands (18), and the Chappuis bands (6).

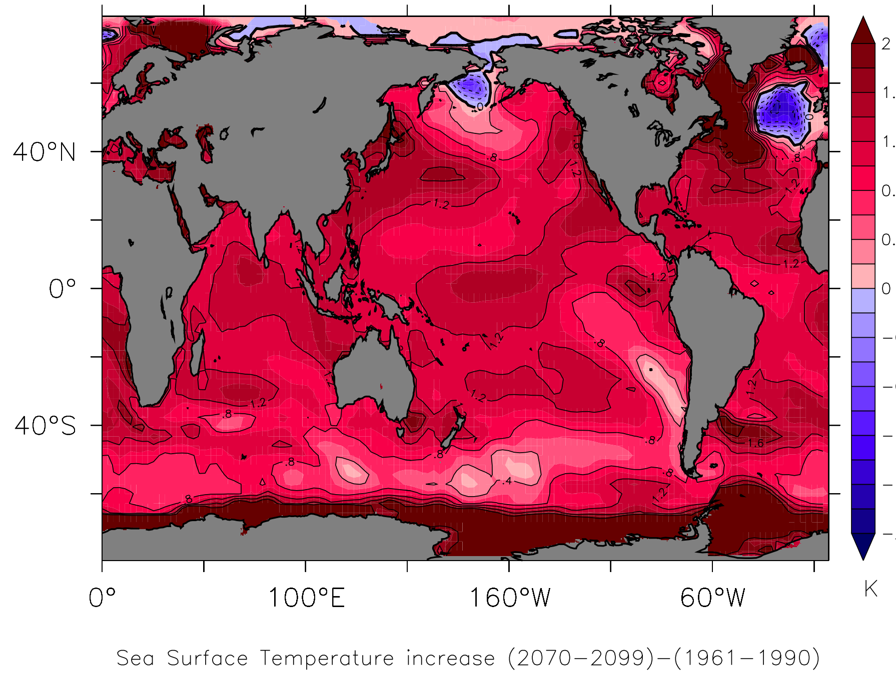

Figure S16: Change of sea surface temperature (SST, in K) between 2070–2099 and 1961–1990 (averages) of the *RC2-oce-01* simulation.

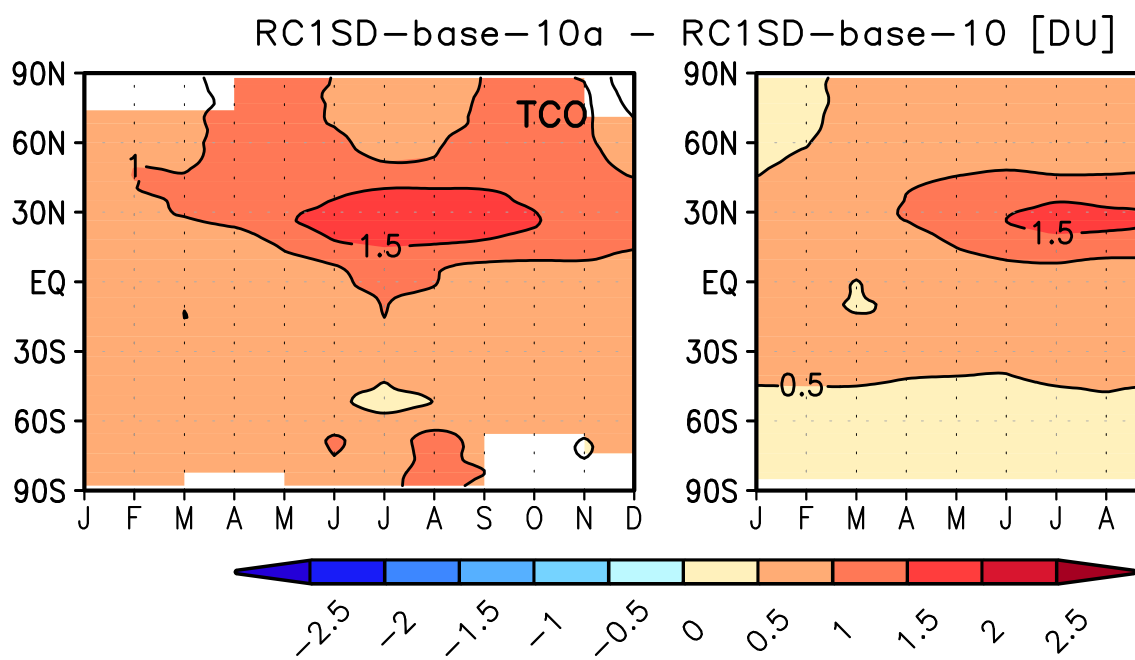

Figure S17: Sensitivity of zonally averaged, monthly total column ozone (TCO, left) and zonally averaged, monthly tropospheric partial column ozone (TPCO, right) to wrong road traffic emissions and wrong stratospheric aerosol optical properties. Shown are the multi-annual (2000 – 2013) differences in DU between *RC1-base-10a* minus *RC1-base-10*. Statistical significance is tested with the paired t-test. Statistically significant changes on the 95% confidence level are coloured.

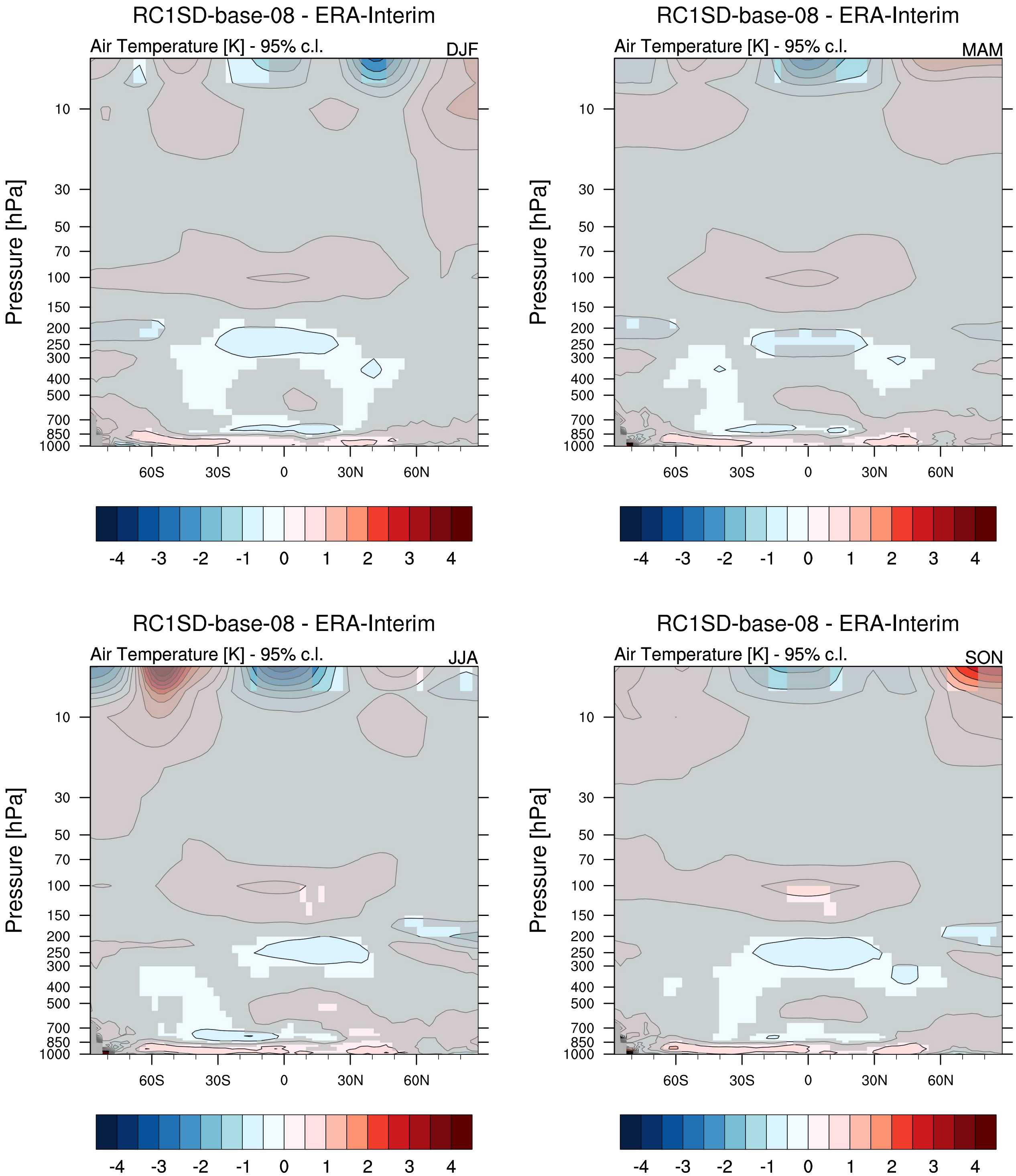

Figure S18: Seasonal temperature differences (in K) of the ESCiMo simulations compared to ERA-Interim data (2000 – 2010). Differences, unless grey shaded, are significant on a 95% confidence level according to a two-sided Welch's test. The number of degrees of freedom are calculated according to the Welch-Satterthwaite equation.

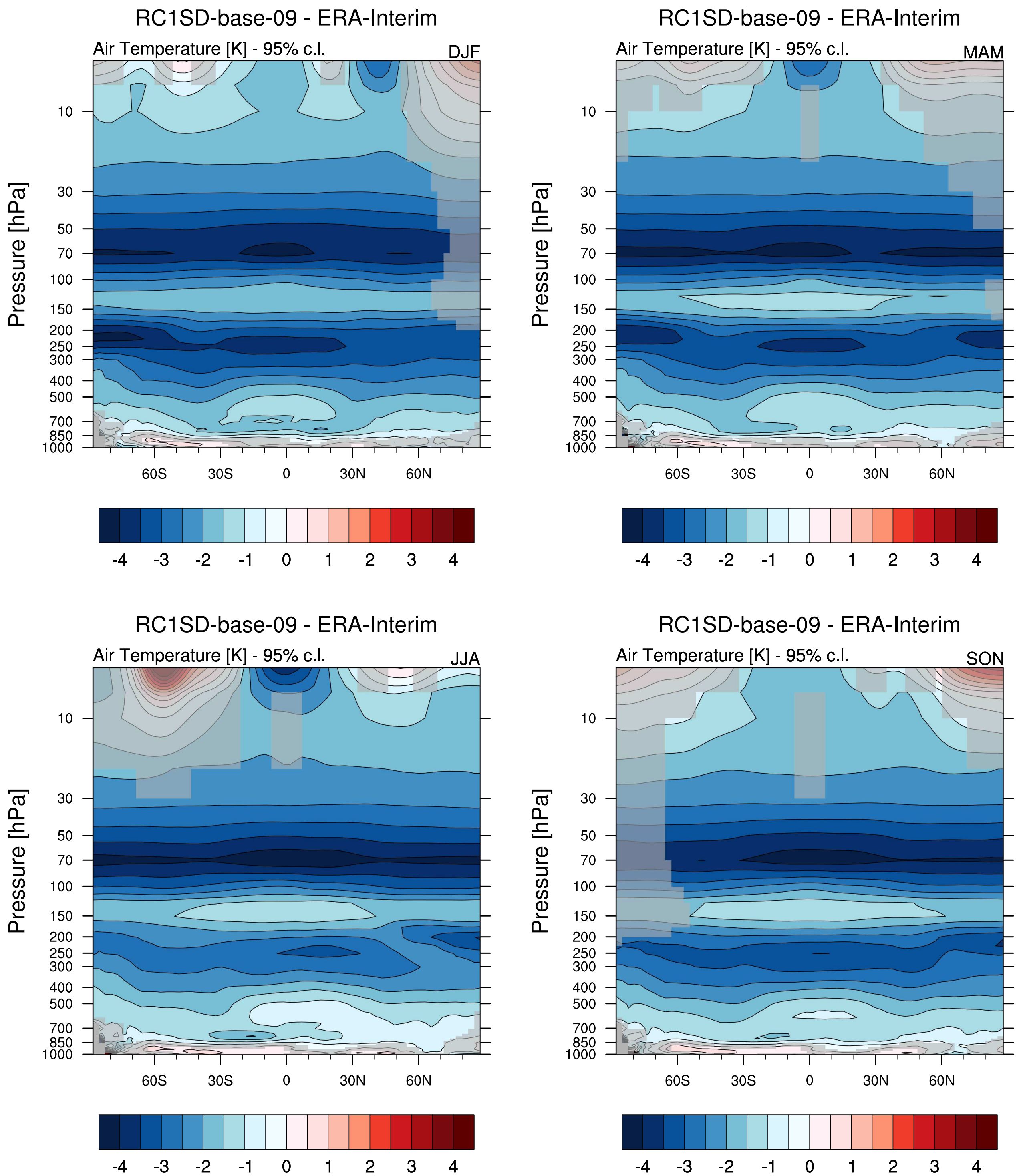

Figure S18: continued

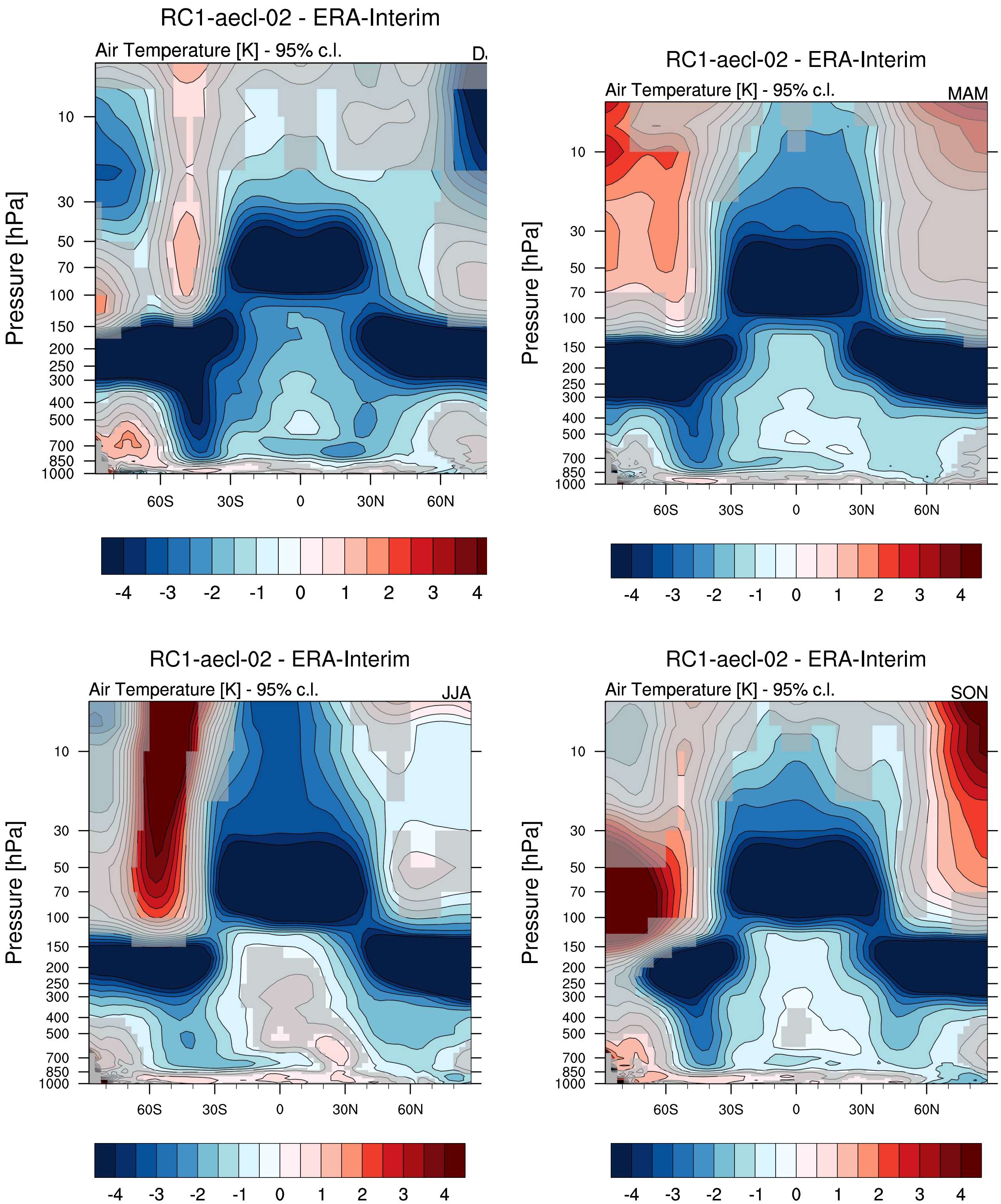

Figure S18: continued

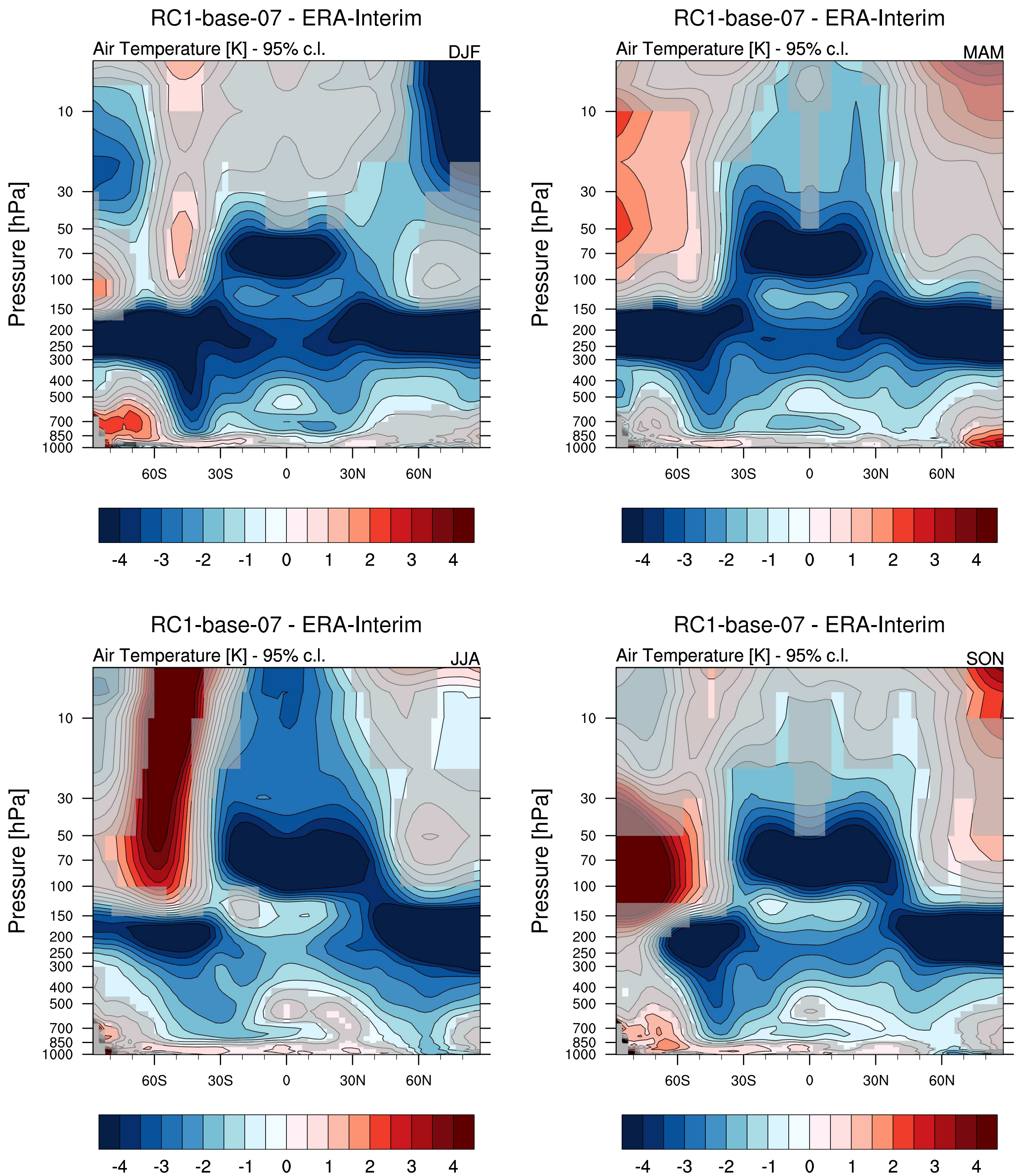

Figure S18: continued

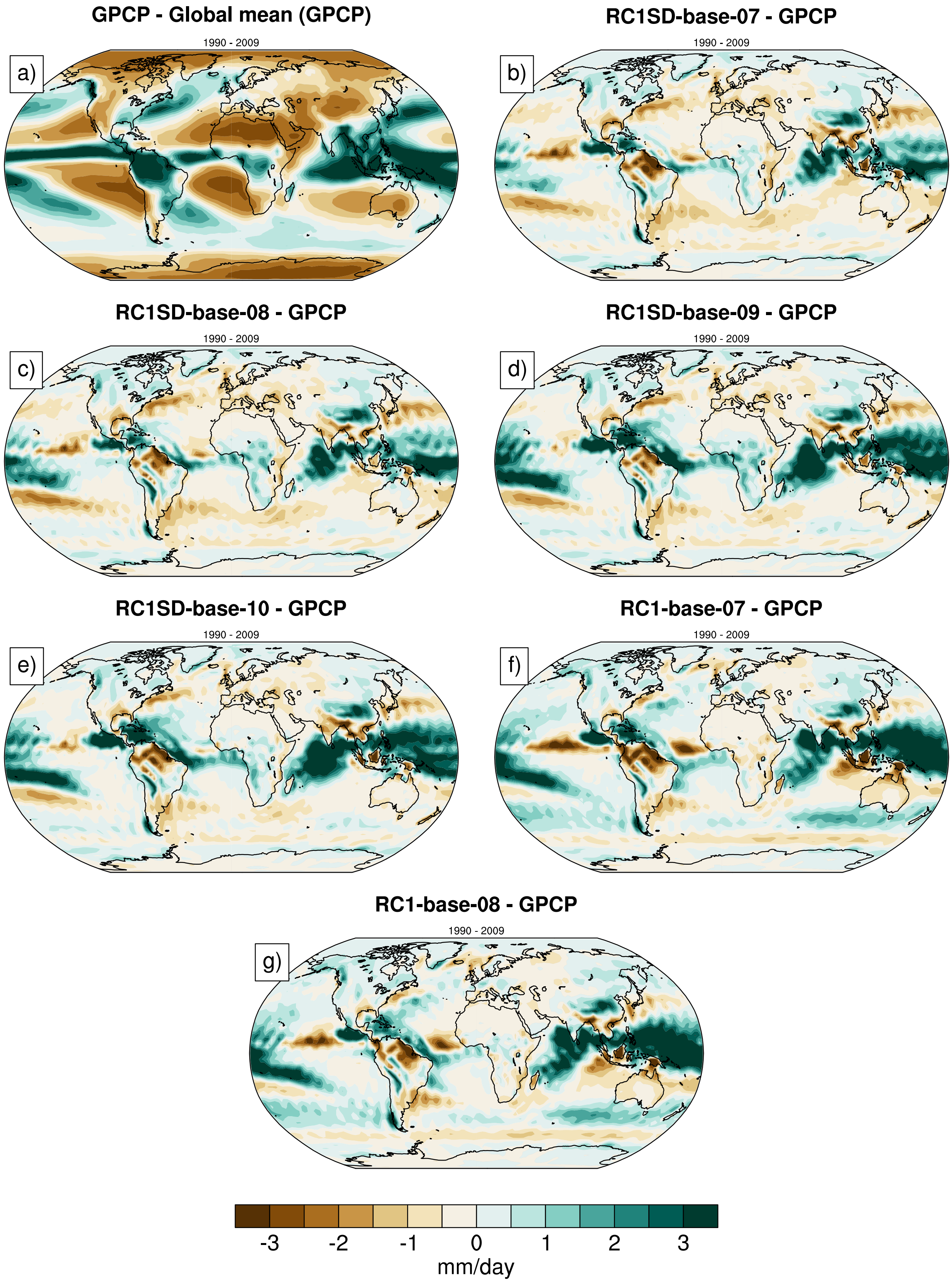

Figure S19: Mean precipitation error (mm/day) for the 20-year period 1990-2009. The differences show the simulation results minus GPCP. Panel a) shows the GPCP data minus the global average (2.68 mm/day).

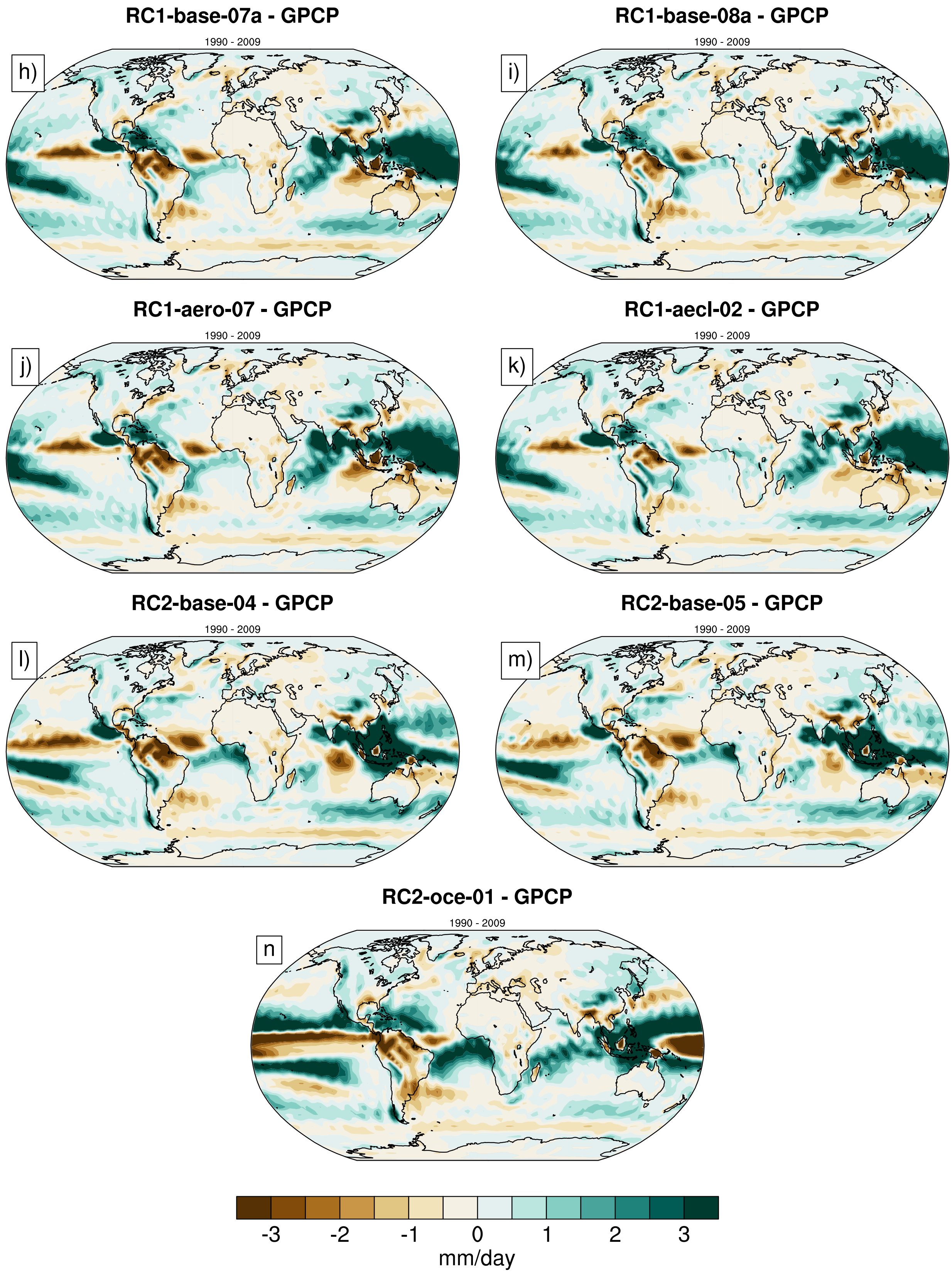

Figure S20: Mean precipitation error (mm/day) for the 20-year period 1990-2009. The differences show the simulation results minus GPCP.

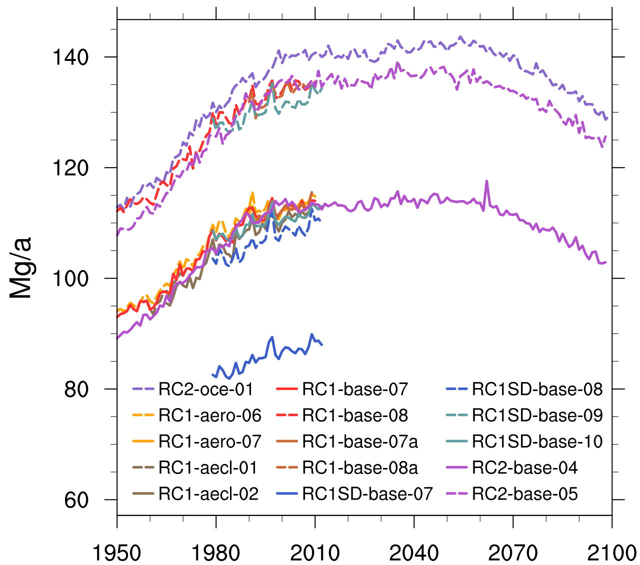

Figure S21: Globally integrated annual ozone wet deposition flux in $\mathrm{Mg\,a^{-1}}$.

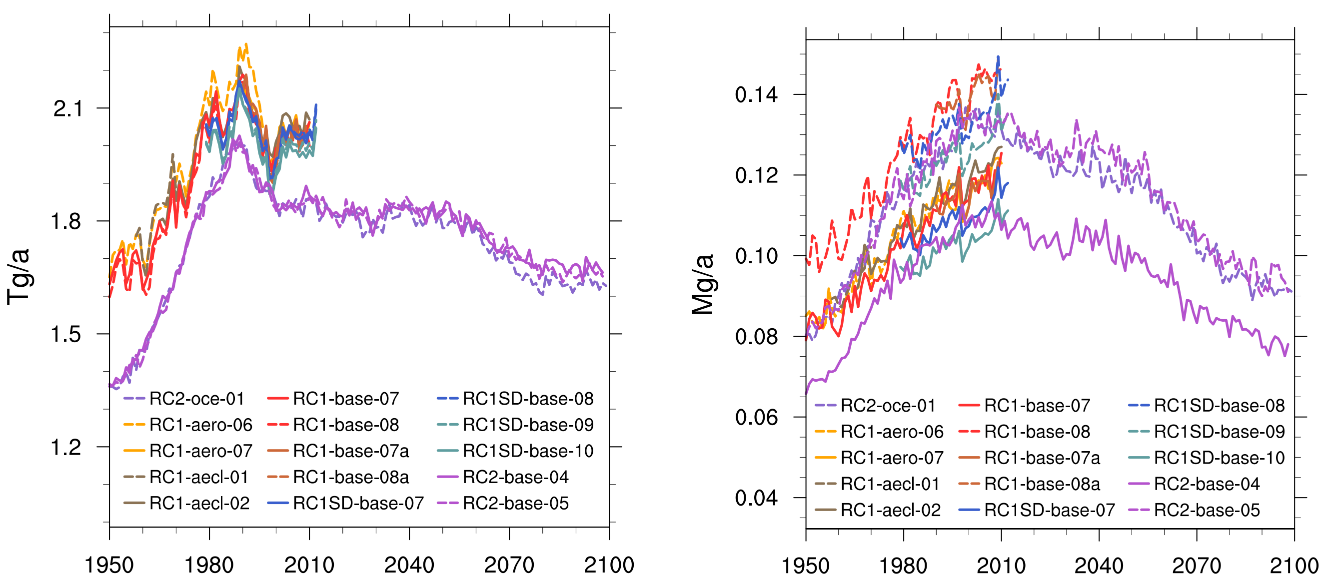

Figure S22: Globally integrated annual NOx (NO + NO_2) dry (left) and wet (right) deposition fluxes in $\mathrm{Tg(N)\,a^{-1}}$ and $\mathrm{Mg(N)\,a^{-1}}$, respectively.

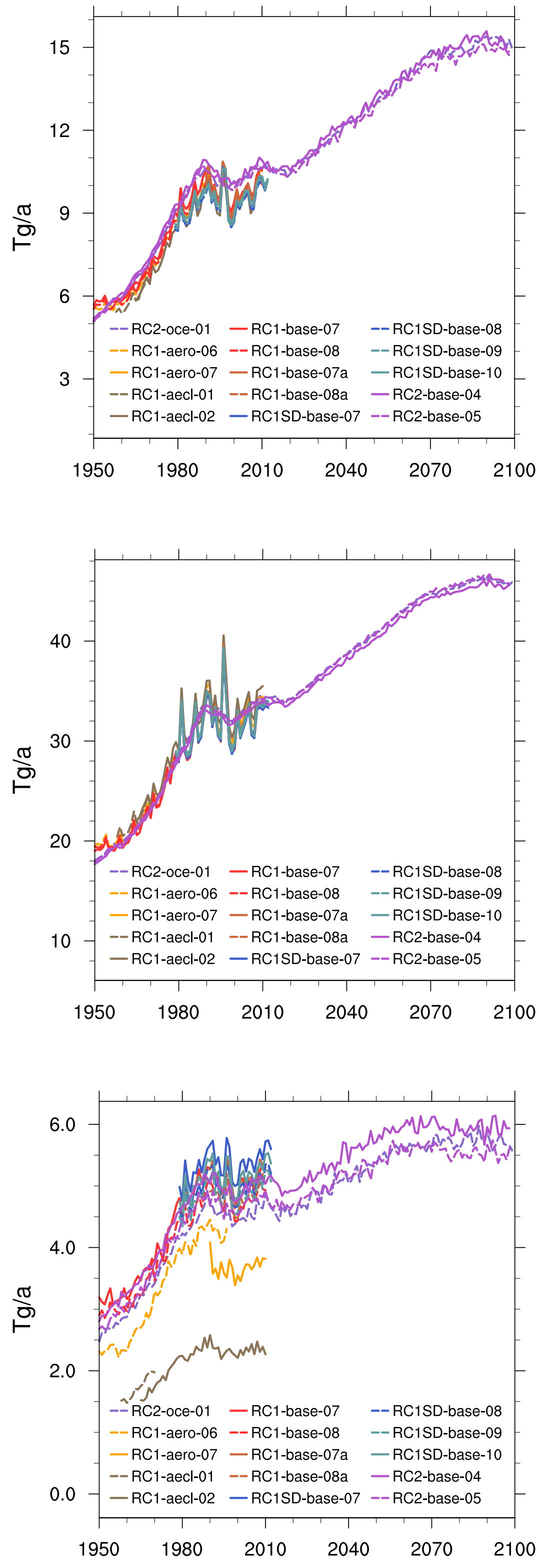

Figure S23: Globally integrated annual ammonium (NH_4^+ + NH_3) dry deposition (upper), wet deposition (middle) and sedimentation (lower) fluxes in $\mathrm{Tg(N)\,a^{-1}}$.

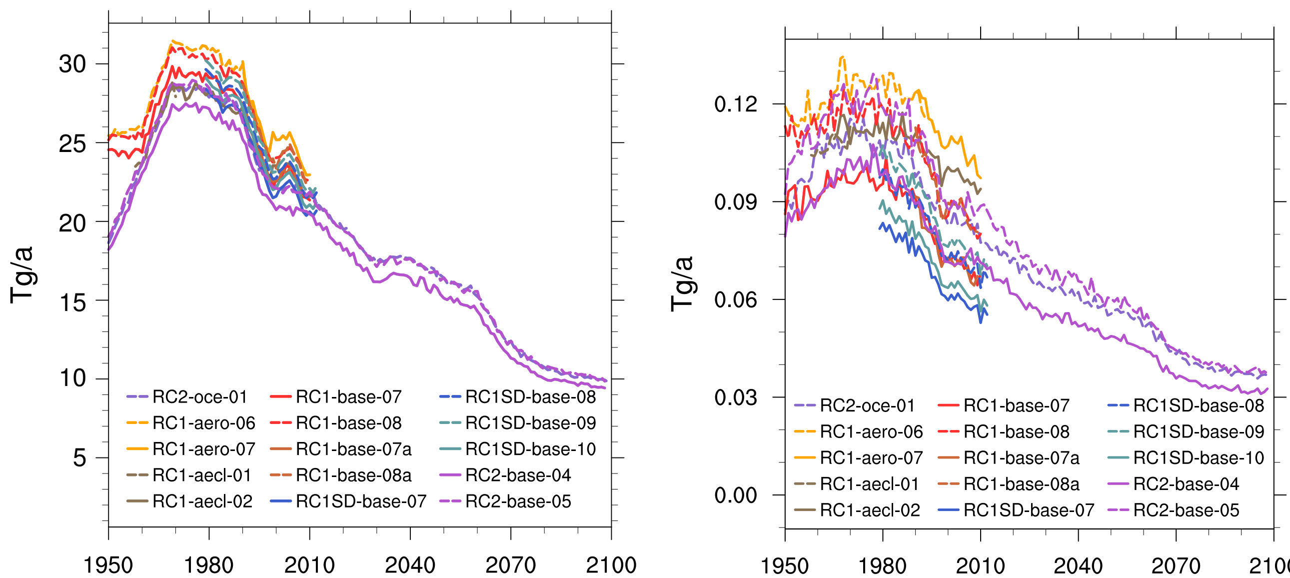

Figure S24: Globally integrated annual sulphite (SO_2 + HSO_3^- + SO_3^{2-}) dry deposition (left) and wet deposition (right) fluxes in $\mathrm{Tg(S)\,a^{-1}}$.

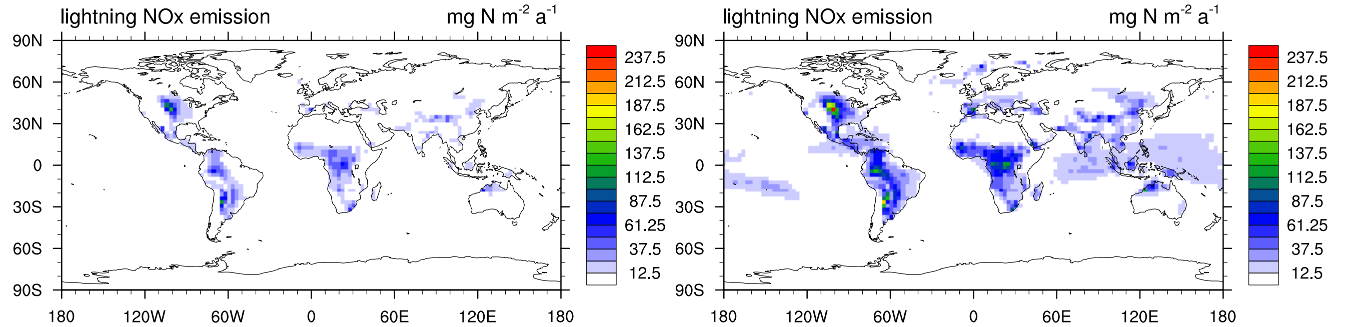

Figure S25: Vertically integrated annual total lightning NOx emissions (in ng(N) m^{-2} a^{-1}) averaged over the years 2000 – 2010 as simulated in *RC1SD-base-07* (left) and *RC1SD-base-10* (right).

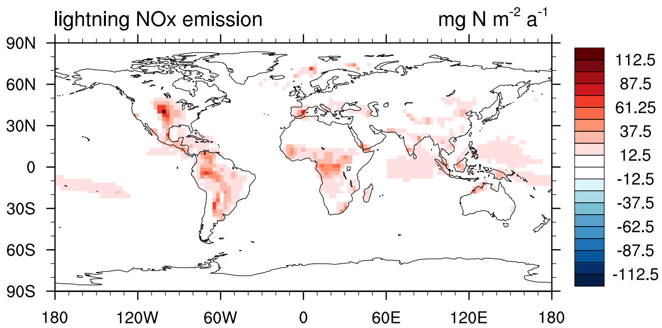

Figure S26: Absolute difference (in ng(N) m^{-2} a^{-1}) between lightning NOx emissions of *RC1SD-base-10* minus *RC1SD-base-07*.

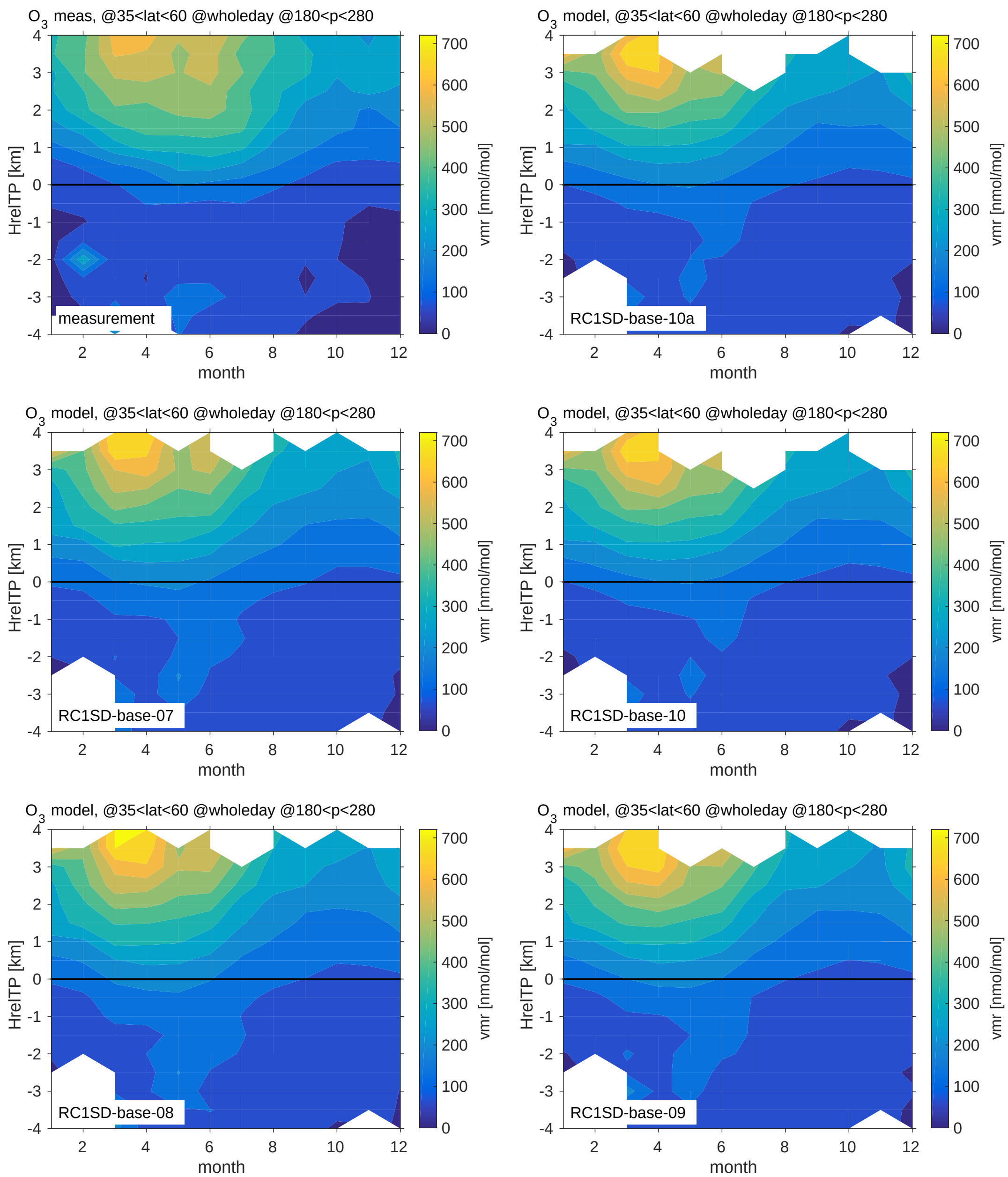

Figure S27: Annual O_3 climatologies derived from CARIBIC observations (upper left) and from nudged model simulations. Vertical coordinate is the distance to the tropopause (here 2 PVU iso-surface).

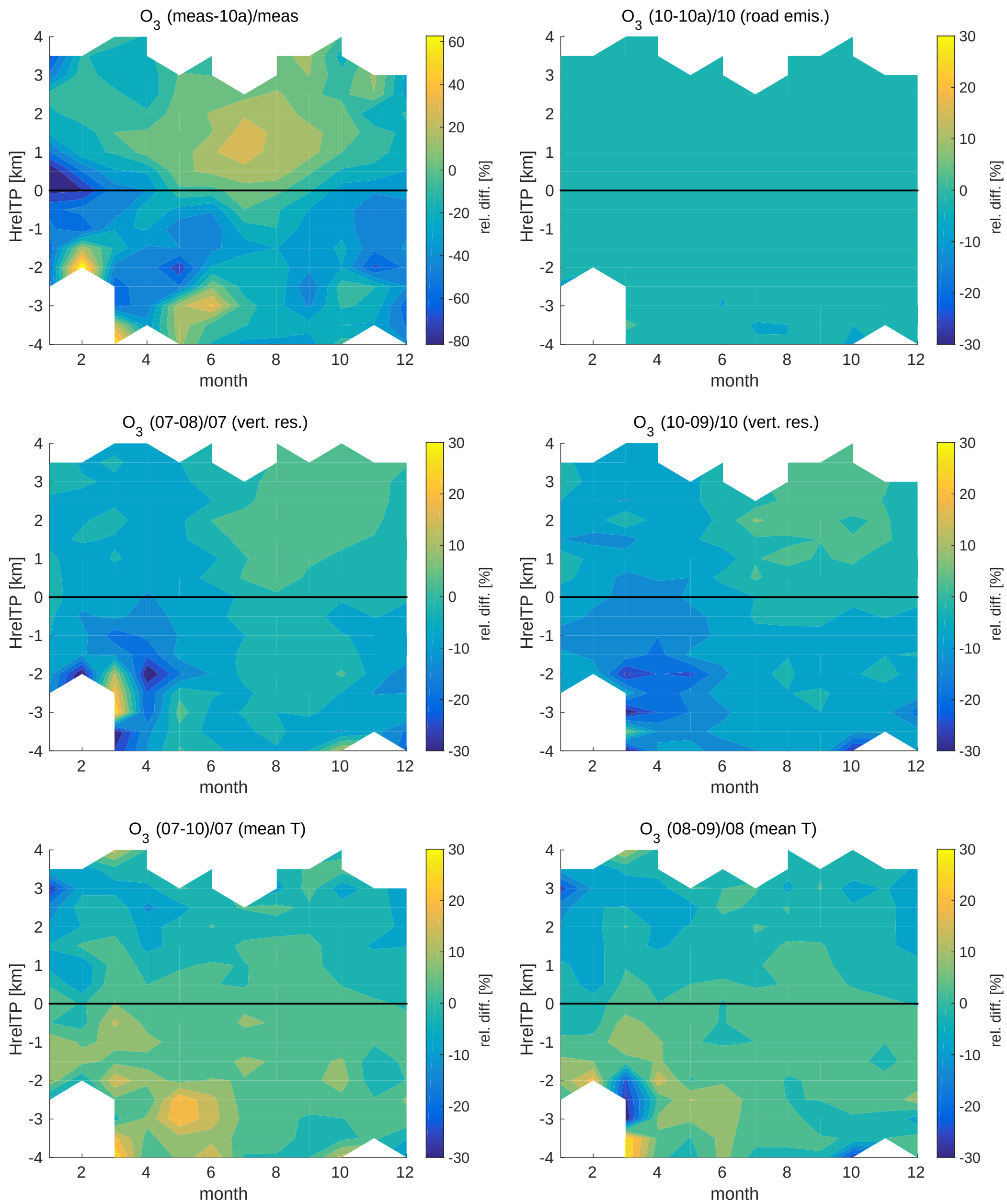

Figure S28: Relative differences between annual O_3 climatologies.

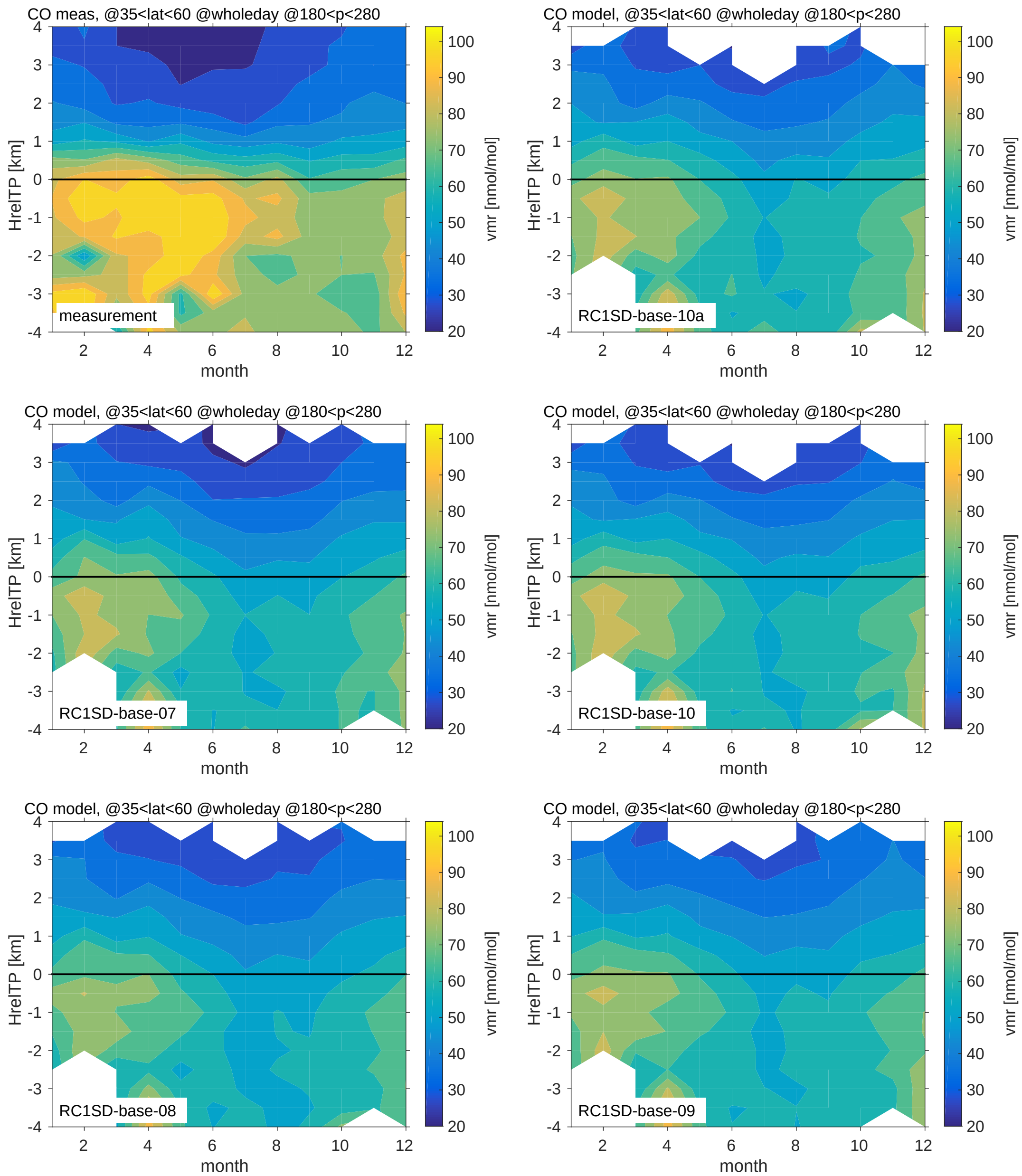

Figure S29: As Figure S27, but for CO.

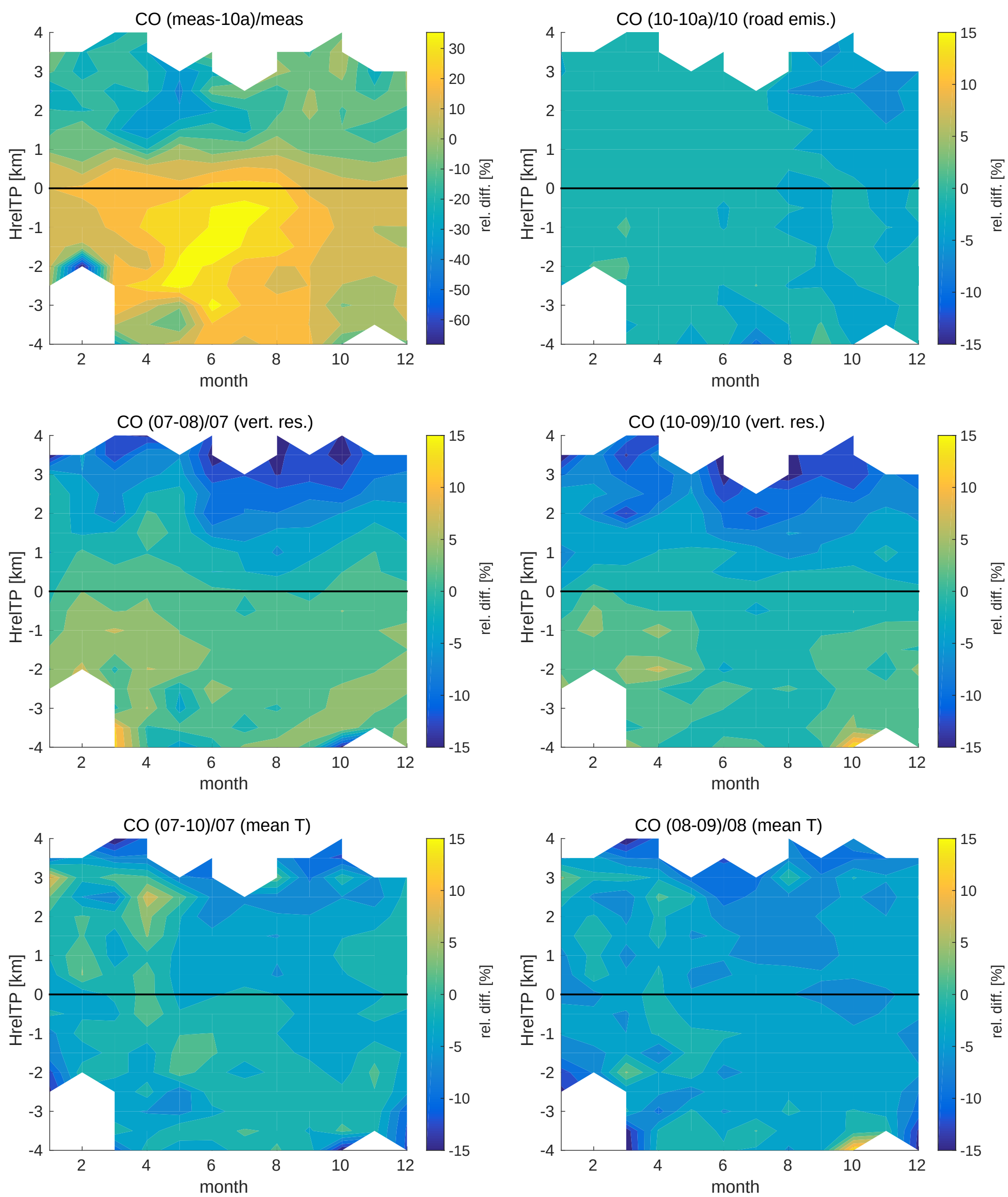

Figure S30: As Figure S28, but for CO.

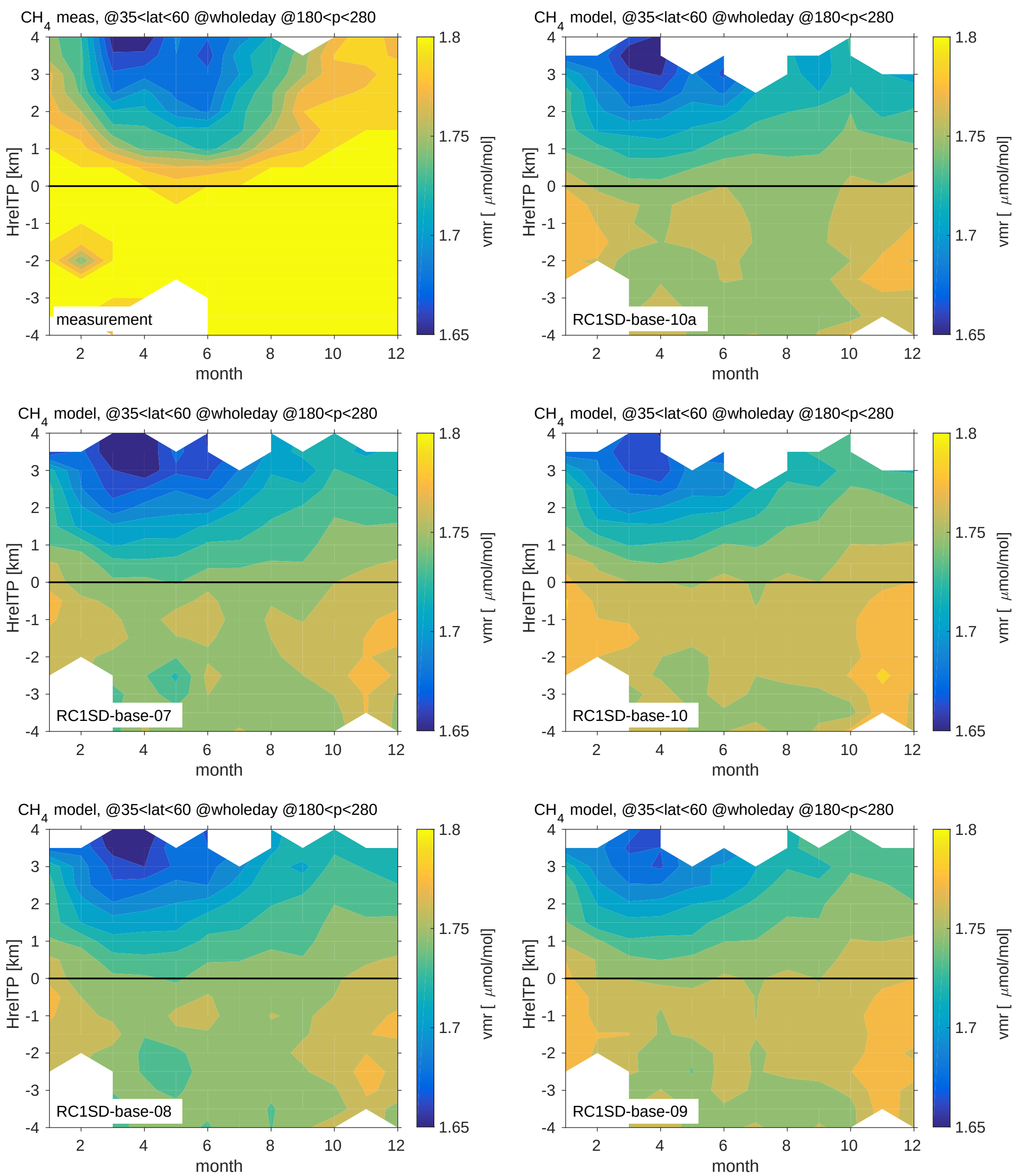

Figure S31: As Figure S27, but for CH_4.

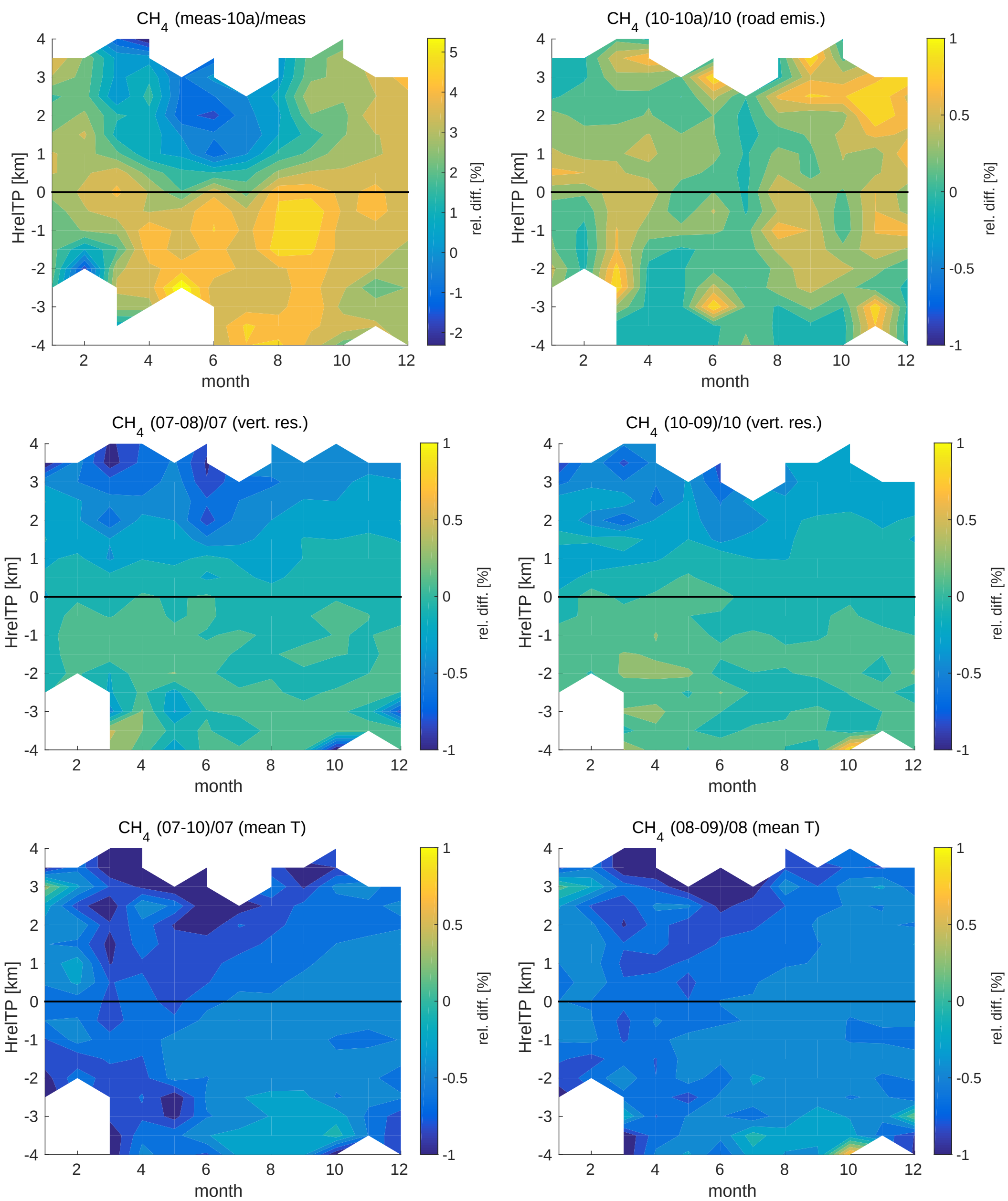

Figure S32: As Figure S28, but for CH_4.

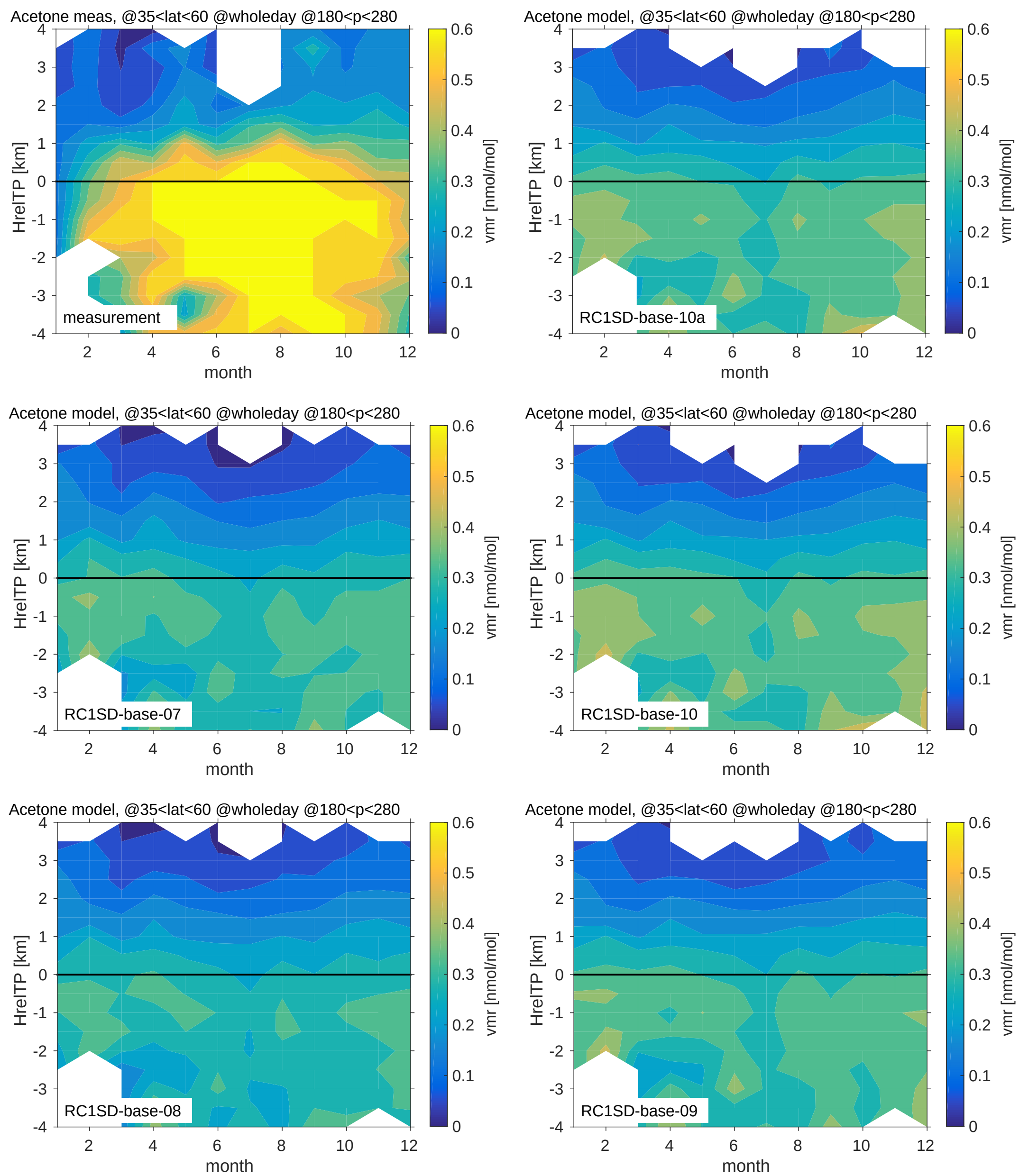

Figure S33: As Figure S27, but for acetone.

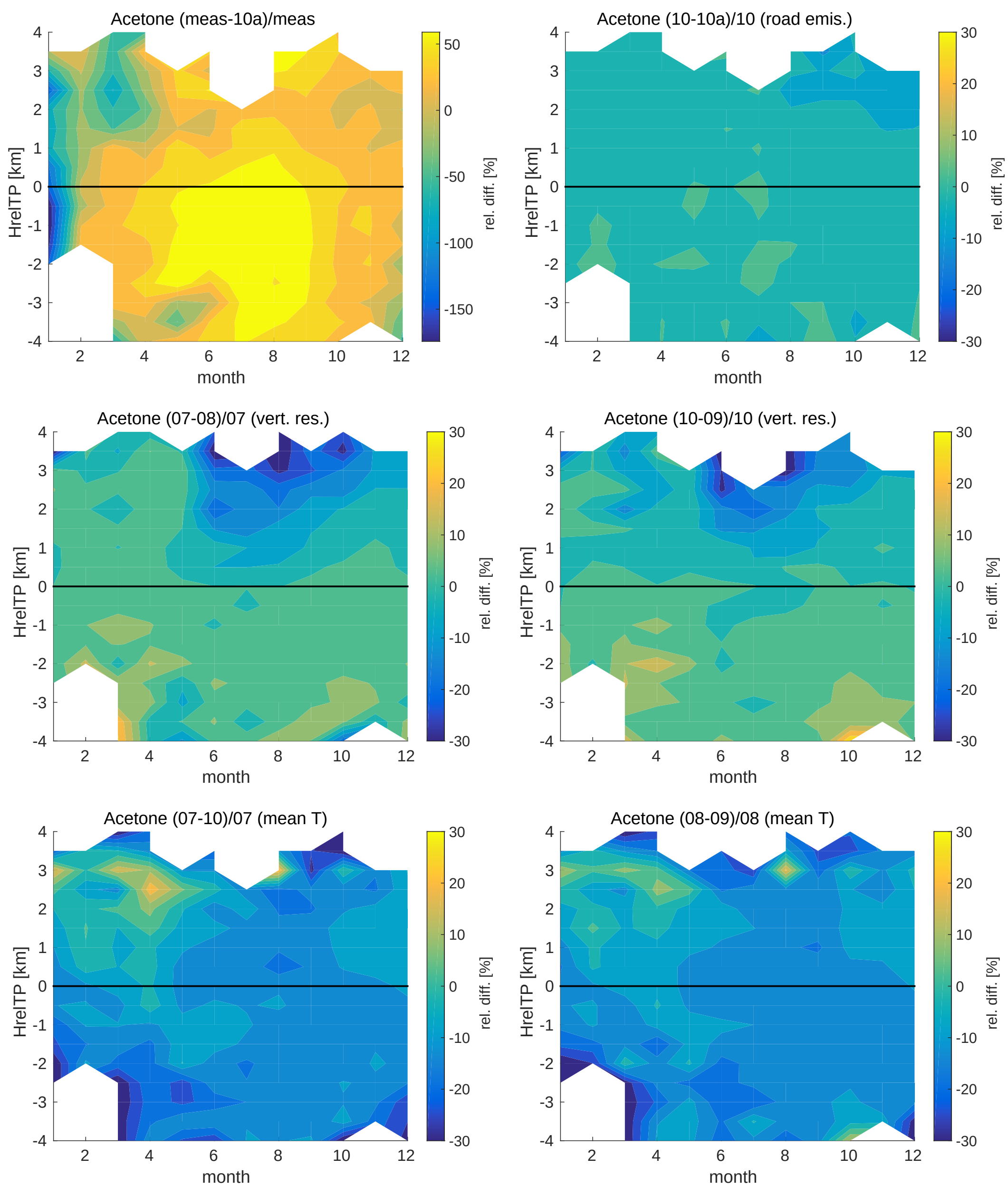

Figure S34: As Figure S28, but for acetone.

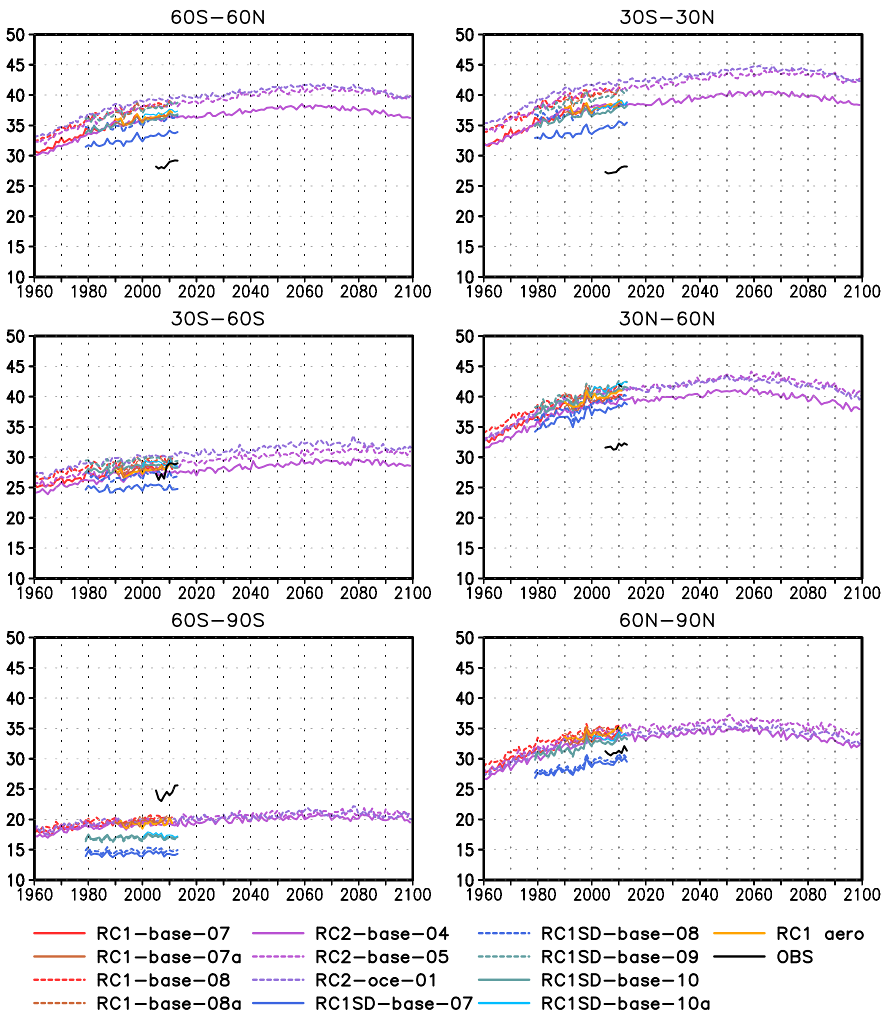

Figure S35: Time series of annual mean tropospheric partial column ozone averaged over different latitude bands. AURA MLS/OMI observations are shown in black.

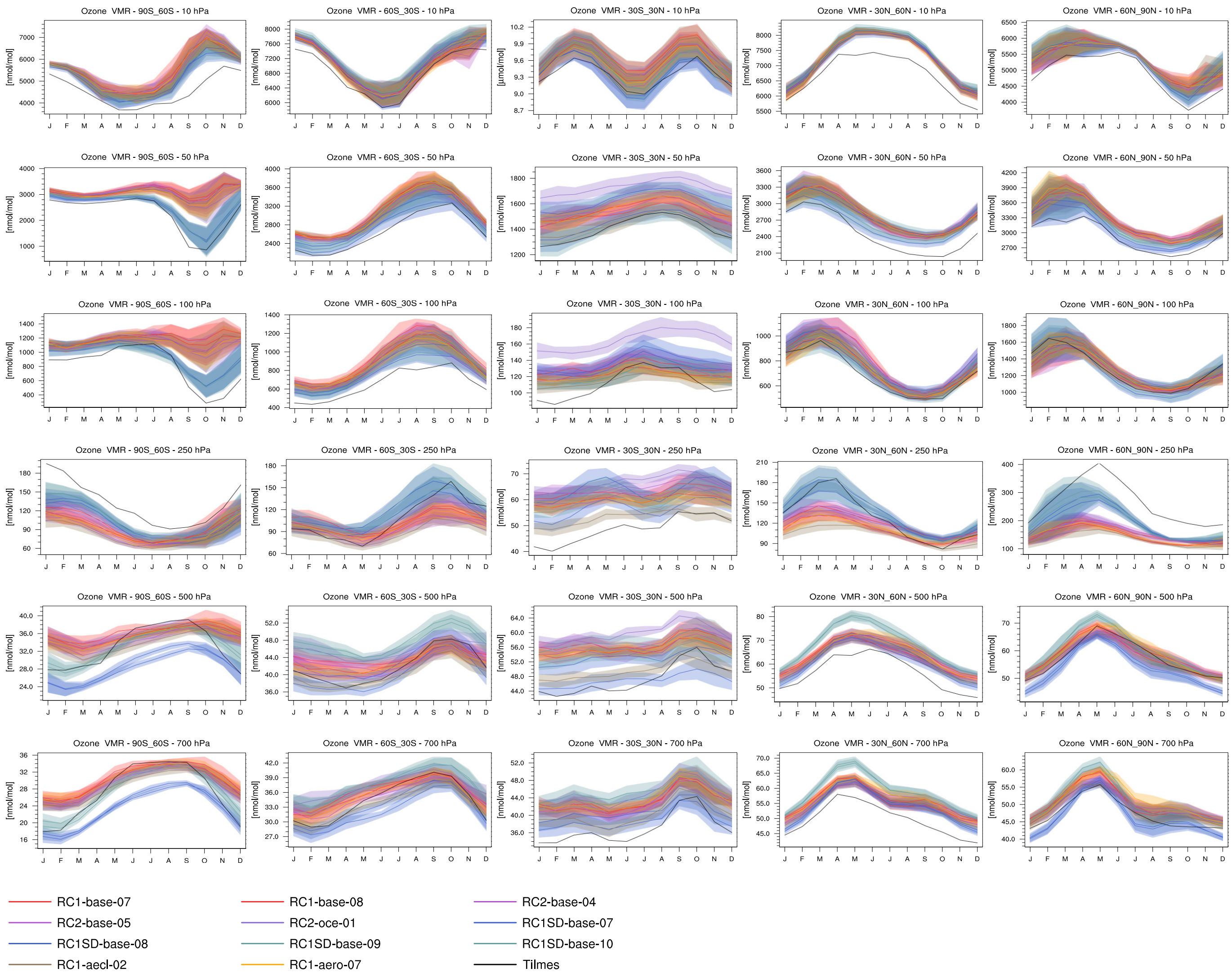

Figure S36: Annual cycle of the ozone climatology in five latitude bands, and at six pressure levels (10, 50, 100, 250, 500 and 700 hPa). Simulation data are first sampled at the ozone-sonde locations. Reference and simulation data are then sorted into three latitude bands and averaged. The shaded areas indicate the $\pm 1\sigma$ inter-annual variability (1995 to 2011, for EMAC only).

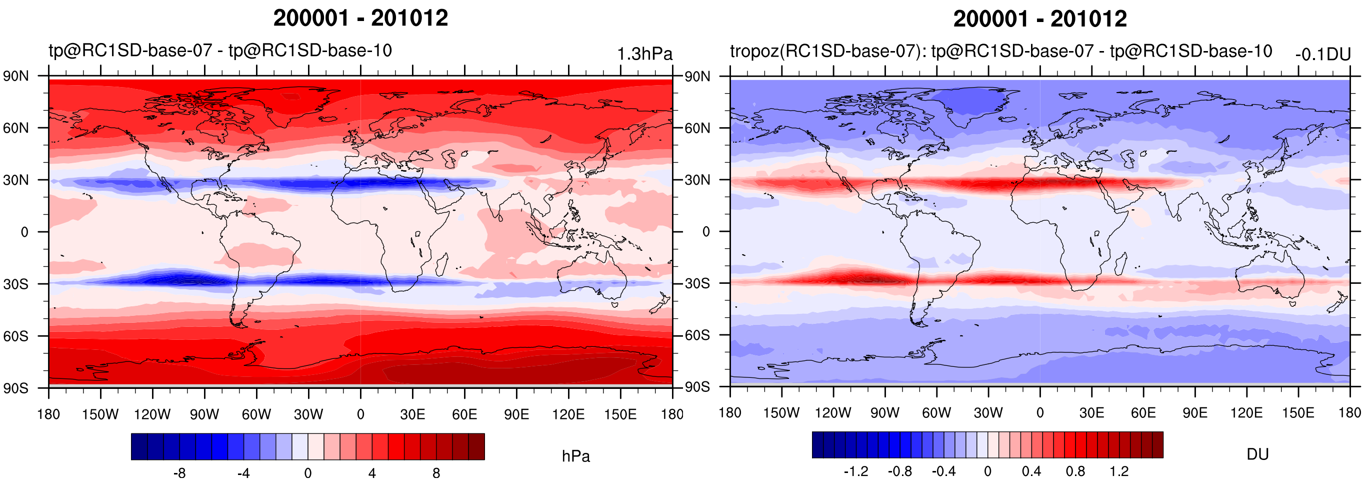

Figure S37: Effect of global mean temperature nudging on tropopause height (in hPa, left) and tropospheric partial ozone column (in DU, right). Shown is the average for the period covering the years 2000 to 2010 as difference between *RC1SD-base-07* (with) minus *RC1SD-base-10* (without mean temperature nudging). The on-line calculated tropopause of submodel TROPOP is considered here (see also Figure S38). In the upper right corner of each panel the respective global average values are shown.

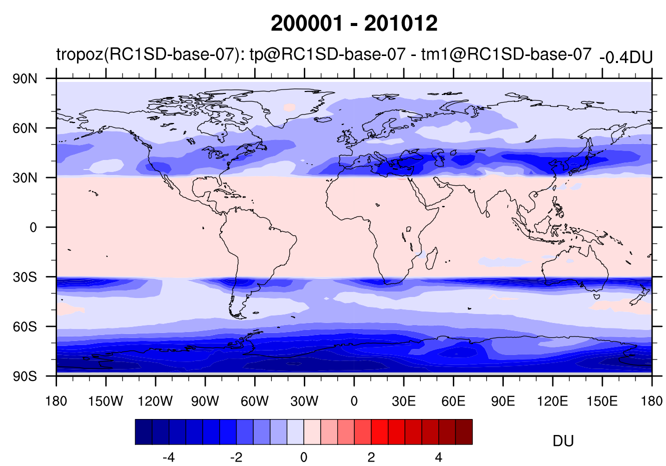

Figure S38: Effect of tropopause definition on analysed tropospheric partial ozone column (TPCO, in DU). Shown is, exemplarily for simulation *RC1SD-base-07*, the (11 year average) difference of the TPCO calculated with the on-line calculated tropopause of submodel TROPOP minus the TPCO calculated with the WMO tropopause at all latitudes. TROPOP defines the tropopause according to the WMO equatorward of 30° latitude (therefore the negligible difference there), and as iso-surface of 3.5 PVU potential vorticity poleward of 30° latitude.

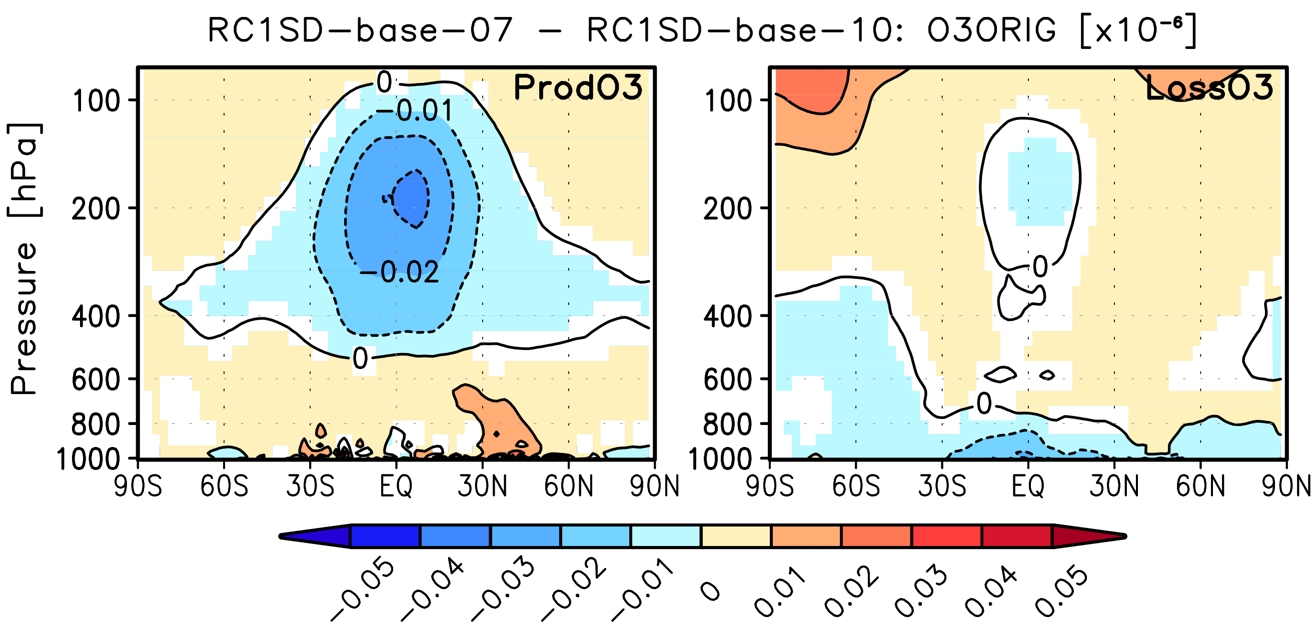

Figure S39: Difference in ozone production (left) and ozone loss (right) between *RC1SD-base-07* and *RC1SD-base-10*, i.e., resulting from the additional mean temperature nudging. Shown is the multi-annual average (1979 - 2013) in 10^{-6} mol/mol/month. Statistically significant changes (according to the paired-t-test) on the 95% confidence level are coloured.

```
&CTRL_FAMILY
...
TF(7) = 'gp',2,F,'Bry','', 'BrNO2','BrCl','Br2:2.0','BrNO3','HOBr','HBr','BrO','Br',
TF(8) = 'gp',2,F,'Cly','','OClO','ClNO2','Cl2:2.0','BrCl','HOCl','ClNO3','ClO','HCl','Cl','Clmres_cs',
...
/
```

Figure S40: Definition of type-2 tracer families for halogen budgeting in CTRL_FAMILY namelist of submodel TRACER.

```
&CPL
...
! provide channel objects (<tracer>_scte) with copies of scavenging tendencies
 te_string = 'HCl;HBr;Br2;HOBr;BrCl;Cl2;HOCl;'
...
/
```

Figure S41: Definition of loss rates (tendencies) in CPL namelist of submodel SCAV for the budgeting of halogen compounds.

```
&CPL
! ### SYNTAX:
! # CALC(.) = 'object-name', 'list-of-channel-objects', \
! #           'operation',
! # list of channel objects = 'ch1:obj1%s1,obj2%s2,...;\
! #                            cha2:obj1%s1,...;'
! # s1, s1, ... optional scaling factors
! # operation = SUM
!
CALC(1) = 'LossBr', 'scav_gp:HBr_scte,Br2_scte%2.0,HOBr_scte,BrCl_scte', 'SUM',
CALC(2) = 'LossCl', 'scav_gp:HCl_scte,Cl2_scte%2.0,HOCl_scte,BrCl_scte', 'SUM',
!
/
```

Figure S42: Summation of loss rates (tendencies from submodel SCAV, see Figure S41) for budgeting of halogen compounds as defined in the CPL namelist of submodel SCALC.

```
&CPL
! ### SYNTAX:
! dtrac(.) = \
!   'new tracer','subname',molar mass, \ ! new diagnostic tracer [A]
!   'tracer','subname',                \ ! total abundance [B]
!   'tracer','subname',                \ ! production (diagtrac.tex) [C]
!   'channel','object',                  ! loss rate [D]
!
! ### Notes:
!    - internally, tendency of [C] is used
!    - [D] must be in [mol/mol/s]
!
dtrac(1) = 'BrL', '', 79.90, 'Bry', '', 'ProdLBr', '', 'scalc', 'LossBr',
dtrac(2) = 'BrS', '', 79.90, 'Bry', '', 'ProdSBr', '', 'scalc', 'LossBr',
dtrac(3) = 'ClL', '', 34.45, 'Cly', '', 'ProdLCl', '', 'scalc', 'LossCl',
dtrac(4) = 'ClS', '', 34.45, 'Cly', '', 'ProdSCl', '', 'scalc', 'LossCl',
!
/
```

Figure S43: Definition of budgeting tracers for short (S) and long (L) lived halogen species (Br, Cl), as defined in the CPL namelist of TBUDGET.

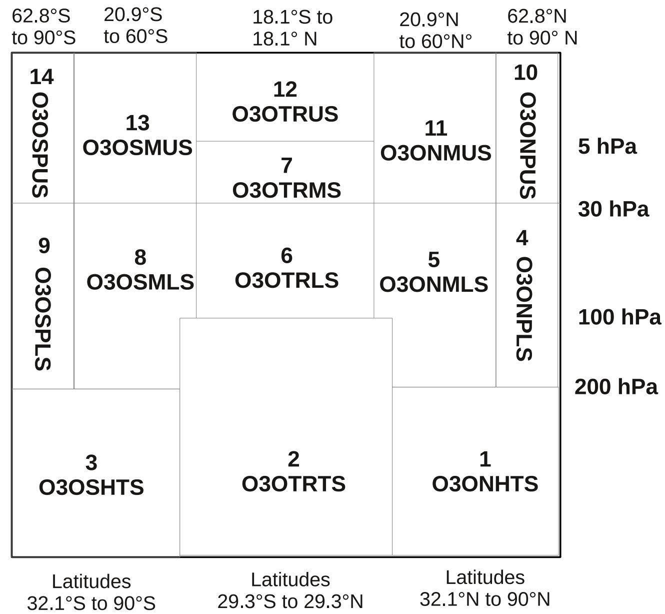

Figure S44: Definition of regions as used for the ozone origin diagnostics in submodel O3ORIG. The horizontal structure is used from file DLR_1.0_X_X_regions4ozone-origin_X.nc.

```
&CPL
!#####################################
!# A. DEFINITION OF ISO-SURFACES
!#####################################
!# NOTES:
!# - channel objects <name>_i, and <name_f> are added for
!#   'index' and 'fraction below'
!# SYNTAX:
!#    ISO-SURFACE name, channel, object, iso-value, index + fraction ?,
!#        reverse search ?, skip levels from top, skip levels from sfc
!#
!# ISENTROPES (THETA=CONST.)
 ISO(6)  = 'isent340',  'ECHAM5',  'tpot',    340.0, T, T,  ,  ,
 ISO(7)  = 'isent380',  'ECHAM5',  'tpot',    380.0, T, T,  ,  ,
 ISO(8)  = 'isent420',  'ECHAM5',  'tpot',    420.0, T, T,  ,  ,
!#
!# CONST. POTENTIAL VORTICITY
 ISO(9)  = 'PV2',        'tropop',  'PV',       2.0, T, T, 1, 4,
 ISO(10) = 'PV3',        'tropop',  'PV',       3.0, T, T, 1, 3,
 ISO(11) = 'PV4',        'tropop',  'PV',       4.0, T, T, 1, 3,
!#
!#####################################
!# B. FIELDS MAPPED TO (ISO-)SURFACES
!#####################################
!# NOTES:
!# - '_i' and '_f' are internally appended to SURFACE(object) name
!#   for 'index' and 'fraction below'; availability of '_f' determines
!#   the mapping method
!# SYNTAX:
!#    MAP name, ISO-SURFACE(channel), ISO-SURFACE(object),
!#              FIELD(channel), FIELD(object)
!#
!# ISENTROPES
 MAP(10) = 'pth340',   'viso',  'isent340', 'ECHAM5', 'press',
 MAP(11) = 'pth380',   'viso',  'isent380', 'ECHAM5', 'press',
 MAP(12) = 'pth420',   'viso',  'isent420', 'ECHAM5', 'press',
 MAP(13) = 'PVth340',  'viso',  'isent340', 'tropop', 'PV',
 MAP(14) = 'PVth380',  'viso',  'isent380', 'tropop', 'PV',
 MAP(15) = 'PVth420',  'viso',  'isent420', 'tropop', 'PV',
!#
!# TROPOPAUSE
 MAP(16) = 'ttp',     'tropop', 'tp',    'ECHAM5', 'tm1',
 MAP(17) = 'ztp',     'tropop', 'tp',    'ECHAM5', 'geopot',
 MAP(18) = 'thtp',    'tropop', 'tp',    'ECHAM5', 'tpot',
!#
!# PLANETARY BOUNDARY LAYER HEIGHT
 MAP(22) = 'ppblh',   'tropop', 'pblh',  'ECHAM5', 'press',
 MAP(23) = 'tpblh',   'tropop', 'pblh',  'ECHAM5', 'tm1',
!#
!# PV
 MAP(24) = 'pPV2',    'viso',   'PV2',   'ECHAM5', 'press',
 MAP(25) = 'pPV3',    'viso',   'PV3',   'ECHAM5', 'press',
 MAP(26) = 'pPV4',    'viso',   'PV4',   'ECHAM5', 'press',
 MAP(27) = 'thPV2',   'viso',   'PV2',   'ECHAM5', 'tpot',
 MAP(28) = 'thPV3',   'viso',   'PV3',   'ECHAM5', 'tpot',
 MAP(29) = 'thPV4',   'viso',   'PV4',   'ECHAM5', 'tpot',
 MAP(30) = 'tPV2',    'viso',   'PV2',   'ECHAM5', 'tm1',
 MAP(31) = 'tPV3',    'viso',   'PV3',   'ECHAM5', 'tm1',
 MAP(32) = 'tPV4',    'viso',   'PV4',   'ECHAM5', 'tm1',
!
/
```

Figure S45: Iso-surface and map definitions as used in the CPL namelist of the submodel VISO.

```
&CPL
!# NAME, LATITUDE, LONGITUDE, LIST OF CHANNEL OBJECTS
!# NOTES:
!#   - NAME <= 5 CHARACTERS
!#   - SYNTAX FOR CHANNEL OBJECT LIST:
!#        "channel:object,object,object;channel:object;"
!#        (in object-names wildcards (*,?) can be used)
!
!
! NOAA/ESRL
!
LOC(20)  = 'ALT',  82.45,  -62.52, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;\scnbuf:vervel;", ! Alert
LOC(21)  = 'ASC',  -6.92,  -14.42, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I, \
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(22)  = 'ASK',  23.18,    5.42, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I, \
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(23)  = 'AZR',  38.75,  -27.08, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I, \
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(24)  = 'BAL',  55.50,   16.67, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(25)  = 'BME',  32.37,  -64.65, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(26)  = 'BMW',  32.27,  -64.88, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
            CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
            g3b:aps;scnbuf:vervel;",
LOC(27)  = 'BRW',  71.32, -156.60, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
            CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
            g3b:aps;scnbuf:vervel;", ! Pt. Barrow
LOC(28)  = 'BSC',  44.17,   28.68, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(29)  = 'CBA',  55.20, -162.72, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(30)  = 'CGO', -40.68,  144.68, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(31)  = 'CHR',   1.70, -157.17, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(32)  = 'CMO',  45.00, -124.00, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(33)  = 'CRZ', -46.45,   51.85, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(34)  = 'EIC', -27.15, -109.45, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(35)  = 'GMI',  13.43,  144.78, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(36)  = 'GOZ',  36.05,   14.18, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(37)  = 'HBA', -75.61,  -27.73, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(38)  = 'HUN',  46.95,   16.65, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(39)  = 'ICE',  63.25,  -20.15, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
```

Figure S46: SCOUT CPL namelist used for hourly sampling of model columns.

```
LOC(40)  = 'ITN',  35.35,  -77.38, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(41)  = 'IZO',  28.30,  -16.48, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;", ! Izana
LOC(42)  = 'KEY',  25.67,  -80.20, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(43)  = 'KUM',  19.52, -154.82, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(44)  = 'KZD',  44.45,   75.57, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(45)  = 'KZM',  43.25,   77.88, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(46)  = 'LEF',  45.93,  -90.27, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(47)  = 'MBC',  76.25, -119.35, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(48)  = 'MHD',  53.33,   -9.90, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(49)  = 'MID',  28.22, -177.37, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(50)  = 'MLO',  19.53, -155.58, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;", ! Mauna Loa
LOC(51)  = 'NWR',  40.05, -105.63, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(52)  = 'PAL',  67.97,   24.12, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(53)  = 'PSA', -64.92,  -64.00, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(54)  = 'PTA',  38.95, -123.73, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(55)  = 'RPB',  13.17,  -59.45, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;", ! Barbados
LOC(56)  = 'SEY',  -4.67,   55.17, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(57)  = 'SHM',  52.72,  174.10, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(58)  = 'SMO', -14.25, -170.57, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;", ! Am. Samoa
LOC(59)  = 'SPO', -89.98,  -24.80, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(60)  = 'STM',  66.00,    2.00, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(61)  = 'SYO', -69.00,   39.58, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(62)  = 'TAP',  36.73,  126.13, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(63)  = 'TDF', -54.87,  -68.48, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
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Figure S46: continued

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LOC(64)  = 'UTA',  39.90, -113.72, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(65)  = 'UUM',  44.45,  111.10, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(66)  = 'WIS',  31.13,   34.88, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(67)  = 'WLG',  36.27,  100.92, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",
LOC(68)  = 'ZEP',  78.90,   11.88, "tracer_gp:CO,C2H4,C2H6,C3H6,C3H8,NC4H10,C5H8,SF6,CO2,CH4,N2O,H2,CH3Br,CH3Cl,CH3I,\
           CH3CCl3,CCl4,CHBr3,CF2ClBr,CF3Br,CF2Cl2,CFCl3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;", ! Ny Aalesund
!
! SHADOZ
!
LOC(80)  = 'Her',  10.00,  -84.11, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Heredia, Costa Rica
LOC(81)  = 'Ala',   9.98,  -84.21, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Alajuela, Costa Rica
LOC(82)  = 'Pag', -14.23, -170.56, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;
           g3b:aps;scnbuf:vervel;",  ! Pago Pago, American Samoa
LOC(83)  = 'Asc',  -7.98,  -14.42, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;
           g3b:aps;scnbuf:vervel;",  ! Ascension Is.
LOC(84)  = 'Fij', -18.13,  178.40, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Suva, Fiji Observatory
LOC(85)  = 'Ire', -25.90,   28.22, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Irene, South Africa
LOC(86)  = 'Kua',   2.73,  101.70, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Kuala Lumpur, Malaysia
LOC(87)  = 'Reu', -21.06,   55.48, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! La Runion
LOC(88)  = 'Nai',  -1.27,   36.80, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Nairobi, Kenya
LOC(89)  = 'Nat',  -5.42,  -35.38, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Natal, Brazil
LOC(90)  = 'Par',   5.81,  -55.21, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Paramaribo, Suriname
LOC(91)  = 'Cri',  -0.92,  -89.60, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! San Cristbal
LOC(92)  = 'Wat',  -7.57,  112.65, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Watukosek, Java
LOC(93)  = 'Mal',  -2.99,   40.19, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Malindi, Kenya
LOC(94)  = 'Pap', -18.00, -149.00, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Papeete Tahiti
LOC(95)  = 'Cot',   6.21,    2.23, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;",  ! Cotonou, Benin
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Figure S46: continued

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!
! selected WOUDC
!
LOC(100)  = 'ST111', -89.983,  -24.800, "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
           g3b:aps;scnbuf:vervel;", ! South Pole (Amundsen Scott)
LOC(101)  = 'ST323', -70.650,   -8.260,  "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
            g3b:aps;scnbuf:vervel;", ! Neumayer
LOC(102)  = 'ST256', -45.044,  169.684, "tracer_gp:O3,O3ONHTS,O3OTRTS,O3OSHTS,O3ONPLS,O3ONMLS,O3OTRLS,O3OTRMS,O3OSMLS,\
            O3OSPLS,O3ONPUS,O3ONMUS,O3OTRUS,O3OSMUS,O3OSPUS ;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,\
            aclc;g3b:aps;scnbuf:vervel;", ! Lauder

LOC(103)  = 'ST026', -38.030,  145.100,  "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
            g3b:aps;scnbuf:vervel;", ! Aspendale
LOC(104)  = 'ST187',  18.533,   73.850,  "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
            g3b:aps;scnbuf:vervel;", ! Poona
LOC(105)  = 'ST109',  19.717, -155.067,  "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
            g3b:aps;scnbuf:vervel;", ! Hilo
LOC(106)  = 'ST014',  36.100,  140.100,  "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
            g3b:aps;scnbuf:vervel;", ! Tateno
LOC(107)  = 'ST067',  40.030, -105.250, "tracer_gp:O3,O3ONHTS,O3OTRTS,O3OSHTS,O3ONPLS,O3ONMLS,O3OTRLS,O3OTRMS,O3OSMLS,\
            O3OSPLS,O3ONPUS,O3ONMUS,O3OTRUS,O3OSMUS,O3OSPUS ;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,\
            aclc;g3b:aps;scnbuf:vervel;", ! Boulder
LOC(108)  = 'ST099',  47.800, 11.020, "tracer_gp:O3,  O3ONHTS,O3OTRTS,O3OSHTS,O3ONPLS,O3ONMLS,O3OTRLS,O3OTRMS,O3OSMLS,\
            O3OSPLS,O3ONPUS,O3ONMUS,O3OTRUS,O3OSMUS,O3OSPUS ;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,\
            aclc;g3b:aps;scnbuf:vervel;", ! Hohenpeissenberg
LOC(109)  = 'ST024',  74.720,  -94.980,  "tracer_gp:O3;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;\
            g3b:aps;scnbuf:vervel;", ! Resolute
LOC(111) = 'SCBAH' , -77.82,  166.65,  "tracer_gp:O3,  O3ONHTS,O3OTRTS,O3OSHTS,O3ONPLS,O3ONMLS,O3OTRLS,O3OTRMS,O3OSMLS,\
           O3OSPLS,O3ONPUS,O3ONMUS,O3OTRUS,O3OSMUS,O3OSPUS ;tropop:tp,PV,pblh;ECHAM5:press,tm1,qm1,vm1,um1,rhum,xlm1,xim1,\
           aclc;g3b:aps;scnbuf:vervel;", ! Scott Base Arrival heights
!
/
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Figure S46: continued (end).

```
&CPL
! T: automatic daily output (highly recommended)
! F: output according to channel.nml (for testing)
lout_auto = T,
! value for re-initialisation at first time step of every day
r_init    = -1.0E+34,
!
!# SYNTAX: - NAME,
!#         - LATITUDE DEPENDENT LOCAL TIME (T,F),
!#           ORBIT INCLINATION (deg),
!#           ASCENDING(+1) (T) OR DESCENDING(-1) (F)
!#         - LOCAL TIME HOUR, LOCAL TIME (MINUTE)
!#           [EQUATOR CROSSING TIME],
!#           LIMIT DT TO LOCAL TIME DISTANCE ? (T,F)
!#         - LIST OF CHANNEL OBJECTS (max 600 characters)
!#
!# NOTES:
!#   - NAME <= 8 CHARACTERS
!#   - SYNTAX FOR CHANNEL OBJECT LIST:
!#        "channel:object,object,object;channel:object;"
!#        (in object-names wildcards (*,?) can be used)
!#
!# Nots:
!#    A:ascending, D:descending
!#    N:nadir, L:limb [f: forward (in flight direction),
!#    b: back]
!
! # ENVISAT: SCIAMACHI(N,Lf), MIPAS(Lb)
!
ORB(1)  = 'ENVI-A1',  T, 98.5451, T, 22,00, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,\
          tm1,vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;lnox_Grewe_gp:xnox,fpsm2cg,fpsm2ic;msbm:phase,\
          H2SO4_liq,N_solid,r_solid,A_liq;tracer_gp:BrNO2,SF6,H2SO4,Cl2O2,CHBr3,OClO,ClNO2,CH3Br,SO2,N2O,N,NH2OH,HONO,PAN,\
          CH3OH,N2O5,Cl2,CO,H2O2,HNO3,CH4,CH3OOH,BrCl,C5H8,H2,BrNO3,HOCl,DMS,Br2,ClNO3,HOBr,O1D,H,HBr,O3,NO3,OH,HO2,NO2,Cl,\
          NO,Br,CH3O2,HCHO,HCl,BrO,ClO,CO2,CO_14C_01,H2O,HNO3_nat*,ClOX,BrOX,NOX,CFCl3,CF2Cl2,CH3CCl3,CCl4,CH3Cl,CH2ClBr,\
          CHCl2Br,CHClBr2,CH2Br2,CF2ClBr,CF3Br;'
!
ORB(2)  = 'ENVI-A2',  T, 98.5451, T, 22,00, F, 'g3b:aps;jval_gp:J_O1D,J_NO2,J_OClO,J_Cl2O2,J_BrO,J_COH2,J_CHOH,J_N2O5,\
          J_HNO3,J_PAN,J_BrCl,J_SO2,J_OCS,J_H2O,J_N2O,J_NO,J_CO2,J_CH4;tracer_gp:*_ns,*_ks,*_as,*_cs,*_ki,*_ai,*_ci,*_l;\
          gmxe_gp:wetrad_M*,densaer_M*;rad01:*;rad01_fubrad:*;'
!
ORB(3)  = 'ENVI-D1',  T, 98.5451, F, 10,00, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,\
          tm1,vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;lnox_Grewe_gp:xnox,fpsm2cg,fpsm2ic;msbm:phase,\
          H2SO4_liq,N_solid,r_solid,A_liq;tracer_gp:BrNO2,SF6,H2SO4,Cl2O2,CHBr3,OClO,ClNO2,CH3Br,SO2,N2O,N,NH2OH,HONO,PAN,\
          CH3OH,N2O5,Cl2,CO,H2O2,HNO3,CH4,CH3OOH,BrCl,C5H8,H2,BrNO3,HOCl,DMS,Br2,ClNO3,HOBr,O1D,H,HBr,O3,NO3,OH,HO2,NO2,Cl,\
          NO,Br,CH3O2,HCHO,HCl,BrO,ClO,CO2,CO_14C_01,H2O,HNO3_nat*,ClOX,BrOX,NOX,CFCl3,CF2Cl2,CH3CCl3,CCl4,CH3Cl,CH2ClBr,\
          CHCl2Br,CHClBr2,CH2Br2,CF2ClBr,CF3Br;'
!
ORB(4)  = 'ENVI-D2',  T, 98.5451, F, 10,00, F, 'g3b:aps;jval_gp:J_O1D,J_NO2,J_OClO,J_Cl2O2,J_BrO,J_COH2,J_CHOH,J_N2O5,\
          J_HNO3,J_PAN,J_BrCl,J_SO2,J_OCS,J_H2O,J_N2O,J_NO,J_CO2,J_CH4;tracer_gp:*_ns,*_ks,*_as,*_cs,*_ki,*_ai,*_ci,*_l;\
          gmxe_gp:wetrad_M*,densaer_M*;rad:*;rad01:*;rad01_fubrad:*;'
!
! # ERS-2: GOME
!
ORB(7)  = 'ERS2-AN',  T, 98.5451, T, 22,30, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,\
          tm1,vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;lnox_Grewe_gp:xnox,fpsm2cg,fpsm2ic;msbm:phase,\
          H2SO4_liq,N_solid,r_solid,A_liq;tracer_gp:H2SO4,Cl2O2,OClO,SO2,H2O2,HNO3,BrCl,O1D,O3,OH,NO2,Cl,NO,Br,HCHO,HCl,\
          BrO,ClO,H2O,HNO3_nat*,ClOX,BrOX,NOX,CFCl3,CF2Cl2,CH3CCl3,CCl4,CH3Cl,CH2ClBr,CHCl2Br,CHClBr2,CH2Br2,CF2ClBr,CF3Br,\
          Br2,BrNO2,BrNO3,CH3Br,CHBr3,HBr,HOBr;jval_gp:J_O1D,J_NO2,J_OClO,J_Cl2O2,J_BrO,J_COH2,J_CHOH,J_N2O5,J_HNO3,J_PAN,\
          J_BrCl,J_SO2,J_OCS,J_H2O,J_N2O,J_NO,J_CO2,J_CH4;tracer_gp:*_ns,*_ks,*_as,*_cs,*_ki,*_ai,*_ci,*_l;\
          gmxe_gp:wetrad_M*,densaer_M*;rad:*;rad01:*;rad01_fubrad:*;'
!
ORB(8)  = 'ERS2-DN',  T, 98.5451, F, 10,30, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,\
          tm1,vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;lnox_Grewe_gp:xnox,fpsm2cg,fpsm2ic;msbm:phase,\
         H2SO4_liq,N_solid,r_solid,A_liq;tracer_gp:H2SO4,Cl2O2,OClO,SO2,H2O2,HNO3,BrCl,O1D,O3,OH,NO2,Cl,NO,Br,HCHO,HCl,\
         BrO,ClO,H2O,HNO3_nat*,ClOX,BrOX,NOX,CFCl3,CF2Cl2,CH3CCl3,CCl4,CH3Cl,CH2ClBr,CHCl2Br,CHClBr2,CH2Br2,CF2ClBr,CF3Br,\
         Br2,BrNO2,BrNO3,CH3Br,CHBr3,HBr,HOBr;jval_gp:J_O1D,J_NO2,J_OClO,J_Cl2O2,J_BrO,J_COH2,J_CHOH,J_N2O5,J_HNO3,J_PAN,\
         J_BrCl,J_SO2,J_OCS,J_H2O,J_N2O,J_NO,J_CO2,J_CH4;tracer_gp:*_ns,*_ks,*_as,*_cs,*_ki,*_ai,*_ci,*_l;\
         gmxe_gp:wetrad_M*,densaer_M*;rad:*;rad01:*;rad01_fubrad:*;'
```

Figure S47: SORBIT CPL namelist used for sampling along sun-synchronous orbits.

```
!
! # MetOp-A: GOME2
!
ORB(9)  = 'MTOPA-AN', T, 98.7,    T, 21,30, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,\
          tm1,vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;lnox_Grewe_gp:xnox,fpsm2cg,fpsm2ic;msbm:phase,\
          H2SO4_liq,N_solid,r_solid,A_liq;tracer_gp:H2SO4,Cl2O2,OClO,SO2,H2O2,HNO3,BrCl,O1D,O3,OH,NO2,Cl,NO,Br,HCHO,HCl,\
          BrO,ClO,H2O,HNO3_nat*,ClOX,BrOX,NOX,CFCl3,CF2Cl2,CH3CCl3,CCl4,CH3Cl,CH3Br,CH2ClBr,CHCl2Br,CHClBr2,CH2Br2,CF2ClBr,\
          CF3Br,Br2,BrNO2,BrNO3,CHBr3,HBr,HOBr;jval_gp:J_O1D,\
          J_NO2,J_OClO,J_Cl2O2,J_BrO,J_COH2,J_CHOH,J_N2O5,J_HNO3,J_PAN,J_BrCl,J_SO2,J_OCS,J_H2O,J_N2O,J_NO,J_CO2,J_CH4;\
          tracer_gp:*_ns,*_ks,*_as,*_cs,*_ki,*_ai,*_ci,*_l;gmxe_gp:wetrad_M*,densaer_M*;rad:*;rad01:*;rad01_fubrad:*;'
!
ORB(10) = 'MTOPA-DN', T, 98.7,    F, 09,30, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,\
          tm1,vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;lnox_Grewe_gp:xnox,fpsm2cg,fpsm2ic;msbm:phase,\
          H2SO4_liq,N_solid,r_solid,A_liq;tracer_gp:H2SO4,Cl2O2,OClO,SO2,H2O2,HNO3,BrCl,O1D,O3,OH,NO2,Cl,NO,Br,HCHO,HCl,\
          BrO,ClO,H2O,HNO3_nat*,ClOX,BrOX,NOX,CFCl3,CF2Cl2,CH3CCl3,CCl4,CH3Cl,CH3Br,CH2ClBr,CHCl2Br,CHClBr2,CH2Br2,CF2ClBr,\
          CF3Br,Br2,BrNO2,BrNO3,CHBr3,HBr,HOBr;jval_gp:J_O1D,\
          J_NO2,J_OClO,J_Cl2O2,J_BrO,J_COH2,J_CHOH,J_N2O5,J_HNO3,J_PAN,J_BrCl,J_SO2,J_OCS,J_H2O,J_N2O,J_NO,J_CO2,J_CH4;\
          tracer_gp:*_ns,*_ks,*_as,*_cs,*_ki,*_ai,*_ci,*_l;gmxe_gp:wetrad_M*,densaer_M*;rad:*;rad01:*;rad01_fubrad:*;'
!
! # AURA: MLS(L), TES(N,L), OMI(N), HIRDLS(L)
!
ORB(11) = 'AURA-A',   T, 98.21,   T, 13,43, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,\
          vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;tracer_gp:CO,O3,ClO,OClO,NO2,SO2,BrO,HCHO,HNO3,Cl2O2,N2O5,\
          BrCl,ClNO3,Cl,NO,Br,HCl,HNO3_nat*,ClOX,BrOX,NOX,CFCl3,CF2Cl2,CH3CCl3,CCl4,CH3Cl,CH3Br,CH2ClBr,CHCl2Br,CHClBr2,\
          CH2Br2,CF2ClBr,CF3Br,Br2,BrNO2,BrNO3,CHBr3,HBr,HOBr;'
!
ORB(12) = 'AURA-D',   T, 98.21,   F, 01,43, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,\
          vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;tracer_gp:CO,O3,ClO,OClO,NO2,SO2,BrO,HCHO,HNO3,Cl2O2,N2O5,\
          BrCl,ClNO3,Cl,NO,Br,HCl,HNO3_nat*,ClOX,BrOX,NOX,CFCl3,CF2Cl2,CH3CCl3,CCl4,CH3Cl,CH3Br,CH2ClBr,CHCl2Br,CHClBr2,\
          CH2Br2,CF2ClBr,CF3Br,Br2,BrNO2,BrNO3,CHBr3,HBr,HOBr;'
!
! # AQUA: AIRS, MODIS
!
ORB(13) = 'AQUA-A',   T, 98.2,    T, 13,30, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,\
          vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;tracer_gp:O3,H2O,CO2;'
ORB(14) = 'AQUA-D',   T, 98.2,    F, 01,30, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,\
          vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;tracer_gp:O3,H2O,CO2;'
!
! # TERRA: MOPITT
!
ORB(15) = 'TERRA-A',  T, 98.2,    T, 22,30, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,\
          vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;tracer_gp:CO,CH4;'
ORB(16) = 'TERRA-D',  T, 98.2,    F, 10,30, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,\
          vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;tracer_gp:CO,CH4;'
!
! # MERLIN
!
ORB(20) = 'MERLIN-A', T, 98.2,    T,  6,00, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,\
          vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;jval_gp:J_CH4;tracer_gp:CO,CH4,CH4_fx,OH,NOX,NO,NO2,Cl,C2H4,\
          C2H6,C3H6,C3H8,NC4H10,CH3COCH3,CH3CO2H,CH3OH,HCHO,HCOOH,MEK,CH3CHO;'
!
ORB(21) = 'MERLIN-D', T, 98.2,    F, 18,00, F, 'g3b:aps,albedo,ws,aprl,aprc,cvs,icecov;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,\
          vm1,um1,aclc,xlm1,xim1,grvol,cossza;tropop:tp,pblh,PV;jval_gp:J_CH4;tracer_gp:CO,CH4,CH4_fx,OH,NOX,NO,NO2,Cl,C2H4,\
          C2H6,C3H6,C3H8,NC4H10,CH3COCH3,CH3CO2H,CH3OH,HCHO,HCOOH,MEK,CH3CHO;'
!
! # CLOUDSAT: CPR
!
ORB(22) = 'CPR-A',    T, 98.2,    T, 13,31, F, 'g3b:aps,aprl,aprc,xi,xl;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,vm1,um1,xlm1,\
          xim1,grvol,cossza;tropop:tp,pblh,PV;cloud:aclc,prec_cover,rainflux,rain_form,rain_evap,snowflux,snow_form,snow_subl,\
          lwc,iwc,mimelt,misedi;convect:cv_precflx,cv_snowflx,cv_cover,cv_lwc,cv_iwc,cv_rform,cv_sform;'
ORB(23) = 'CPR-D',    T, 98.2,    F, 01,31, F, 'g3b:aps,aprl,aprc,xi,xl;geoloc:gboxarea;ECHAM5:geopot,qm1,tm1,vm1,um1,xlm1,\
          xim1,grvol,cossza;tropop:tp,pblh,PV;cloud:aclc,prec_cover,rainflux,rain_form,rain_evap,snowflux,snow_form,snow_subl,\
          lwc,iwc,mimelt,misedi;convect:cv_precflx,cv_snowflx,cv_cover,cv_lwc,cv_iwc,cv_rform,cv_sform;'
!
/
```

Figure S47: continued (end).

```
&CPL
!###############################################################################
!# SYNTAX: NAME, TRACK-DATA FILE BASE, UPDATE-SWITCH, COLUMN OUTPUT ?,
!#         OUTPUT ALL MODEL TIME STEPS ALONG TRACK, FILL VALUE
!#         LIST OF CHANNEL OBJECTS
!#
!# NOTES:
!#   - NAME <= 8 CHARACTERS
!#   - UPDATE SWITCH: -1: NEVER (SWITCHED OFF)
!#                     0: DAILY
!#                     1: MONTHLY
!#   - TRACK-DATA FILE NAMES
!#                <path>/<prefix><YYYY><MM><DD>.pos  (daily)   -> 0 !
!#                <path>/<prefix><YYYY><MM>.pos      (monthly) -> 1 !
!#   - SYNTAX FOR CHANNEL OBJECT LIST:
!#        "channel:object,object,object;channel:object;"
!#        (in object-names wildcards (*,?) can be used)
!#
!#   - THE TRACK-DATA FILES MUST CONTAIN:
!#       year month day hour minute second longitude latitude pressure [hPa]
!#
!###############################################################################
!
!# CARIBIC-1: daily position files
TRACK(1) = 'CARIBIC1', '$INPUTDIR_MESSY/s4d/misc/CARIBIC-1/C1F_', 0, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,\
           tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
!
!# CARIBIC-2: monthly position files
TRACK(2) = 'CARIBIC2', '$INPUTDIR_MESSY/s4d/misc/CARIBIC-2/C2F_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,\
           tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
!
!# TROICA: monthly position files
TRACK(3) = 'TROICA', '$INPUTDIR_MESSY/s4d/misc/TROICA/TROICA_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,\
           tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
!
!# MOZAIC: monthly position files; 5 different aircraft !!! unzip !!!
TRACK(4) = 'MOZAIC01','$INPUTDIR_MESSY/s4d/misc/MOZAIC/MOZAIC_01_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,\
           tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(5) = 'MOZAIC02','$INPUTDIR_MESSY/s4d/misc/MOZAIC/MOZAIC_02_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,\
           tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(6) = 'MOZAIC03','$INPUTDIR_MESSY/s4d/misc/MOZAIC/MOZAIC_03_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,\
           tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(7) = 'MOZAIC04','$INPUTDIR_MESSY/s4d/misc/MOZAIC/MOZAIC_04_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,\
           tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(8) = 'MOZAIC05','$INPUTDIR_MESSY/s4d/misc/MOZAIC/MOZAIC_05_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,\
           tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
!
!# HALOE: monthly position files
TRACK(10) = 'HALOESR','$INPUTDIR_MESSY/s4d/misc/HALOE/HALOE_Version19_SR_', 1, T, F, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;m7_gp:wetrad_M*,densaer_M*;",
TRACK(11) = 'HALOESS','$INPUTDIR_MESSY/s4d/misc/HALOE/HALOE_Version19_SS_', 1, T, F, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;m7_gp:wetrad_M*,densaer_M*;",
!
!# DADLR: HALO
!
TRACK(12) = 'DADLR','$INPUTDIR_MESSY/s4d/misc/DADLR/LR/DADLR_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
!
!# N677F: GV, HIAPER
!
TRACK(13) = 'N677F','$INPUTDIR_MESSY/s4d/misc/N677F/LR/N677F_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
!
!# DCMET: DLR-Falcon
!
TRACK(14) = 'DCMET','$INPUTDIR_MESSY/s4d/misc/DCMET/LR/DCMET_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
```

Figure S48: S4D CPL namelist used for sampling along tracks of various research platforms in the *RC1SD-base* simulations.

```
!
!# DCGFD: GFD-Lear Jet
!
TRACK(15) = 'DCGFD','$INPUTDIR_MESSY/s4d/misc/DCGFD/LR/DCGFD_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
!
!# MXCHINA: monthly position files
!
TRACK(16) = 'MXCHINA', '$INPUTDIR_MESSY/s4d/misc/MXCHINA/MXCHINA_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV,pblh;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;rad4all:srad*,trad*;",
!
!# MXCHINA2: monthly position files
!
TRACK(17) = 'MXCHINA2', '$INPUTDIR_MESSY/s4d/misc/MXCHINA2/MXCHINA2_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV,pblh;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;rad4all:srad*,trad*;",
!
!# PHLAB: National Aerospace Laboratory (NLR) Cessna Citation II (Netherlands)
!
TRACK(18) = 'PHLAB','$INPUTDIR_MESSY/s4d/misc/PHLAB/LR/PHLAB_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
!
!# M55205: Geophysica
!
TRACK(19) = 'M55204','$INPUTDIR_MESSY/s4d/misc/M55204/LR/M55204_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
!
!
!# ER2-809: NASA ER-2 #809
!
TRACK(20) = 'ER2-809','$INPUTDIR_MESSY/s4d/misc/ER2-809/LR/ER2-809_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,tm1,qm1,vm
!
!
!# VH-ARA: Egrett
!
TRACK(21) = 'VHARA','$INPUTDIR_MESSY/s4d/misc/VHARA/LR/VHARA_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
!
!
!# G-ENVR: NERC Dornier Do228-101
!
TRACK(22) = 'GENVR','$INPUTDIR_MESSY/s4d/misc/GENVR/LR/GENVR_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,tm1,qm1,vm1,um1,
!
!
!# N926: NASA WB-57
!
TRACK(23) = 'N926','$INPUTDIR_MESSY/s4d/misc/N926/LR/N926_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;ECHAM5:geopot,tm1,qm1,vm1,um1,rhu
!
!
!# MarionDufresne: research vessel
!
TRACK(24) = 'MaDuf','$INPUTDIR_MESSY/s4d/misc/MarionDufresne/LR/MarionDufresne_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
!
!
!# RonBrown: research vessel
!
TRACK(25) = 'RonBr','$INPUTDIR_MESSY/s4d/misc/RonBrown/LR/RonBrown_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
!
!
!# Sonne: research vessel
!
TRACK(26) = 'Sonne','$INPUTDIR_MESSY/s4d/misc/Sonne/LR/Sonne_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;lnox_Grewe_gp:*;",
```

Figure S48: continued

```
!
!# NOXAR
!
TRACK(27) = 'NOXAR', '$INPUTDIR_MESSY/s4d/misc/NOXAR/NOXAR_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
!
!# CONTRAIL
TRACK(28) = 'CONTRAIL', '$INPUTDIR_MESSY/s4d/misc/CONTRAIL/CONTRAIL_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
!
!# IAGOS: monthly position files (LR); 10 different aircraft
TRACK(31) = 'IAGOS01','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/01/IAGOS_01_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(32) = 'IAGOS02','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/02/IAGOS_02_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(33) = 'IAGOS03','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/03/IAGOS_03_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(34) = 'IAGOS04','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/04/IAGOS_04_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(35) = 'IAGOS05','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/05/IAGOS_05_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(36) = 'IAGOS06','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/06/IAGOS_06_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(37) = 'IAGOS07','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/07/IAGOS_07_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(38) = 'IAGOS08','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/08/IAGOS_08_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(39) = 'IAGOS09','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/09/IAGOS_09_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
TRACK(40) = 'IAGOS10','$INPUTDIR_MESSY/s4d/misc/IAGOS/LR/10/IAGOS_10_', 1, T, T, -1.E+34, "tracer_gp:*;tropop:tp,PV;\
            ECHAM5:geopot,tpot,tm1,qm1,vm1,um1,rhum,xlm1,xim1,aclc;g3b:aps;scnbuf:vervel;",
!
/
```

Figure S48: continued (end).

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