Supplementary material to: Global cloud and precipitation chemistry and wet deposition: tropospheric model simulations with ECHAM5/MESSy1

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1 Chemical Reaction Sets

1.1 Gas phase chemistry

Table 1: Gas phase reactions

#	reaction	rate coefficient
G1000	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	3.2E-11*EXP(70./temp)
G1001	$O_2 + O(^3P) \rightarrow O_3$	6.E-34*((temp/300.)**(-2.4)) *cair
G1002	$O_3 + O(^1D) \rightarrow 2\ O_2$	1.2E-10
G1003	$O_3 + O(^3P) \rightarrow 2\ O_2$	8.E-12*EXP(-2060./temp)
G01Diag	$O_3(s) \rightarrow LO_3(s)$	k_O3s
G2100	$H + O_2 \rightarrow HO_2$	k_3rd(temp,cair,5.7E-32,1.6, 7.5E-11,0.,0.6)
G2101	$H + O_3 \rightarrow OH$	1.4E-10*EXP(-470./temp)
G2102	$H_2 + O(^1D) \rightarrow H + OH$	1.1E-10
G2103	$OH + O(^3P) \rightarrow H$	2.2E-11*EXP(120./temp)
G2104	$OH + O_3 \rightarrow HO_2$	1.7E-12*EXP(-940./temp)
G2105	$OH + H_2 \rightarrow H_2O + H$	5.5E-12*EXP(-2000./temp)
G2106	$HO_2 + O(^3P) \rightarrow OH$	3.E-11*EXP(200./temp)
G2107	$HO_2 + O_3 \rightarrow OH$	1.E-14*EXP(-490./temp)
G2108a	$HO_2 + H \rightarrow 2\ OH$	0.69*8.1E-11
G2108b	$HO_2 + H \rightarrow H_2$	0.29*8.1E-11
G2108c	$HO_2 + H \rightarrow O(^3P) + H_2O$	0.02*8.1E-11
G2109	$HO_2 + OH \rightarrow H_2O$	4.8E-11*EXP(250./temp)
G2110	$HO_2 + HO_2 \rightarrow H_2O_2$	k_HO2_HO2
G2111	$H_2O + O(^1D) \rightarrow 2\ OH$	2.2E-10
G2112	$H_2O_2 + OH \rightarrow H_2O + HO_2$	2.9E-12*EXP(-160./temp)
G3100	$N + O_2 \rightarrow NO + O(^3P)$	1.5E-11*EXP(-3600./temp)
G3101	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	1.8E-11*EXP(110./temp)
G3102a	$N_2O + O(^1D) \rightarrow 2\ NO$	6.7E-11
G3102b	$N_2O + O(^1D) \rightarrow N_2 + O_2$	4.9E-11
G3103	$NO + O_3 \rightarrow NO_2 + O_2$	3.E-12*EXP(-1500./temp)
G3104	$NO + N \rightarrow O(^3P) + N_2$	2.1E-11*EXP(100./temp)
G3105	$NO_2 + O(^3P) \rightarrow NO + O_2$	5.6E-12*EXP(180./temp)
G3106	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)
G3107	$NO_2 + N \rightarrow N_2O + O(^3P)$	5.8E-12*EXP(220./temp)
G3108	$NO_3 + NO \rightarrow 2\ NO_2$	1.5E-11*EXP(170./temp)
G3109	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2
G3110	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(3.E-27*EXP(10990./ temp))
G3200	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.E-31,2.6, 3.6E-11,0.1,0.6)
G3201	$NO + HO_2 \rightarrow NO_2 + OH$	3.5E-12*EXP(250./temp)
G3202	$NO_2 + OH \rightarrow HNO_3$	k_3rd(temp,cair,2.E-30,3., 2.5E-11,0.,0.6)
G3203	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2
G3204	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12
G3205	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)
G3206	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH
G3207	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*EXP(10900./ temp))
G3208	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)

Table 1: Gas phase reactions (... continued)

#	reaction	rate coefficient
G4100	CH_4 + $O(^1D)$ → .75 CH_3O_2 + .75 OH + .25 HCHO + .4 H + .05 H_2	1.5E-10
G4101	CH_4 + OH → CH_3O_2 + H_2O	1.85E-20*EXP(2.82*log(temp) -987./temp)
G4102	CH_3OH + OH → HCHO + HO_2	7.3E-12*EXP(-620./temp)
G4103a	CH_3O_2 + HO_2 → CH_3OOH	4.1E-13*EXP(750./temp) /(1.+1./497.7*EXP(1160./temp))
G4103b	CH_3O_2 + HO_2 → HCHO + H_2O + O_2	4.1E-13*EXP(750./temp) /(1.+497.7*EXP(-1160./temp))
G4104	CH_3O_2 + NO → HCHO + NO_2 + HO_2	2.8E-12*EXP(300./temp)
G4105	CH_3O_2 + NO_3 → HCHO + HO_2 + NO_2	1.3E-12
G4106a	CH_3O_2 + CH_3O_2 → 2 HCHO + 2 HO_2	9.5E-14*EXP(390./temp) /(1.+1./26.2*EXP(1130./temp))
G4106b	CH_3O_2 + CH_3O_2 → HCHO + CH_3OH	9.5E-14*EXP(390./temp) /(1.+26.2*EXP(-1130./temp))
G4107	CH_3OOH + OH → .7 CH_3O_2 + .3 HCHO + .3 OH + H_2O	k_CH3OOH_OH
G4108	HCHO + OH → CO + H_2O + HO_2	9.52E-18*EXP(2.03*log(temp) +636./temp)
G4109	HCHO + NO_3 → HNO_3 + CO + HO_2	3.4E-13*EXP(-1900./temp)
G4110	CO + OH → H + CO_2	1.57E-13 + cair*3.54E-33
G4111	HCOOH + OH → HO_2	4.E-13
G4200	C_2H_6 + OH → $C_2H_5O_2$ + H_2O	1.49E-17*temp*temp*EXP(-499./ temp)
G4201	C_2H_4 + O_3 → HCHO + .22 HO_2 + .12 OH + .23 CO + .54 HCOOH + .1 H_2	1.2E-14*EXP(-2630./temp)
G4202	C_2H_4 + OH → .6666667 $CH_3CH(O_2)CH_2OH$	k_3rd(temp,cair,1.E-28,0.8, 8.8E-12,0.,0.6)
G4203	$C_2H_5O_2$ + HO_2 → C_2H_5OOH	7.5E-13*EXP(700./temp)
G4204	$C_2H_5O_2$ + NO → CH_3CHO + HO_2 + NO_2	2.6E-12*EXP(365./temp)
G4205	$C_2H_5O_2$ + NO_3 → CH_3CHO + HO_2 + NO_2	2.3E-12
G4206	$C_2H_5O_2$ + CH_3O_2 → .75 HCHO + HO_2 + .75 CH_3CHO + .25 CH_3OH	1.6E-13*EXP(195./temp)
G4207	C_2H_5OOH + OH → .3 $C_2H_5O_2$ + .7 CH_3CHO + .7 OH	k_CH3OOH_OH
G4208	CH_3CHO + OH → $CH_3C(O)OO$ + H_2O	5.6E-12*EXP(270./temp)
G4209	CH_3CHO + NO_3 → $CH_3C(O)OO$ + HNO_3	1.4E-12*EXP(-1900./temp)
G4210	CH_3COOH + OH → CH_3O_2	4.E-13*EXP(200./temp)
G4211a	$CH_3C(O)OO$ + HO_2 → $CH_3C(O)OOH$	4.3E-13*EXP(1040./temp) /(1.+1./37.*EXP(660./temp))
G4211b	$CH_3C(O)OO$ + HO_2 → CH_3COOH + O_3	4.3E-13*EXP(1040./temp) /(1.+37.*EXP(-660./temp))
G4212	$CH_3C(O)OO$ + NO → CH_3O_2 + NO_2	8.1E-12*EXP(270./temp)
G4213	$CH_3C(O)OO$ + NO_2 → PAN	k_PA_NO2
G4214	$CH_3C(O)OO$ + NO_3 → CH_3O_2 + NO_2	4.E-12
G4215a	$CH_3C(O)OO$ + CH_3O_2 → HCHO + HO_2 + CH_3O_2 + CO_2	0.9*2.E-12*EXP(500./temp)
G4215b	$CH_3C(O)OO$ + CH_3O_2 → CH_3COOH + HCHO + CO_2	0.1*2.E-12*EXP(500./temp)
G4216	$CH_3C(O)OO$ + $C_2H_5O_2$ → .82 CH_3O_2 + CH_3CHO + .82 HO_2 + .18 CH_3COOH	4.9E-12*EXP(211./temp)

Table 1: Gas phase reactions (... continued)

#	reaction	rate coefficient
G4217	$CH_3C(O)OO + CH_3C(O)OO \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	2.5E-12*EXP(500./temp)
G4218	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO$	k_CH3OOH_OH
G4219	$NACA + OH \rightarrow NO_2 + HCHO + CO$	5.6E-12*EXP(270./temp)
G4220	$PAN + OH \rightarrow HCHO + NO_2$	2.E-14
G4221	$PAN \rightarrow CH_3C(O)OO + NO_2$	k_PAN_M
G4300	$C_3H_8 + OH \rightarrow .82\ C_3H_7O_2 + .18\ C_2H_5O_2 + H_2O$	1.65E-17*temp*temp*EXP(-87./temp)
G4301	$C_3H_6 + O_3 \rightarrow .57\ HCHO + .47\ CH_3CHO + .33\ OH + .26\ HO_2 + .07\ CH_3O_2 + .06\ C_2H_5O_2 + .23\ CH_3C(O)OO + .04\ CH_3COCHO + .06\ CH_4 + .31\ CO + .22\ HCOOH + .03\ CH_3OH$	6.5E-15*EXP(-1900./temp)
G4302	$C_3H_6 + OH \rightarrow CH_3CH(O_2)CH_2OH$	k_3rd(temp,cair,8.E-27,3.5,3.E-11,0.,0.5)
G4303	$C_3H_6 + NO_3 \rightarrow ONIT$	4.6E-13*EXP(-1155./temp)
G4304	$C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH$	k_PrO2_HO2
G4305	$C_3H_7O_2 + NO \rightarrow .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ C_3H_7ONO_2$	k_PrO2_NO
G4306	$C_3H_7O_2 + CH_3O_2 \rightarrow CH_3COCH_3 + .8\ HCHO + .8\ HO_2 + .2\ CH_3OH$	k_PrO2_CH3O2
G4307	$C_3H_7OOH + OH \rightarrow .3\ C_3H_7O_2 + .7\ CH_3COCH_3 + .7\ OH$	k_CH3OOH_OH
G4308	$CH_3CH(O_2)CH_2OH + HO_2 \rightarrow CH_3CH(OOH)CH_2OH$	6.5E-13*EXP(650./temp)
G4309	$CH_3CH(O_2)CH_2OH + NO \rightarrow .98\ CH_3CHO + .98\ HCHO + .98\ HO_2 + .98\ NO_2 + .02\ ONIT$	4.2E-12*EXP(180./temp)
G4310	$CH_3CH(OOH)CH_2OH + OH \rightarrow .5\ CH_3CH(O_2)CH_2OH + .5\ CH_3COCH_2OH + .5\ OH + H_2O$	3.8E-12*EXP(200./temp)
G4311	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2 + H_2O$	1.33E-13+3.82E-11*EXP(-2000./temp)
G4312	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	8.6E-13*EXP(700./temp)
G4313	$CH_3COCH_2O_2 + NO \rightarrow NO_2 + CH_3C(O)OO + HCHO$	2.9E-12*EXP(300./temp)
G4314	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow .5\ CH_3COCHO + .5\ CH_3OH + .3\ CH_3C(O)OO + .8\ HCHO + .3\ HO_2 + .2\ CH_3COCH_2OH$	7.5E-13*EXP(500./temp)
G4315	$CH_3COCH_2O_2H + OH \rightarrow .3\ CH_3COCH_2O_2 + .7\ CH_3COCHO + .7\ OH$	k_CH3OOH_OH
G4316	$CH_3COCH_2OH + OH \rightarrow CH_3COCHO + HO_2$	3.E-12
G4317	$CH_3COCHO + OH \rightarrow CH_3C(O)OO + CO$	8.4E-13*EXP(830./temp)
G4318	$MPAN + OH \rightarrow CH_3COCH_2OH + NO_2$	3.2E-11
G4319	$MPAN \rightarrow MVKO2 + NO_2$	k_PAN_M
G4320	$C_3H_7ONO_2 + OH \rightarrow CH_3COCH_3 + NO_2$	6.2E-13*EXP(-230./temp)
G4400	$C_4H_{10} + OH \rightarrow C_4H_9O_2 + H_2O$	1.81E-17*temp*temp*EXP(114./temp)
G4401	$C_4H_9O_2 + CH_3O_2 \rightarrow .88\ CH_3COC_2H_5 + .68\ HCHO + 1.23\ HO_2 + .12\ CH_3CHO + .12\ C_2H_5O_2 + .18\ CH_3OH$	k_PrO2_CH3O2
G4402	$C_4H_9O_2 + HO_2 \rightarrow C_4H_9OOH$	k_PrO2_HO2

Table 1: Gas phase reactions (... continued)

#	reaction	rate coefficient
G4403	$C_4H_9O_2$ + NO → .84 NO_2 + .56 $CH_3COC_2H_5$ + .56 HO_2 + .28 $C_2H_5O_2$ + .84 CH_3CHO + .16 ONIT	k_PrO2_NO
G4404	C_4H_9OOH + OH → .15 $C_4H_9O_2$ + .85 $CH_3COC_2H_5$ + .85 OH + .85 H_2O	k_CH3OOH_OH
G4405	MVK + O_3 → .45 HCOOH + .9 CH_3COCHO + .1 $CH_3C(O)OO$ + .19 OH + .22 CO + .32 HO_2	.5*(1.36E-15*EXP(-2112./temp) +7.51E-16*EXP(-1521./temp))
G4406	MVK + OH → MVKO2	.5*(4.1E-12*EXP(452./temp) +1.9E-11*EXP(175./temp))
G4407	MVKO2 + HO_2 → MVKOOH	1.82E-13*EXP(1300./temp)
G4408	MVKO2 + NO → NO_2 + .25 $CH_3C(O)OO$ + .25 CH_3COCH_2OH + .75 HCHO + .25 CO + .75 HO_2 + .5 CH_3COCHO	2.54E-12*EXP(360./temp)
G4409	MVKO2 + NO_2 → MPAN	.25*k_3rd(temp,cair,9.7E-29, 5.6,9.3E-12,1.5,0.6)
G4410	MVKO2 + CH_3O_2 → .5 CH_3COCHO + .375 CH_3COCH_2OH + .125 $CH_3C(O)OO$ + 1.125 HCHO + .875 HO_2 + .125 CO + .25 CH_3OH	2.E-12
G4411	MVKO2 + MVKO2 → CH_3COCH_2OH + CH_3COCHO + .5 CO + .5 HCHO + HO_2	2.E-12
G4412	MVKOOH + OH → MVKO2	3.E-11
G4413	$CH_3COC_2H_5$ + OH → MEKO2	1.3E-12*EXP(-25./temp)
G4414	MEKO2 + HO_2 → MEKOOH	k_PrO2_HO2
G4415	MEKO2 + NO → .985 CH_3CHO + .985 $CH_3C(O)OO$ + .985 NO_2 + .015 ONIT	k_PrO2_NO
G4416	MEKOOH + OH → .8 MeCOCO + .8 OH + .2 MEKO2	k_CH3OOH_OH
G4417	ONIT + OH → $CH_3COC_2H_5$ + NO_2 + H_2O	1.7E-12
G4500	ISOP + O_3 → .28 HCOOH + .65 MVK + .1 MVKO2 + .1 $CH_3C(O)OO$ + .14 CO + .58 HCHO + .09 H_2O_2 + .08 CH_3O_2 + .25 OH + .25 HO_2	7.86E-15*EXP(-1913./temp)
G4501	ISOP + OH → ISO2	2.54E-11*EXP(410./temp)
G4502	ISOP + NO_3 → ISON	3.03E-12*EXP(-446./temp)
G4503	ISO2 + HO_2 → ISOOH	2.22E-13*EXP(1300./temp)
G4504	ISO2 + NO → .88 NO_2 + .88 MVK + .88 HCHO + .88 HO_2 + .12 ISON	2.54E-12*EXP(360./temp)
G4505	ISO2 + CH_3O_2 → .5 MVK + 1.25 HCHO + HO_2 + .25 CH_3COCHO + .25 CH_3COCH_2OH + .25 CH_3OH	2.E-12
G4506	ISO2 + ISO2 → 2 MVK + HCHO + HO_2	2.E-12
G4507	ISOOH + OH → MVK + OH	1.E-10
G4508	ISON + OH → CH_3COCH_2OH + NACA	1.3E-11
G6100	Cl + O_3 → ClO	2.3E-11*EXP(-200./temp)
G6101	ClO + O(^{3}P) → Cl	3.E-11*EXP(70./temp)
G6102	ClO + ClO → Cl_2O_2	k_ClO_ClO
G6103	Cl_2O_2 → ClO + ClO	k_ClO_ClO/(1.27E-27*EXP(8744./ temp))
G6200	Cl + H_2 → HCl + H	3.7E-11*EXP(-2300./temp)
G6201a	Cl + HO_2 → HCl	1.8E-11*EXP(170./temp)
G6201b	Cl + HO_2 → ClO + OH	4.1E-11*EXP(-450./temp)

Table 1: Gas phase reactions (... continued)

#	reaction	rate coefficient
G6202	$Cl + H_2O_2 \rightarrow HCl + HO_2$	`1.1E-11*EXP(-980./temp)`
G6203a	$ClO + OH \rightarrow Cl + HO_2$	`7.4E-12*EXP(270./temp)`
G6203b	$ClO + OH \rightarrow HCl$	`6.E-13*EXP(230./temp)`
G6204	$ClO + HO_2 \rightarrow HOCl$	`2.7E-12*EXP(220./temp)`
G6205	$HCl + OH \rightarrow Cl + H_2O$	`2.6E-12*EXP(-350./temp)`
G6206	$HOCl+ OH \rightarrow ClO + H_2O$	`3.E-12*EXP(-500./temp)`
G6300	$ClO + NO \rightarrow NO_2 + Cl$	`6.4E-12*EXP(290./temp)`
G6301	$ClO + NO_2 \rightarrow ClNO_3$	`k_3rd(temp,cair,1.8E-31,3.4, 1.5E-11,1.9,0.6)`
G6303	$ClNO_3 + O(^3P) \rightarrow ClO + NO_3$	`2.9E-12*EXP(-800./temp)`
G6304	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	`6.5E-12*EXP(135./temp)`
G6400	$Cl + CH_4 \rightarrow HCl + CH_3O_2$	`9.6E-12*EXP(-1360./temp)`
G6401	$Cl + HCHO \rightarrow HCl + CO + HO_2$	`8.1E-11*EXP(-30./temp)`
G6402	$Cl + CH_3OOH \rightarrow CH_3O_2 + HCl$	`5.7E-11`
G6403	$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	`3.3E-12*EXP(-115./temp)`
G6404	$CCl_4 + O(^1D) \rightarrow ClO + 3\ Cl$	`3.3E-10`
G6405	$CH_3Cl + O(^1D) \rightarrow OH + Cl$	`1.65E-10`
G6406	$CH_3Cl + OH \rightarrow H_2O + Cl$	`2.4E-12*EXP(-1250./temp)`
G6407	$CH_3CCl_3 + O(^1D) \rightarrow OH + 3\ Cl$	`3.E-10`
G6408	$CH_3CCl_3 + OH \rightarrow H_2O + 3\ Cl$	`1.6E-12*EXP(-1520./temp)`
G6500	$CF_2Cl_2 + O(^1D) \rightarrow ClO + Cl$	`1.4E-10`
G6501	$CFCl_3 + O(^1D) \rightarrow ClO + 2\ Cl$	`2.3E-10`
G7100	$Br + O_3 \rightarrow BrO$	`1.7E-11*EXP(-800./temp)`
G7101	$BrO + O(^3P) \rightarrow Br + O_2$	`1.9E-11*EXP(230./temp)`
G7102a	$BrO + BrO \rightarrow Br + Br$	`2.4E-12*EXP(40./temp)`
G7102b	$BrO + BrO \rightarrow Br_2$	`2.8E-14*EXP(869./temp)`
G7200	$Br + HO_2 \rightarrow HBr$	`1.5E-11*EXP(-600./temp)`
G7201	$BrO + HO_2 \rightarrow HOBr$	`3.4E-12*EXP(540./temp)`
G7202	$HBr + OH \rightarrow Br + H_2O$	`1.1E-11`
G7203	$HOBr + O(^3P) \rightarrow OH + BrO$	`1.2E-10*EXP(-430./temp)`
G7301	$BrO + NO \rightarrow Br + NO_2$	`8.8E-12*EXP(260./temp)`
G7302	$BrO + NO_2 \rightarrow BrNO_3$	`k_BrO_NO2`
G7400	$Br + HCHO \rightarrow HBr + CO + HO_2$	`1.7E-11*EXP(-800./temp)`
G7403	$CH_3Br + OH \rightarrow H_2O + Br$	`2.35E-12*EXP(-1300./temp)`
G7603a	$BrO + ClO \rightarrow Br + OClO$	`9.5E-13*EXP(550./temp)`
G7603b	$BrO + ClO \rightarrow Br + Cl$	`2.3E-12*EXP(260./temp)`
G7603c	$BrO + ClO \rightarrow BrCl$	`4.1E-13*EXP(290./temp)`
G9200	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	`k_3rd(temp,cair,3.E-31,3.3, 1.5E-12,0.,0.6)`
G9400a	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	`1.13E-11*EXP(-253./temp)`
G9400b	$DMS + OH \rightarrow DMSO + HO_2$	`k_DMS_OH`
G9401	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	`1.9E-13*EXP(520./temp)`
G9402	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	`1.E-10`
G9403	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	`1.9E13*EXP(-8661./temp)`
G9404	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	`3.E-13`
G9405	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	`5.E-11`

Notes:
Rate coefficients for three-body reactions are defined via the function `k_3rd`(T, M, k_0^{300}, n, k_{inf}^{300}, m, f_c). In the code, the temperature T is called `temp` and the concentration of "air molecules" M is called `cair`.

Using the auxiliary variables $k_0(T)$, $k_{\rm inf}(T)$, and $k_{\rm ratio}$, `k_3rd` is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \tag{1}$$

$$k_{\rm inf}(T) = k_{\rm inf}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \tag{2}$$

$$k_{\rm ratio} = \frac{k_0(T)M}{k_{\rm inf}(T)} \tag{3}$$

$$\texttt{k\_3rd} = \frac{k_0(T)M}{1+k_{\rm ratio}} \times f_{\rm c}^{\left(\frac{1}{1+(\log_{10}(k_{\rm ratio}))^2}\right)} \tag{4}$$

A similar function, called `k_3rd_iupac` here, is used by Atkinson et al. (2005) for three-body reactions. It has the same function parameters as `k_3rd` and it is defined as:

$$k_0(T) = k_0^{300} \times \left(\frac{300\text{K}}{T}\right)^n \tag{5}$$

$$k_{\rm inf}(T) = k_{\rm inf}^{300} \times \left(\frac{300\text{K}}{T}\right)^m \tag{6}$$

$$k_{\rm ratio} = \frac{k_0(T)M}{k_{\rm inf}(T)} \tag{7}$$

$$N = 0.75 - 1.27 \times \log_{10}(f_{\rm c}) \tag{8}$$

$$\texttt{k\_3rd\_iupac} = \frac{k_0(T)M}{1+k_{\rm ratio}} \times f_{\rm c}^{\left(\frac{1}{1+(\log_{10}(k_{\rm ratio})/N)^2}\right)} \tag{9}$$

G1000: Sander et al. (2003)
G1001: Sander et al. (2003)
G1002: Sander et al. (2003), path leading to 2 $O(^3P)$ + O_2 neglected
G1003: Sander et al. (2003)
G01Diag: Roelofs and Lelieveld (1997), `k_O3s = (1.7E-12*EXP(-940./temp))*C(KPP_OH)+(1.E-14*EXP(-490./temp))*C(KPP_HO2)+J_O1D*2.2E-10*C(KPP_H2O)/(3.2E-11*EXP(70./temp)*C(KPP_O2)+1.8E-11*EXP(110./temp)*C(KPP_N2)+2.2E-10*C(KPP_H2O))`
G2100: Sander et al. (2003)
G2101: Sander et al. (2003)
G2102: Sander et al. (2003)
G2103: Sander et al. (2003)
G2104: Sander et al. (2003)
G2105: Sander et al. (2003)
G2106: Sander et al. (2003)
G2107: Sander et al. (2003)
G2108a,b,c: Sander et al. (2003), branching ratio from Hack et al., see note B5 of Sander et al. (2003)
G2109: Sander et al. (2003)
G2110: Christensen et al. (2002), Kircher and Sander (1984), The rate coefficient is: `k_HO2_HO2 = (1.5E-12*EXP(19./temp)+1.7E-33*EXP(1000./temp)*cair)* (1.+1.4E-21*EXP(2200./temp)*C(KPP_H2O))`. The value for the first (pressure-independent) part is from Christensen et al. (2002), the water term from Kircher and Sander (1984)
G2111: Sander et al. (2003)
G2112: Sander et al. (2003)
G3100: Sander et al. (2003)
G3101: Sander et al. (2003)
G3102a: Sander et al. (2003)
G3102b: Sander et al. (2003)
G3103: Sander et al. (2003)
G3104: Sander et al. (2003)
G3105: Sander et al. (2003)
G3106: Sander et al. (2003)
G3107: Sander et al. (2003)
G3108: Sander et al. (2003)
G3109: Sander et al. (2003). The rate coefficient is: `k_NO3_NO2 = k_3rd(temp,cair,2.E-30,4.4,1.4E-12,0.7,0.6)`.
G3110: Sander et al. (2003). The rate coefficient is defined as backward reaction divided by equilibrium constant.
G3200: Sander et al. (2003)
G3201: Sander et al. (2003)
G3202: Sander et al. (2003)
G3203: Sander et al. (2003). The rate coefficient is: `k_NO2_HO2 = k_3rd(temp,cair,1.8E-31,3.2,4.7E-12,1.4,0.6)`.
G3204: Sander et al. (2003)
G3205: Sander et al. (2003)
G3206: Sander et al. (2003). The rate coefficient is: `k_HNO3_OH = 2.4E-14 * EXP(460./temp) + 1./ ( 1./(6.5E-34 * EXP(1335./temp)*cair) + 1./(2.7E-17 * EXP(2199./temp)) )`
G3207: Sander et al. (2003). The rate coefficient is defined as backward reaction divided by equilibrium constant.

G3208: Sander et al. (2003)
G4100: Sander et al. (2003)
G4101: Atkinson (2003)
G4102: Sander et al. (2003)
G4103a,b: Sander et al. (2003), product distribution is from Elrod et al. (2001)
G4104: Sander et al. (2003)
G4105: Atkinson et al. (1999)
G4106a: Sander et al. (2003)
G4106b: Sander et al. (2003)
G4107: Sander et al. (2003). The rate coefficient is: `k_CH3OOH_OH = 3.8E-12*EXP(200./temp)`
G4108: Sivakumaran et al. (2003)
G4109: Sander et al. (2003), same temperature dependence assumed as for CH_3CHO+NO_3
G4110: McCabe et al. (2001)
G4111: Sander et al. (2003)
G4200: Atkinson (2003)
G4201: Sander et al. (2003), product distribution is from von Kuhlmann (2001) (see also Neeb et al. (1998))
G4202: Sander et al. (2003)
G4203: Sander et al. (2003)
G4204: Sander et al. (2003)
G4205: Atkinson et al. (1999)
G4206: Rate coefficient calculated by von Kuhlmann (pers. comm. 2004) using self reactions of CH_3OO and C_2H_5OO from Sander et al. (2003) and geometric mean as suggested by Madronich and Calvert (1990) and Kirchner and Stockwell (1996). The product distribution (branching=0.5/0.25/0.25) is calculated by von Kuhlmann (pers. comm. 2004) based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).
G4207: Same value as for **G4107:** CH_3OOH+OH assumed.
G4208: Sander et al. (2003)
G4209: Sander et al. (2003)
G4210: Sander et al. (2003)
G4211a: Tyndall et al. (2001)
G4211b: Tyndall et al. (2001)
G4212: Tyndall et al. (2001)
G4213: Tyndall et al. (2001). The rate coefficient is: `k_PA_NO2 = k_3rd(temp,cair,8.5E-29, 6.5,1.1E-11,1.,0.6)`.
G4214: Canosa-Mas et al. (1996)
G4215a: Sander et al. (2003)
G4215b: Sander et al. (2003)
G4216: `1.0E-11` from Atkinson et al. (1999), temperature dependence from Kirchner and Stockwell (1996)
G4217: Tyndall et al. (2001)
G4218: Same value as for **G4107:** CH_3OOH+OH assumed.
G4219: According to Pöschl et al. (2000), the same value as for CH_3CHO+OH can be assumed.
G4220: 50% of the upper limit given by Sander et al. (2003), as suggested by von Kuhlmann (2001)
G4221: Sander et al. (2003). The rate coefficient is: `k_PAN_M = k_PA_NO2/9.E-29*EXP(-14000./temp)`, i.e. the rate coefficient is defined as backward reaction divided by equilibrium constant.
G4300: Atkinson (2003)
G4301: Sander et al. (2003), product distribution is for terminal olefin carbons from Zaveri and Peters (1999)
G4302: Atkinson et al. (1999)
G4303: Atkinson et al. (1999)
G4304: Atkinson (1997). The rate coefficient is: `k_PrO2_HO2 = 1.9E-13*EXP(1300./temp)`. Value for generic RO_2 + HO_2 reaction from Atkinson (1997) is used.
G4305: Atkinson et al. (1999). The rate coefficient is: `k_PrO2_NO = 2.7E-12*EXP(360./temp)`
G4306: Kirchner and Stockwell (1996). The rate coefficient is: `k_PrO2_CH3O2 = 9.46E-14*EXP(431./temp)`. The product distribution is from von Kuhlmann (2001).
G4307: Same value as for **G4107:** CH_3OOH+OH assumed.
G4308: Müller and Brasseur (1995)
G4309: Müller and Brasseur (1995), products are from von Kuhlmann (2001)
G4310: Müller and Brasseur (1995)
G4311: Sander et al. (2003)
G4312: Tyndall et al. (2001)
G4313: Sander et al. (2003)
G4314: Tyndall et al. (2001)
G4315: Same value as for **G4107:** CH_3OOH+OH assumed.
G4316: Atkinson et al. (1999)
G4317: Tyndall et al. (1995)
G4318: Orlando et al. (2002)
G4319: Same value as for PAN assumed.
G4320: Atkinson et al. (1999)
G4400: Atkinson (2003)
G4401: Same value as for propyl group assumed (`k_PrO2_CH3O2`).
G4402: Same value as for propyl group assumed (`k_PrO2_HO2`).
G4403: Same value as for propyl group assumed (`k_PrO2_NO`).
G4404: Same value as for **G4107:** CH_3OOH+OH assumed.
G4405: Pöschl et al. (2000)
G4406: Pöschl et al. (2000)
G4407: Pöschl et al. (2000)
G4408: Pöschl et al. (2000)
G4409: Pöschl et al. (2000). The factor 0.25 was recommended by Uli Poeschl (pers. comm. 2004).
G4410: von Kuhlmann (2001)
G4411: Pöschl et al. (2000)
G4412: Pöschl et al. (2000)
G4413: Atkinson et al. (1999)
G4414: Same value as for propyl group assumed (`k_PrO2_HO2`).
G4415: Same value as for propyl group assumed (`k_PrO2_NO`).

G4416: Same value as for **G4107:** CH_3OOH+OH assumed.
G4417: Atkinson et al. (1999), value for $C_4H_9ONO_2$ used here.
G4500: Pöschl et al. (2000)
G4501: Pöschl et al. (2000)
G4502: Pöschl et al. (2000)
G4503: Boyd et al. (2003), same temperature dependence assumed as for other RO_2+HO_2 reactions
G4504: Pöschl et al. (2000), yield of 12 % $RONO_2$ assumed as suggested in Table 2 of Sprengnether et al. (2002).
G4505: von Kuhlmann (2001)
G4506: Pöschl et al. (2000)
G4507: Pöschl et al. (2000)
G4508: Pöschl et al. (2000)
G6100: Sander et al. (2003)
G6101: Sander et al. (2003)
G6102: Atkinson et al. (2005). The rate coefficient is: `k_ClO_ClO = k_3rd_iupac(temp,cair,2.E-32, 4.,1.E-11,0.,0.45)`.
G6103: Sander et al. (2003). The rate coefficient is defined as backward reaction divided by equilibrium constant.
G6200: Sander et al. (2003)
G6201a: Sander et al. (2003)
G6201b: Sander et al. (2003)
G6202: Sander et al. (2003)
G6203a: Sander et al. (2003)
G6203b: Sander et al. (2003)
G6204: Sander et al. (2003). At low temperatures, there may be a minor reaction channel leading to O_3+HCl. See Finkbeiner et al. (1995) for details. It is neglected here.
G6205: Sander et al. (2003)
G6206: Sander et al. (2003)
G6300: Sander et al. (2003)
G6301: Sander et al. (2003)
G6303: Sander et al. (2003)
G6304: Sander et al. (2003)
G6400: Sander et al. (2003)
G6401: Sander et al. (2003)
G6402: Sander et al. (2003)
G6403: Sander et al. (2003)
G6404: Sander et al. (2003)
G6405: Sander et al. (2003), average of reactions with CH_3Br and CH_3F (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).
G6406: Sander et al. (2003)
G6407: Sander et al. (2003), extrapolated from reactions with CH_3CF_3, CH_3CClF_2, and CH_3CCl_2F (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).
G6408: Sander et al. (2003)
G6500: Sander et al. (2003)
G6501: Sander et al. (2003)
G7100: Sander et al. (2003)
G7101: Sander et al. (2003)
G7102a: Sander et al. (2003)
G7102b: Sander et al. (2003)
G7200: Sander et al. (2003)
G7201: Sander et al. (2003)
G7202: Sander et al. (2003)
G7203: Sander et al. (2003)
G7301: Sander et al. (2003)
G7302: Sander et al. (2003). The rate coefficient is: `k_BrO_NO2 = k_3rd(temp,cair,5.2E-31,3.2, 6.9E-12,2.9,0.6)`.
G7400: Sander et al. (2003)
G7403: Sander et al. (2003)
G7603a: Sander et al. (2003)
G7603b: Sander et al. (2003)
G7603c: Sander et al. (2003)
G9200: Sander et al. (2003)
G9400a: Atkinson et al. (2003); Abstraction path. The assumed reaction sequence (omitting H_2O and O_2 as products) according to Yin et al. (1990) is:

$$\begin{aligned}
\mathrm{DMS + OH} &\rightarrow \mathrm{CH_3SCH_2} \\
\mathrm{CH_3SCH_2 + O_2} &\rightarrow \mathrm{CH_3SCH_2OO} \\
\mathrm{CH_3SCH_2OO + NO} &\rightarrow \mathrm{CH_3SCH_2O + NO_2} \\
\mathrm{CH_3SCH_2O} &\rightarrow \mathrm{CH_3S + HCHO} \\
\mathrm{CH_3S + O_3} &\rightarrow \mathrm{CH_3SO} \\
\mathrm{CH_3SO + O_3} &\rightarrow \mathrm{CH_3SO_2} \\
\hline
\mathrm{DMS + OH} & \quad \mathrm{CH_3SO_2 + HCHO} \\
\mathrm{+NO + 2O_3} &\rightarrow \mathrm{+NO_2}
\end{aligned}$$

Neglecting the effect on O_3 and NO_x, the remaining reaction is:

$$\mathrm{DMS + OH + O_3 \rightarrow CH_3SO_2 + HCHO}$$

G9400b: Atkinson et al. (2003); Addition path. The rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(KPP_O2)/ (1.+ 5.0E-30*EXP(6280./temp)*C(KPP_O2))`.
G9401: Atkinson et al. (2003)
G9402: Hynes and Wine (1996)
G9403: Barone et al. (1995)
G9404: Barone et al. (1995)
G9405: Barone et al. (1995)

Table 2: Photolysis reactions

#	reaction	rate coefficient
J1000	O_2 + hν → $O(^3P)$ + $O(^3P)$	`JX(ip_O2)`
J1001a	O_3 + hν → $O(^1D)$	`JX(ip_O1D)`

Table 2: Photolysis reactions (... continued)

#	reaction	rate coefficient
J1001b	O_3 + hν → $O(^3P)$	JX(ip_O3P)
J2100	H_2O + hν → H + OH	JX(ip_H2O)
J2101	H_2O_2 + hν → 2 OH	JX(ip_H2O2)
J3100	N_2O + hν → $O(^1D)$	JX(ip_N2O)
J3101	NO_2 + hν → NO + $O(^3P)$	JX(ip_NO2)
J3102	NO + hν → N + $O(^3P)$	JX(ip_NO)
J3103a	NO_3 + hν → NO_2 + $O(^3P)$	JX(ip_NO2O)
J3103b	NO_3 + hν → NO	JX(ip_NOO2)
J3104	N_2O_5 + hν → NO_2 + NO_3	JX(ip_N2O5)
J3200	HONO + hν → NO + OH	JX(ip_HONO)
J3201	HNO_3 + hν → NO_2 + OH	JX(ip_HNO3)
J3202	HNO_4 + hν → .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH	JX(ip_HNO4)
J4100	CH_3OOH + hν → HCHO + OH + HO_2	JX(ip_CH3OOH)
J4101a	HCHO + hν → H_2 + CO	JX(ip_COH2)
J4101b	HCHO + hν → H + CO + HO_2	JX(ip_CHOH)
J4102	CO_2 + hν → CO + $O(^3P)$	JX(ip_CO2)
J4200	C_2H_5OOH + hν → CH_3CHO + HO_2 + OH	JX(ip_CH3OOH)
J4201	CH_3CHO + hν → CH_3O_2 + HO_2 + CO	JX(ip_CH3CHO)
J4202	$CH_3C(O)OOH$ + hν → CH_3O_2 + OH	JX(ip_PAA)
J4203	NACA + hν → NO_2 + HCHO + CO	0.19*JX(ip_CHOH)
J4204	PAN + hν → $CH_3C(O)OO$ + NO_2	JX(ip_PAN)
J4300	C_3H_7OOH + hν → CH_3COCH_3 + HO_2 + OH	JX(ip_CH3OOH)
J4301	CH_3COCH_3 + hν → $CH_3C(O)OO$ + CH_3O_2	JX(ip_CH3COCH3)
J4302	CH_3COCH_2OH + hν → $CH_3C(O)OO$ + HCHO + HO_2	0.074*JX(ip_CHOH)
J4303	CH_3COCHO + hν → $CH_3C(O)OO$ + CO + HO_2	JX(ip_CH3COCHO)
J4304	$CH_3COCH_2O_2H$ + hν → $CH_3C(O)OO$ + HO_2 + OH	JX(ip_CH3OOH)
J4305	MPAN + hν → CH_3COCH_2OH + NO_2	JX(ip_PAN)
J4306	$C_3H_7ONO_2$ + hν → CH_3COCH_3 + NO_2 + HO_2	3.7*JX(ip_PAN)
J4400	C_4H_9OOH + hν → OH + .67 $CH_3COC_2H_5$ + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	JX(ip_CH3OOH)
J4401	MVK + hν → $CH_3C(O)OO$ + HCHO + CO + HO_2	0.019*JX(ip_COH2) +.015*JX(ip_ CH3COCHO)
J4402	MVKOOH + hν → OH + .5 CH_3COCHO + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 $CH_3C(O)OO$ + .25 CO	JX(ip_CH3OOH)
J4403	$CH_3COC_2H_5$ + hν → $CH_3C(O)OO$ + $C_2H_5O_2$	0.42*JX(ip_CHOH)
J4404	MEKOOH + hν → $CH_3C(O)OO$ + CH_3CHO + OH	JX(ip_CH3OOH)
J4405	MeCOCO + hν → 2 $CH_3C(O)OO$	2.15*JX(ip_ CH3COCHO)
J4406	ONIT + hν → NO_2 + .67 $CH_3COC_2H_5$ + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	3.7*JX(ip_PAN)
J4500	ISOOH + hν → MVK + HCHO + HO_2 + OH	JX(ip_CH3OOH)
J4501	ISON + hν → MVK + HCHO + NO_2 + HO_2	3.7*JX(ip_PAN)
J6000	Cl_2 + hν → Cl + Cl	JX(ip_Cl2)
J6100	Cl_2O_2 + hν → 2 Cl	1.4*JX(ip_Cl2O2)
J6101	OClO + hν → ClO + $O(^3P)$	JX(ip_OClO)
J6200	HCl + hν → Cl + H	JX(ip_HCl)
J6201	HOCl + hν → OH + Cl	JX(ip_HOCl)
J6301	$ClNO_3$ + hν → Cl + NO_3	JX(ip_ClNO3)

Table 2: Photolysis reactions (... continued)

#	reaction	rate coefficient
J6400	$CH_3Cl + h\nu \rightarrow Cl + CH_3O_2$	`JX(ip_CH3Cl)`
J6401	$CCl_4 + h\nu \rightarrow 4\ Cl$	`JX(ip_CCl4)`
J6402	$CH_3CCl_3 + h\nu \rightarrow 3\ Cl$	`JX(ip_CH3CCl3)`
J6500	$CFCl_3 + h\nu \rightarrow 3\ Cl$	`JX(ip_CFCl3)`
J6501	$CF_2Cl_2 + h\nu \rightarrow 2\ Cl$	`JX(ip_CF2Cl2)`
J7000	$Br_2 + h\nu \rightarrow Br + Br$	`JX(ip_Br2)`
J7200	$HOBr + h\nu \rightarrow Br + OH$	`JX(ip_HOBr)`
J7301	$BrNO_3 + h\nu \rightarrow Br + NO_3$	`JX(ip_BrNO3)`
J7400	$CH_3Br + h\nu \rightarrow Br + CH_3O_2$	`JX(ip_CH3Br)`
J7500	$CF_3Br + h\nu \rightarrow Br$	`JX(ip_CF3Br)`
J7600	$BrCl + h\nu \rightarrow Br + Cl$	`JX(ip_BrCl)`
J7601	$CF_2ClBr + h\nu \rightarrow Br + Cl$	`JX(ip_CF2ClBr)`

Notes: J-values are calculated with an external submodel and then supplied to the MECCA chemistry
J6100: Stimpfle et al. (2004) state that the combination of absorption cross sections from Burkholder et al. (1990) and the Cl_2O_2 formation rate coefficient by Sander et al. (2003) can approximately reproduce the observed Cl_2O_2/ClO ratios and ozone depletion. They give an almost zenith-angle independent ratio of 1.4 for Burkholder et al. (1990) to Sander et al. (2003) J-values. The IUPAC recommendation for the Cl_2O_2 formation rate is about 5 to 15 % less than the value by Sander et al. (2003) but more than 20 % larger than the value by Sander et al. (2000). The J-values by Burkholder et al. (1990) are within the uncertainty range of the IUPAC recommendation.

Table 3: Heterogeneous reactions on climatological aerosols

#	reaction	rate coefficient
PSC200	$N_2O_5 + H_2O \rightarrow HNO_3 + HNO_3$	`khet_N2O5_H2O`
PSC410	$HOCl + HCl \rightarrow Cl_2 + H_2O$	`khet_HOCl_HCl`
PSC420	$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	`khet_ClNO3_HCl`
PSC421	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	`khet_ClNO3_H2O`
PSC510	$HOBr + HBr \rightarrow Br_2 + H_2O$	`khet_HOBr_HBr`
PSC520	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	`khet_BrNO3_H2O`
PSC540	$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	`khet_ClNO3_HBr`
PSC541	$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	`khet_BrNO3_HCl`
PSC542	$HOCl + HBr \rightarrow BrCl + H_2O$	`khet_HOCl_HBr`
PSC543	$HOBr + HCl \rightarrow BrCl + H_2O$	`khet_HOBr_HCl`

Notes: These reaction rates are calculated with the HETCHEM submodel and then supplied to the MECCA chemistry (see `http://www.messy-interface.org` for details).

1.2 Cloud and precipitation chemistry

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient
H1000f	Sc	$O_2 \rightarrow O_2(aq)$	`k_exf(KPP_O2)`
H1000b	Sc	$O_2(aq) \rightarrow O_2$	`k_exb(KPP_O2)`
H1001f	ScScm	$O_3 \rightarrow O_3(aq)$	`k_exf(KPP_O3)`
H1001b	ScScm	$O_3(aq) \rightarrow O_3$	`k_exb(KPP_O3)`
H2100f	Sc	$OH \rightarrow OH(aq)$	`k_exf(KPP_OH)`
H2100b	Sc	$OH(aq) \rightarrow OH$	`k_exb(KPP_OH)`
H2101f	Sc	$HO_2 \rightarrow HO_2(aq)$	`k_exf(KPP_HO2)`
H2101b	Sc	$HO_2(aq) \rightarrow HO_2$	`k_exb(KPP_HO2)`
H2102f	ScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	`k_exf(KPP_H2O2)`
H2102b	ScScm	$H_2O_2(aq) \rightarrow H_2O_2$	`k_exb(KPP_H2O2)`
H3100f	Sc	$NO \rightarrow NO(aq)$	`k_exf(KPP_NO)`
H3100b	Sc	$NO(aq) \rightarrow NO$	`k_exb(KPP_NO)`
H3101f	Sc	$NO_2 \rightarrow NO_2(aq)$	`k_exf(KPP_NO2)`
H3101b	Sc	$NO_2(aq) \rightarrow NO_2$	`k_exb(KPP_NO2)`
H3102f	Sc	$NO_3 \rightarrow NO_3(aq)$	`k_exf(KPP_NO3)`
H3102b	Sc	$NO_3(aq) \rightarrow NO_3$	`k_exb(KPP_NO3)`
H3200f	ScScm	$NH_3 \rightarrow NH_3(aq)$	`k_exf(KPP_NH3)`
H3200b	ScScm	$NH_3(aq) \rightarrow NH_3$	`k_exb(KPP_NH3)`
H3201	ScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	`k_exf_N2O5 * C(KPP_H2O_l)`
H3202f	Sc	$HONO \rightarrow HONO(aq)$	`k_exf(KPP_HONO)`
H3202b	Sc	$HONO(aq) \rightarrow HONO$	`k_exb(KPP_HONO)`
H3203f	ScScm	$HNO_3 \rightarrow HNO_3(aq)$	`k_exf(KPP_HNO3)`
H3203b	ScScm	$HNO_3(aq) \rightarrow HNO_3$	`k_exb(KPP_HNO3)`
H3204f	Sc	$HNO_4 \rightarrow HNO_4(aq)$	`k_exf(KPP_HNO4)`
H3204b	Sc	$HNO_4(aq) \rightarrow HNO_4$	`k_exb(KPP_HNO4)`
H4100f	ScScm	$CO_2 \rightarrow CO_2(aq)$	`k_exf(KPP_CO2)`
H4100b	ScScm	$CO_2(aq) \rightarrow CO_2$	`k_exb(KPP_CO2)`
H4101f	ScScm	$HCHO \rightarrow HCHO(aq)$	`k_exf(KPP_HCHO)`
H4101b	ScScm	$HCHO(aq) \rightarrow HCHO$	`k_exb(KPP_HCHO)`
H4102f	Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	`k_exf(KPP_CH3O2)`
H4102b	Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	`k_exb(KPP_CH3O2)`
H4103f	ScScm	$HCOOH \rightarrow HCOOH(aq)$	`k_exf(KPP_HCOOH)`
H4103b	ScScm	$HCOOH(aq) \rightarrow HCOOH$	`k_exb(KPP_HCOOH)`
H4104f	ScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	`k_exf(KPP_CH3OOH)`
H4104b	ScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	`k_exb(KPP_CH3OOH)`
H4105f	Sc	$CH_3OH \rightarrow CH_3OH(aq)$	`k_exf(KPP_CH3OH)`
H4105b	Sc	$CH_3OH(aq) \rightarrow CH_3OH$	`k_exb(KPP_CH3OH)`
H4200f	ScScm	$CH_3COOH \rightarrow CH_3COOH(aq)$	`k_exf(KPP_CH3COOH)`
H4200b	ScScm	$CH_3COOH(aq) \rightarrow CH_3COOH$	`k_exb(KPP_CH3COOH)`
H4201f	Sc	$CH_3CHO \rightarrow CH_3CHO(aq)$	`k_exf(KPP_CH3CHO)`
H4201b	Sc	$CH_3CHO(aq) \rightarrow CH_3CHO$	`k_exb(KPP_CH3CHO)`
H4202f	Sc	$PAN \rightarrow PAN(aq)$	`k_exf(KPP_PAN)`
H4202b	Sc	$PAN(aq) \rightarrow PAN$	`k_exb(KPP_PAN)`
H4300f	Sc	$CH_3COCH_3 \rightarrow CH_3COCH_3(aq)$	`k_exf(KPP_CH3COCH3)`
H4300f	Sc	$CH_3COCH_3(aq) \rightarrow CH_3COCH_3$	`k_exb(KPP_CH3COCH3)`
H6000f	Sc	$Cl_2 \rightarrow Cl_2(aq)$	`k_exf(KPP_Cl2)`
H6000b	Sc	$Cl_2(aq) \rightarrow Cl_2$	`k_exb(KPP_Cl2)`
H6200f	ScScm	$HCl \rightarrow HCl(aq)$	`k_exf(KPP_HCl)`
H6200b	ScScm	$HCl(aq) \rightarrow HCl$	`k_exb(KPP_HCl)`

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient
H6201f	Sc	$HOCl \rightarrow HOCl(aq)$	`k_exf(KPP_HOCl)`
H6201b	Sc	$HOCl(aq) \rightarrow HOCl$	`k_exb(KPP_HOCl)`
H7000f	Sc	$Br_2 \rightarrow Br_2(aq)$	`k_exf(KPP_Br2)`
H7000b	Sc	$Br_2(aq) \rightarrow Br_2$	`k_exb(KPP_Br2)`
H7200f	ScScm	$HBr \rightarrow HBr(aq)$	`k_exf(KPP_HBr)`
H7200b	ScScm	$HBr(aq) \rightarrow HBr$	`k_exb(KPP_HBr)`
H7201f	Sc	$HOBr \rightarrow HOBr(aq)$	`k_exf(KPP_HOBr)`
H7201b	Sc	$HOBr(aq) \rightarrow HOBr$	`k_exb(KPP_HOBr)`
H7600f	Sc	$BrCl \rightarrow BrCl(aq)$	`k_exf(KPP_BrCl)`
H7600b	Sc	$BrCl(aq) \rightarrow BrCl$	`k_exb(KPP_BrCl)`
H9100f	ScScm	$SO_2 \rightarrow SO_2(aq)$	`k_exf(KPP_SO2)`
H9100b	ScScm	$SO_2(aq) \rightarrow SO_2$	`k_exb(KPP_SO2)`
H9200	ScScm	$H_2SO_4 \rightarrow H_2SO_4(aq)$	`k_exf(KPP_H2SO4)`

Notes:
The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_scav_base.f90` using the accommodation coefficients (Table 6) and Henry's law coefficients (Table 5) as described by Tost et al. (2006).

Table 5: Henry's Law Coefficients

Species	$K_0[M/atm]$	$-\Delta_{sol}H/R[K]$	Reference
HNO_3	$1.7 \cdot 10^5$	8694	Lelieveld and Crutzen (1991)
H_2O_2	$1.0 \cdot 10^5$	6338	Lind and Kok (1994)
CH_3OOH	$3.0 \cdot 10^2$	5322	Lind and Kok (1994)
HCHO	$7.0 \cdot 10^3$	6425	Chameides (1984)
HCOOH	$3.7 \cdot 10^3$	5700	Lelieveld and Crutzen (1991)
CH_3COOH	$5.5 \cdot 10^3$	5894	Khan et al. (1995)
O_3	$1.2 \cdot 10^{-2}$	2560	Chameides (1984)
SO_2	1.2	3120	Chameides (1984)
H_2SO_4	$1.0 \cdot 10^{11}$	-	
N_2O_5	1.4	-	Ervens et al. (2003)
PAN	5.0	-	Holdren et al. (1984)
OH	$3.0 \cdot 10^1$	4300	Hanson et al. (1992)
HONO	$4.9 \cdot 10^1$	4780	Chameides (1984)
CO_2	$3.1 \cdot 10^{-2}$	2423	Chameides (1984)
NH_3	58.0	4085	Chameides (1984)
HO_2	$3.9 \cdot 10^3$	5900	Hanson et al. (1992)
NO_3	2.0	2000	Thomas et al. (1993)
NO_2	$6.4 \cdot 10^{-3}$	2500	Lee and Schwartz (1981), for temperature dependence Chameides (1984)
HNO_4	$1.2 \cdot 10^4$	6900	Régimbal and Mozurkewich (1997)
CH_3OH	$2.20 \cdot 10^2$	5390	Snider and Dawson (1985)
CH_3CHO	$1.14 \cdot 10^1$	6254	Betterton and Hoffmann (1988a)
CH_3O_2	6.0	5600	Lelieveld and Crutzen (1991)
$C_2H_5O_2$	6.0	87	Ervens et al. (2003)
NO	$1.9 \cdot 10^{-3}$	1480	Schwartz and White (1981)
CH_3COCH_3	$3.52 \cdot 10^1$	3800	Zhou and Mopper (1990)
HCl	1.2	9001	Brimblecombe and Clegg (1989)
HBr	1.3	10239	Brimblecombe and Clegg (1989)
HOCl	$6.7 \cdot 10^2$	5862	Huthwelker et al. (1995)
HOBr	$9.3 \cdot 10^1$	5862	Vogt et al. (1996)

Table 5: Henry's Law Coefficients

Species	$K_0[M/atm]$	-$\Delta_{sol}H/R[K]$	Reference
BrCl	$9.4 \cdot 10^{-1}$	5600	Bartlett and Margerum (1999)
Cl_2	$9.1 \cdot 10^{-2}$	2500	Wilhelm et al. (1977)
Br_2	$7.6 \cdot 10^{-1}$	4094	Dean (1992)
DMSO	$5.0 \cdot 10^{4}$	6425	De Bruyn et al. (1994)
O_2	$1.3 \cdot 10^{-3}$	1500	Lide and Frederikse (1995)

Table 6: Accommodation Coefficients

Species	α^0	-$\Delta_{sol}H/R[K]$	Reference
HNO_3	0.5	-	Abbatt and Waschewsky (1998)
H_2O_2	0.077	2769	Worsnop et al. (1989)
CH_3OOH	$4.5 \cdot 10^{-3}$	3273	Magi et al. (1997)
HCHO	0.043	-	DeMore et al. (1997)
HCOOH	0.014	3978	DeMore et al. (1997)
CH_3COOH	$1.9 \cdot 10^{-2}$	5894	
O_3	$2.0 \cdot 10^{-3}$	-	DeMore et al. (1997)
SO_2	0.11	-	DeMore et al. (1997)
H_2SO_4	0.65	-	Pöschl et al. (1998)
N_2O_5	0.1	-	DeMore et al. (1997)
PAN	0.1	-	estimated
OH	$1.0 \cdot 10^{-2}$	-	Takami et al. (1998)
HONO	$4.0 \cdot 10^{-2}$	-	DeMore et al. (1997)
CO_2	0.01	2000	estimated
NH_3	$6.0 \cdot 10^{-2}$	-	DeMore et al. (1997)
HO_2	0.2	-	DeMore et al. (1997)
NO_3	$4.0 \cdot 10^{-2}$	-	Rudich et al. (1996)
NO_2	$1.5 \cdot 10^{-3}$	-	Ponche et al. (1993)
HNO_4	0.1	-	DeMore et al. (1997)
CH_3OH	0.1	-	estimated
CH_3CHO	0.03	-	estimated, Ervens et al. (2003)
CH_3O_2	0.01	2000	estimated
$C_2H_5O_2$	$8.2 \cdot 10^{-3}$	-	estimated, Ervens et al. (2003)
NO	0.1	-	estimated
CH_3COCH_3	$1.9 \cdot 10^{-2}$	-	Ervens et al. (2003)
HCl	0.074	3072	Schweitzer et al. (2000)
HBr	0.031	3940	Schweitzer et al. (2000)
HOCl	0.5	-	estimated
HOBr	0.5	-	estimated
BrCl	0.033	-	estimated
Cl_2	0.038	6546	Hu et al. (1995)
Br_2	0.038	6546	Hu et al. (1995)
DMSO	0.048	2578	De Bruyn et al. (1994)
O_2	0.01	2000	estimated

Table 7: Acid-base and other eqilibria

#	labels	reaction	$K_0[M^{m-n}]$	-$\Delta H/R[K]$
EQ20	Sc	$HO_2 \rightleftharpoons O_2^- + H^+$	1.6E-5	
EQ21	ScScm	$H_2O \rightleftharpoons H^+ + OH^-$	1.0E-16	-6716
EQ30	ScScm	$NH_4^+ \rightleftharpoons H^+ + NH_3$	5.88E-10	-2391

Table 7: Acid-base and other eqilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$
EQ31	Sc	$HONO \rightleftharpoons H^+ + NO_2^-$	5.1E-4	-1260
EQ32	ScScm	$HNO_3 \rightleftharpoons H^+ + NO_3^-$	15	8700
EQ33	Sc	$HNO_4 \rightleftharpoons NO_4^- + H^+$	1.E-5	
EQ40	ScScm	$CO_2 \rightleftharpoons H^+ + HCO_3^-$	4.3E-7	-913
EQ41	ScScm	$HCOOH \rightleftharpoons H^+ + HCOO^-$	1.8E-4	
EQ42	ScScm	$CH_3COOH \rightleftharpoons H^+ + CH_3COO^-$	1.75E-5	-46
EQ61	ScScm	$HCl \rightleftharpoons H^+ + Cl^-$	1.7E6	6896
EQ62	Sc	$HOCl \rightleftharpoons H^+ + ClO^-$	3.2E-8	
EQ71	ScScm	$HBr \rightleftharpoons H^+ + Br^-$	1.0E9	
EQ72	Sc	$HOBr \rightleftharpoons H^+ + BrO^-$	2.3E-9	-3091
EQ90	ScScm	$SO_2 \rightleftharpoons H^+ + HSO_3^-$	1.7E-2	2090
EQ91	ScScm	$HSO_3^- \rightleftharpoons H^+ + SO_3^{2-}$	6.0E-8	1120
EQ92	ScScm	$HSO_4^- \rightleftharpoons H^+ + SO_4^{2-}$	1.2E-2	2720
EQ93	ScScm	$H_2SO_4 \rightleftharpoons H^+ + HSO_4^-$	1.0E3	

Notes:

EQ20 Weinstein-Lloyd and Schwartz (1991)
EQ21 Chameides (1984)
EQ30 Chameides (1984)
EQ31 Schwartz and White (1981)
EQ32 Davis and de Bruin (1964)
EQ33 Warneck (1999)
EQ40 Chameides (1984)
EQ41 Weast (1980)
EQ42 see note
EQ61 Marsh and McElroy (1985)
EQ62 Lax (1969)
EQ71 Lax (1969)
EQ72 Kelley and Tartar (1956)
EQ90 Chameides (1984)
EQ91 Chameides (1984)
EQ92 Seinfeld and Pandis (1998)
EQ93 Seinfeld and Pandis (1998)

Table 8: Aqueous phase reactions

#	labels	reaction	$k_0\ [M^{1-n}s^{-1}]$	$-E_a/R[K]$
A1000	Sc	$O_3 + O_2^- \rightarrow OH + OH^-$	1.5E9	
A2100	Sc	$OH + O_2^- \rightarrow OH^-$	1.0E10	
A2101	Sc	$OH + OH \rightarrow H_2O_2$	5.5E9	
A2102	Sc	$HO_2 + O_2^- \rightarrow H_2O_2 + OH^-$	1.0E8	-900
A2103	Sc	$HO_2 + OH \rightarrow H_2O$	7.1E9	
A2104	Sc	$HO_2 + HO_2 \rightarrow H_2O_2$	9.7E5	-2500
A2105	Sc	$H_2O_2 + OH \rightarrow HO_2$	2.7E7	-1684
A3100	Sc	$NO_2^- + O_3 \rightarrow NO_3^-$	5.0E5	-6950
A3101	Sc	$NO_2 + NO_2 \rightarrow HNO_3 + HONO$	1.0E8	
A3102	Sc	$NO_4^- \rightarrow NO_2^-$	8.0E1	
A3200	Sc	$NO_2 + HO_2 \rightarrow HNO_4$	1.8E9	
A3201	Sc	$NO_2^- + OH \rightarrow NO_2 + OH^-$	1.0E10	
A3202	Sc	$NO_3 + OH^- \rightarrow NO_3^- + OH$	8.2E7	-2700
A3203	Sc	$HONO + OH \rightarrow NO_2$	1.0E10	
A3204	Sc	$HONO + H_2O_2 \rightarrow HNO_3$	4.6E3	-6800
A4100	Sc	$CO_3^- + O_2^- \rightarrow HCO_3^- + OH^-$	6.5E8	
A4101	Sc	$CO_3^- + H_2O_2 \rightarrow HCO_3^- + HO_2$	4.3E5	
A4102	Sc	$HCOO^- + CO_3^- \rightarrow 2\ HCO_3^- + HO_2$	1.5E5	
A4103	Sc	$HCOO^- + OH \rightarrow OH^- + HO_2 + CO_2$	3.1E9	-1240
A4104	Sc	$HCO_3^- + OH \rightarrow CO_3^-$	8.5E6	
A4105	Sc	$HCHO + OH \rightarrow HCOOH + HO_2$	7.7E8	-1020

Table 8: Aqueous phase reactions (...continued)

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$
A4106	Sc	$HCOOH + OH \rightarrow HO_2 + CO_2$	1.1E8	-991
A4107	Sc	$CH_3OO + O_2^- \rightarrow CH_3OOH + OH^-$	5.0E7	
A4108	Sc	$CH_3OO + HO_2 \rightarrow CH_3OOH$	4.3E5	
A4109	Sc	$CH_3OH + OH \rightarrow HCHO + HO_2$	9.7E8	
A4110a	Sc	$CH_3OOH + OH \rightarrow CH_3OO$	2.7E7	-1715
A4110b	Sc	$CH_3OOH + OH \rightarrow HCHO + OH$	1.1E7	-1715
A9100	Sc	$SO_3^- + O_2 \rightarrow SO_5^-$	1.5E9	
A9101	ScScm	$SO_3^{2-} + O_3 \rightarrow SO_4^{2-}$	1.5E9	-5300
A9102	Sc	$SO_4^- + O_2^- \rightarrow SO_4^{2-}$	3.5E9	
A9103	Sc	$SO_4^- + SO_3^{2-} \rightarrow SO_3^- + SO_4^{2-}$	4.6E8	
A9104	Sc	$SO_5^- + O_2^- \rightarrow HSO_5^- + OH^-$	2.3E8	
A9200	Sc	$SO_3^{2-} + OH \rightarrow SO_3^- + OH^-$	5.5E9	
A9201	Sc	$SO_4^- + OH \rightarrow HSO_5^-$	1.0E9	
A9202	Sc	$SO_4^- + HO_2 \rightarrow SO_4^{2-} + H^+$	3.5E9	
A9203	Sc	$SO_4^- + H_2O \rightarrow SO_4^{2-} + H^+ + OH$	1.1E1	-1110
A9204	Sc	$SO_4^- + H_2O_2 \rightarrow SO_4^{2-} + H^+ + HO_2$	1.2E7	
A9205	Sc	$HSO_3^- + O_2^- \rightarrow SO_4^{2-} + OH$	3.0E3	
A9206	ScScm	$HSO_3^- + O_3 \rightarrow SO_4^{2-} + H^+$	3.7E5	-5500
A9207	Sc	$HSO_3^- + OH \rightarrow SO_3^-$	4.5E9	
A9208	Sc	$HSO_3^- + HO_2 \rightarrow SO_4^{2-} + OH + H^+$	3.0E3	
A9209	ScScm	$HSO_3^- + H_2O_2 \rightarrow SO_4^{2-} + H^+$	5.2E6	-3650
A9210	Sc	$HSO_3^- + SO_4^- \rightarrow SO_3^- + SO_4^{2-} + H^+$	8.0E8	
A9212	Sc	$HSO_3^- + HSO_5^- \rightarrow 2\ SO_4^{2-} + 2\ H^+$	7.1E6	
A9300	Sc	$SO_3^{2-} + NO_2 \rightarrow SO_4^{2-} + 2\ HONO - NO_2$	2.0E7	
A9301	Sc	$SO_4^- + NO_3^- \rightarrow SO_4^{2-} + NO_3$	5.0E4	
A9302	Sc	$SO_4^{2-} + NO_3 \rightarrow NO_3^- + SO_4^-$	1.0E5	
A9303	Sc	$HSO_3^- + NO_2 \rightarrow HSO_4^- + 2\ HONO - NO_2$	2.0E7	
A9304	Sc	$HSO_3^- + NO_3 \rightarrow SO_3^- + NO_3^- + H^+$	1.4E9	-2000
A9305	Sc	$HSO_3^- + HNO_4 \rightarrow HSO_4^- + NO_3^- + H^+$	3.1E5	
A9400	Sc	$SO_3^{2-} + HCHO \rightarrow CH_2OHSO_3^- + OH^-$	1.4E4	
A9401	Sc	$SO_3^{2-} + CH_3OOH \rightarrow SO_4^{2-} + CH_3OH$	1.6E7	-3800
A9402	Sc	$HSO_3^- + HCHO \rightarrow CH_2OHSO_3^-$	4.3E-1	
A9403	Sc	$HSO_3^- + CH_3OOH \rightarrow SO_4^{2-} + H^+ + CH_3OH$	1.6E7	-3800
A9404	Sc	$CH_2OHSO_3^- + OH^- \rightarrow SO_3^{2-} + HCHO$	3.6E3	

Notes:

A1000: Sehested et al. (1983)
A2100: Sehested et al. (1968)
A2101: Buxton et al. (1988)
A2102: Christensen and Sehested (1988)
A2103: Sehested et al. (1968)
A2104: Christensen and Sehested (1988)
A2105: Christensen et al. (1982)
A3100: Damschen and Martin (1983)
A3101: Lee and Schwartz (1981)
A3102: Warneck (1999)
A3200: Warneck (1999)
A3201: Wingenter et al. (1999)
A3202: Exner et al. (1992)
A3203: Barker et al. (1970)
A3204: Damschen and Martin (1983)
A4100: Ross et al. (1992)
A4101: Ross et al. (1992)
A4102: Ross et al. (1992)
A4103: Chin and Wine (1994)
A4104: Ross et al. (1992)
A4105: Chin and Wine (1994)
A4106: Chin and Wine (1994)
A4107: Jacob (1986)
A4108: Jacob (1986)
A4109: Buxton et al. (1988)
A4110a,b: Jacob (1986)
A9100: Huie and Neta (1987)
A9101: Hoffmann (1986)
A9102: Jiang et al. (1992)
A9103: Huie and Neta (1987)

A9104: Buxton et al. (1996)
A9200: Buxton et al. (1988)
A9201: Jiang et al. (1992)
A9202: Jiang et al. (1992)
A9203: Herrmann et al. (1995)
A9204: Wine et al. (1989)
A9205: D. Sedlak, pers. comm. (1993)
A9206: Hoffmann (1986)
A9207: Buxton et al. (1988)
A9208: D. Sedlak, pers. comm. (1993)
A9209: Martin and Damschen (1981)
A9210: Huie and Neta (1987)
A9212: Betterton and Hoffmann (1988b)
A9300: Clifton et al. (1988)
A9301: Exner et al. (1992)
A9302: Logager et al. (1993)
A9303: Clifton et al. (1988)
A9304: Exner et al. (1992)
A9305: Warneck (1999)
A9400: Boyce and Hoffmann (1984)
A9401: Lind et al. (1987)
A9402: Boyce and Hoffmann (1984)
A9403: Lind et al. (1987)
A9404: Seinfeld and Pandis (1998)

Table 9: Photolysis reactions

#	labels	reaction	rate coefficient
PH2100	Sc	$H_2O_2 + h\nu \rightarrow 2\ OH$	`JX(ip_H2O2) * 2.33`

Notes: J-values are calculated with an external submodel and then supplied to the SCAV chemistry.

2 pH values for the NADP network

In this section the comparison of the pH values of the model simulation and the NADP network are shown.

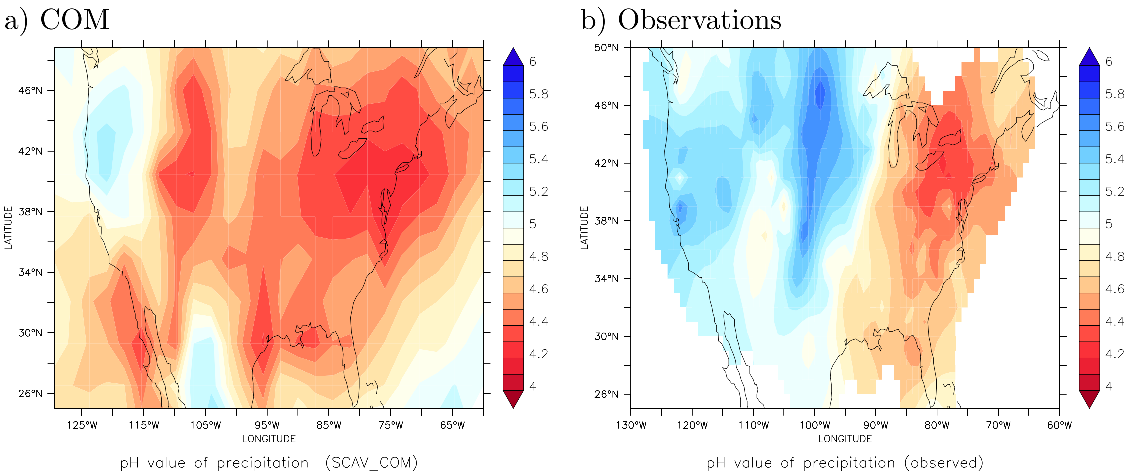
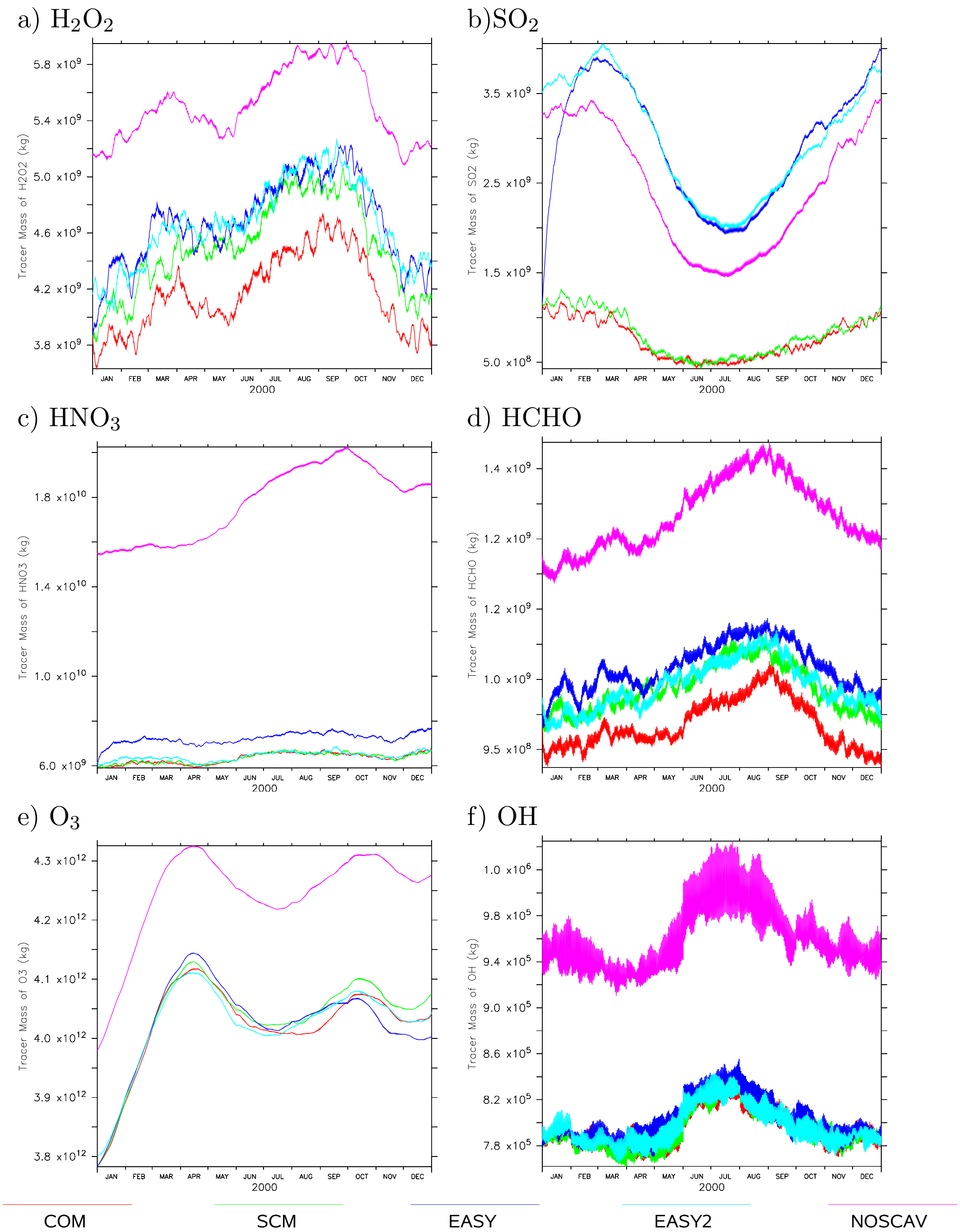


Figure 1: Average pH values for the year 2000 in the for the COM model simulation and the NADP network.

3 Global tracer masses

In this section the globally integrated tracer mass for the four sensitivity studies is presented for hydrogen peroxide (H_2O_2), sulphur dioxide (SO_2), nitric acid (HNO_3), formaldehyde (HCHO) and ozone (O_3). The red lines denote the COM simulation, green the SCM, blue the EASY, turquoise the EASY2 and magenta the NOSCAV simulation, respectively.

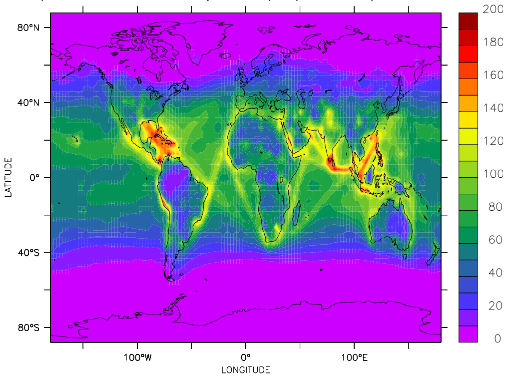


4 Surface layer distributions, comparing the individual simulations additional species

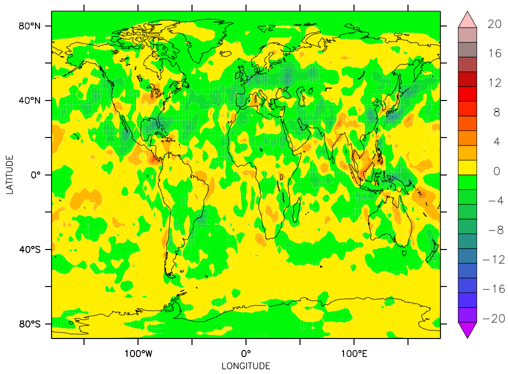
4.1 Hydroxyl radical (OH)

In this section the annual average surface layer trace gas mixing ratios of OH are presented. The upper left panel shows the absolute values of the COM simulation, and the other panels the absolute differences to the COM simulation.

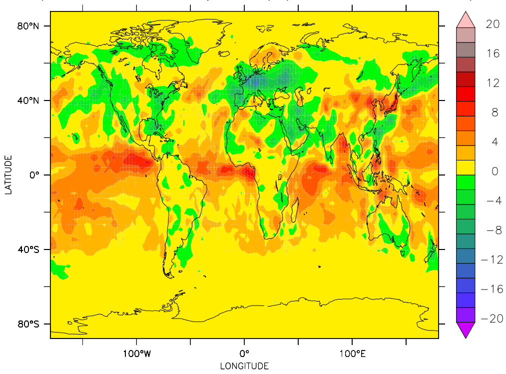
a) OH surface layer mixing ratio
(in 10^{-15} mol/mol) (COM)



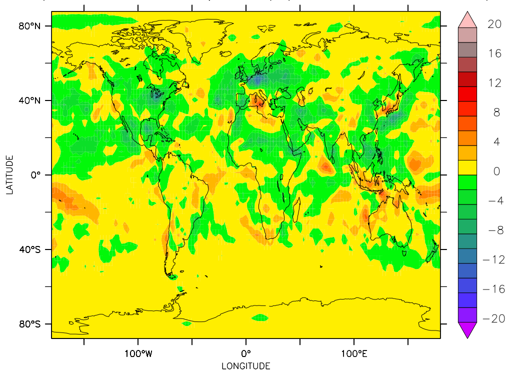
b) absolute difference
(in 10^{-15} mol/mol) (SCM - COM)



c) absolute difference
(in 10^{-15} mol/mol)(EASY - COM)

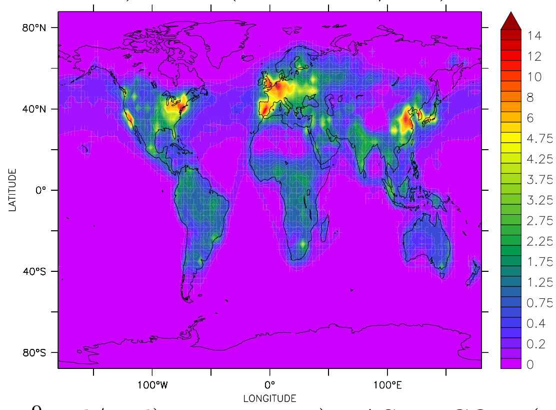


d) absolute difference
(in 10^{-15} mol/mol)(EASY2 - COM)

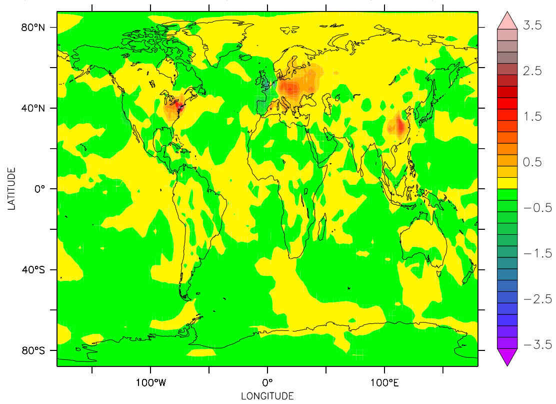


4.2 NO_x

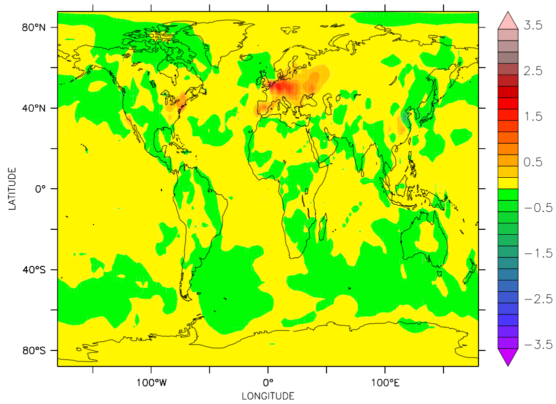
a) COM (in 10^{-9}mol/mol)



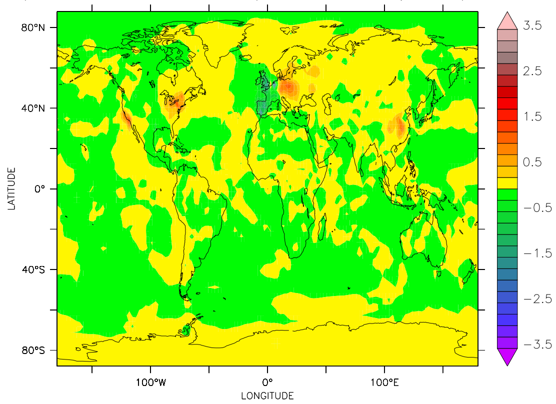
b) SCM - COM (in 10^{-9}mol/mol)



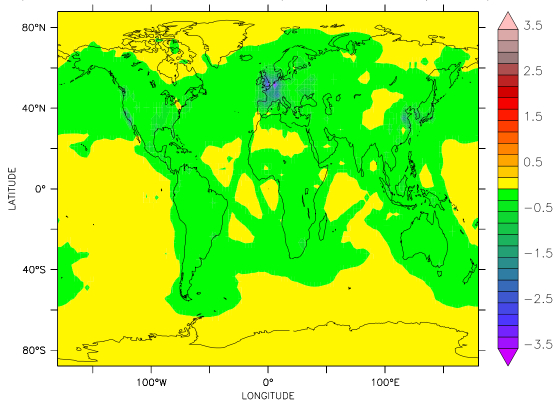
c) EASY - COM (in 10^{-9}mol/mol)



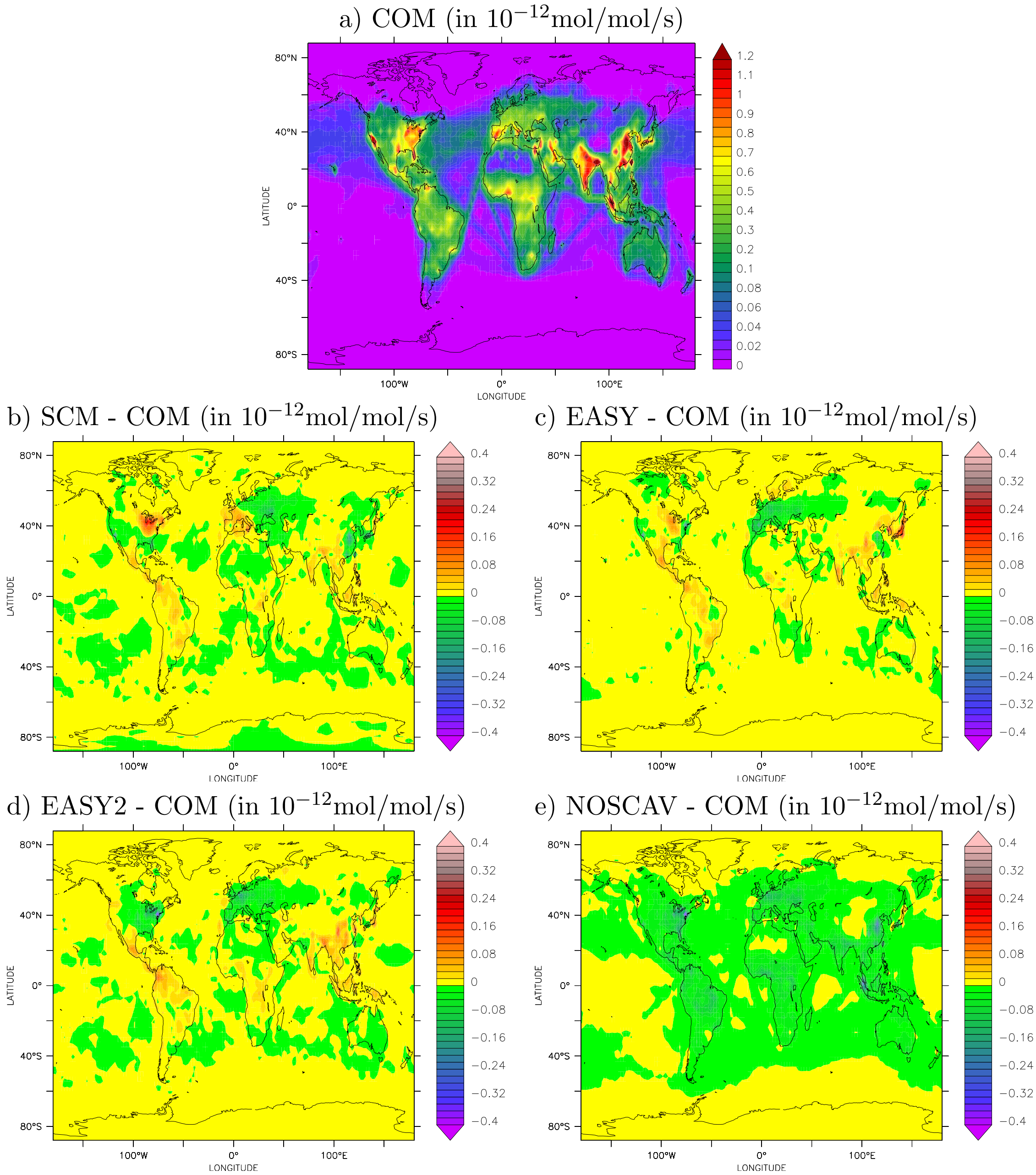
d) EASY2 - COM (in 10^{-9}mol/mol)



e) NOSCAV - COM (in 10^{-9}mol/mol)



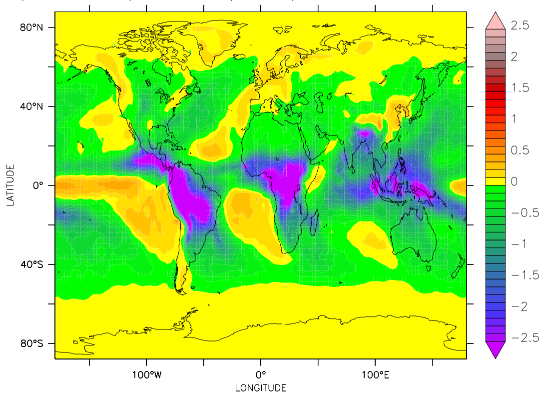
4.3 O_3 production from NO



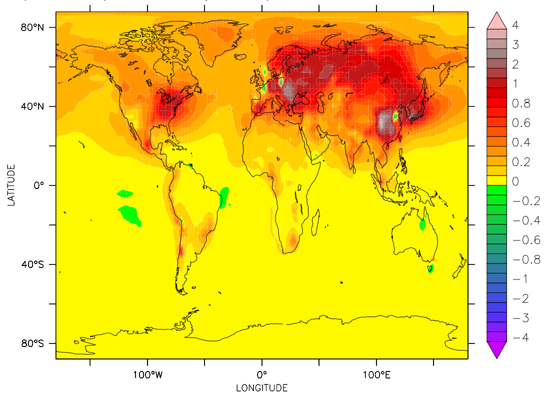
5 Surface layer trace gas distributions of the NOSCAV simulation

In this section the annual average surface layer trace gas mixing ratio differences (NOSCAV - COM) of the NOSCAV simulation are presented. Since this simulation setup without a sink in the liquid phase is hardly realistic, the Figures are shown here in the supplement, completing the Figures 6, 8, 10, 12 and 14 of the main manuscript.

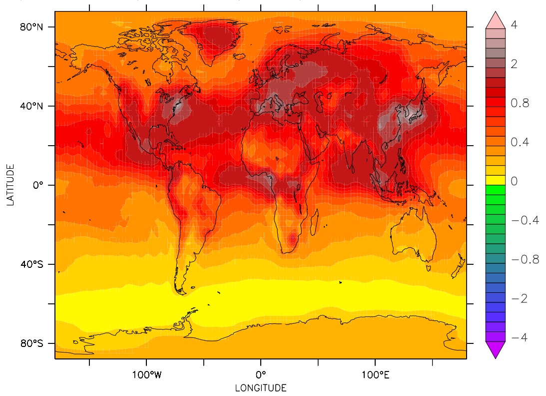
a) H_2O_2 (in nmol/mol)



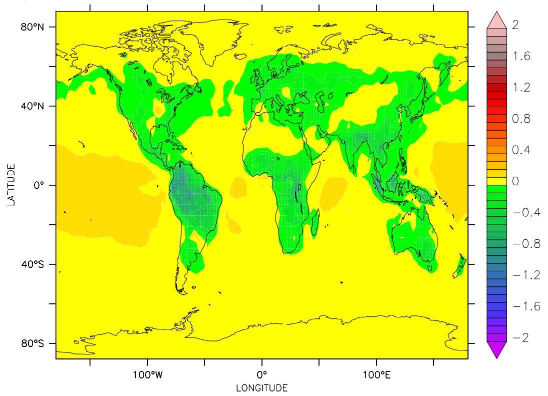
b)SO_2 (in nmol/mol)



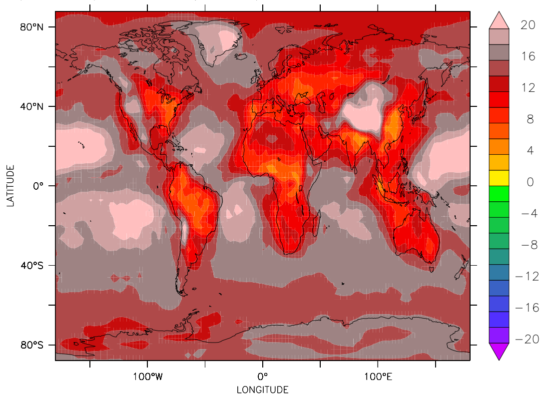
c) HNO_3 (in nmol/mol)



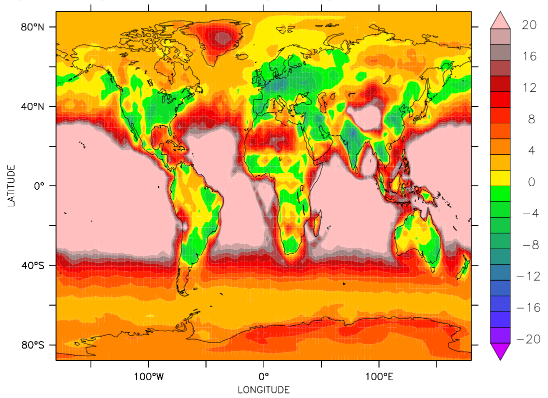
d) HCHO (in nmol/mol)



e) O_3 (in nmol/mol)



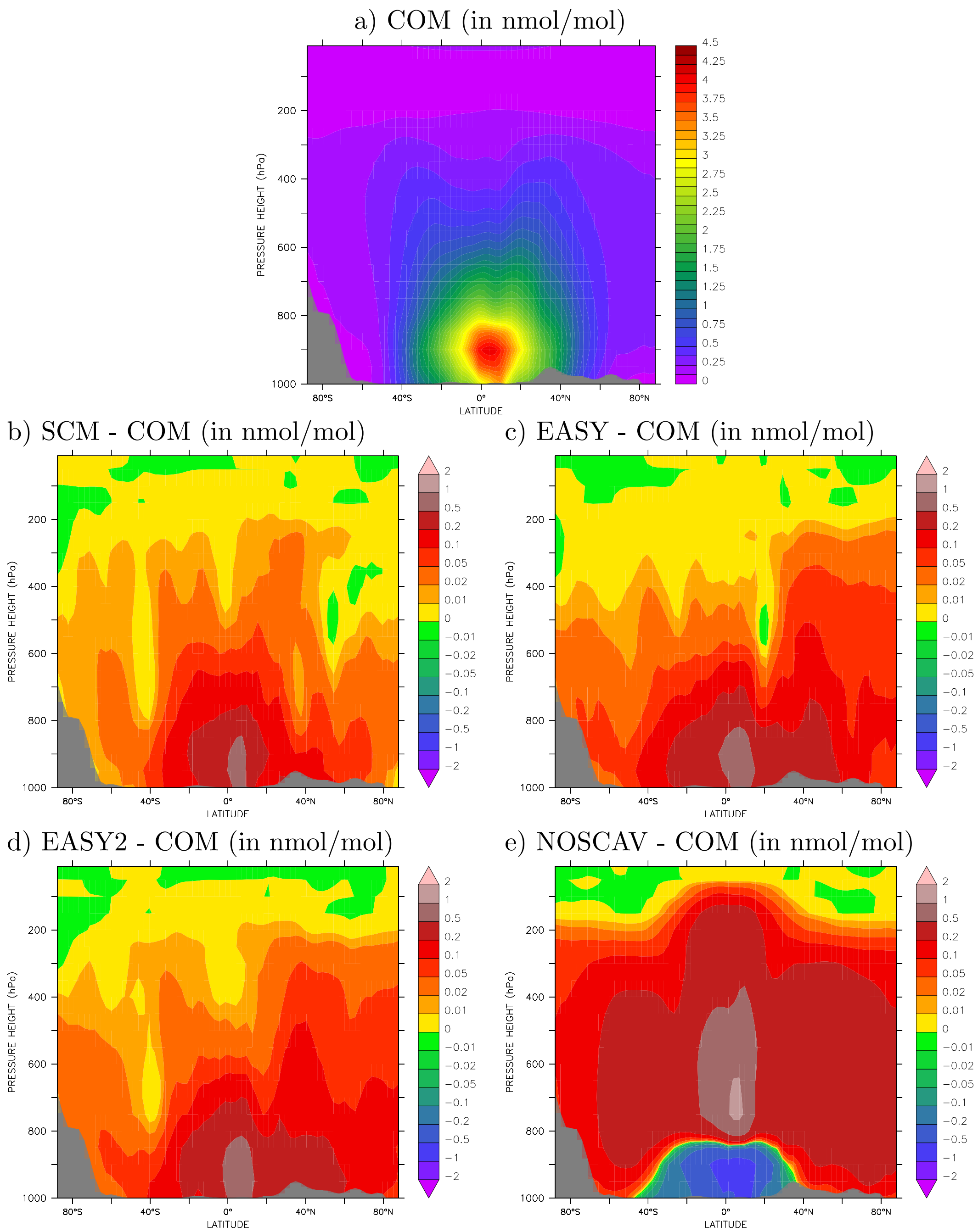
f) OH (in 10^{-15} mol/mol)



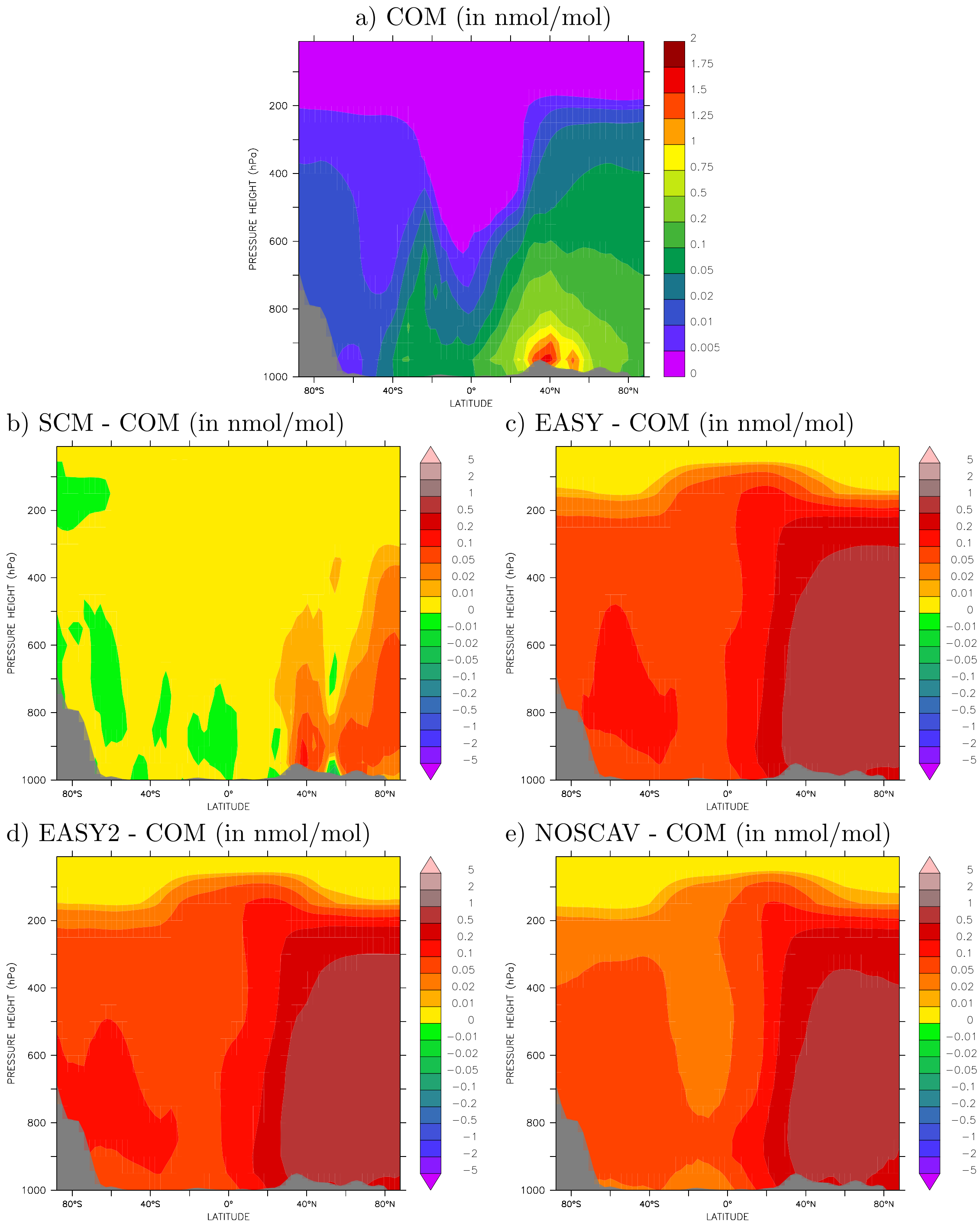
6 Zonal average trace gas distributions, comparing the individual simulations

In this section the zonal annual average trace gas mixing ratios are shown. For the COM simulation the absolute values are presented and the absolute differences for the other four sensitivity runs.

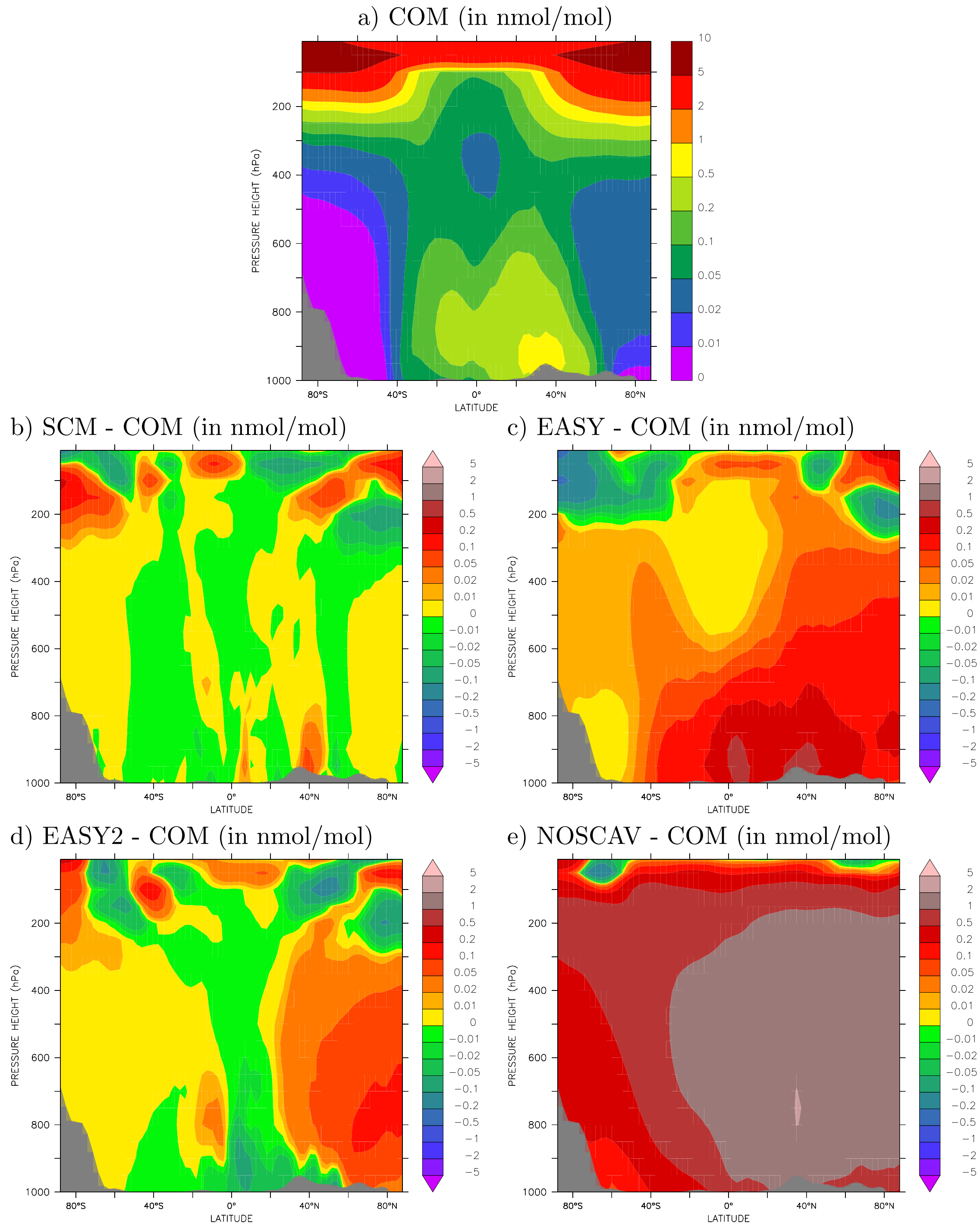
6.1 Hydrogen peroxide (H_2O_2)



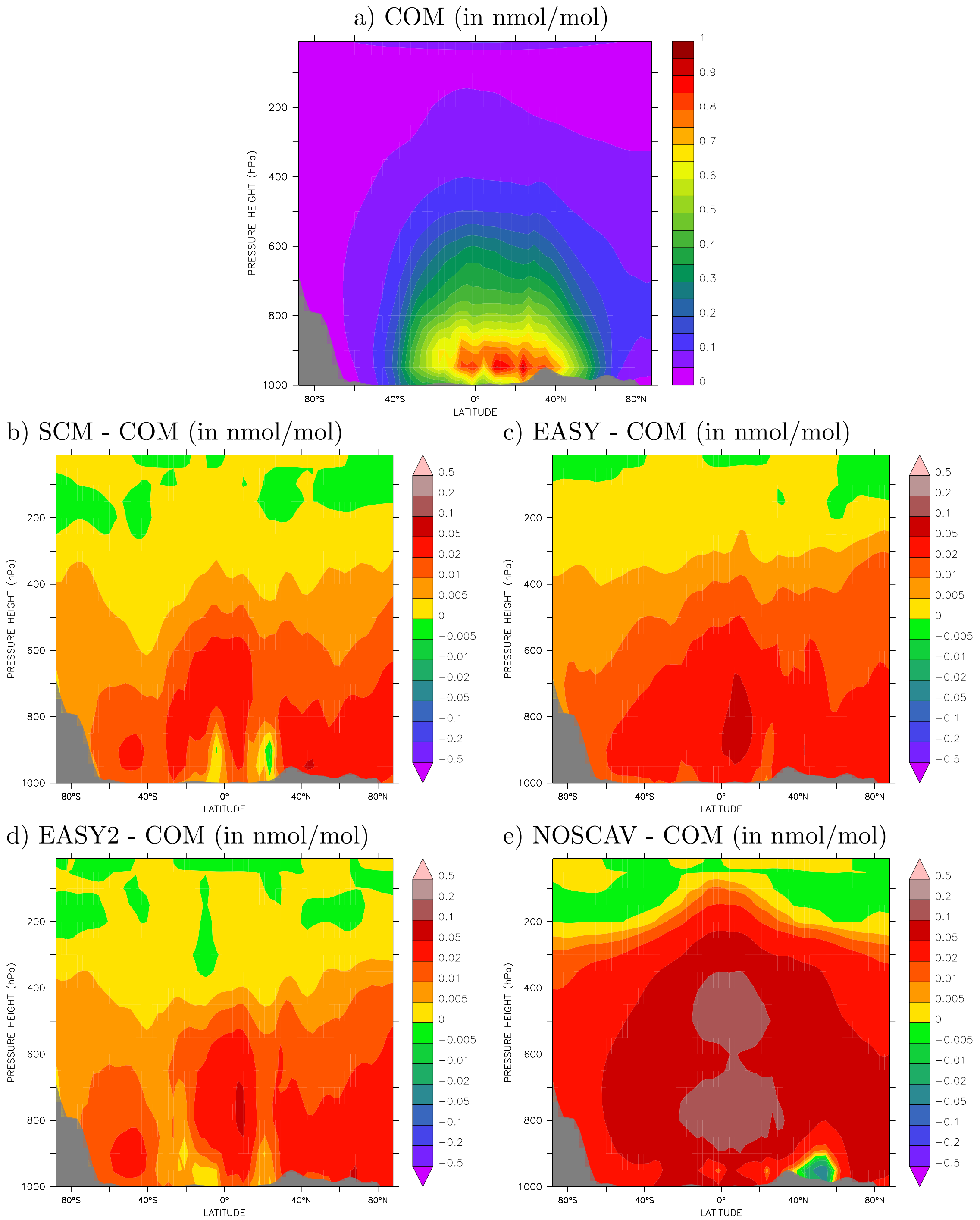
6.2 Sulphur dioxide (SO_2)



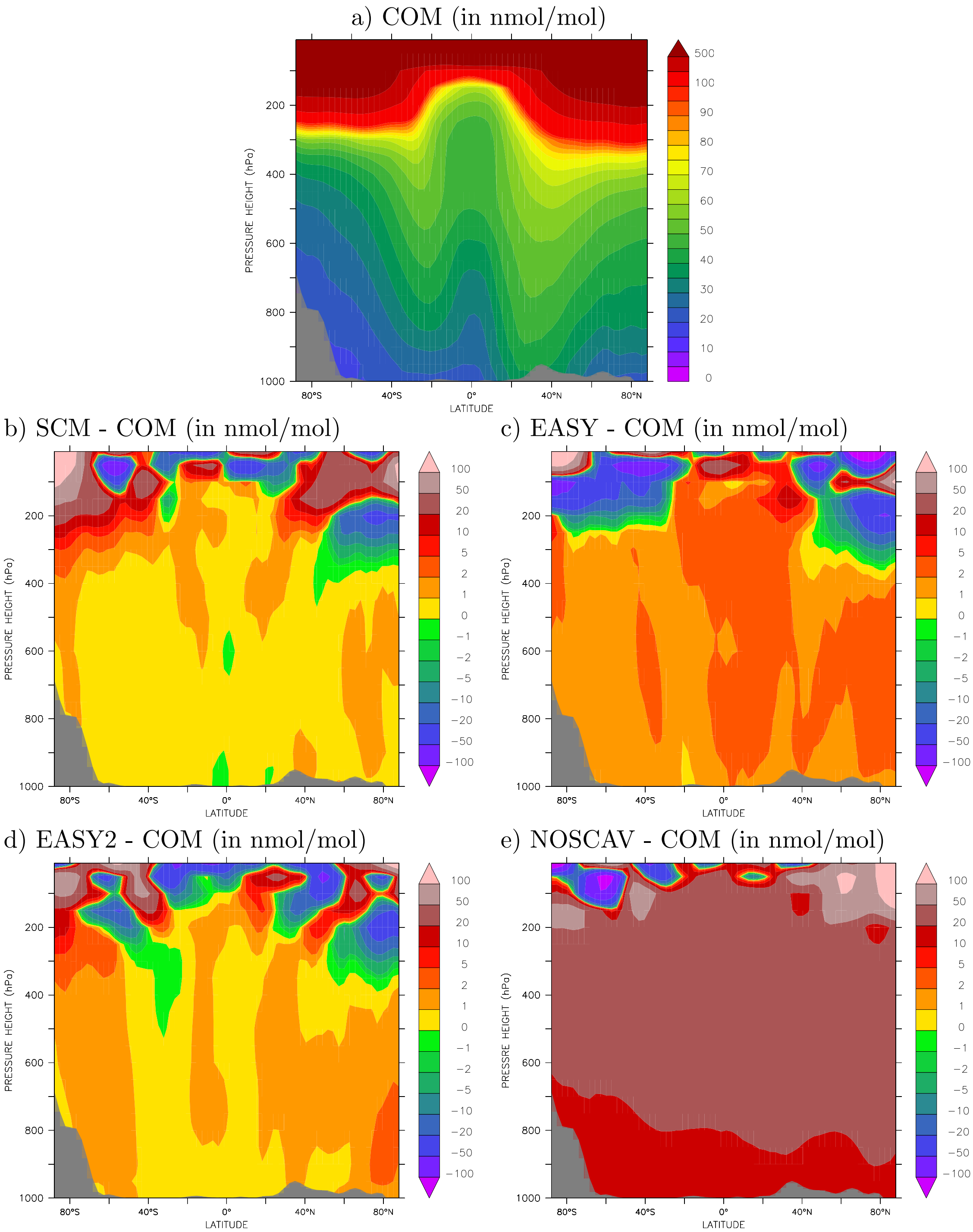
6.3 Nitric acid (HNO_3)



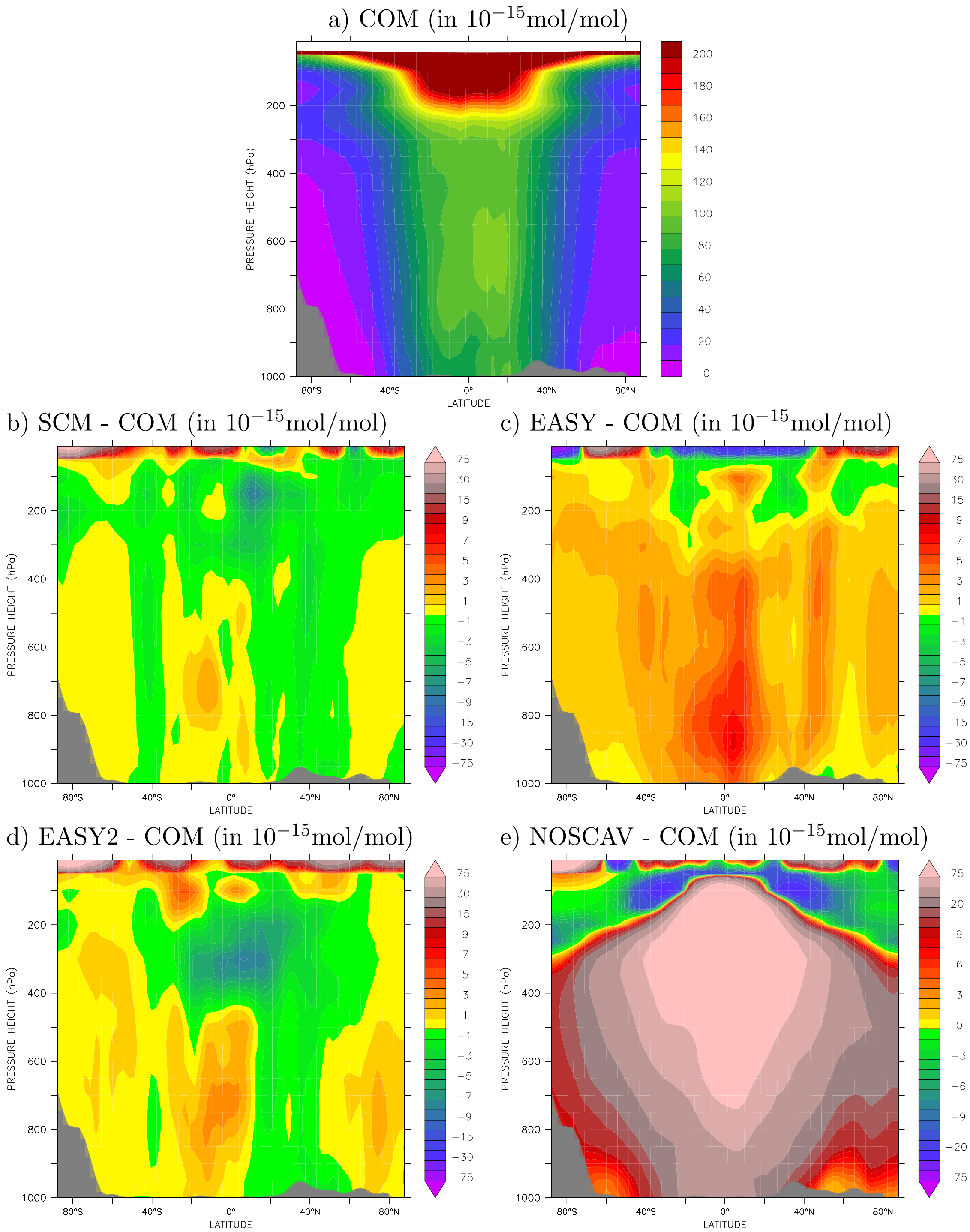
6.4 Formaldehyde (HCHO)



6.5 Ozone (O_3)


a) COM (in nmol/mol)
b) SCM - COM (in nmol/mol)
c) EASY - COM (in nmol/mol)
d) EASY2 - COM (in nmol/mol)
e) NOSCAV - COM (in nmol/mol)
PRESSURE HEIGHT (hPa)
LATITUDE
80°S
40°S
0°
40°N
80°N
200
400
600
800
1000
500
100
90
80
70
60
50
40
30
20
10
0
100
50
20
10
5
2
1
0
−1
−2
−5
−10
−20
−50
−100

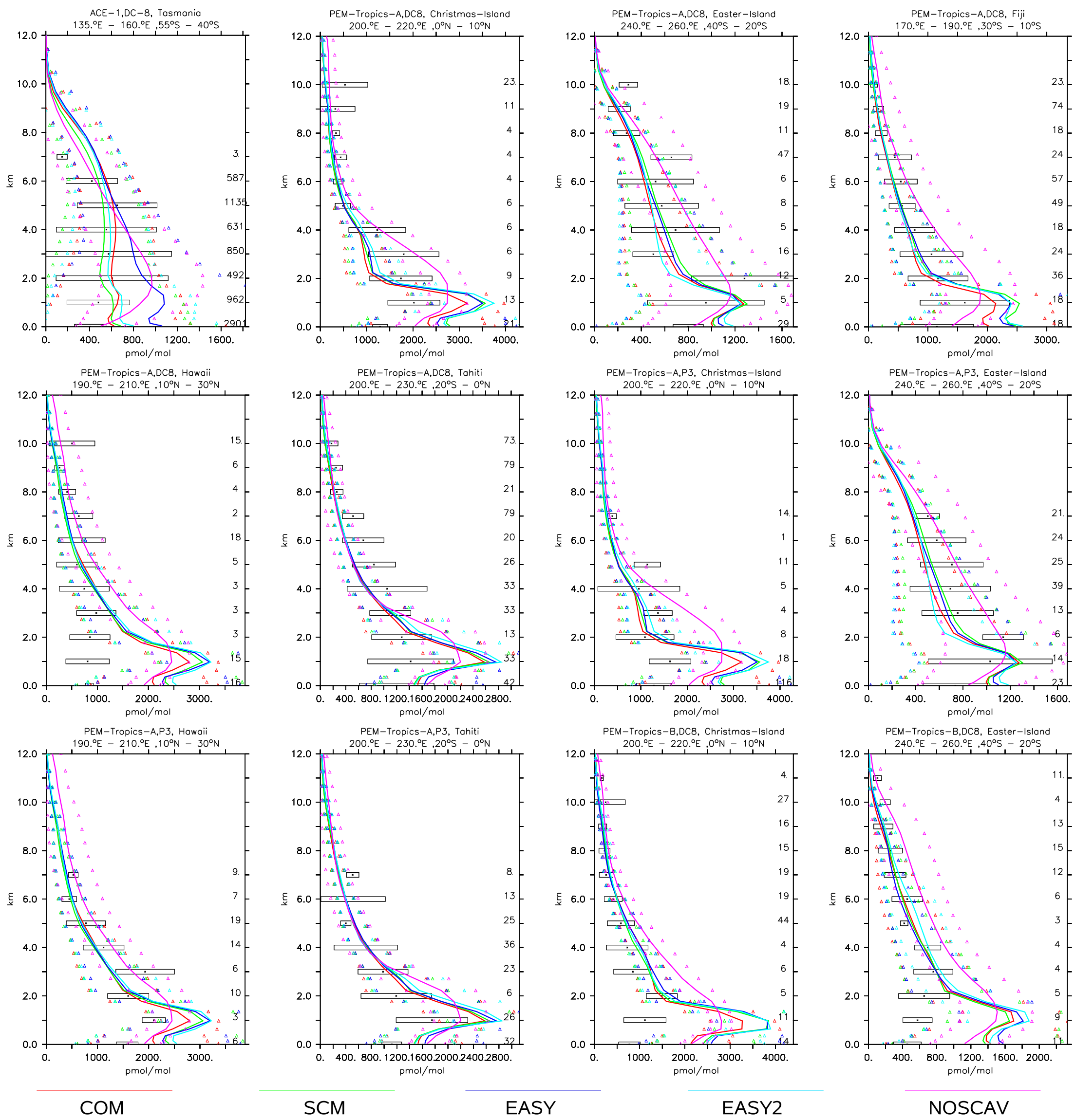
6.6 Hydroxyl radical (OH)

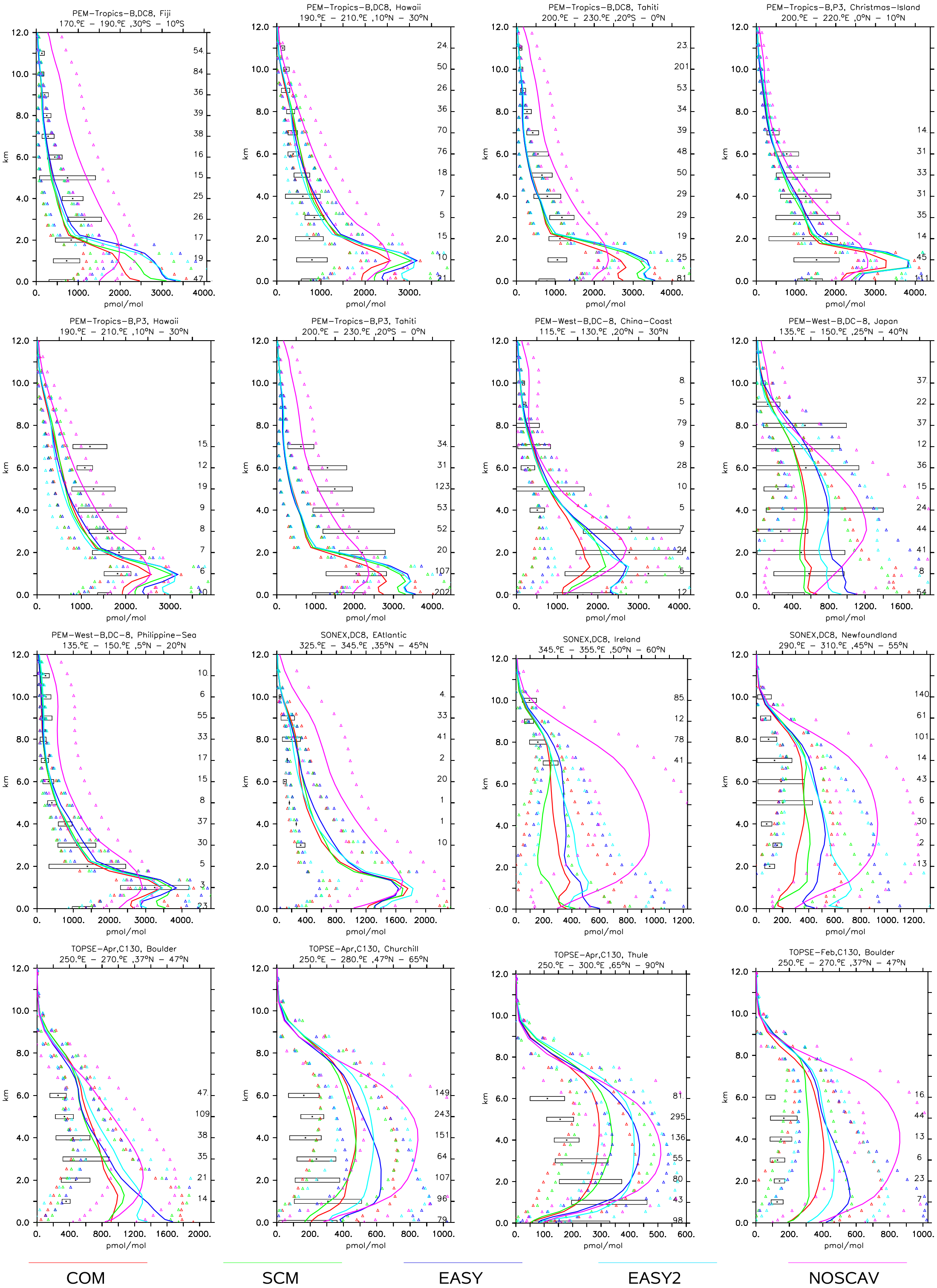


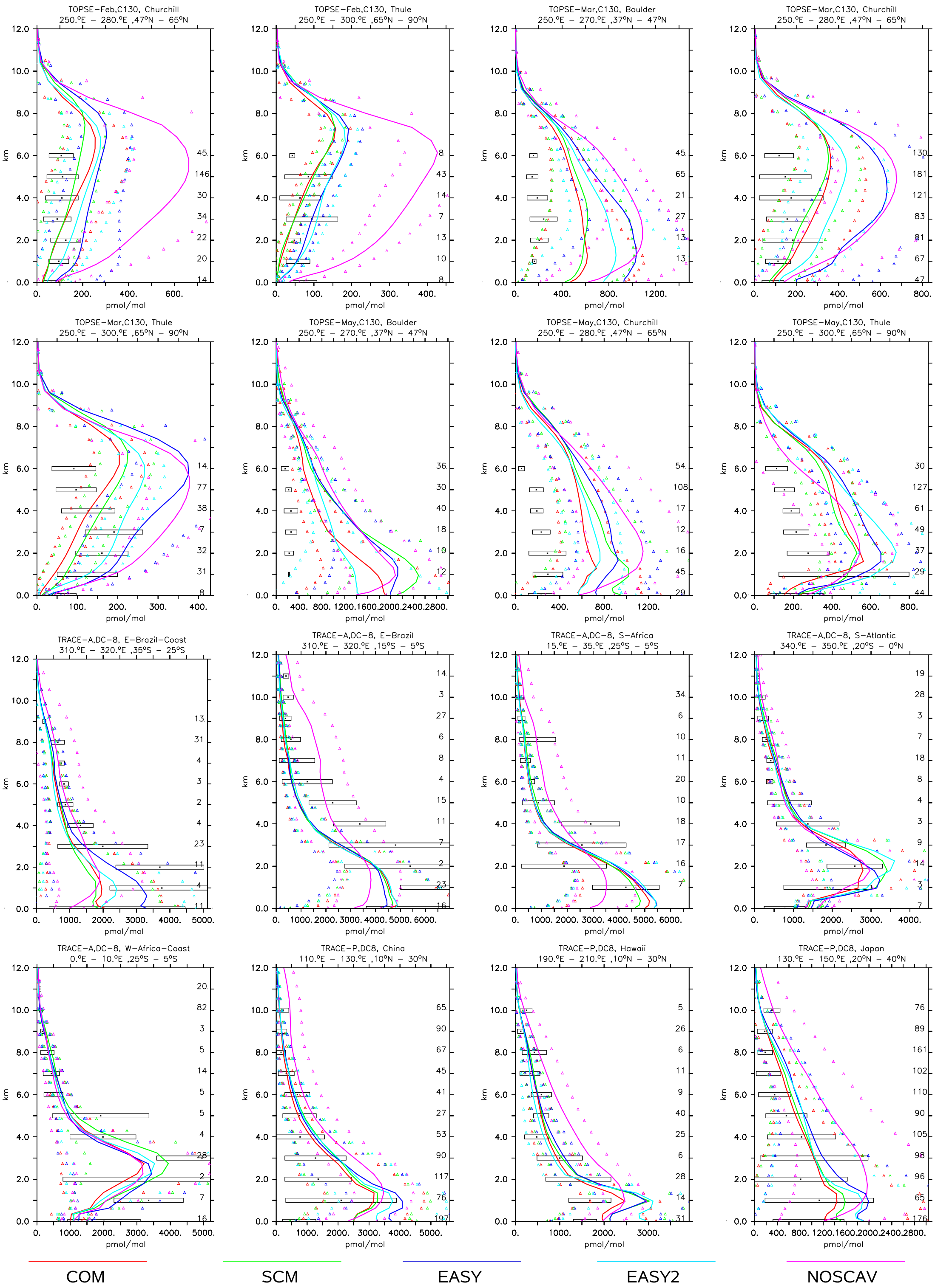
7 Comparison of the simulation results with the Emmons et al. (2000) observation dataset

In this section additional results of the analysed species are presented to achieve a more comprehensive view. All following figures show the observations as the black boxes (the center is the average value from the measurements and the box width the standard deviation), and the coloured lines the simulations (the continuous line represents the mean value and the dotted lines the mean value $\pm$ σ (one standard deviation)); red denotes the COM simulation, green the SCM, blue the EASY, turquoise the EASY2 and magenta the NOSCAV simulation, respectively. The scaling is selected such that the observations are properly represented. However, this may lead to simulated values running off scale, showing that these model simulations do not represent the measurements.

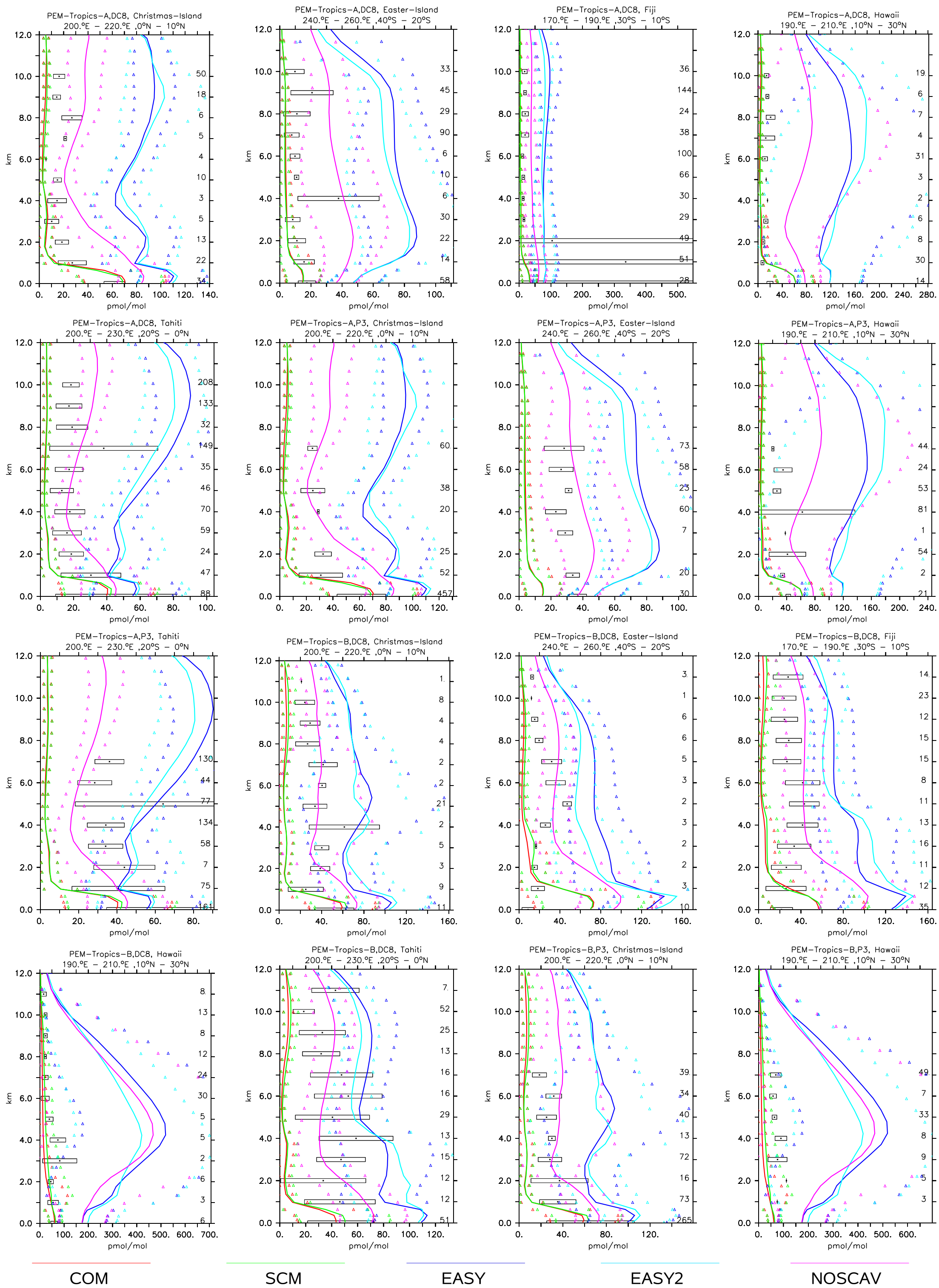
7.1 Hydrogen peroxide (H_2O_2)

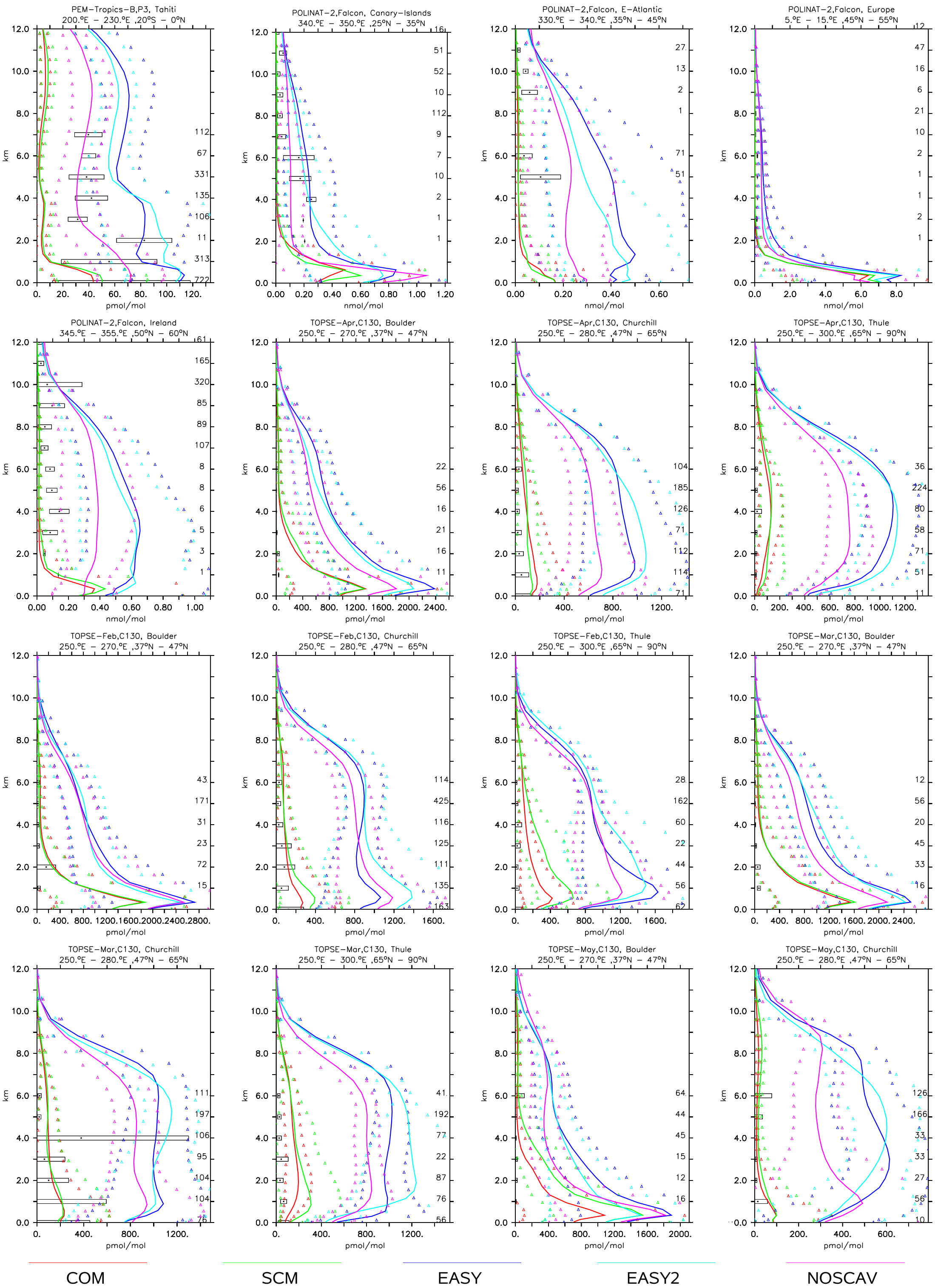


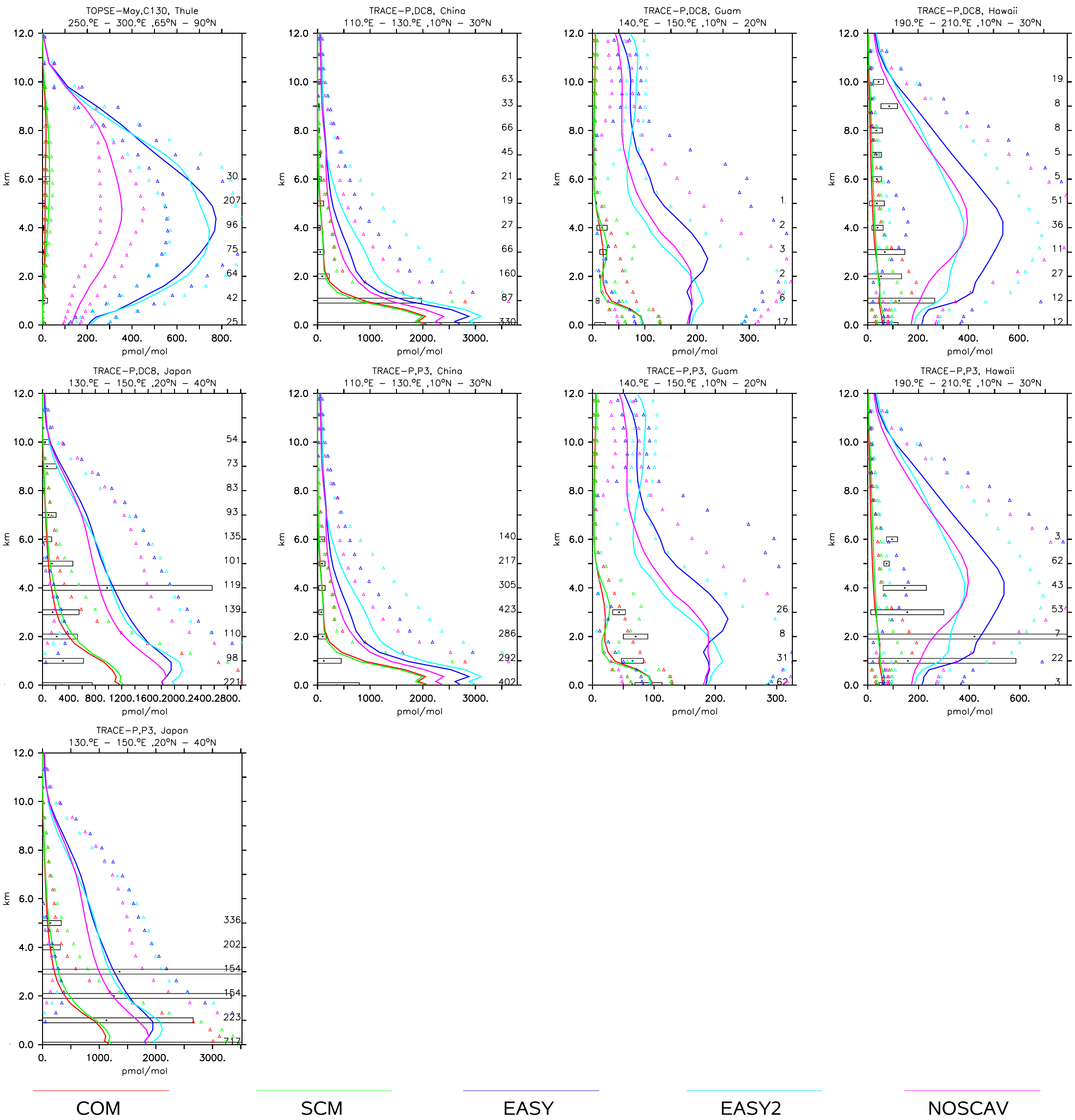

PEM−Tropics−B,DC8, Fiji
170.°E − 190.°E ,30°S − 10°S
PEM−Tropics−B,DC8, Hawaii
190.°E − 210.°E ,10°N − 30°N
PEM−Tropics−B,DC8, Tahiti
200.°E − 230.°E ,20°S − 0°N
PEM−Tropics−B,P3, Christmas−Island
200.°E − 220.°E ,0°N − 10°N
PEM−Tropics−B,P3, Hawaii
190.°E − 210.°E ,10°N − 30°N
PEM−Tropics−B,P3, Tahiti
200.°E − 230.°E ,20°S − 0°N
PEM−West−B,DC−8, China−Coast
115.°E − 130.°E ,20°N − 30°N
PEM−West−B,DC−8, Japan
135.°E − 150.°E ,25°N − 40°N
PEM−West−B,DC−8, Philippine−Sea
135.°E − 150.°E ,5°N − 20°N
SONEX,DC8, EAtlantic
325.°E − 345.°E ,35°N − 45°N
SONEX,DC8, Ireland
345.°E − 355.°E ,50°N − 60°N
SONEX,DC8, Newfoundland
290.°E − 310.°E ,45°N − 55°N
TOPSE−Apr,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Apr,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Apr,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−Feb,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
km
pmol/mol
COM
SCM
EASY
EASY2
NOSCAV


TOPSE−Feb,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Feb,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−Mar,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Mar,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Mar,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−May,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−May,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−May,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TRACE−A,DC−8, E−Brazil−Coast
310.°E − 320.°E ,35°S − 25°S
TRACE−A,DC−8, E−Brazil
310.°E − 320.°E ,15°S − 5°S
TRACE−A,DC−8, S−Africa
15.°E − 35.°E ,25°S − 5°S
TRACE−A,DC−8, S−Atlantic
340.°E − 350.°E ,20°S − 0°N
TRACE−A,DC−8, W−Africa−Coast
0.°E − 10.°E ,25°S − 5°S
TRACE−P,DC8, China
110.°E − 130.°E ,10°N − 30°N
TRACE−P,DC8, Hawaii
190.°E − 210.°E ,10°N − 30°N
TRACE−P,DC8, Japan
130.°E − 150.°E ,20°N − 40°N
km
pmol/mol
COM
SCM
EASY
EASY2
NOSCAV

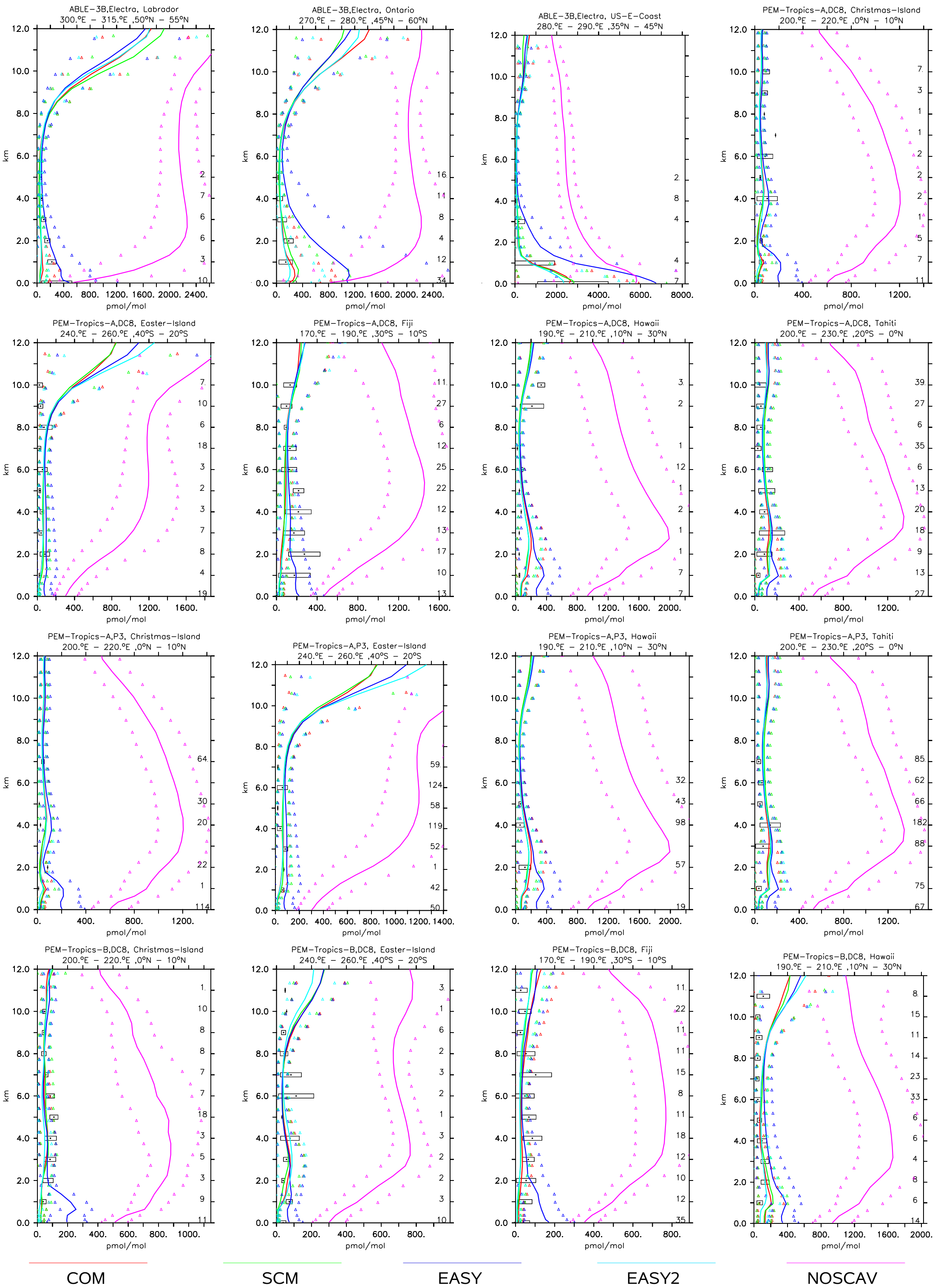
7.2 Sulphur dioxide (SO_2)

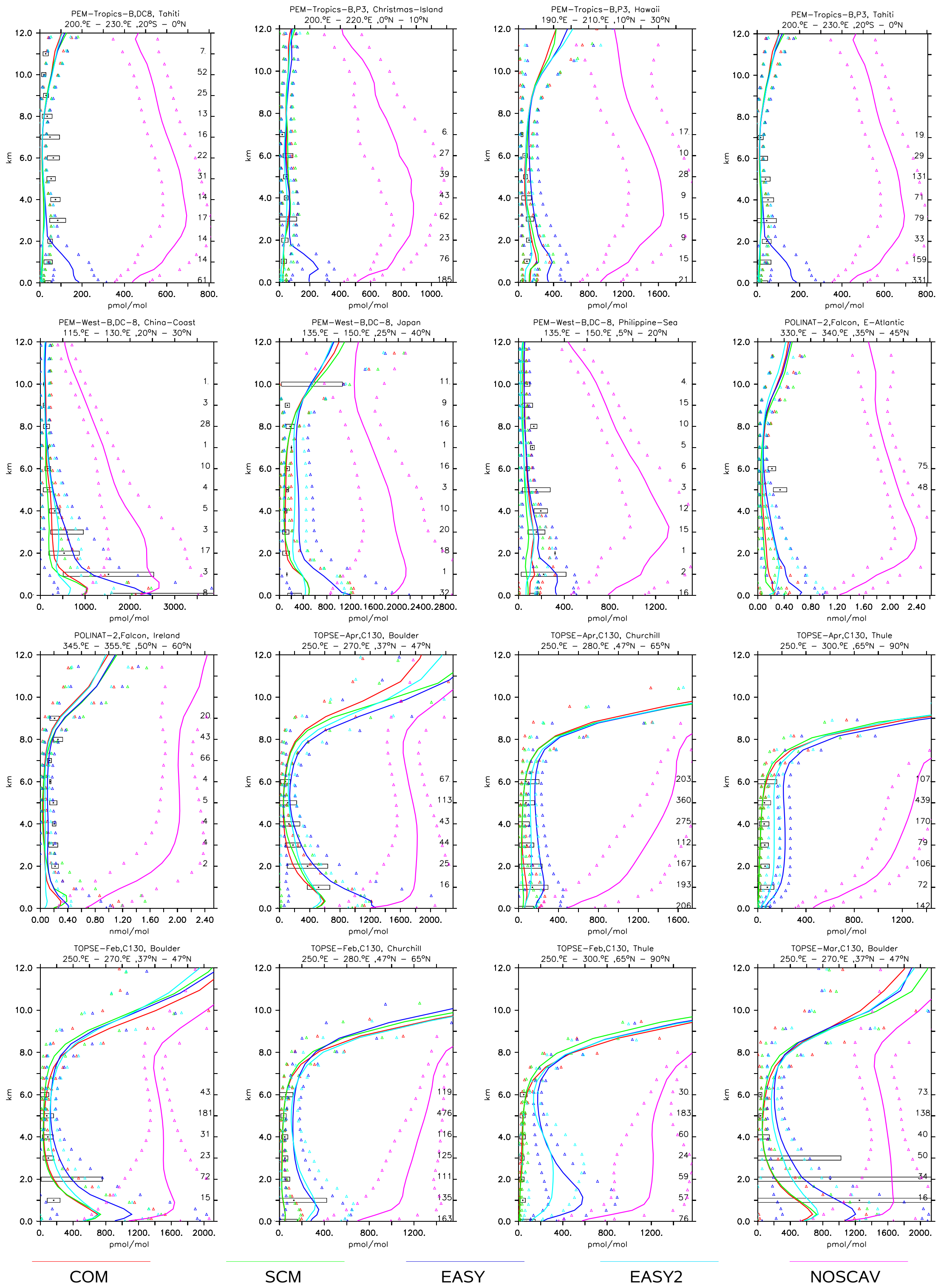


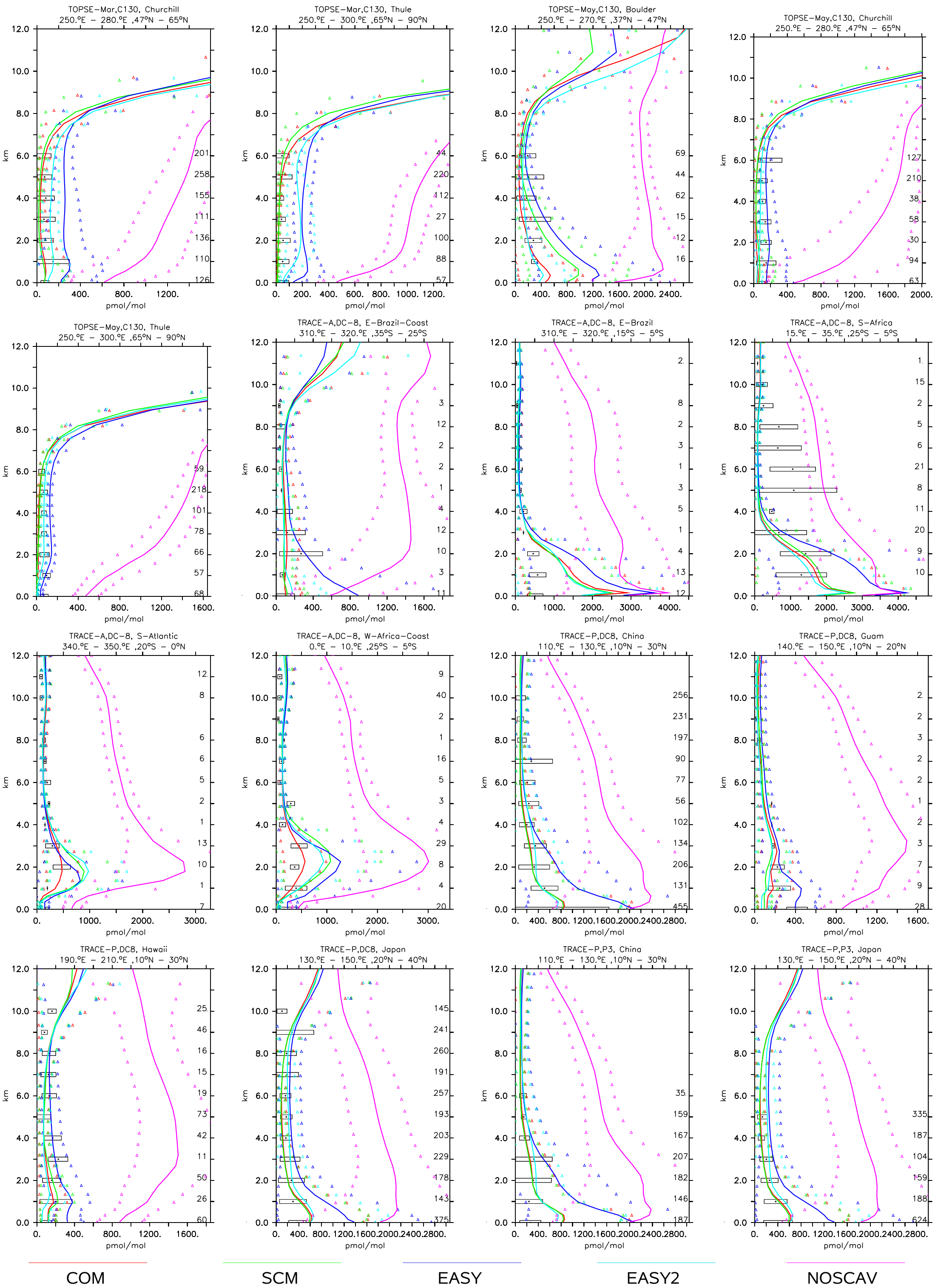

PEM−Tropics−B,P3, Tahiti
200.°E − 230.°E ,20°S − 0°N
POLINAT−2,Falcon, Canary−Islands
340.°E − 350.°E ,25°N − 35°N
POLINAT−2,Falcon, E−Atlantic
330.°E − 340.°E ,35°N − 45°N
POLINAT−2,Falcon, Europe
5.°E − 15.°E ,45°N − 55°N
POLINAT−2,Falcon, Ireland
345.°E − 355.°E ,50°N − 60°N
TOPSE−Apr,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Apr,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Apr,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−Feb,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Feb,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Feb,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−Mar,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Mar,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Mar,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−May,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−May,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
km
pmol/mol
nmol/mol
COM
SCM
EASY
EASY2
NOSCAV


TOPSE−May,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TRACE−P,DC8, China
110.°E − 130.°E ,10°N − 30°N
TRACE−P,DC8, Guam
140.°E − 150.°E ,10°N − 20°N
TRACE−P,DC8, Hawaii
190.°E − 210.°E ,10°N − 30°N
TRACE−P,DC8, Japan
130.°E − 150.°E ,20°N − 40°N
TRACE−P,P3, China
110.°E − 130.°E ,10°N − 30°N
TRACE−P,P3, Guam
140.°E − 150.°E ,10°N − 20°N
TRACE−P,P3, Hawaii
190.°E − 210.°E ,10°N − 30°N
TRACE−P,P3, Japan
130.°E − 150.°E ,20°N − 40°N
km
pmol/mol
COM
SCM
EASY
EASY2
NOSCAV

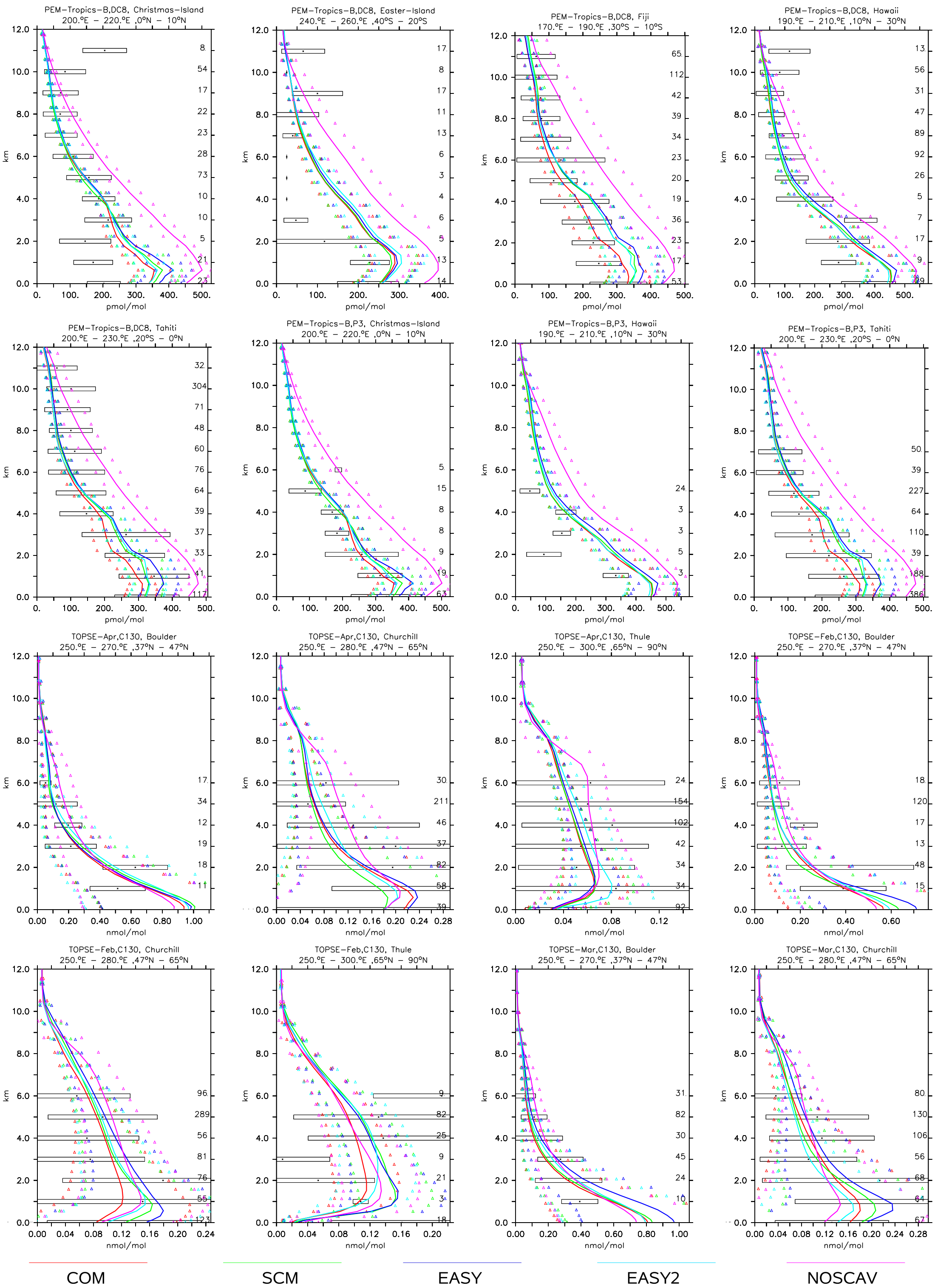
7.3 Nitric Acid (HNO_3)

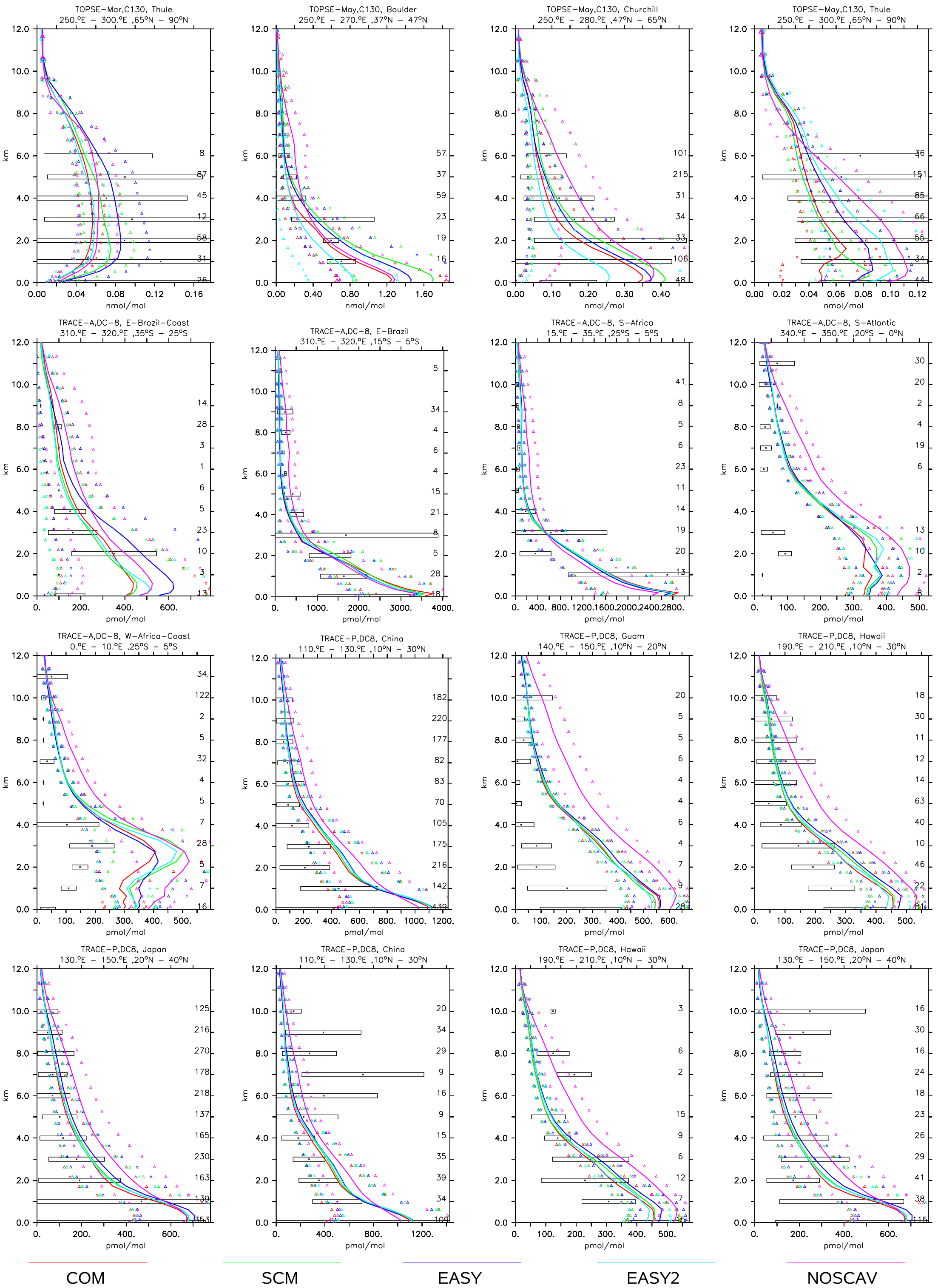



PEM−Tropics−B,DC8, Tahiti
200.°E − 230.°E ,20°S − 0°N
PEM−Tropics−B,P3, Christmas−Island
200.°E − 220.°E ,0°N − 10°N
PEM−Tropics−B,P3, Hawaii
190.°E − 210.°E ,10°N − 30°N
PEM−Tropics−B,P3, Tahiti
200.°E − 230.°E ,20°S − 0°N
PEM−West−B,DC−8, China−Coast
115.°E − 130.°E ,20°N − 30°N
PEM−West−B,DC−8, Japan
135.°E − 150.°E ,25°N − 40°N
PEM−West−B,DC−8, Philippine−Sea
135.°E − 150.°E ,5°N − 20°N
POLINAT−2,Falcon, E−Atlantic
330.°E − 340.°E ,35°N − 45°N
POLINAT−2,Falcon, Ireland
345.°E − 355.°E ,50°N − 60°N
TOPSE−Apr,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Apr,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Apr,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−Feb,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Feb,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Feb,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−Mar,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
km
pmol/mol
nmol/mol
COM
SCM
EASY
EASY2
NOSCAV

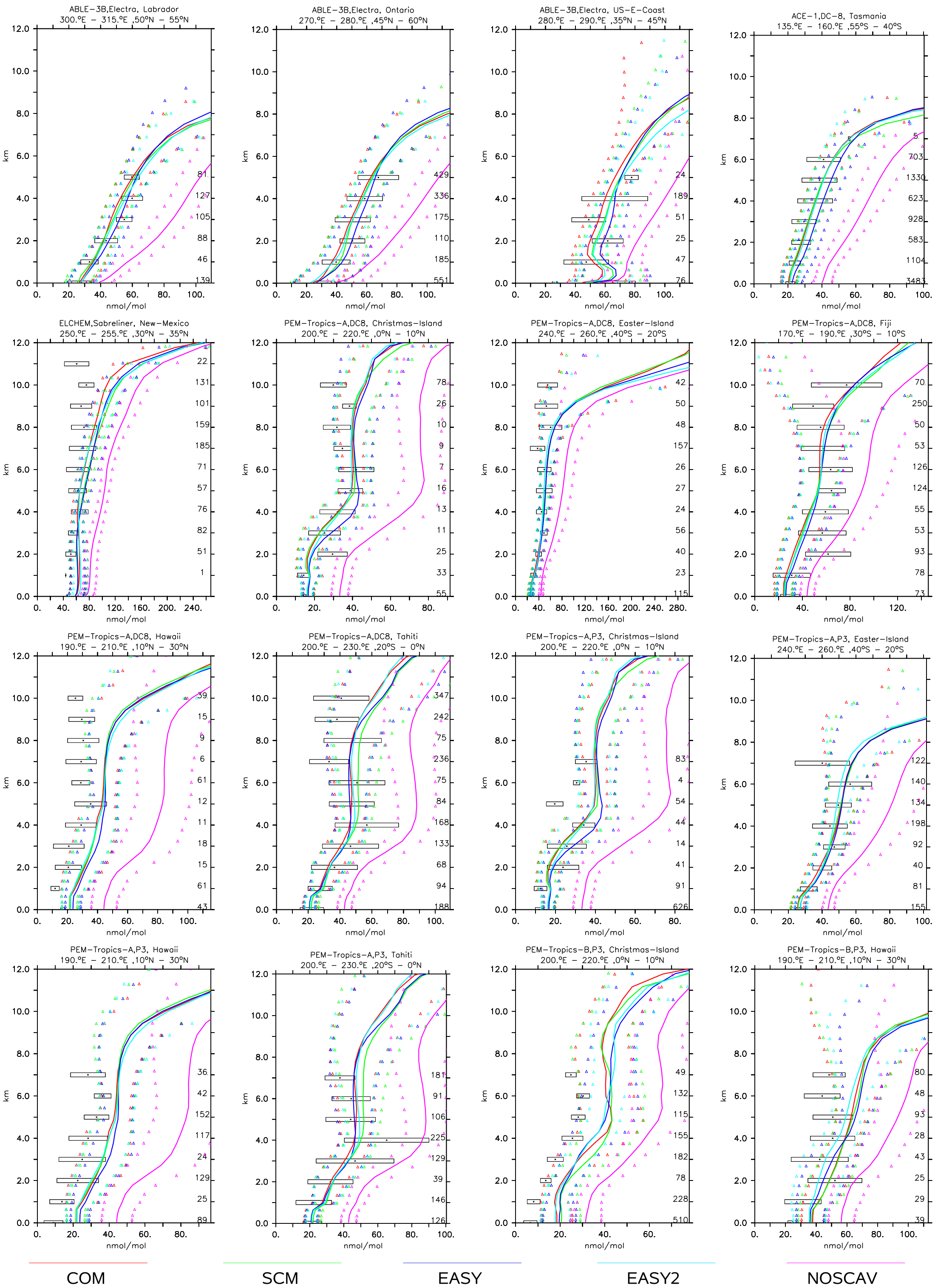

TOPSE−Mar,C130, Churchill
TOPSE−Mar,C130, Thule
TOPSE−May,C130, Boulder
TOPSE−May,C130, Churchill
TOPSE−May,C130, Thule
TRACE−A,DC−8, E−Brazil−Coast
TRACE−A,DC−8, E−Brazil
TRACE−A,DC−8, S−Africa
TRACE−A,DC−8, S−Atlantic
TRACE−A,DC−8, W−Africa−Coast
TRACE−P,DC8, China
TRACE−P,DC8, Guam
TRACE−P,DC8, Hawaii
TRACE−P,DC8, Japan
TRACE−P,P3, China
TRACE−P,P3, Japan
km
pmol/mol
COM
SCM
EASY
EASY2
NOSCAV

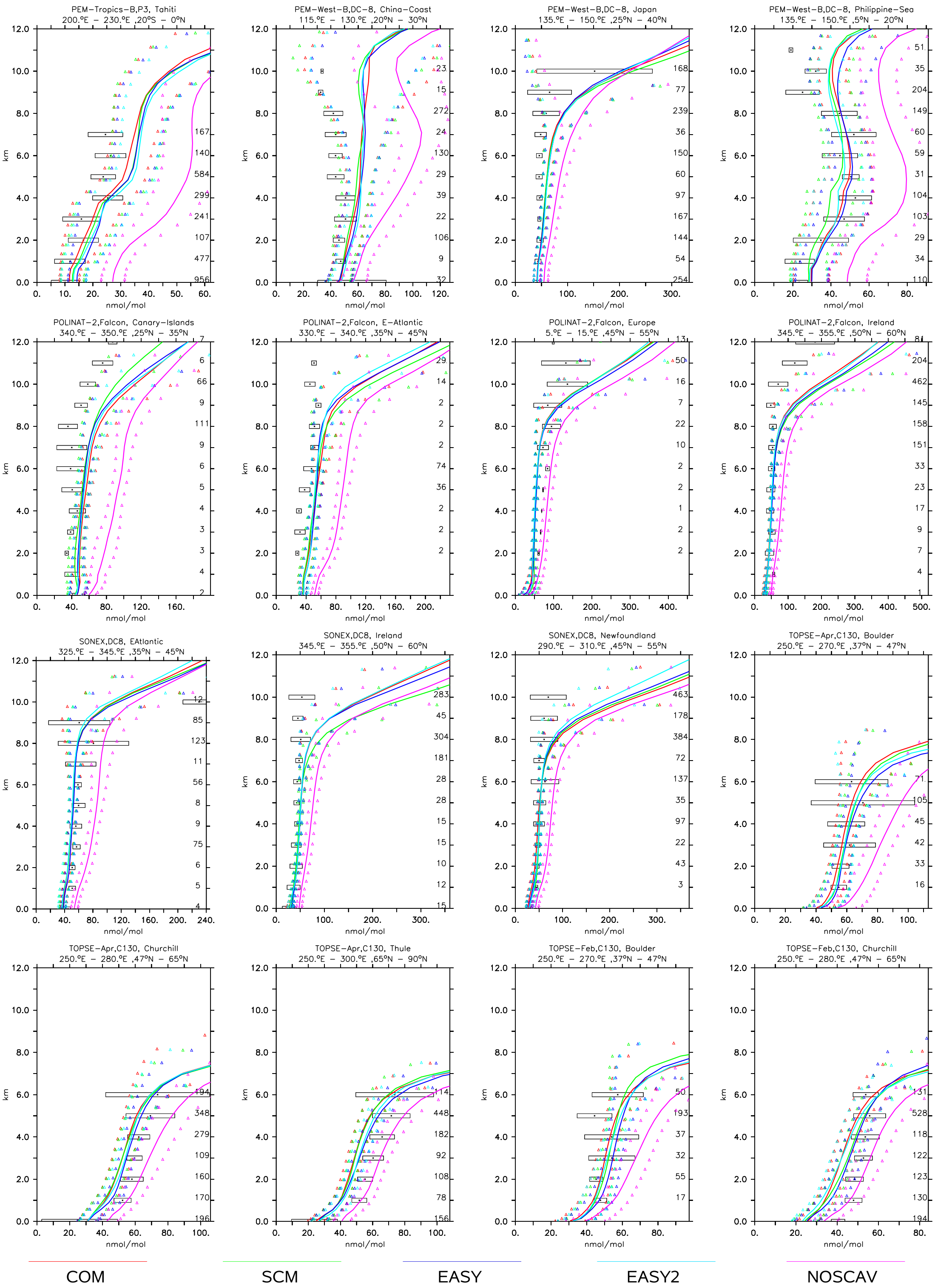
7.4 Formaldehyde (HCHO)




TOPSE−Mar,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−May,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−May,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−May,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TRACE−A,DC−8, E−Brazil−Coast
310.°E − 320.°E ,35°S − 25°S
TRACE−A,DC−8, E−Brazil
310.°E − 320.°E ,15°S − 5°S
TRACE−A,DC−8, S−Africa
15.°E − 35.°E ,25°S − 5°S
TRACE−A,DC−8, S−Atlantic
340.°E − 350.°E ,20°S − 0°N
TRACE−A,DC−8, W−Africa−Coast
0.°E − 10.°E ,25°S − 5°S
TRACE−P,DC8, China
110.°E − 130.°E ,10°N − 30°N
TRACE−P,DC8, Guam
140.°E − 150.°E ,10°N − 20°N
TRACE−P,DC8, Hawaii
190.°E − 210.°E ,10°N − 30°N
TRACE−P,DC8, Japan
130.°E − 150.°E ,20°N − 40°N
TRACE−P,DC8, China
110.°E − 130.°E ,10°N − 30°N
TRACE−P,DC8, Hawaii
190.°E − 210.°E ,10°N − 30°N
TRACE−P,DC8, Japan
130.°E − 150.°E ,20°N − 40°N
km
nmol/mol
pmol/mol
COM
SCM
EASY
EASY2
NOSCAV

7.5 Ozone (O_3)


ABLE−3B,Electra, Labrador
300.°E − 315.°E ,50°N − 55°N
ABLE−3B,Electra, Ontario
270.°E − 280.°E ,45°N − 60°N
ABLE−3B,Electra, US−E−Coast
280.°E − 290.°E ,35°N − 45°N
ACE−1,DC−8, Tasmania
135.°E − 160.°E ,55°S − 40°S
ELCHEM,Sabreliner, New−Mexico
250.°E − 255.°E ,30°N − 35°N
PEM−Tropics−A,DC8, Christmas−Island
200.°E − 220.°E ,0°N − 10°N
PEM−Tropics−A,DC8, Easter−Island
240.°E − 260.°E ,40°S − 20°S
PEM−Tropics−A,DC8, Fiji
170.°E − 190.°E ,30°S − 10°S
PEM−Tropics−A,DC8, Hawaii
190.°E − 210.°E ,10°N − 30°N
PEM−Tropics−A,DC8, Tahiti
200.°E − 230.°E ,20°S − 0°N
PEM−Tropics−A,P3, Christmas−Island
200.°E − 220.°E ,0°N − 10°N
PEM−Tropics−A,P3, Easter−Island
240.°E − 260.°E ,40°S − 20°S
PEM−Tropics−A,P3, Hawaii
190.°E − 210.°E ,10°N − 30°N
PEM−Tropics−A,P3, Tahiti
200.°E − 230.°E ,20°S − 0°N
PEM−Tropics−B,P3, Christmas−Island
200.°E − 220.°E ,0°N − 10°N
PEM−Tropics−B,P3, Hawaii
190.°E − 210.°E ,10°N − 30°N
km
nmol/mol
COM
SCM
EASY
EASY2
NOSCAV



PEM−Tropics−B,P3, Tahiti
200.°E − 230.°E ,20°S − 0°N
PEM−West−B,DC−8, China−Coast
115.°E − 130.°E ,20°N − 30°N
PEM−West−B,DC−8, Japan
135.°E − 150.°E ,25°N − 40°N
PEM−West−B,DC−8, Philippine−Sea
135.°E − 150.°E ,5°N − 20°N
POLINAT−2,Falcon, Canary−Islands
340.°E − 350.°E ,25°N − 35°N
POLINAT−2,Falcon, E−Atlantic
330.°E − 340.°E ,35°N − 45°N
POLINAT−2,Falcon, Europe
5.°E − 15.°E ,45°N − 55°N
POLINAT−2,Falcon, Ireland
345.°E − 355.°E ,50°N − 60°N
SONEX,DC8, EAtlantic
325.°E − 345.°E ,35°N − 45°N
SONEX,DC8, Ireland
345.°E − 355.°E ,50°N − 60°N
SONEX,DC8, Newfoundland
290.°E − 310.°E ,45°N − 55°N
TOPSE−Apr,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Apr,C130, Churchill
250.°E − 280.°E ,47°N − 65°N
TOPSE−Apr,C130, Thule
250.°E − 300.°E ,65°N − 90°N
TOPSE−Feb,C130, Boulder
250.°E − 270.°E ,37°N − 47°N
TOPSE−Feb,C130, Churchill
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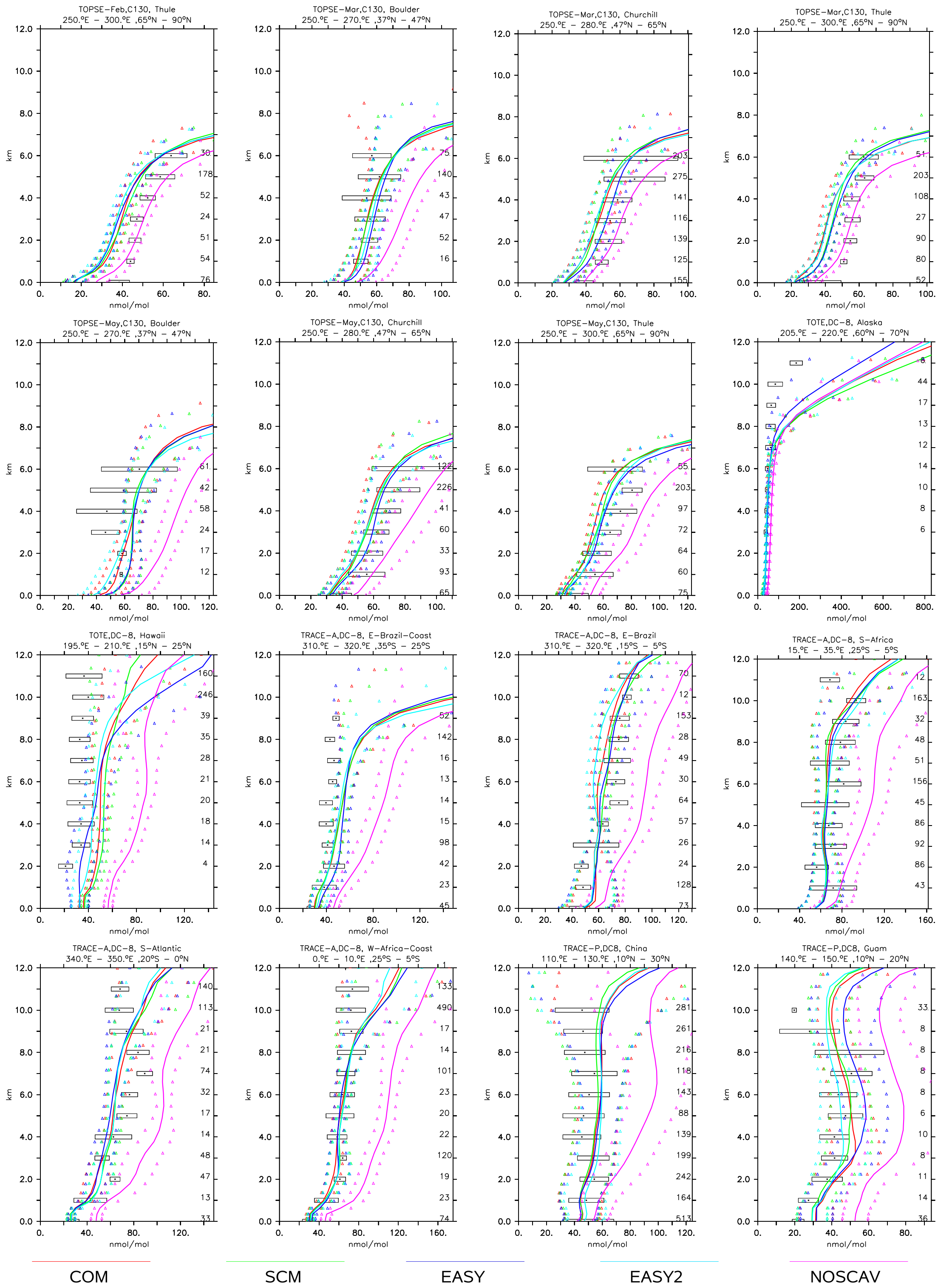
km
nmol/mol
COM
SCM
EASY
EASY2
NOSCAV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TOPSE−May,C130, Thule
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TOTE,DC−8, Alaska
205.°E − 220.°E ,60°N − 70°N
TOTE,DC−8, Hawaii
195.°E − 210.°E ,15°N − 25°N
TRACE−A,DC−8, E−Brazil−Coast
310.°E − 320.°E ,35°S − 25°S
TRACE−A,DC−8, E−Brazil
310.°E − 320.°E ,15°S − 5°S
TRACE−A,DC−8, S−Africa
15.°E − 35.°E ,25°S − 5°S
TRACE−A,DC−8, S−Atlantic
340.°E − 350.°E ,20°S − 0°N
TRACE−A,DC−8, W−Africa−Coast
0.°E − 10.°E ,25°S − 5°S
TRACE−P,DC8, China
110.°E − 130.°E ,10°N − 30°N
TRACE−P,DC8, Guam
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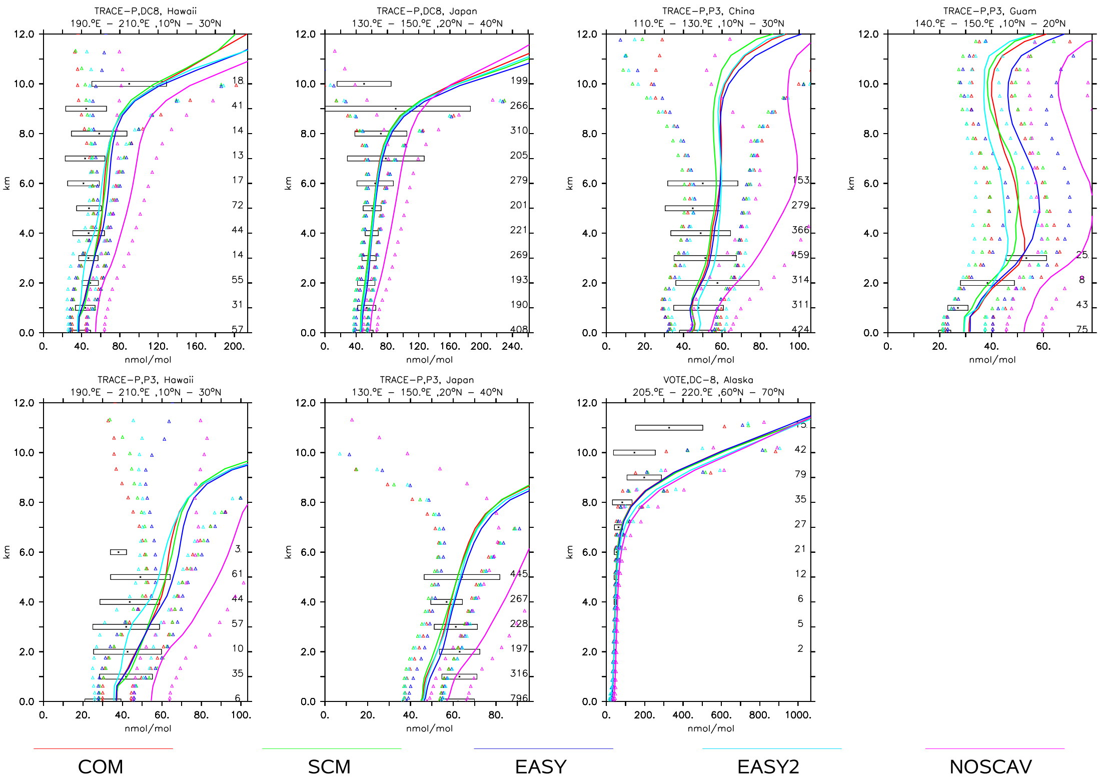
km
nmol/mol
COM
SCM
EASY
EASY2
NOSCAV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TRACE−P,P3, Guam
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TRACE−P,P3, Hawaii
190.°E − 210.°E ,10°N − 30°N
TRACE−P,P3, Japan
130.°E − 150.°E ,20°N − 40°N
VOTE,DC−8, Alaska
205.°E − 220.°E ,60°N − 70°N
km
nmol/mol
COM
SCM
EASY
EASY2
NOSCAV

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