

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_03s
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	$\text{CH}_4 + \text{O}(^1\text{D}) \rightarrow .75 \text{CH}_3\text{O}_2 + .75 \text{OH} + .25 \text{HCHO} + .4 \text{H} + .05 \text{H}_2$	1.5E-10
G4101	$\text{CH}_4 + \text{OH} \rightarrow \text{CH}_3\text{O}_2 + \text{H}_2\text{O}$	$1.85\text{E}-20 * \text{EXP}(2.82 * \log(\text{temp}) - 987./\text{temp})$
G4102	$\text{CH}_3\text{OH} + \text{OH} \rightarrow \text{HCHO} + \text{HO}_2$	$7.3\text{E}-12 * \text{EXP}(-620./\text{temp})$
G4103a	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{OOH}$	$4.1\text{E}-13 * \text{EXP}(750./\text{temp}) / (1.+1./497.7 * \text{EXP}(1160./\text{temp}))$
G4103b	$\text{CH}_3\text{O}_2 + \text{HO}_2 \rightarrow \text{HCHO} + \text{H}_2\text{O} + \text{O}_2$	$4.1\text{E}-13 * \text{EXP}(750./\text{temp}) / (1.+497.7 * \text{EXP}(-1160./\text{temp}))$
G4104	$\text{CH}_3\text{O}_2 + \text{NO} \rightarrow \text{HCHO} + \text{NO}_2 + \text{HO}_2$	$2.8\text{E}-12 * \text{EXP}(300./\text{temp})$
G4105	$\text{CH}_3\text{O}_2 + \text{NO}_3 \rightarrow \text{HCHO} + \text{HO}_2 + \text{NO}_2$	1.3E-12
G4106a	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow 2 \text{HCHO} + 2 \text{HO}_2$	$9.5\text{E}-14 * \text{EXP}(390./\text{temp}) / (1.+1./26.2 * \text{EXP}(1130./\text{temp}))$
G4106b	$\text{CH}_3\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{CH}_3\text{OH}$	$9.5\text{E}-14 * \text{EXP}(390./\text{temp}) / (1.+26.2 * \text{EXP}(-1130./\text{temp}))$
G4107	$\text{CH}_3\text{OOH} + \text{OH} \rightarrow .7 \text{CH}_3\text{O}_2 + .3 \text{HCHO} + .3 \text{OH} + \text{H}_2\text{O}$	k_CH300H_OH
G4108	$\text{HCHO} + \text{OH} \rightarrow \text{CO} + \text{H}_2\text{O} + \text{HO}_2$	$9.52\text{E}-18 * \text{EXP}(2.03 * \log(\text{temp}) + 636./\text{temp})$
G4109	$\text{HCHO} + \text{NO}_3 \rightarrow \text{HNO}_3 + \text{CO} + \text{HO}_2$	$3.4\text{E}-13 * \text{EXP}(-1900./\text{temp})$
G4110	$\text{CO} + \text{OH} \rightarrow \text{H} + \text{CO}_2$	$1.57\text{E}-13 + \text{cair} * 3.54\text{E}-33$
G4111	$\text{HCOOH} + \text{OH} \rightarrow \text{HO}_2$	4.E-13
G4200	$\text{C}_2\text{H}_6 + \text{OH} \rightarrow \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.49\text{E}-17 * \text{temp} * \text{temp} * \text{EXP}(-499./\text{temp})$
G4201	$\text{C}_2\text{H}_4 + \text{O}_3 \rightarrow \text{HCHO} + .22 \text{HO}_2 + .12 \text{OH} + .23 \text{CO} + .54 \text{HCOOH} + .1 \text{H}_2$	$1.2\text{E}-14 * \text{EXP}(-2630./\text{temp})$
G4202	$\text{C}_2\text{H}_4 + \text{OH} \rightarrow .6666667 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	k_3rd(temp, cair, 1.E-28, 0.8, 8.8E-12, 0., 0.6)
G4203	$\text{C}_2\text{H}_5\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_2\text{H}_5\text{OOH}$	$7.5\text{E}-13 * \text{EXP}(700./\text{temp})$
G4204	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO} \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	$2.6\text{E}-12 * \text{EXP}(365./\text{temp})$
G4205	$\text{C}_2\text{H}_5\text{O}_2 + \text{NO}_3 \rightarrow \text{CH}_3\text{CHO} + \text{HO}_2 + \text{NO}_2$	2.3E-12
G4206	$\text{C}_2\text{H}_5\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .75 \text{HCHO} + \text{HO}_2 + .75 \text{CH}_3\text{CHO} + .25 \text{CH}_3\text{OH}$	$1.6\text{E}-13 * \text{EXP}(195./\text{temp})$
G4207	$\text{C}_2\text{H}_5\text{OOH} + \text{OH} \rightarrow .3 \text{C}_2\text{H}_5\text{O}_2 + .7 \text{CH}_3\text{CHO} + .7 \text{OH}$	k_CH300H_OH
G4208	$\text{CH}_3\text{CHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{H}_2\text{O}$	$5.6\text{E}-12 * \text{EXP}(270./\text{temp})$
G4209	$\text{CH}_3\text{CHO} + \text{NO}_3 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HNO}_3$	$1.4\text{E}-12 * \text{EXP}(-1900./\text{temp})$
G4210	$\text{CH}_3\text{COOH} + \text{OH} \rightarrow \text{CH}_3\text{O}_2$	$4.\text{E}-13 * \text{EXP}(200./\text{temp})$
G4211a	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{C}(\text{O})\text{OOH}$	$4.3\text{E}-13 * \text{EXP}(1040./\text{temp}) / (1.+1./37.*\text{EXP}(660./\text{temp}))$
G4211b	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{HO}_2 \rightarrow \text{CH}_3\text{COOH} + \text{O}_3$	$4.3\text{E}-13 * \text{EXP}(1040./\text{temp}) / (1.+37.*\text{EXP}(-660./\text{temp}))$
G4212	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO} \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	$8.1\text{E}-12 * \text{EXP}(270./\text{temp})$
G4213	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2 \rightarrow \text{PAN}$	k_PA_N02
G4214	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_3 \rightarrow \text{CH}_3\text{O}_2 + \text{NO}_2$	4.E-12
G4215a	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{HCHO} + \text{HO}_2 + \text{CH}_3\text{O}_2 + \text{CO}_2$	$0.9 * 2.\text{E}-12 * \text{EXP}(500./\text{temp})$
G4215b	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COOH} + \text{HCHO} + \text{CO}_2$	$0.1 * 2.\text{E}-12 * \text{EXP}(500./\text{temp})$
G4216	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{C}_2\text{H}_5\text{O}_2 \rightarrow .82 \text{CH}_3\text{O}_2 + \text{CH}_3\text{CHO} + .82 \text{HO}_2 + .18 \text{CH}_3\text{COOH}$	$4.9\text{E}-12 * \text{EXP}(211./\text{temp})$

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

#	reaction	rate coefficient
G4217	$\text{CH}_3\text{C}(\text{O})\text{OO} + \text{CH}_3\text{C}(\text{O})\text{OO} \rightarrow 2 \text{CH}_3\text{O}_2 + 2 \text{CO}_2 + \text{O}_2$	$2.5\text{E-}12 * \text{EXP}(500./\text{temp})$
G4218	$\text{CH}_3\text{C}(\text{O})\text{OOH} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO}$	k_CH300H_OH
G4219	$\text{NACA} + \text{OH} \rightarrow \text{NO}_2 + \text{HCHO} + \text{CO}$	$5.6\text{E-}12 * \text{EXP}(270./\text{temp})$
G4220	$\text{PAN} + \text{OH} \rightarrow \text{HCHO} + \text{NO}_2$	2.E-14
G4221	$\text{PAN} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{NO}_2$	k_PAN_M
G4300	$\text{C}_3\text{H}_8 + \text{OH} \rightarrow .82 \text{C}_3\text{H}_7\text{O}_2 + .18 \text{C}_2\text{H}_5\text{O}_2 + \text{H}_2\text{O}$	$1.65\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(-87./\text{temp})$
G4301	$\text{C}_3\text{H}_6 + \text{O}_3 \rightarrow .57 \text{HCHO} + .47 \text{CH}_3\text{CHO} + .33 \text{OH} + .26 \text{HO}_2 + .07 \text{CH}_3\text{O}_2 + .06 \text{C}_2\text{H}_5\text{O}_2 + .23 \text{CH}_3\text{C}(\text{O})\text{OO} + .04 \text{CH}_3\text{COCHO} + .06 \text{CH}_4 + .31 \text{CO} + .22 \text{HCOOH} + .03 \text{CH}_3\text{OH}$	$6.5\text{E-}15 * \text{EXP}(-1900./\text{temp})$
G4302	$\text{C}_3\text{H}_6 + \text{OH} \rightarrow \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH}$	k_3rd(temp, cair, 8.E-27, 3.5, 3.E-11, 0., 0.5)
G4303	$\text{C}_3\text{H}_6 + \text{NO}_3 \rightarrow \text{ONIT}$	$4.6\text{E-}13 * \text{EXP}(-1155./\text{temp})$
G4304	$\text{C}_3\text{H}_7\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_3\text{H}_7\text{OOH}$	k_Pr02_HO2
G4305	$\text{C}_3\text{H}_7\text{O}_2 + \text{NO} \rightarrow .96 \text{CH}_3\text{COCH}_3 + .96 \text{HO}_2 + .96 \text{NO}_2 + .04 \text{C}_3\text{H}_7\text{ONO}_2$	k_Pr02_NO
G4306	$\text{C}_3\text{H}_7\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow \text{CH}_3\text{COCH}_3 + .8 \text{HCHO} + .8 \text{HO}_2 + .2 \text{CH}_3\text{OH}$	k_Pr02_CH3O2
G4307	$\text{C}_3\text{H}_7\text{OOH} + \text{OH} \rightarrow .3 \text{C}_3\text{H}_7\text{O}_2 + .7 \text{CH}_3\text{COCH}_3 + .7 \text{OH}$	k_CH300H_OH
G4308	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{HO}_2 \rightarrow \text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{OH}$	$6.5\text{E-}13 * \text{EXP}(650./\text{temp})$
G4309	$\text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + \text{NO} \rightarrow .98 \text{CH}_3\text{CHO} + .98 \text{HCHO} + .98 \text{HO}_2 + .98 \text{NO}_2 + .02 \text{ONIT}$	$4.2\text{E-}12 * \text{EXP}(180./\text{temp})$
G4310	$\text{CH}_3\text{CH}(\text{OOH})\text{CH}_2\text{OH} + \text{OH} \rightarrow .5 \text{CH}_3\text{CH}(\text{O}_2)\text{CH}_2\text{OH} + .5 \text{CH}_3\text{COCH}_2\text{OH} + .5 \text{OH} + \text{H}_2\text{O}$	$3.8\text{E-}12 * \text{EXP}(200./\text{temp})$
G4311	$\text{CH}_3\text{COCH}_3 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	$1.33\text{E-}13 + 3.82\text{E-}11 * \text{EXP}(-2000./\text{temp})$
G4312	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2 \rightarrow \text{CH}_3\text{COCH}_2\text{O}_2\text{H}$	$8.6\text{E-}13 * \text{EXP}(700./\text{temp})$
G4313	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{NO} \rightarrow \text{NO}_2 + \text{CH}_3\text{C}(\text{O})\text{OO} + \text{HCHO}$	$2.9\text{E-}12 * \text{EXP}(300./\text{temp})$
G4314	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .5 \text{CH}_3\text{COCHO} + .5 \text{CH}_3\text{OH} + .3 \text{CH}_3\text{C}(\text{O})\text{OO} + .8 \text{HCHO} + .3 \text{HO}_2 + .2 \text{CH}_3\text{COCH}_2\text{OH}$	$7.5\text{E-}13 * \text{EXP}(500./\text{temp})$
G4315	$\text{CH}_3\text{COCH}_2\text{O}_2\text{H} + \text{OH} \rightarrow .3 \text{CH}_3\text{COCH}_2\text{O}_2 + .7 \text{CH}_3\text{COCHO} + .7 \text{OH}$	k_CH300H_OH
G4316	$\text{CH}_3\text{COCH}_2\text{OH} + \text{OH} \rightarrow \text{CH}_3\text{COCHO} + \text{HO}_2$	3.E-12
G4317	$\text{CH}_3\text{COCHO} + \text{OH} \rightarrow \text{CH}_3\text{C}(\text{O})\text{OO} + \text{CO}$	$8.4\text{E-}13 * \text{EXP}(830./\text{temp})$
G4318	$\text{MPAN} + \text{OH} \rightarrow \text{CH}_3\text{COCH}_2\text{OH} + \text{NO}_2$	3.2E-11
G4319	$\text{MPAN} \rightarrow \text{MVKO}_2 + \text{NO}_2$	k_PAN_M
G4320	$\text{C}_3\text{H}_7\text{ONO}_2 + \text{OH} \rightarrow \text{CH}_3\text{COCH}_3 + \text{NO}_2$	$6.2\text{E-}13 * \text{EXP}(-230./\text{temp})$
G4400	$\text{C}_4\text{H}_{10} + \text{OH} \rightarrow \text{C}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$1.81\text{E-}17 * \text{temp} * \text{temp} * \text{EXP}(114./\text{temp})$
G4401	$\text{C}_4\text{H}_9\text{O}_2 + \text{CH}_3\text{O}_2 \rightarrow .88 \text{CH}_3\text{COC}_2\text{H}_5 + .68 \text{HCHO} + 1.23 \text{HO}_2 + .12 \text{CH}_3\text{CHO} + .12 \text{C}_2\text{H}_5\text{O}_2 + .18 \text{CH}_3\text{OH}$	k_Pr02_CH3O2
G4402	$\text{C}_4\text{H}_9\text{O}_2 + \text{HO}_2 \rightarrow \text{C}_4\text{H}_9\text{OOH}$	k_Pr02_HO2

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

#	reaction	rate coefficient
G4403	$C_4H_9O_2 + NO \rightarrow .84 NO_2 + .56 CH_3COC_2H_5 + .56 HO_2 + .28 C_2H_5O_2 + .84 CH_3CHO + .16 ONIT$	k_Pr02_NO
G4404	$C_4H_9OOH + OH \rightarrow .15 C_4H_9O_2 + .85 CH_3COC_2H_5 + .85 OH + .85 H_2O$	k_CH300H_OH
G4405	$MVK + O_3 \rightarrow .45 HCOOH + .9 CH_3COCHO + .1 CH_3C(O)OO + .19 OH + .22 CO + .32 HO_2$	$.5*(1.36E-15*EXP(-2112./temp) + 7.51E-16*EXP(-1521./temp))$
G4406	$MVK + OH \rightarrow MVKO2$	$.5*(4.1E-12*EXP(452./temp) + 1.9E-11*EXP(175./temp))$
G4407	$MVKO2 + HO_2 \rightarrow MVKOOH$	$1.82E-13*EXP(1300./temp)$
G4408	$MVKO2 + NO \rightarrow NO_2 + .25 CH_3C(O)OO + .25 CH_3COCH_2OH + .75 HCHO + .25 CO + .75 HO_2 + .5 CH_3COCHO$	$2.54E-12*EXP(360./temp)$
G4409	$MVKO2 + NO_2 \rightarrow MPAN$	$.25*k_3rd(temp, cair, 9.7E-29, 5.6, 9.3E-12, 1.5, 0.6)$
G4410	$MVKO2 + CH_3O_2 \rightarrow .5 CH_3COCHO + .375 CH_3COCH_2OH + .125 CH_3C(O)OO + 1.125 HCHO + .875 HO_2 + .125 CO + .25 CH_3OH$	$2.E-12$
G4411	$MVKO2 + MVKO2 \rightarrow CH_3COCH_2OH + CH_3COCHO + .5 CO + .5 HCHO + HO_2$	$2.E-12$
G4412	$MVKOOH + OH \rightarrow MVKO2$	$3.E-11$
G4413	$CH_3COC_2H_5 + OH \rightarrow MEKO2$	$1.3E-12*EXP(-25./temp)$
G4414	$MEKO2 + HO_2 \rightarrow MEKOOH$	k_Pr02_HO2
G4415	$MEKO2 + NO \rightarrow .985 CH_3CHO + .985 CH_3C(O)OO + .985 NO_2 + .015 ONIT$	k_Pr02_NO
G4416	$MEKOOH + OH \rightarrow .8 MeCOCO + .8 OH + .2 MEKO2$	k_CH300H_OH
G4417	$ONIT + OH \rightarrow CH_3COC_2H_5 + NO_2 + H_2O$	$1.7E-12$
G4500	$ISOP + O_3 \rightarrow .28 HCOOH + .65 MVK + .1 MVKO2 + .1 CH_3C(O)OO + .14 CO + .58 HCHO + .09 H_2O_2 + .08 CH_3O_2 + .25 OH + .25 HO_2$	$7.86E-15*EXP(-1913./temp)$
G4501	$ISOP + OH \rightarrow ISO2$	$2.54E-11*EXP(410./temp)$
G4502	$ISOP + NO_3 \rightarrow ISON$	$3.03E-12*EXP(-446./temp)$
G4503	$ISO2 + HO_2 \rightarrow ISOOH$	$2.22E-13*EXP(1300./temp)$
G4504	$ISO2 + NO \rightarrow .88 NO_2 + .88 MVK + .88 HCHO + .88 HO_2 + .12 ISON$	$2.54E-12*EXP(360./temp)$
G4505	$ISO2 + CH_3O_2 \rightarrow .5 MVK + 1.25 HCHO + HO_2 + .25 CH_3COCHO + .25 CH_3COCH_2OH + .25 CH_3OH$	$2.E-12$
G4506	$ISO2 + ISO2 \rightarrow 2 MVK + HCHO + HO_2$	$2.E-12$
G4507	$ISOOH + OH \rightarrow MVK + OH$	$1.E-10$
G4508	$ISON + OH \rightarrow CH_3COCH_2OH + NACA$	$1.3E-11$
G6100	$Cl + O_3 \rightarrow ClO$	$2.3E-11*EXP(-200./temp)$
G6101	$ClO + O(^3P) \rightarrow Cl$	$3.E-11*EXP(70./temp)$
G6102	$ClO + ClO \rightarrow Cl_2O_2$	k_ClO_ClO
G6103	$Cl_2O_2 \rightarrow ClO + ClO$	$k_ClO_ClO/(1.27E-27*EXP(8744./temp))$
G6200	$Cl + H_2 \rightarrow HCl + H$	$3.7E-11*EXP(-2300./temp)$
G6201a	$Cl + HO_2 \rightarrow HCl$	$1.8E-11*EXP(170./temp)$
G6201b	$Cl + HO_2 \rightarrow ClO + OH$	$4.1E-11*EXP(-450./temp)$

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

#	reaction	rate coefficient
G6202	$\text{Cl} + \text{H}_2\text{O}_2 \rightarrow \text{HCl} + \text{HO}_2$	$1.1\text{E-}11 * \text{EXP}(-980./\text{temp})$
G6203a	$\text{ClO} + \text{OH} \rightarrow \text{Cl} + \text{HO}_2$	$7.4\text{E-}12 * \text{EXP}(270./\text{temp})$
G6203b	$\text{ClO} + \text{OH} \rightarrow \text{HCl}$	$6.\text{E-}13 * \text{EXP}(230./\text{temp})$
G6204	$\text{ClO} + \text{HO}_2 \rightarrow \text{HOCl}$	$2.7\text{E-}12 * \text{EXP}(220./\text{temp})$
G6205	$\text{HCl} + \text{OH} \rightarrow \text{Cl} + \text{H}_2\text{O}$	$2.6\text{E-}12 * \text{EXP}(-350./\text{temp})$
G6206	$\text{HOCl} + \text{OH} \rightarrow \text{ClO} + \text{H}_2\text{O}$	$3.\text{E-}12 * \text{EXP}(-500./\text{temp})$
G6300	$\text{ClO} + \text{NO} \rightarrow \text{NO}_2 + \text{Cl}$	$6.4\text{E-}12 * \text{EXP}(290./\text{temp})$
G6301	$\text{ClO} + \text{NO}_2 \rightarrow \text{ClNO}_3$	$k_3\text{rd}(\text{temp}, \text{cair}, 1.8\text{E-}31, 3.4, 1.5\text{E-}11, 1.9, 0.6)$
G6303	$\text{ClNO}_3 + \text{O}(^3\text{P}) \rightarrow \text{ClO} + \text{NO}_3$	$2.9\text{E-}12 * \text{EXP}(-800./\text{temp})$
G6304	$\text{ClNO}_3 + \text{Cl} \rightarrow \text{Cl}_2 + \text{NO}_3$	$6.5\text{E-}12 * \text{EXP}(135./\text{temp})$
G6400	$\text{Cl} + \text{CH}_4 \rightarrow \text{HCl} + \text{CH}_3\text{O}_2$	$9.6\text{E-}12 * \text{EXP}(-1360./\text{temp})$
G6401	$\text{Cl} + \text{HCHO} \rightarrow \text{HCl} + \text{CO} + \text{HO}_2$	$8.1\text{E-}11 * \text{EXP}(-30./\text{temp})$
G6402	$\text{Cl} + \text{CH}_3\text{OOH} \rightarrow \text{CH}_3\text{O}_2 + \text{HCl}$	$5.7\text{E-}11$
G6403	$\text{ClO} + \text{CH}_3\text{O}_2 \rightarrow \text{HO}_2 + \text{Cl} + \text{HCHO}$	$3.3\text{E-}12 * \text{EXP}(-115./\text{temp})$
G6404	$\text{CCl}_4 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 3 \text{Cl}$	$3.3\text{E-}10$
G6405	$\text{CH}_3\text{Cl} + \text{O}(^1\text{D}) \rightarrow \text{OH} + \text{Cl}$	$1.65\text{E-}10$
G6406	$\text{CH}_3\text{Cl} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Cl}$	$2.4\text{E-}12 * \text{EXP}(-1250./\text{temp})$
G6407	$\text{CH}_3\text{CCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{OH} + 3 \text{Cl}$	$3.\text{E-}10$
G6408	$\text{CH}_3\text{CCl}_3 + \text{OH} \rightarrow \text{H}_2\text{O} + 3 \text{Cl}$	$1.6\text{E-}12 * \text{EXP}(-1520./\text{temp})$
G6500	$\text{CF}_2\text{Cl}_2 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + \text{Cl}$	$1.4\text{E-}10$
G6501	$\text{CFCl}_3 + \text{O}(^1\text{D}) \rightarrow \text{ClO} + 2 \text{Cl}$	$2.3\text{E-}10$
G7100	$\text{Br} + \text{O}_3 \rightarrow \text{BrO}$	$1.7\text{E-}11 * \text{EXP}(-800./\text{temp})$
G7101	$\text{BrO} + \text{O}(^3\text{P}) \rightarrow \text{Br} + \text{O}_2$	$1.9\text{E-}11 * \text{EXP}(230./\text{temp})$
G7102a	$\text{BrO} + \text{BrO} \rightarrow \text{Br} + \text{Br}$	$2.4\text{E-}12 * \text{EXP}(40./\text{temp})$
G7102b	$\text{BrO} + \text{BrO} \rightarrow \text{Br}_2$	$2.8\text{E-}14 * \text{EXP}(869./\text{temp})$
G7200	$\text{Br} + \text{HO}_2 \rightarrow \text{HBr}$	$1.5\text{E-}11 * \text{EXP}(-600./\text{temp})$
G7201	$\text{BrO} + \text{HO}_2 \rightarrow \text{HOBr}$	$3.4\text{E-}12 * \text{EXP}(540./\text{temp})$
G7202	$\text{HBr} + \text{OH} \rightarrow \text{Br} + \text{H}_2\text{O}$	$1.1\text{E-}11$
G7203	$\text{HOBr} + \text{O}(^3\text{P}) \rightarrow \text{OH} + \text{BrO}$	$1.2\text{E-}10 * \text{EXP}(-430./\text{temp})$
G7301	$\text{BrO} + \text{NO} \rightarrow \text{Br} + \text{NO}_2$	$8.8\text{E-}12 * \text{EXP}(260./\text{temp})$
G7302	$\text{BrO} + \text{NO}_2 \rightarrow \text{BrNO}_3$	k_BrO_NO2
G7400	$\text{Br} + \text{HCHO} \rightarrow \text{HBr} + \text{CO} + \text{HO}_2$	$1.7\text{E-}11 * \text{EXP}(-800./\text{temp})$
G7403	$\text{CH}_3\text{Br} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{Br}$	$2.35\text{E-}12 * \text{EXP}(-1300./\text{temp})$
G7603a	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{OClO}$	$9.5\text{E-}13 * \text{EXP}(550./\text{temp})$
G7603b	$\text{BrO} + \text{ClO} \rightarrow \text{Br} + \text{Cl}$	$2.3\text{E-}12 * \text{EXP}(260./\text{temp})$
G7603c	$\text{BrO} + \text{ClO} \rightarrow \text{BrCl}$	$4.1\text{E-}13 * \text{EXP}(290./\text{temp})$
G9200	$\text{SO}_2 + \text{OH} \rightarrow \text{H}_2\text{SO}_4 + \text{HO}_2$	$k_3\text{rd}(\text{temp}, \text{cair}, 3.\text{E-}31, 3.3, 1.5\text{E-}12, 0., 0.6)$
G9400a	$\text{DMS} + \text{OH} \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$	$1.13\text{E-}11 * \text{EXP}(-253./\text{temp})$
G9400b	$\text{DMS} + \text{OH} \rightarrow \text{DMSO} + \text{HO}_2$	k_DMS_OH
G9401	$\text{DMS} + \text{NO}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HNO}_3 + \text{HCHO}$	$1.9\text{E-}13 * \text{EXP}(520./\text{temp})$
G9402	$\text{DMSO} + \text{OH} \rightarrow .6 \text{SO}_2 + \text{HCHO} + .6 \text{CH}_3\text{O}_2 + .4 \text{HO}_2 + .4 \text{CH}_3\text{SO}_3\text{H}$	$1.\text{E-}10$
G9403	$\text{CH}_3\text{SO}_2 \rightarrow \text{SO}_2 + \text{CH}_3\text{O}_2$	$1.9\text{E}13 * \text{EXP}(-8661./\text{temp})$
G9404	$\text{CH}_3\text{SO}_2 + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_3$	$3.\text{E-}13$
G9405	$\text{CH}_3\text{SO}_3 + \text{HO}_2 \rightarrow \text{CH}_3\text{SO}_3\text{H}$	$5.\text{E-}11$

Notes:

Rate coefficients for three-body reactions are defined via the function $k_3\text{rd}(T, M, k_0^{300}, n, k_{\text{inf}}^{300}, m, f_c)$. In the code, the temperature T is called `temp` and the concentration of “air molecules” M is called `cair`.

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

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

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

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (3)$$

$$\mathbf{k_3rd} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c \left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}}))^2} \right) \quad (4)$$

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

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

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

$$k_{\text{ratio}} = \frac{k_0(T)M}{k_{\text{inf}}(T)} \quad (7)$$

$$N = 0.75 - 1.27 \times \log_{10}(f_c) \quad (8)$$

$$\mathbf{k_3rd_iupac} = \frac{k_0(T)M}{1 + k_{\text{ratio}}} \times f_c \left(\frac{1}{1 + (\log_{10}(k_{\text{ratio}})/N)^2} \right) \quad (9)$$

G1000: Sander et al. (2003)

G1001: Sander et al. (2003)

G1002: Sander et al. (2003), path leading to 2 O(³P) + O₂ neglected

G1003: Sander et al. (2003)

G01Diag: Roelofs and Lelieveld (1997), $\mathbf{k_03s} = (1.7\text{E-}12 \cdot \text{EXP}(-940./\text{temp})) \cdot \text{C}(\text{KPP_OH}) + (1.\text{E-}14 \cdot \text{EXP}(-490./\text{temp})) \cdot \text{C}(\text{KPP_H02}) + \text{J_01D} \cdot 2.2\text{E-}10 \cdot \text{C}(\text{KPP_H2O}) / (3.2\text{E-}11 \cdot \text{EXP}(70./\text{temp})) \cdot \text{C}(\text{KPP_O2}) + 1.8\text{E-}11 \cdot \text{EXP}(110./\text{temp}) \cdot \text{C}(\text{KPP_N2}) + 2.2\text{E-}10 \cdot \text{C}(\text{KPP_H2O})$

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: $\mathbf{k_H02_H02} = (1.5\text{E-}12 \cdot \text{EXP}(19./\text{temp}) + 1.7\text{E-}33 \cdot \text{EXP}(1000./\text{temp}) \cdot \text{cair}) \cdot (1 + 1.4\text{E-}21 \cdot \text{EXP}(2200./\text{temp})) \cdot \text{C}(\text{KPP_H2O})$. 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: $\mathbf{k_N03_N02} = \mathbf{k_3rd}(\text{temp}, \text{cair}, 2.\text{E-}30, 4.4, 1.4\text{E-}12, 0.7, 0.6)$.

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: $\mathbf{k_N02_H02} = \mathbf{k_3rd}(\text{temp}, \text{cair}, 1.8\text{E-}31, 3.2, 4.7\text{E-}12, 1.4, 0.6)$.

G3204: Sander et al. (2003)

G3205: Sander et al. (2003)

G3206: Sander et al. (2003). The rate coefficient is: $\mathbf{k_HN03_OH} = 2.4\text{E-}14 \cdot \text{EXP}(460./\text{temp}) + 1./ (1./ (6.5\text{E-}34 \cdot \text{EXP}(1335./\text{temp})) \cdot \text{cair}) + 1./ (2.7\text{E-}17 \cdot \text{EXP}(2199./\text{temp})))$

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: $k_{\text{CH3OOH_OH}} = 3.8\text{E-}12 * \text{EXP}(200./\text{temp})$
G4108: Sivakumaran et al. (2003)
G4109: Sander et al. (2003), same temperature dependence assumed as for $\text{CH}_3\text{CHO} + \text{NO}_3$
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 $\text{C}_2\text{H}_5\text{OO}$ 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**: $\text{CH}_3\text{OOH} + \text{OH}$ 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: $k_{\text{PA_NO2}} = k_{\text{3rd}}(\text{temp}, \text{cair}, 8.5\text{E-}29, 6.5, 1.1\text{E-}11, 1., 0.6)$.
G4214: Canosa-Mas et al. (1996)
G4215a: Sander et al. (2003)
G4215b: Sander et al. (2003)
G4216: $1.0\text{E-}11$ from Atkinson et al. (1999), temperature dependence from Kirchner and Stockwell (1996)
G4217: Tyndall et al. (2001)
G4218: Same value as for **G4107**: $\text{CH}_3\text{OOH} + \text{OH}$ assumed.
G4219: According to Pöschl et al. (2000), the same value as for $\text{CH}_3\text{CHO} + \text{OH}$ 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: $k_{\text{PAN_M}} = k_{\text{PA_NO2}} / 9.\text{E-}29 * \text{EXP}(-14000./\text{temp})$, 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: $k_{\text{PrO2_HO2}} = 1.9\text{E-}13 * \text{EXP}(1300./\text{temp})$. Value for generic $\text{RO}_2 + \text{HO}_2$ reaction from Atkinson (1997) is used.
G4305: Atkinson et al. (1999). The rate coefficient is: $k_{\text{PrO2_NO}} = 2.7\text{E-}12 * \text{EXP}(360./\text{temp})$
G4306: Kirchner and Stockwell (1996). The rate coefficient is: $k_{\text{PrO2_CH3O2}} = 9.46\text{E-}14 * \text{EXP}(431./\text{temp})$. The product distribution is from von Kuhlmann (2001).
G4307: Same value as for **G4107**: $\text{CH}_3\text{OOH} + \text{OH}$ 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**: $\text{CH}_3\text{OOH} + \text{OH}$ 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 ($k_{\text{PrO2_CH3O2}}$).
G4402: Same value as for propyl group assumed ($k_{\text{PrO2_HO2}}$).
G4403: Same value as for propyl group assumed ($k_{\text{PrO2_NO}}$).
G4404: Same value as for **G4107**: $\text{CH}_3\text{OOH} + \text{OH}$ 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 ($k_{\text{PrO2_HO2}}$).
G4415: Same value as for propyl group assumed ($k_{\text{PrO2_NO}}$).

- G4416:** Same value as for **G4107**: $\text{CH}_3\text{OOH} + \text{OH}$ assumed.
- G4417:** Atkinson et al. (1999), value for $\text{C}_4\text{H}_9\text{ONO}_2$ 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 $\text{RO}_2 + \text{HO}_2$ 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: $k_{\text{C10}_\text{C10}} = k_{\text{3rd_iupac}}(\text{temp}, \text{cair}, 2.\text{E}-32, 4., 1.\text{E}-11, 0., 0.45)$.
- 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 $\text{O}_3 + \text{HCl}$. 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 $\text{CH}_3\text{CCl}_2\text{F}$ (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: $k_{\text{BrO}_\text{NO2}} = k_{\text{3rd}}(\text{temp}, \text{cair}, 5.2\text{E}-31, 3.2, 6.9\text{E}-12, 2.9, 0.6)$.
- 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:
- $$\begin{array}{lcl} \text{DMS} + \text{OH} & \rightarrow & \text{CH}_3\text{SCH}_2 \\ \text{CH}_3\text{SCH}_2 + \text{O}_2 & \rightarrow & \text{CH}_3\text{SCH}_2\text{OO} \\ \text{CH}_3\text{SCH}_2\text{OO} + \text{NO} & \rightarrow & \text{CH}_3\text{SCH}_2\text{O} + \text{NO}_2 \\ \text{CH}_3\text{SCH}_2\text{O} & \rightarrow & \text{CH}_3\text{S} + \text{HCHO} \\ \text{CH}_3\text{S} + \text{O}_3 & \rightarrow & \text{CH}_3\text{SO} \\ \text{CH}_3\text{SO} + \text{O}_3 & \rightarrow & \text{CH}_3\text{SO}_2 \end{array}$$
-
- $$\begin{array}{lcl} \text{DMS} + \text{OH} & & \text{CH}_3\text{SO}_2 + \text{HCHO} \\ + \text{NO} + 2\text{O}_3 & \rightarrow & + \text{NO}_2 \end{array}$$
- Neglecting the effect on O_3 and NO_x , the remaining reaction is:
- $$\text{DMS} + \text{OH} + \text{O}_3 \rightarrow \text{CH}_3\text{SO}_2 + \text{HCHO}$$
- G9400b:** Atkinson et al. (2003); Addition path. The rate coefficient is: $k_{\text{DMS}_\text{OH}} = 1.0\text{E}-39 * \text{EXP}(5820./\text{temp}) * \text{C}(\text{KPP}_\text{O2}) / (1. + 5.0\text{E}-30 * \text{EXP}(6280./\text{temp}) * \text{C}(\text{KPP}_\text{O2}))$.
- 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	$\text{O}_2 + h\nu \rightarrow \text{O}(^3\text{P}) + \text{O}(^3\text{P})$	JX(ip_02)
J1001a	$\text{O}_3 + h\nu \rightarrow \text{O}(^1\text{D})$	JX(ip_01D)

Table 2: Photolysis reactions (... continued)

#	reaction	rate coefficient
J1001b	$O_3 + h\nu \rightarrow O(^3P)$	JX(ip_03P)
J2100	$H_2O + h\nu \rightarrow H + OH$	JX(ip_H2O)
J2101	$H_2O_2 + h\nu \rightarrow 2 OH$	JX(ip_H2O2)
J3100	$N_2O + h\nu \rightarrow O(^1D)$	JX(ip_N2O)
J3101	$NO_2 + h\nu \rightarrow NO + O(^3P)$	JX(ip_NO2)
J3102	$NO + h\nu \rightarrow N + O(^3P)$	JX(ip_NO)
J3103a	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	JX(ip_NO2O)
J3103b	$NO_3 + h\nu \rightarrow NO$	JX(ip_NO02)
J3104	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	JX(ip_N2O5)
J3200	$HONO + h\nu \rightarrow NO + OH$	JX(ip_HONO)
J3201	$HNO_3 + h\nu \rightarrow NO_2 + OH$	JX(ip_HNO3)
J3202	$HNO_4 + h\nu \rightarrow .667 NO_2 + .667 HO_2 + .333 NO_3 + .333 OH$	JX(ip_HNO4)
J4100	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	JX(ip_CH300H)
J4101a	$HCHO + h\nu \rightarrow H_2 + CO$	JX(ip_COH2)
J4101b	$HCHO + h\nu \rightarrow H + CO + HO_2$	JX(ip_CHOH)
J4102	$CO_2 + h\nu \rightarrow CO + O(^3P)$	JX(ip_CO2)
J4200	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	JX(ip_CH300H)
J4201	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	JX(ip_CH3CHO)
J4202	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	JX(ip_PAA)
J4203	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	0.19*JX(ip_CHOH)
J4204	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	JX(ip_PAN)
J4300	$C_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	JX(ip_CH300H)
J4301	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	JX(ip_CH3COCH3)
J4302	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	0.074*JX(ip_CHOH)
J4303	$CH_3COCHO + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	JX(ip_CH3COCHO)
J4304	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HO_2 + OH$	JX(ip_CH300H)
J4305	$MPAN + h\nu \rightarrow CH_3COCH_2OH + NO_2$	JX(ip_PAN)
J4306	$C_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	3.7*JX(ip_PAN)
J4400	$C_4H_9OOH + h\nu \rightarrow OH + .67 CH_3COC_2H_5 + .67 HO_2 + .33 C_2H_5O_2 + .33 CH_3CHO$	JX(ip_CH300H)
J4401	$MVK + h\nu \rightarrow CH_3C(O)OO + HCHO + CO + HO_2$	0.019*JX(ip_COH2) +0.015*JX(ip_CH3COCHO)
J4402	$MVKOOH + h\nu \rightarrow OH + .5 CH_3COCHO + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 CH_3C(O)OO + .25 CO$	JX(ip_CH300H)
J4403	$CH_3COC_2H_5 + h\nu \rightarrow CH_3C(O)OO + C_2H_5O_2$	0.42*JX(ip_CHOH)
J4404	$MEKOOH + h\nu \rightarrow CH_3C(O)OO + CH_3CHO + OH$	JX(ip_CH300H)
J4405	$MeCOCO + h\nu \rightarrow 2 CH_3C(O)OO$	2.15*JX(ip_CH3COCHO)
J4406	$ONIT + h\nu \rightarrow NO_2 + .67 CH_3COC_2H_5 + .67 HO_2 + .33 C_2H_5O_2 + .33 CH_3CHO$	3.7*JX(ip_PAN)
J4500	$ISOOH + h\nu \rightarrow MVK + HCHO + HO_2 + OH$	JX(ip_CH300H)
J4501	$ISON + h\nu \rightarrow MVK + HCHO + NO_2 + HO_2$	3.7*JX(ip_PAN)
J6000	$Cl_2 + h\nu \rightarrow Cl + Cl$	JX(ip_Cl2)
J6100	$Cl_2O_2 + h\nu \rightarrow 2 Cl$	1.4*JX(ip_Cl2O2)
J6101	$OCIO + h\nu \rightarrow ClO + O(^3P)$	JX(ip_OC10)
J6200	$HCl + h\nu \rightarrow Cl + H$	JX(ip_HCl)
J6201	$HOCl + h\nu \rightarrow OH + Cl$	JX(ip_HOCl)
J6301	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	JX(ip_ClNO3)

Table 2: Photolysis reactions (... continued)

#	reaction	rate coefficient
J6400	$\text{CH}_3\text{Cl} + h\nu \rightarrow \text{Cl} + \text{CH}_3\text{O}_2$	JX(ip_CH3Cl)
J6401	$\text{CCl}_4 + h\nu \rightarrow 4 \text{Cl}$	JX(ip_CCl4)
J6402	$\text{CH}_3\text{CCl}_3 + h\nu \rightarrow 3 \text{Cl}$	JX(ip_CH3CCl3)
J6500	$\text{CFCl}_3 + h\nu \rightarrow 3 \text{Cl}$	JX(ip_CFC13)
J6501	$\text{CF}_2\text{Cl}_2 + h\nu \rightarrow 2 \text{Cl}$	JX(ip_CF2Cl2)
J7000	$\text{Br}_2 + h\nu \rightarrow \text{Br} + \text{Br}$	JX(ip_Br2)
J7200	$\text{HOBr} + h\nu \rightarrow \text{Br} + \text{OH}$	JX(ip_HOBr)
J7301	$\text{BrNO}_3 + h\nu \rightarrow \text{Br} + \text{NO}_3$	JX(ip_BrNO3)
J7400	$\text{CH}_3\text{Br} + h\nu \rightarrow \text{Br} + \text{CH}_3\text{O}_2$	JX(ip_CH3Br)
J7500	$\text{CF}_3\text{Br} + h\nu \rightarrow \text{Br}$	JX(ip_CF3Br)
J7600	$\text{BrCl} + h\nu \rightarrow \text{Br} + \text{Cl}$	JX(ip_BrCl)
J7601	$\text{CF}_2\text{ClBr} + h\nu \rightarrow \text{Br} + \text{Cl}$	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 $\text{Cl}_2\text{O}_2/\text{ClO}$ 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	$\text{N}_2\text{O}_5 + \text{H}_2\text{O} \rightarrow \text{HNO}_3 + \text{HNO}_3$	khet_N2O5_H2O
PSC410	$\text{HOCl} + \text{HCl} \rightarrow \text{Cl}_2 + \text{H}_2\text{O}$	khet_HOCl_HCl
PSC420	$\text{ClNO}_3 + \text{HCl} \rightarrow \text{Cl}_2 + \text{HNO}_3$	khet_ClNO3_HCl
PSC421	$\text{ClNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOCl} + \text{HNO}_3$	khet_ClNO3_H2O
PSC510	$\text{HOBr} + \text{HBr} \rightarrow \text{Br}_2 + \text{H}_2\text{O}$	khet_HOBr_HBr
PSC520	$\text{BrNO}_3 + \text{H}_2\text{O} \rightarrow \text{HOBr} + \text{HNO}_3$	khet_BrNO3_H2O
PSC540	$\text{ClNO}_3 + \text{HBr} \rightarrow \text{BrCl} + \text{HNO}_3$	khet_ClNO3_HBr
PSC541	$\text{BrNO}_3 + \text{HCl} \rightarrow \text{BrCl} + \text{HNO}_3$	khet_BrNO3_HCl
PSC542	$\text{HOCl} + \text{HBr} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	khet_HOCl_HBr
PSC543	$\text{HOBr} + \text{HCl} \rightarrow \text{BrCl} + \text{H}_2\text{O}$	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	$O_2 \rightarrow O_2(aq)$	$k_{\text{exf}}(\text{KPP_O2})$
H1000b	Sc	$O_2(aq) \rightarrow O_2$	$k_{\text{exb}}(\text{KPP_O2})$
H1001f	ScScm	$O_3 \rightarrow O_3(aq)$	$k_{\text{exf}}(\text{KPP_O3})$
H1001b	ScScm	$O_3(aq) \rightarrow O_3$	$k_{\text{exb}}(\text{KPP_O3})$
H2100f	Sc	$OH \rightarrow OH(aq)$	$k_{\text{exf}}(\text{KPP_OH})$
H2100b	Sc	$OH(aq) \rightarrow OH$	$k_{\text{exb}}(\text{KPP_OH})$
H2101f	Sc	$HO_2 \rightarrow HO_2(aq)$	$k_{\text{exf}}(\text{KPP_HO2})$
H2101b	Sc	$HO_2(aq) \rightarrow HO_2$	$k_{\text{exb}}(\text{KPP_HO2})$
H2102f	ScScm	$H_2O_2 \rightarrow H_2O_2(aq)$	$k_{\text{exf}}(\text{KPP_H2O2})$
H2102b	ScScm	$H_2O_2(aq) \rightarrow H_2O_2$	$k_{\text{exb}}(\text{KPP_H2O2})$
H3100f	Sc	$NO \rightarrow NO(aq)$	$k_{\text{exf}}(\text{KPP_NO})$
H3100b	Sc	$NO(aq) \rightarrow NO$	$k_{\text{exb}}(\text{KPP_NO})$
H3101f	Sc	$NO_2 \rightarrow NO_2(aq)$	$k_{\text{exf}}(\text{KPP_NO2})$
H3101b	Sc	$NO_2(aq) \rightarrow NO_2$	$k_{\text{exb}}(\text{KPP_NO2})$
H3102f	Sc	$NO_3 \rightarrow NO_3(aq)$	$k_{\text{exf}}(\text{KPP_NO3})$
H3102b	Sc	$NO_3(aq) \rightarrow NO_3$	$k_{\text{exb}}(\text{KPP_NO3})$
H3200f	ScScm	$NH_3 \rightarrow NH_3(aq)$	$k_{\text{exf}}(\text{KPP_NH3})$
H3200b	ScScm	$NH_3(aq) \rightarrow NH_3$	$k_{\text{exb}}(\text{KPP_NH3})$
H3201	ScScm	$N_2O_5 \rightarrow HNO_3(aq) + HNO_3(aq)$	$k_{\text{exf_N2O5}} * C(\text{KPP_H2O_1})$
H3202f	Sc	$HONO \rightarrow HONO(aq)$	$k_{\text{exf}}(\text{KPP_HONO})$
H3202b	Sc	$HONO(aq) \rightarrow HONO$	$k_{\text{exb}}(\text{KPP_HONO})$
H3203f	ScScm	$HNO_3 \rightarrow HNO_3(aq)$	$k_{\text{exf}}(\text{KPP_HNO3})$
H3203b	ScScm	$HNO_3(aq) \rightarrow HNO_3$	$k_{\text{exb}}(\text{KPP_HNO3})$
H3204f	Sc	$HNO_4 \rightarrow HNO_4(aq)$	$k_{\text{exf}}(\text{KPP_HNO4})$
H3204b	Sc	$HNO_4(aq) \rightarrow HNO_4$	$k_{\text{exb}}(\text{KPP_HNO4})$
H4100f	ScScm	$CO_2 \rightarrow CO_2(aq)$	$k_{\text{exf}}(\text{KPP_CO2})$
H4100b	ScScm	$CO_2(aq) \rightarrow CO_2$	$k_{\text{exb}}(\text{KPP_CO2})$
H4101f	ScScm	$HCHO \rightarrow HCHO(aq)$	$k_{\text{exf}}(\text{KPP_HCHO})$
H4101b	ScScm	$HCHO(aq) \rightarrow HCHO$	$k_{\text{exb}}(\text{KPP_HCHO})$
H4102f	Sc	$CH_3O_2 \rightarrow CH_3OO(aq)$	$k_{\text{exf}}(\text{KPP_CH3O2})$
H4102b	Sc	$CH_3OO(aq) \rightarrow CH_3O_2$	$k_{\text{exb}}(\text{KPP_CH3O2})$
H4103f	ScScm	$HCOOH \rightarrow HCOOH(aq)$	$k_{\text{exf}}(\text{KPP_HCOOH})$
H4103b	ScScm	$HCOOH(aq) \rightarrow HCOOH$	$k_{\text{exb}}(\text{KPP_HCOOH})$
H4104f	ScScm	$CH_3OOH \rightarrow CH_3OOH(aq)$	$k_{\text{exf}}(\text{KPP_CH3OOH})$
H4104b	ScScm	$CH_3OOH(aq) \rightarrow CH_3OOH$	$k_{\text{exb}}(\text{KPP_CH3OOH})$
H4105f	Sc	$CH_3OH \rightarrow CH_3OH(aq)$	$k_{\text{exf}}(\text{KPP_CH3OH})$
H4105b	Sc	$CH_3OH(aq) \rightarrow CH_3OH$	$k_{\text{exb}}(\text{KPP_CH3OH})$
H4200f	ScScm	$CH_3COOH \rightarrow CH_3COOH(aq)$	$k_{\text{exf}}(\text{KPP_CH3COOH})$
H4200b	ScScm	$CH_3COOH(aq) \rightarrow CH_3COOH$	$k_{\text{exb}}(\text{KPP_CH3COOH})$
H4201f	Sc	$CH_3CHO \rightarrow CH_3CHO(aq)$	$k_{\text{exf}}(\text{KPP_CH3CHO})$
H4201b	Sc	$CH_3CHO(aq) \rightarrow CH_3CHO$	$k_{\text{exb}}(\text{KPP_CH3CHO})$
H4202f	Sc	$PAN \rightarrow PAN(aq)$	$k_{\text{exf}}(\text{KPP_PAN})$
H4202b	Sc	$PAN(aq) \rightarrow PAN$	$k_{\text{exb}}(\text{KPP_PAN})$
H4300f	Sc	$CH_3COCH_3 \rightarrow CH_3COCH_3(aq)$	$k_{\text{exf}}(\text{KPP_CH3COCH3})$
H4300b	Sc	$CH_3COCH_3(aq) \rightarrow CH_3COCH_3$	$k_{\text{exb}}(\text{KPP_CH3COCH3})$
H6000f	Sc	$Cl_2 \rightarrow Cl_2(aq)$	$k_{\text{exf}}(\text{KPP_Cl2})$
H6000b	Sc	$Cl_2(aq) \rightarrow Cl_2$	$k_{\text{exb}}(\text{KPP_Cl2})$
H6200f	ScScm	$HCl \rightarrow HCl(aq)$	$k_{\text{exf}}(\text{KPP_HCl})$
H6200b	ScScm	$HCl(aq) \rightarrow HCl$	$k_{\text{exb}}(\text{KPP_HCl})$

Table 4: Heterogeneous reactions

#	labels	reaction	rate coefficient
H6201f	Sc	$\text{HOCl} \rightarrow \text{HOCl(aq)}$	$k_{\text{exf}}(\text{KPP_HOCl})$
H6201b	Sc	$\text{HOCl(aq)} \rightarrow \text{HOCl}$	$k_{\text{exb}}(\text{KPP_HOCl})$
H7000f	Sc	$\text{Br}_2 \rightarrow \text{Br}_2(\text{aq})$	$k_{\text{exf}}(\text{KPP_Br}_2)$
H7000b	Sc	$\text{Br}_2(\text{aq}) \rightarrow \text{Br}_2$	$k_{\text{exb}}(\text{KPP_Br}_2)$
H7200f	ScScm	$\text{HBr} \rightarrow \text{HBr(aq)}$	$k_{\text{exf}}(\text{KPP_HBr})$
H7200b	ScScm	$\text{HBr(aq)} \rightarrow \text{HBr}$	$k_{\text{exb}}(\text{KPP_HBr})$
H7201f	Sc	$\text{HOBr} \rightarrow \text{HOBr(aq)}$	$k_{\text{exf}}(\text{KPP_HOBr})$
H7201b	Sc	$\text{HOBr(aq)} \rightarrow \text{HOBr}$	$k_{\text{exb}}(\text{KPP_HOBr})$
H7600f	Sc	$\text{BrCl} \rightarrow \text{BrCl(aq)}$	$k_{\text{exf}}(\text{KPP_BrCl})$
H7600b	Sc	$\text{BrCl(aq)} \rightarrow \text{BrCl}$	$k_{\text{exb}}(\text{KPP_BrCl})$
H9100f	ScScm	$\text{SO}_2 \rightarrow \text{SO}_2(\text{aq})$	$k_{\text{exf}}(\text{KPP_SO}_2)$
H9100b	ScScm	$\text{SO}_2(\text{aq}) \rightarrow \text{SO}_2$	$k_{\text{exb}}(\text{KPP_SO}_2)$
H9200	ScScm	$\text{H}_2\text{SO}_4 \rightarrow \text{H}_2\text{SO}_4(\text{aq})$	$k_{\text{exf}}(\text{KPP_H}_2\text{SO}_4)$

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	$K_0[M/atm]$	$-\Delta_{\text{sol}}H/R[K]$	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)
$\text{C}_2\text{H}_5\text{O}_2$	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 ₂ O ₂	0.077	2769	Worsnop et al. (1989)
CH ₃ OOH	$4.5 \cdot 10^{-3}$	3273	Magi et al. (1997)
HCHO	0.043	-	DeMore et al. (1997)
HCOOH	0.014	3978	DeMore et al. (1997)
CH ₃ COOH	$1.9 \cdot 10^{-2}$	5894	
O ₃	$2.0 \cdot 10^{-3}$	-	DeMore et al. (1997)
SO ₂	0.11	-	DeMore et al. (1997)
H ₂ SO ₄	0.65	-	Pöschl et al. (1998)
N ₂ O 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 ₃ OH	0.1	-	estimated
CH ₃ CHO	0.03	-	estimated, Ervens et al. (2003)
CH ₃ O ₂	0.01	2000	estimated
C ₂ H ₅ O ₂	$8.2 \cdot 10^{-3}$	-	estimated, Ervens et al. (2003)
NO	0.1	-	estimated
CH ₃ COCH 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 equilibria

#	labels	reaction	$K_0[M^{m-n}]$	$-\Delta H/R[K]$
EQ20	Sc	$\text{HO}_2 \rightleftharpoons \text{O}_2^- + \text{H}^+$	1.6E-5	
EQ21	ScScm	$\text{H}_2\text{O} \rightleftharpoons \text{H}^+ + \text{OH}^-$	1.0E-16	-6716
EQ30	ScScm	$\text{NH}_4^+ \rightleftharpoons \text{H}^+ + \text{NH}_3$	5.88E-10	-2391

Table 7: Acid-base and other equilibria

#	labels	reaction	$K_0 [M^{m-n}]$	$-\Delta H/R [K]$
EQ31	Sc	$\text{HONO} \rightleftharpoons \text{H}^+ + \text{NO}_2^-$	5.1E-4	-1260
EQ32	ScScm	$\text{HNO}_3 \rightleftharpoons \text{H}^+ + \text{NO}_3^-$	15	8700
EQ33	Sc	$\text{HNO}_4 \rightleftharpoons \text{NO}_4^- + \text{H}^+$	1.E-5	
EQ40	ScScm	$\text{CO}_2 \rightleftharpoons \text{H}^+ + \text{HCO}_3^-$	4.3E-7	-913
EQ41	ScScm	$\text{HCOOH} \rightleftharpoons \text{H}^+ + \text{HCOO}^-$	1.8E-4	
EQ42	ScScm	$\text{CH}_3\text{COOH} \rightleftharpoons \text{H}^+ + \text{CH}_3\text{COO}^-$	1.75E-5	-46
EQ61	ScScm	$\text{HCl} \rightleftharpoons \text{H}^+ + \text{Cl}^-$	1.7E6	6896
EQ62	Sc	$\text{HOCl} \rightleftharpoons \text{H}^+ + \text{ClO}^-$	3.2E-8	
EQ71	ScScm	$\text{HBr} \rightleftharpoons \text{H}^+ + \text{Br}^-$	1.0E9	
EQ72	Sc	$\text{HOBr} \rightleftharpoons \text{H}^+ + \text{BrO}^-$	2.3E-9	-3091
EQ90	ScScm	$\text{SO}_2 \rightleftharpoons \text{H}^+ + \text{HSO}_3^-$	1.7E-2	2090
EQ91	ScScm	$\text{HSO}_3^- \rightleftharpoons \text{H}^+ + \text{SO}_3^{2-}$	6.0E-8	1120
EQ92	ScScm	$\text{HSO}_4^- \rightleftharpoons \text{H}^+ + \text{SO}_4^{2-}$	1.2E-2	2720
EQ93	ScScm	$\text{H}_2\text{SO}_4 \rightleftharpoons \text{H}^+ + \text{HSO}_4^-$	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	$\text{O}_3 + \text{O}_2^- \rightarrow \text{OH} + \text{OH}^-$	1.5E9	
A2100	Sc	$\text{OH} + \text{O}_2^- \rightarrow \text{OH}^-$	1.0E10	
A2101	Sc	$\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O}_2$	5.5E9	
A2102	Sc	$\text{HO}_2 + \text{O}_2^- \rightarrow \text{H}_2\text{O}_2 + \text{OH}^-$	1.0E8	-900
A2103	Sc	$\text{HO}_2 + \text{OH} \rightarrow \text{H}_2\text{O}$	7.1E9	
A2104	Sc	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2$	9.7E5	-2500
A2105	Sc	$\text{H}_2\text{O}_2 + \text{OH} \rightarrow \text{HO}_2$	2.7E7	-1684
A3100	Sc	$\text{NO}_2^- + \text{O}_3 \rightarrow \text{NO}_3^-$	5.0E5	-6950
A3101	Sc	$\text{NO}_2 + \text{NO}_2 \rightarrow \text{HNO}_3 + \text{HONO}$	1.0E8	
A3102	Sc	$\text{NO}_4^- \rightarrow \text{NO}_2^-$	8.0E1	
A3200	Sc	$\text{NO}_2 + \text{HO}_2 \rightarrow \text{HNO}_4$	1.8E9	
A3201	Sc	$\text{NO}_2^- + \text{OH} \rightarrow \text{NO}_2 + \text{OH}^-$	1.0E10	
A3202	Sc	$\text{NO}_3 + \text{OH}^- \rightarrow \text{NO}_3^- + \text{OH}$	8.2E7	-2700
A3203	Sc	$\text{HONO} + \text{OH} \rightarrow \text{NO}_2$	1.0E10	
A3204	Sc	$\text{HONO} + \text{H}_2\text{O}_2 \rightarrow \text{HNO}_3$	4.6E3	-6800
A4100	Sc	$\text{CO}_3^- + \text{O}_2^- \rightarrow \text{HCO}_3^- + \text{OH}^-$	6.5E8	
A4101	Sc	$\text{CO}_3^- + \text{H}_2\text{O}_2 \rightarrow \text{HCO}_3^- + \text{HO}_2$	4.3E5	
A4102	Sc	$\text{HCOO}^- + \text{CO}_3^- \rightarrow 2 \text{HCO}_3^- + \text{HO}_2$	1.5E5	
A4103	Sc	$\text{HCOO}^- + \text{OH} \rightarrow \text{OH}^- + \text{HO}_2 + \text{CO}_2$	3.1E9	-1240
A4104	Sc	$\text{HCO}_3^- + \text{OH} \rightarrow \text{CO}_3^-$	8.5E6	
A4105	Sc	$\text{HCHO} + \text{OH} \rightarrow \text{HCOOH} + \text{HO}_2$	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) | A4100: Ross et al. (1992) |
| A2100: Sehested et al. (1968) | A4101: Ross et al. (1992) |
| A2101: Buxton et al. (1988) | A4102: Ross et al. (1992) |
| A2102: Christensen and Sehested (1988) | A4103: Chin and Wine (1994) |
| A2103: Sehested et al. (1968) | A4104: Ross et al. (1992) |
| A2104: Christensen and Sehested (1988) | A4105: Chin and Wine (1994) |
| A2105: Christensen et al. (1982) | A4106: Chin and Wine (1994) |
| A3100: Damschen and Martin (1983) | A4107: Jacob (1986) |
| A3101: Lee and Schwartz (1981) | A4108: Jacob (1986) |
| A3102: Warneck (1999) | A4109: Buxton et al. (1988) |
| A3200: Warneck (1999) | A4110a,b: Jacob (1986) |
| A3201: Wingenter et al. (1999) | A9100: Huie and Neta (1987) |
| A3202: Exner et al. (1992) | A9101: Hoffmann (1986) |
| A3203: Barker et al. (1970) | A9102: Jiang et al. (1992) |
| A3204: Damschen and Martin (1983) | A9103: Huie and Neta (1987) |

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

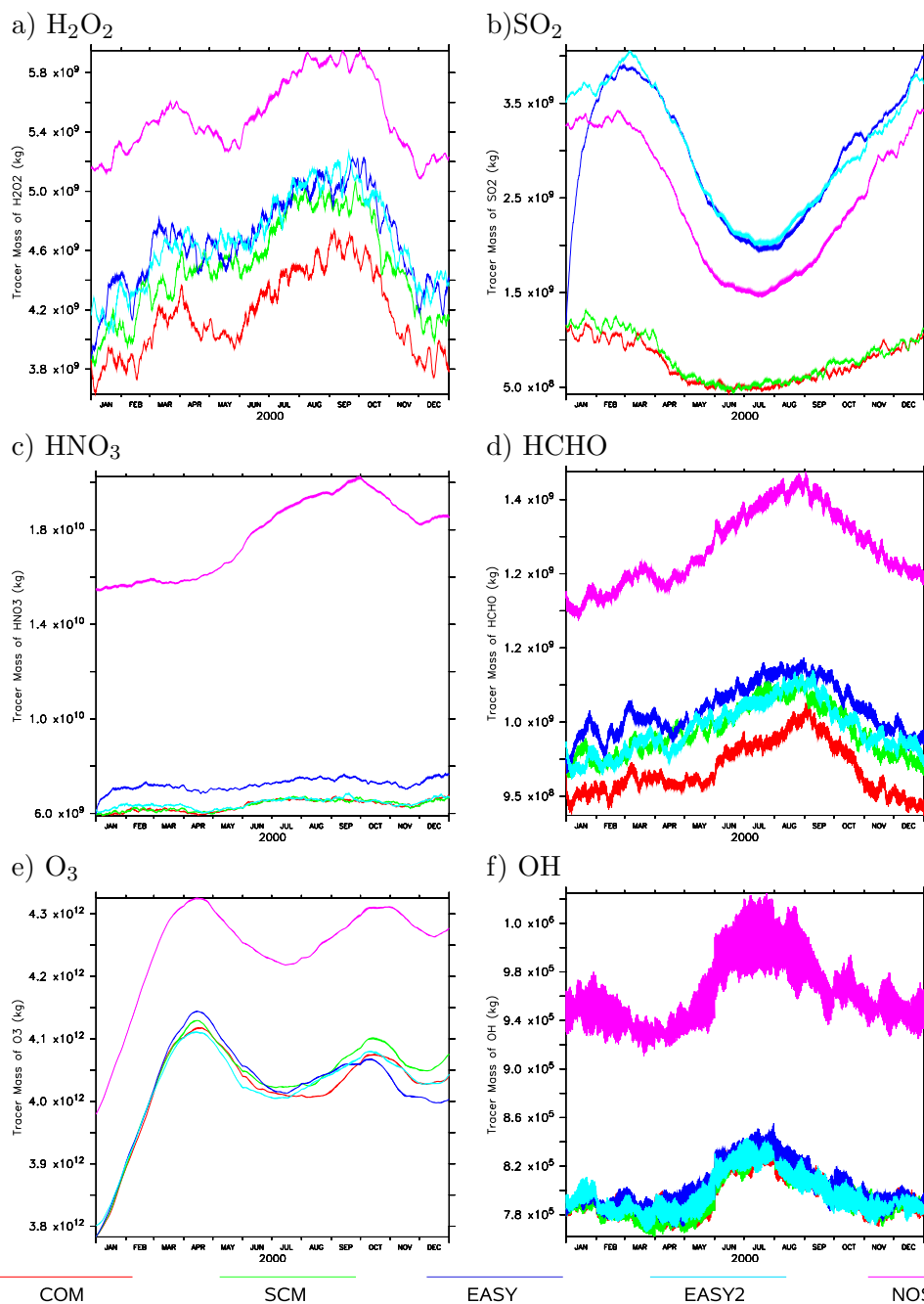
Table 9: Photolysis reactions

#	labels	reaction	rate coefficient
PH2100	Sc	$\text{H}_2\text{O}_2 + h\nu \rightarrow 2 \text{OH}$	$\text{JX}(\text{ip_H2O2}) * 2.33$

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

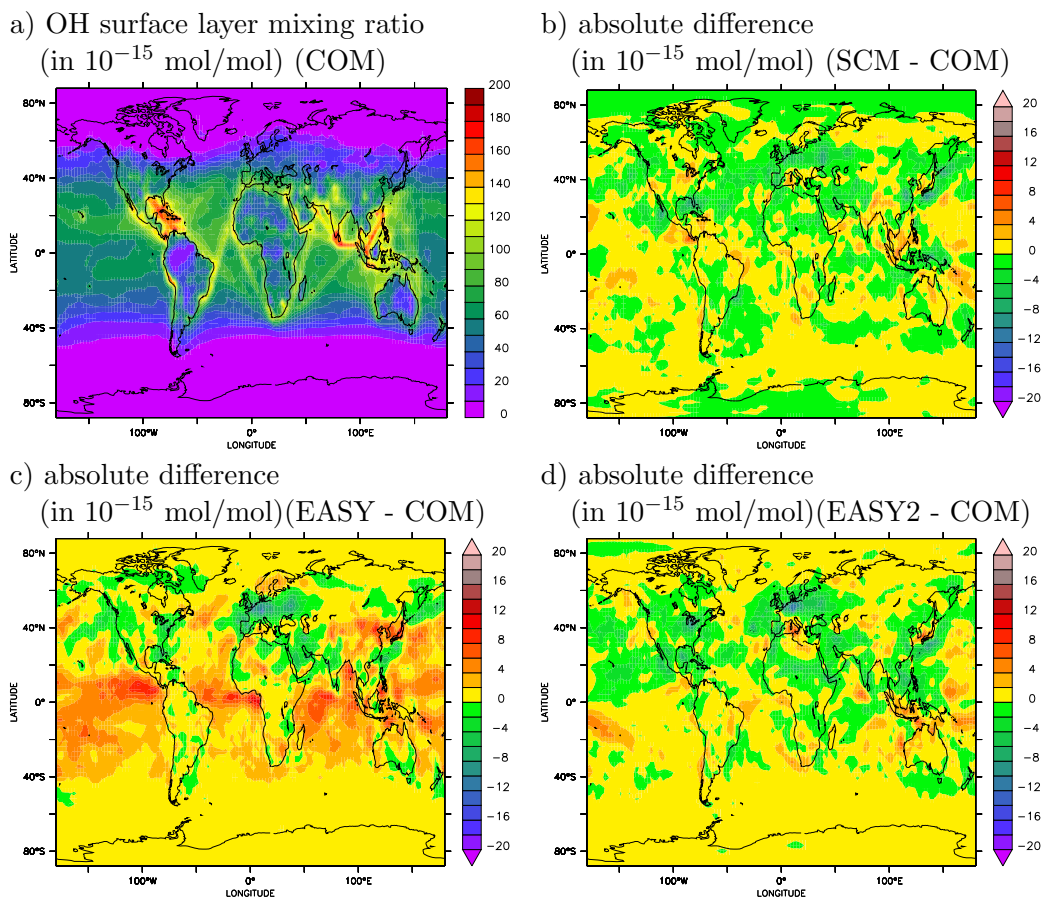
2 Global tracer masses

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.



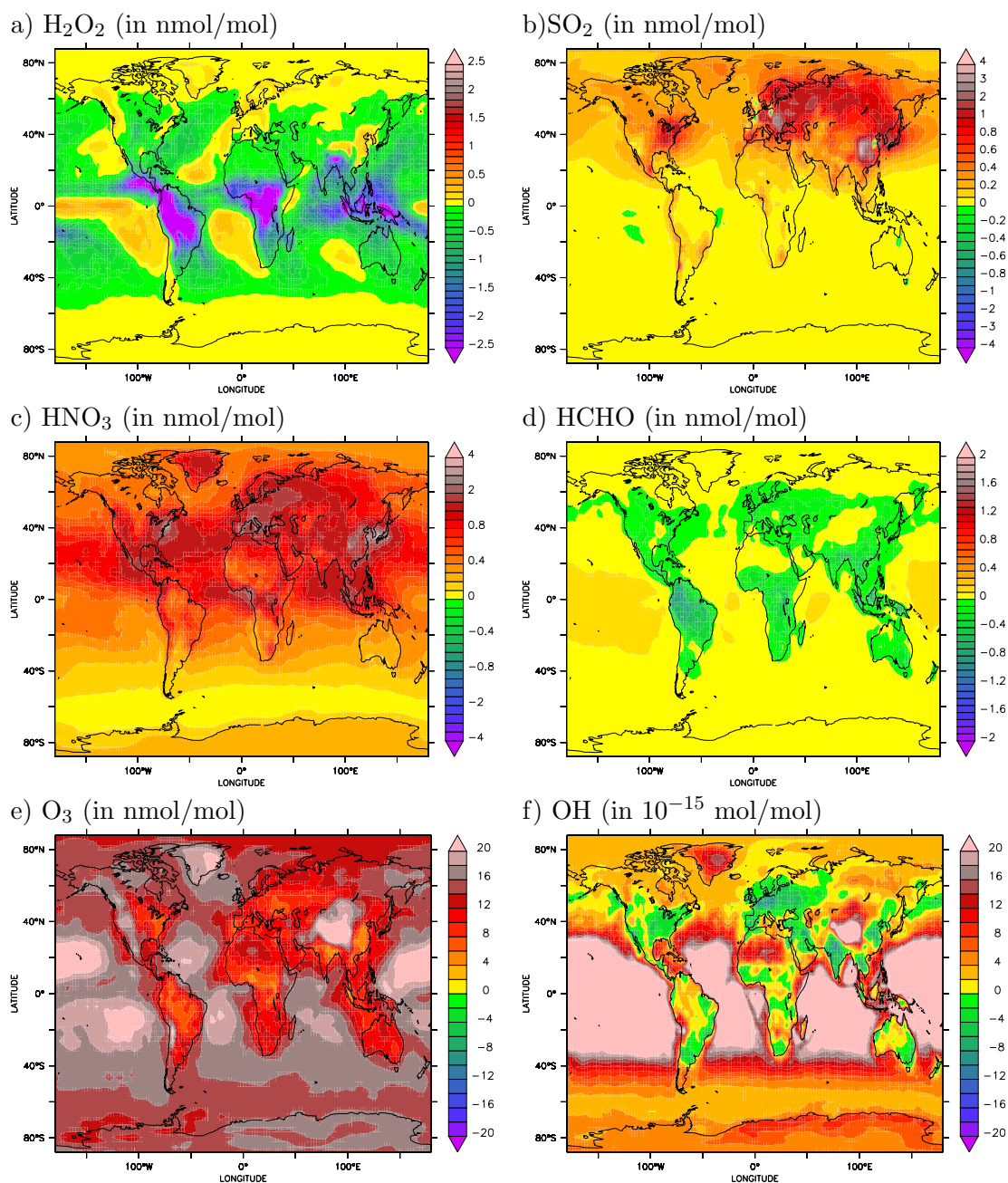
3 Surface layer OH distributions, comparing the individual simulations

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.



4 Surface layer trace gas distributions of the NOSCAV simulation

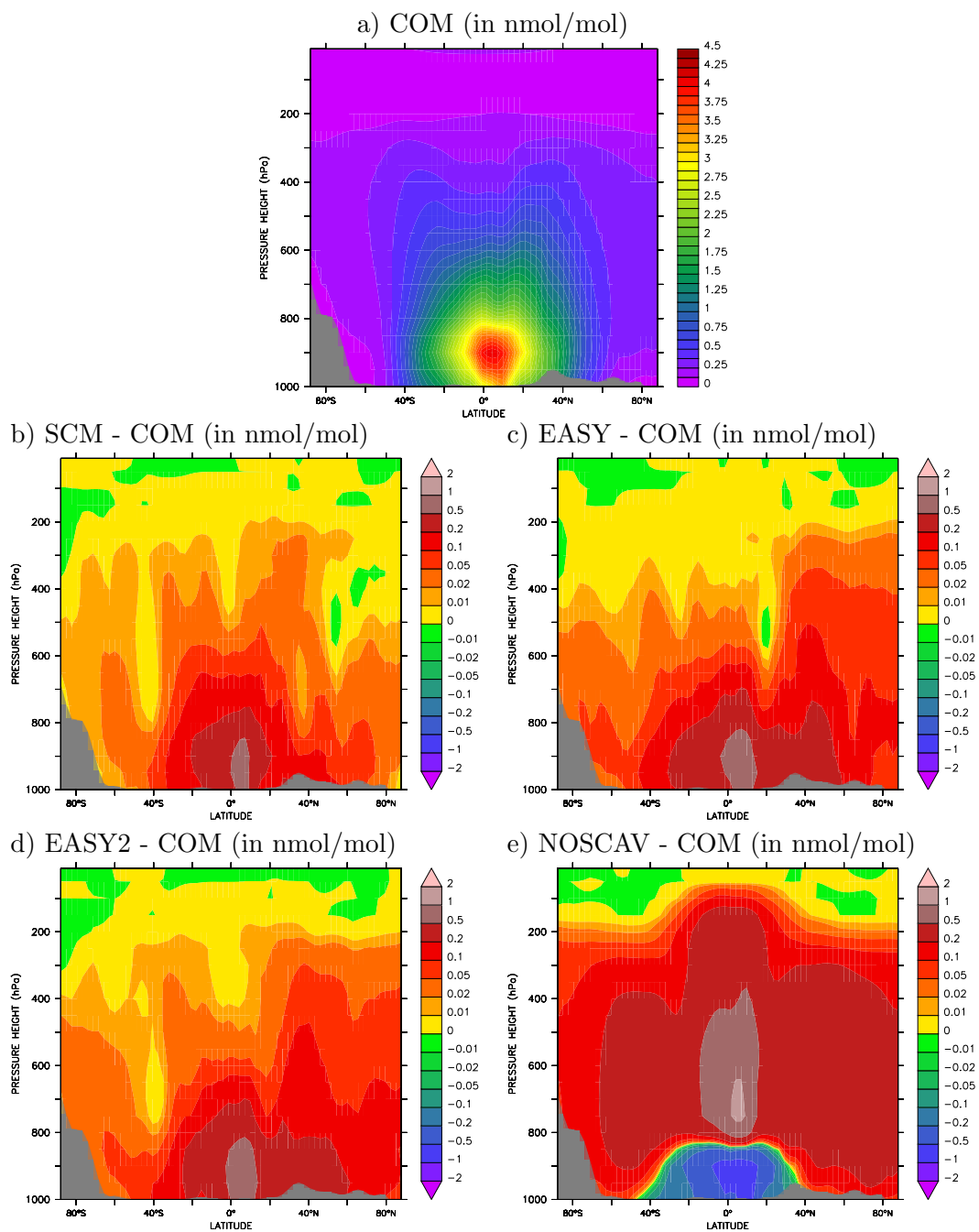
In this section the annual average surface layer trace gas mixing ratio differences (NOSCAV - COM) of the NOSCAV simulation are presented. Since this simulation setup without a sink in the liquid phase is hardly realistic, the Figures are shown here in the supplement, completing the Figures 6, 8, 10,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



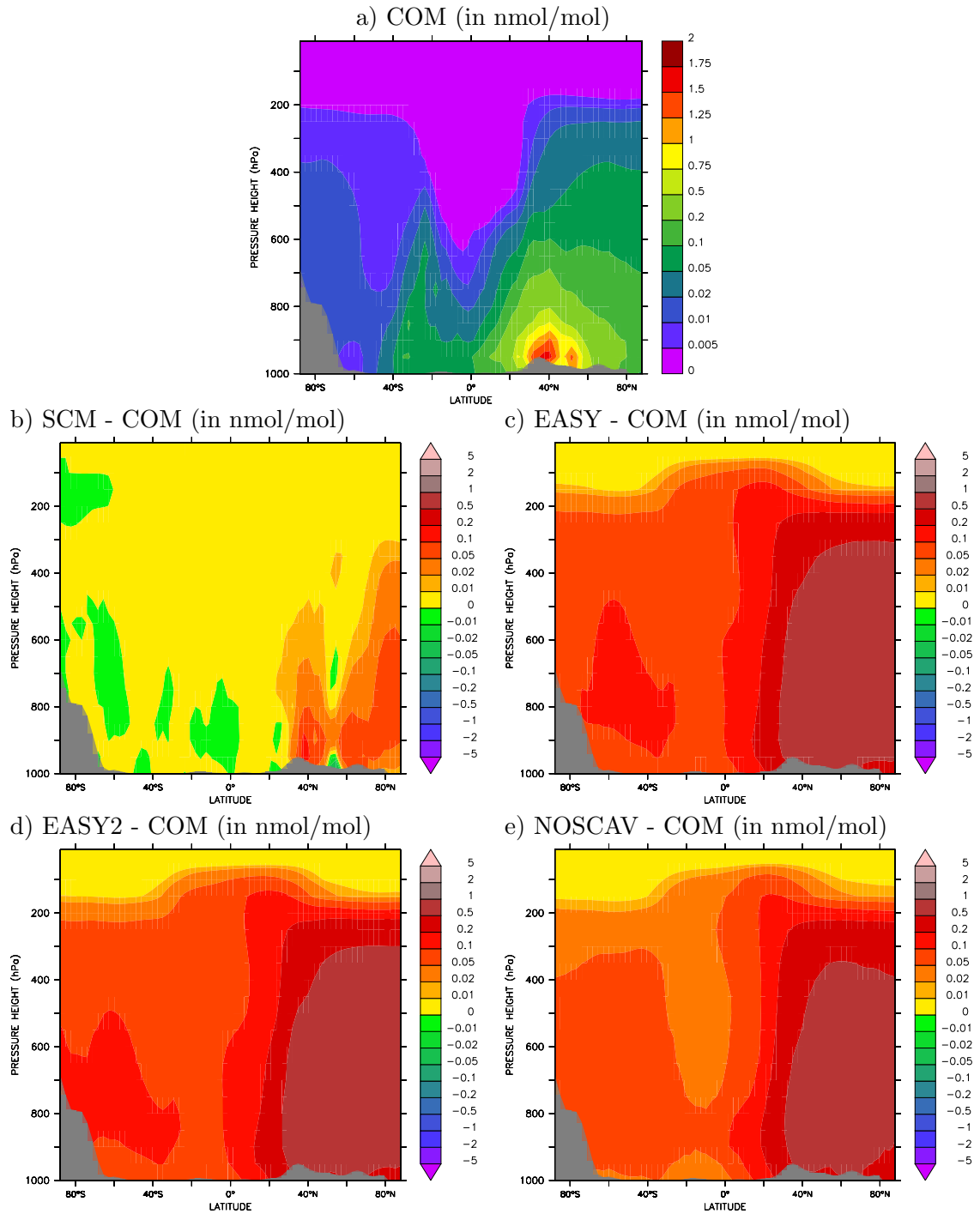
5 Zonal average trace gas distributions, comparing the individual simulations

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.

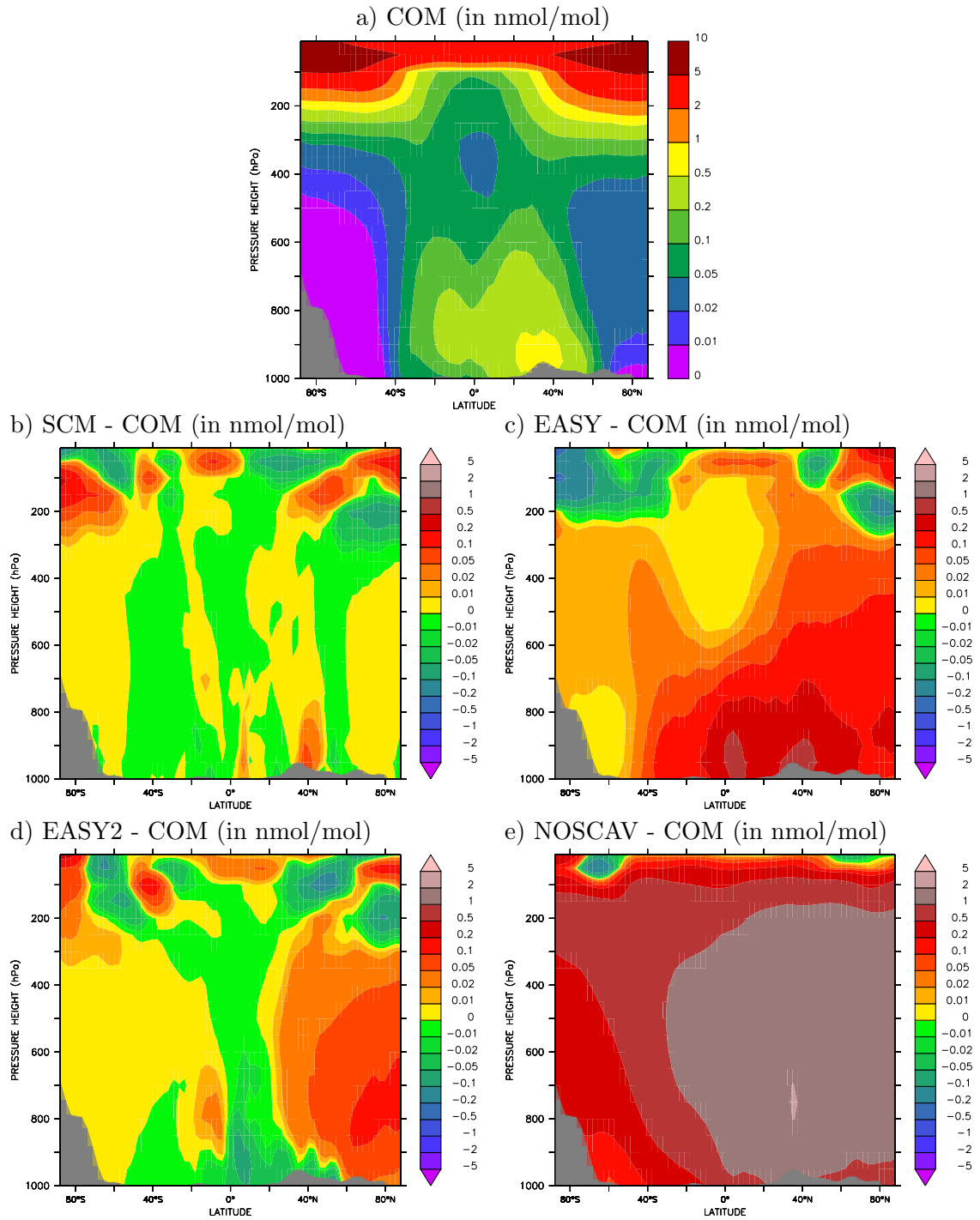
5.1 Hydrogen peroxide (H_2O_2)



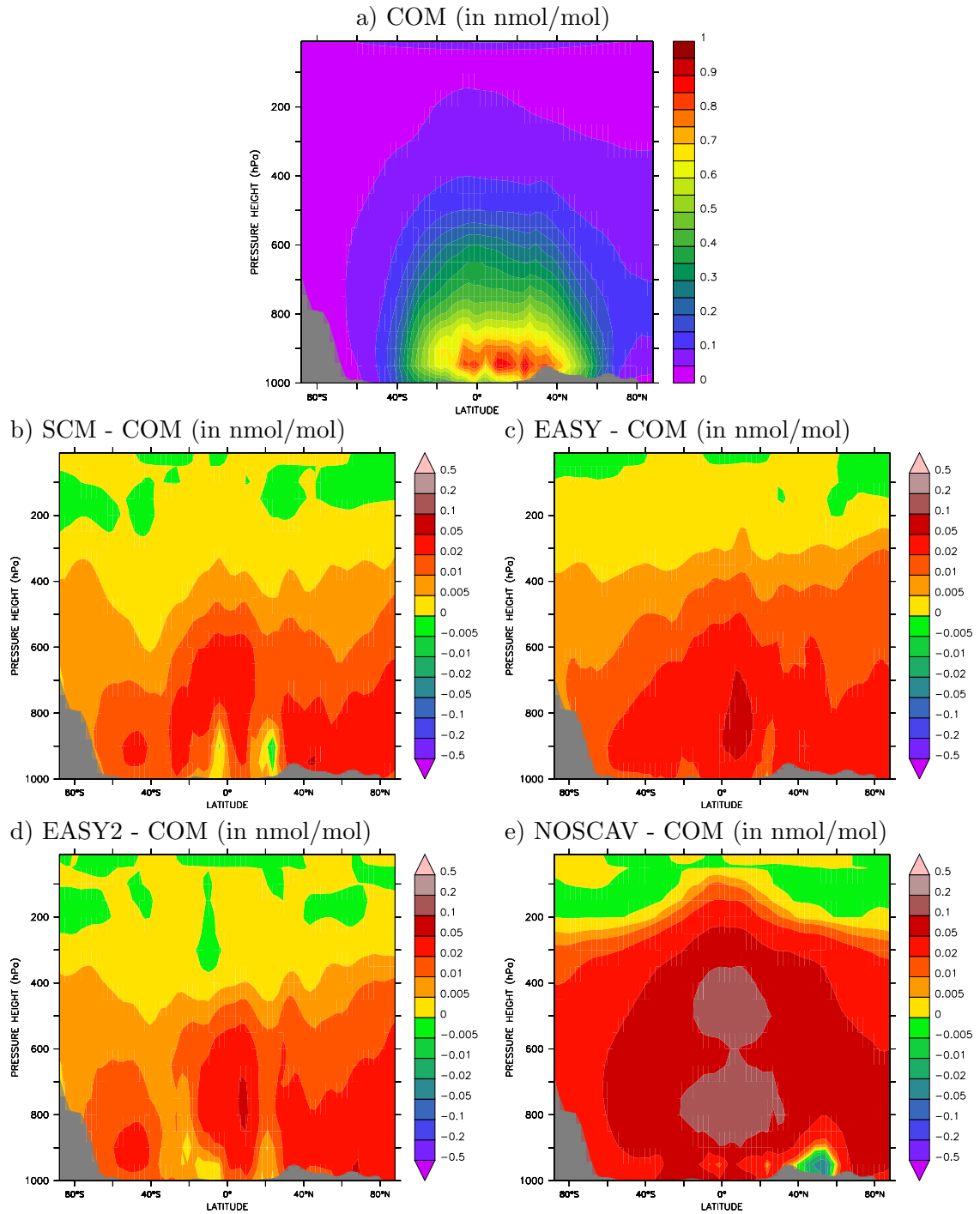
5.2 Sulphur dioxide (SO₂)



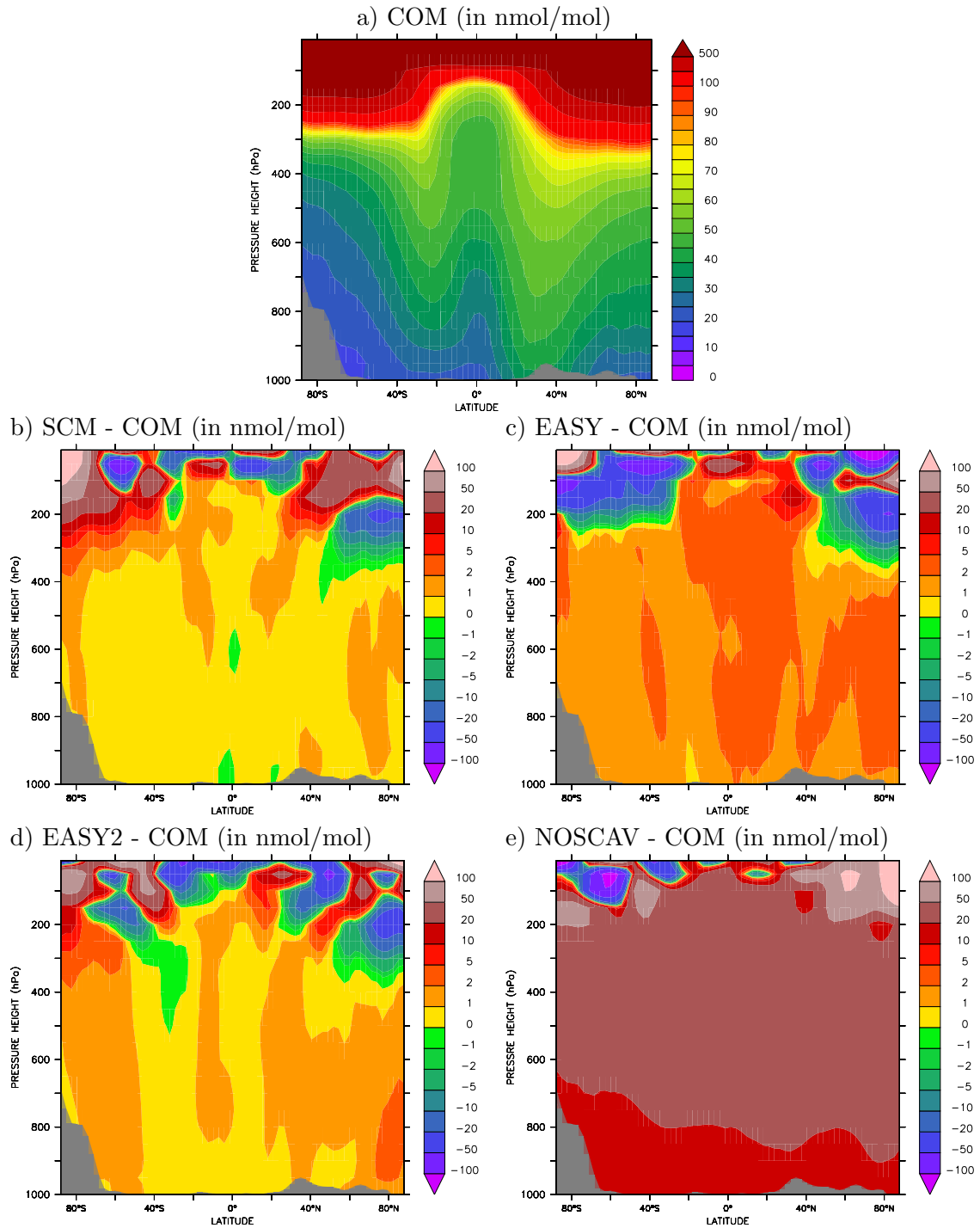
5.3 Nitric acid (HNO₃)



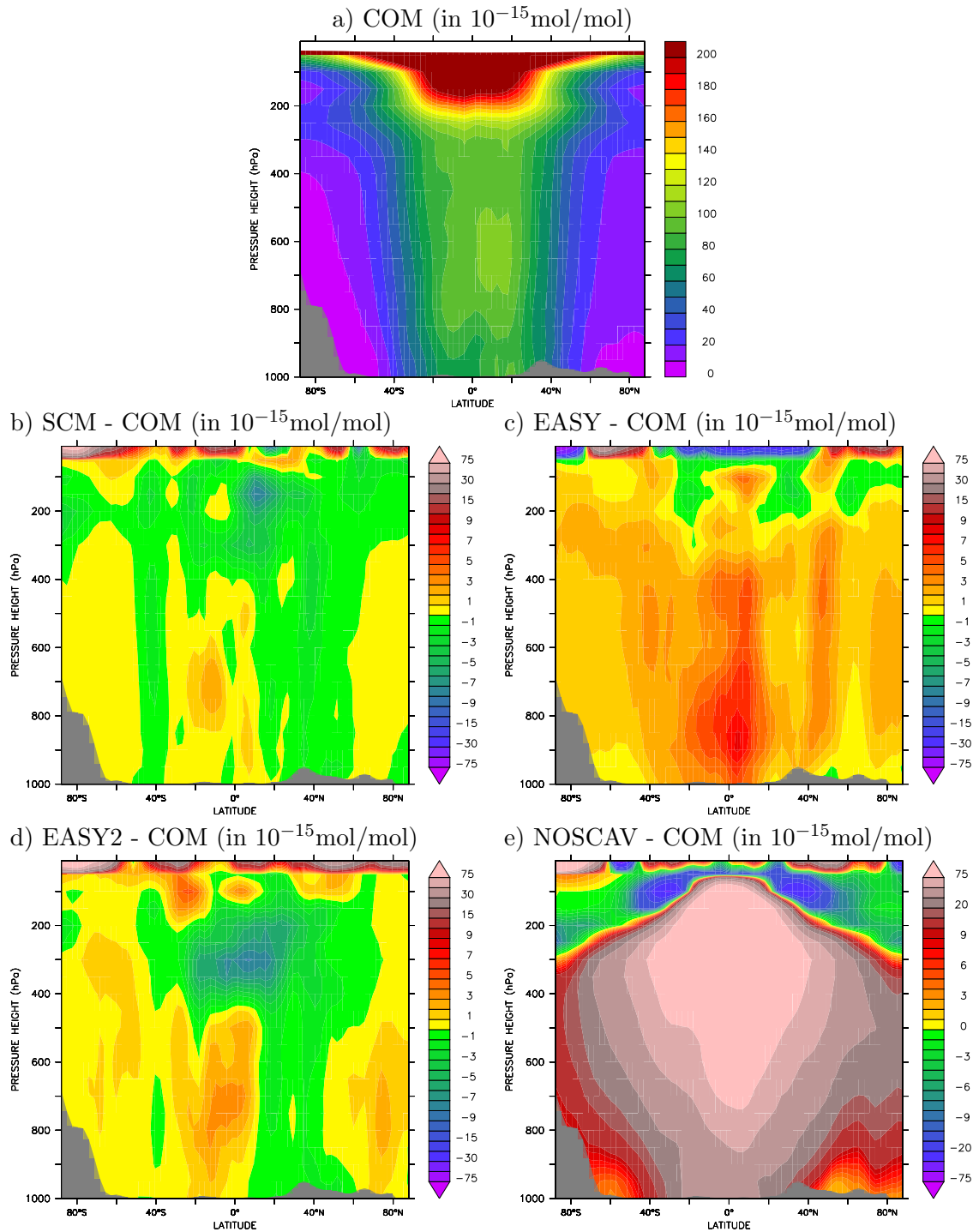
5.4 Formaldehyde (HCHO)



5.5 Ozone (O_3)



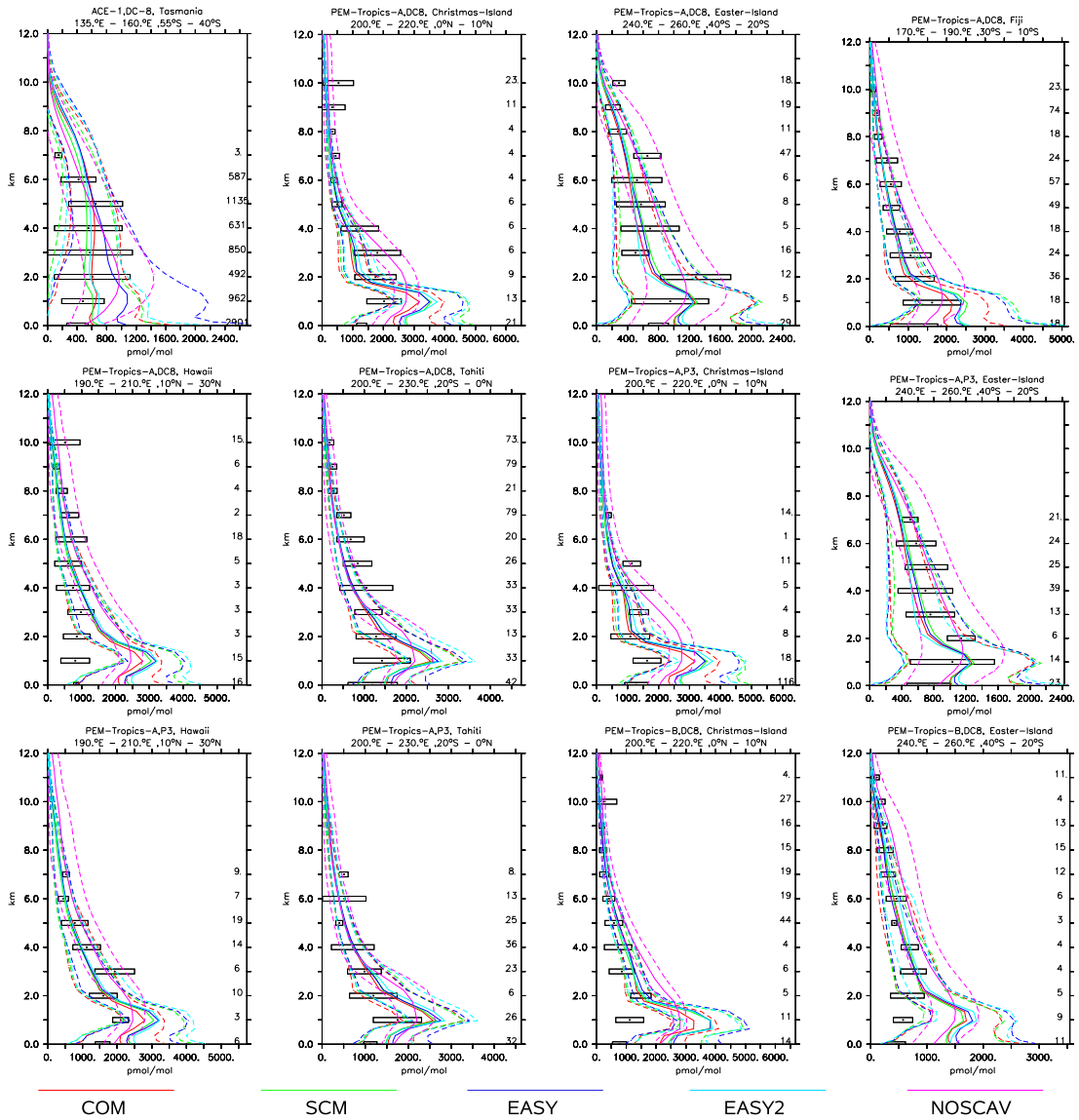
5.6 Hydroxyl radical (OH)

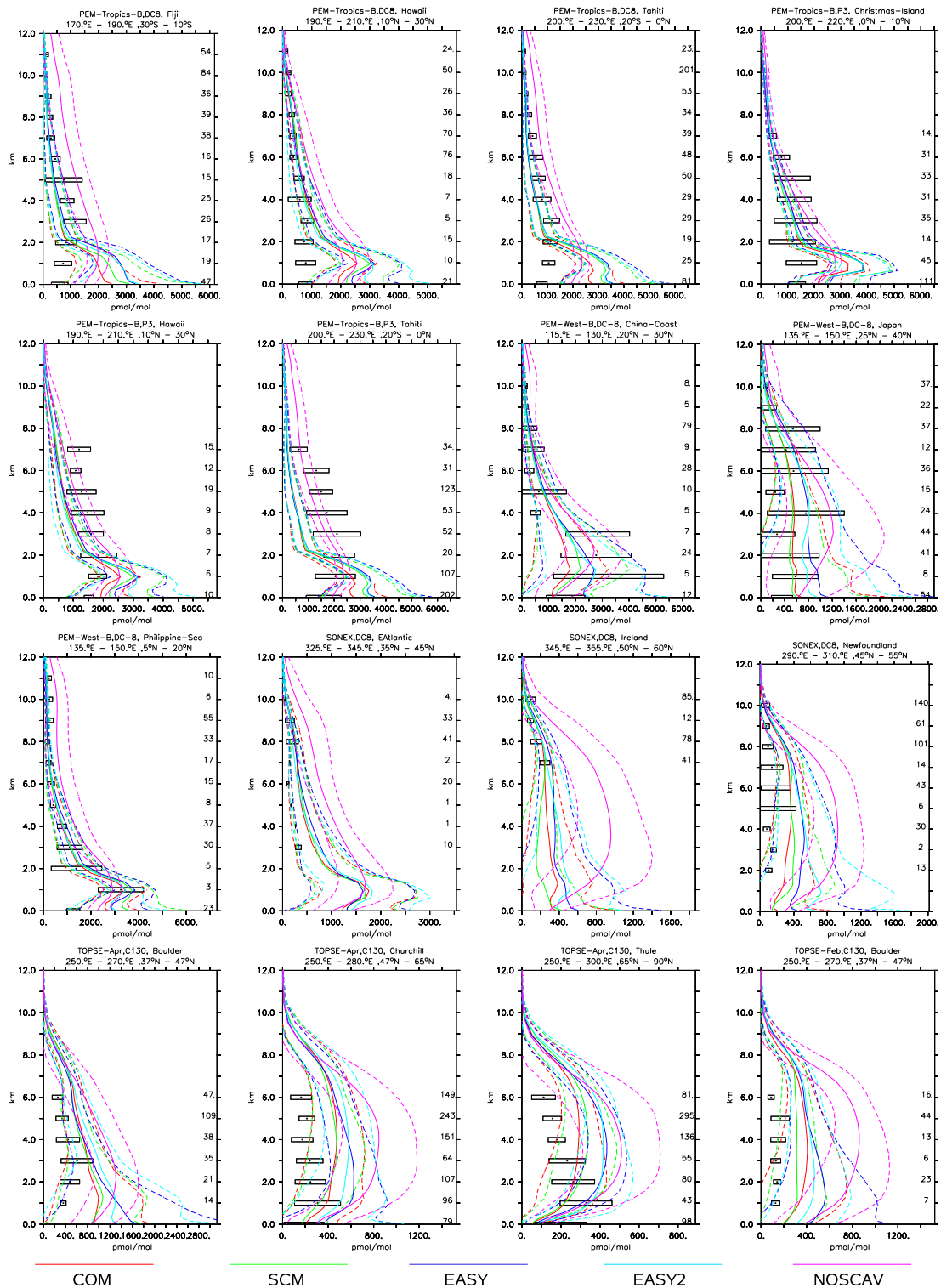


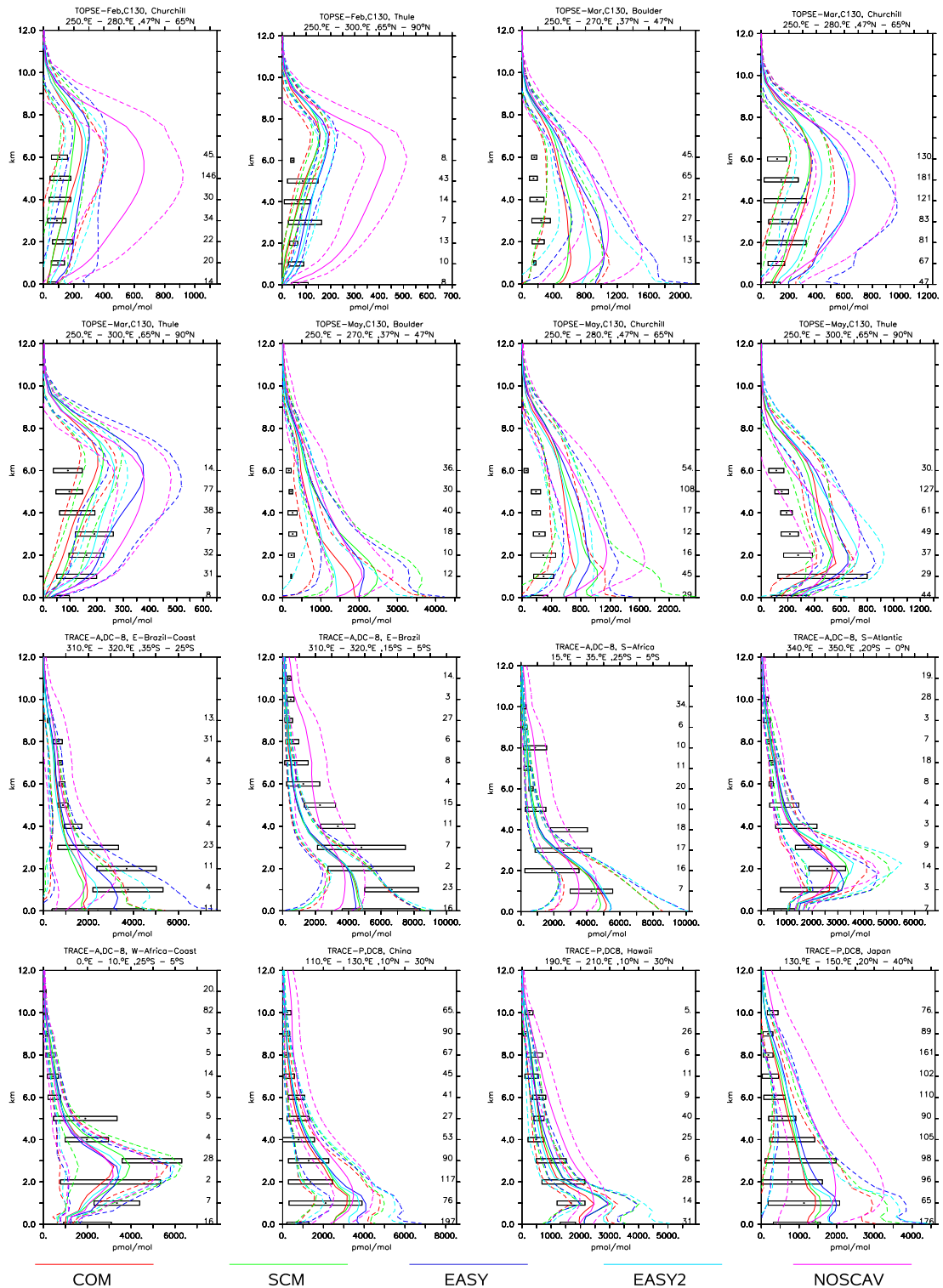
6 Comparison of the simulation results with the Emmons et al. (2000) observation dataset

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 $\pm \sigma$ (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.

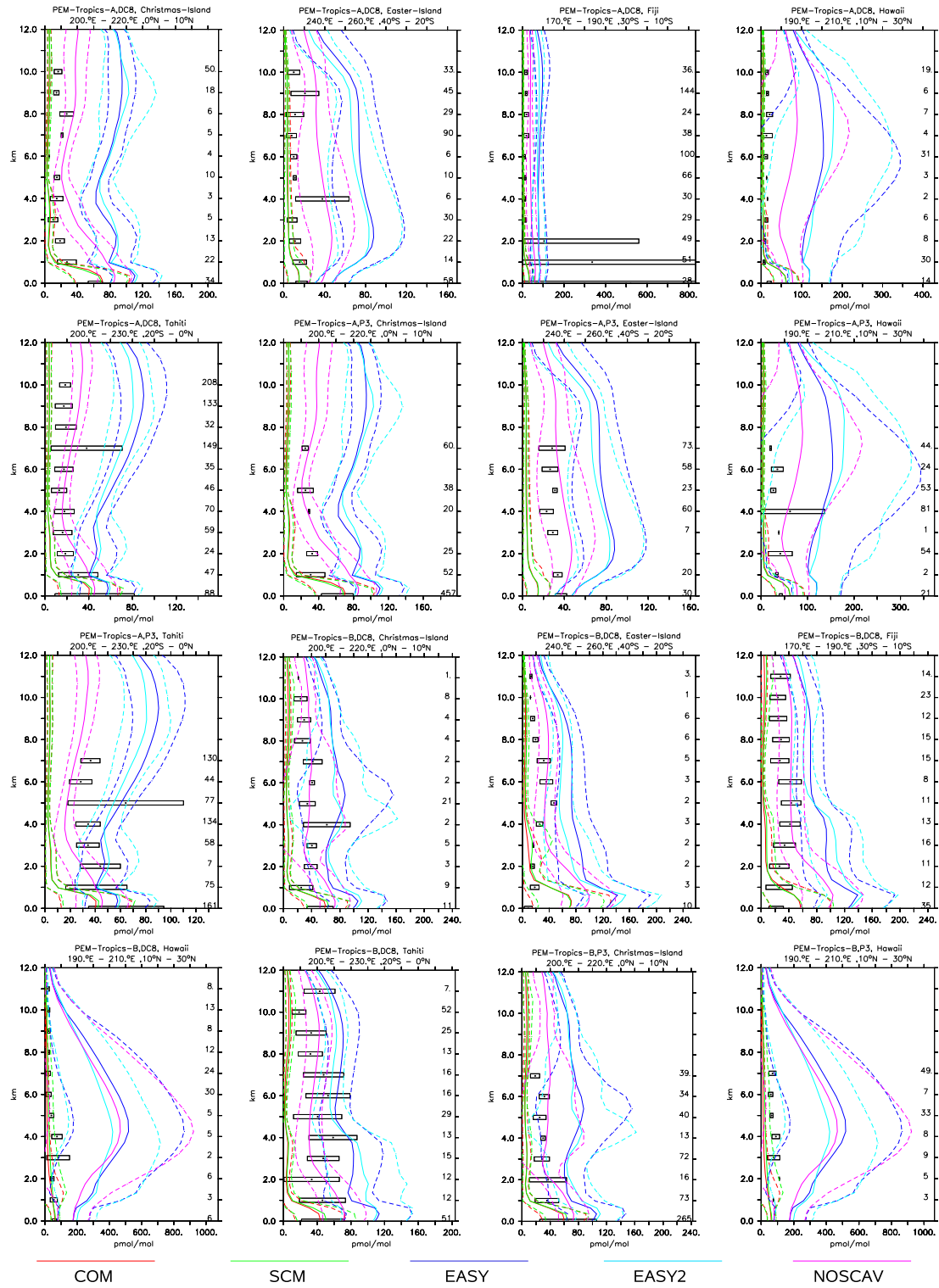
6.1 Hydrogen peroxide (H_2O_2)

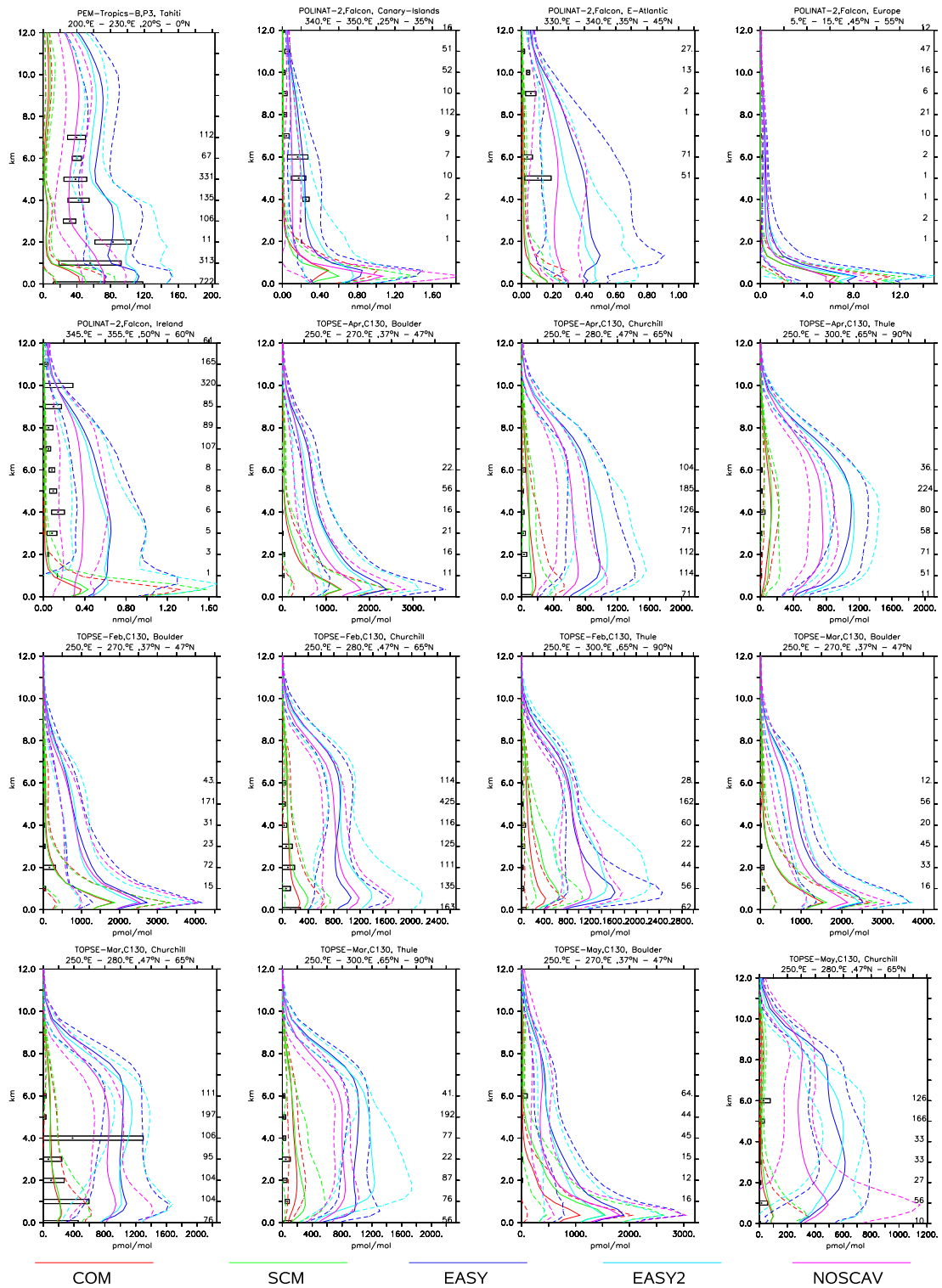


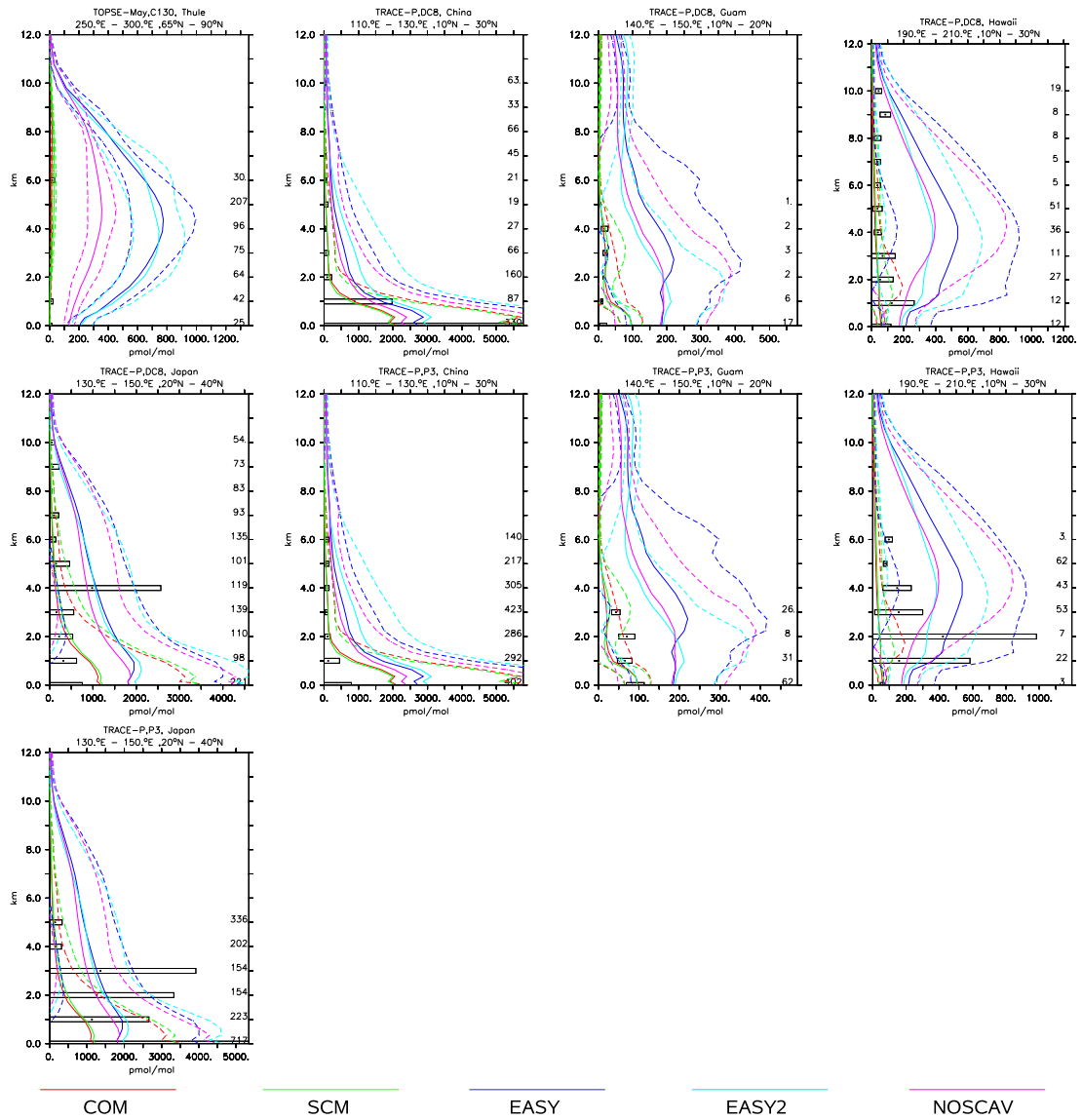




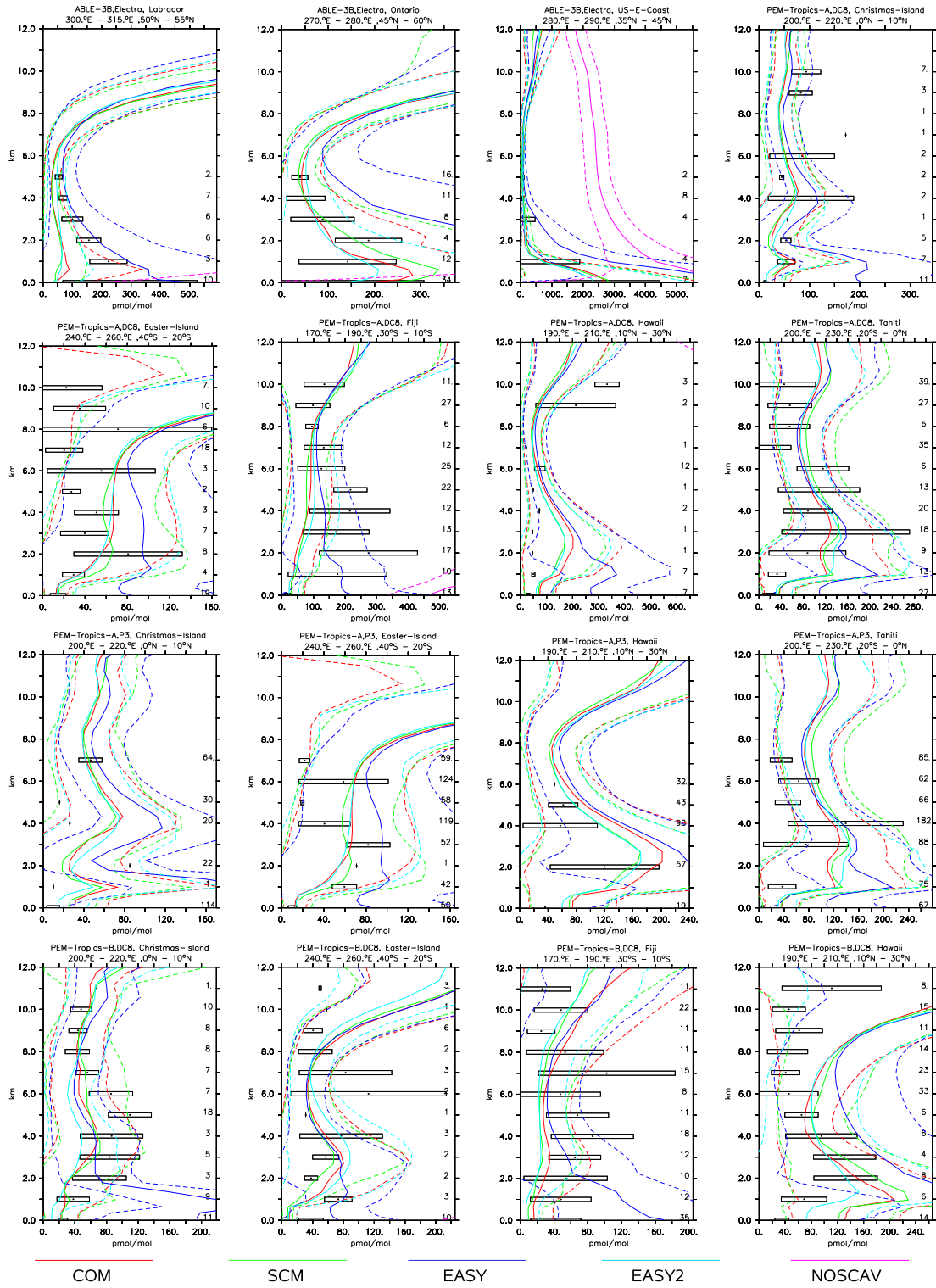
6.2 Sulphur dioxide (SO₂)

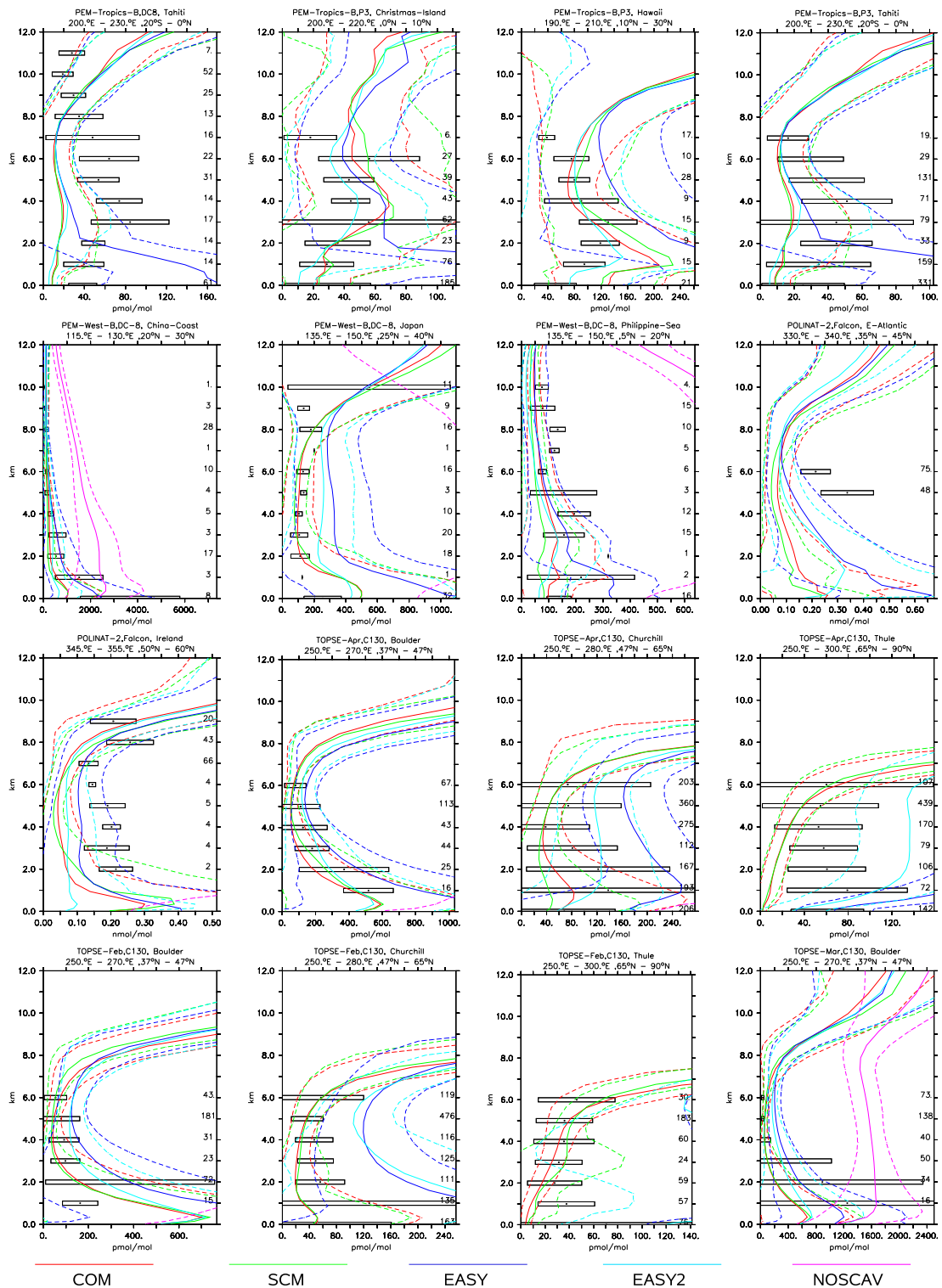


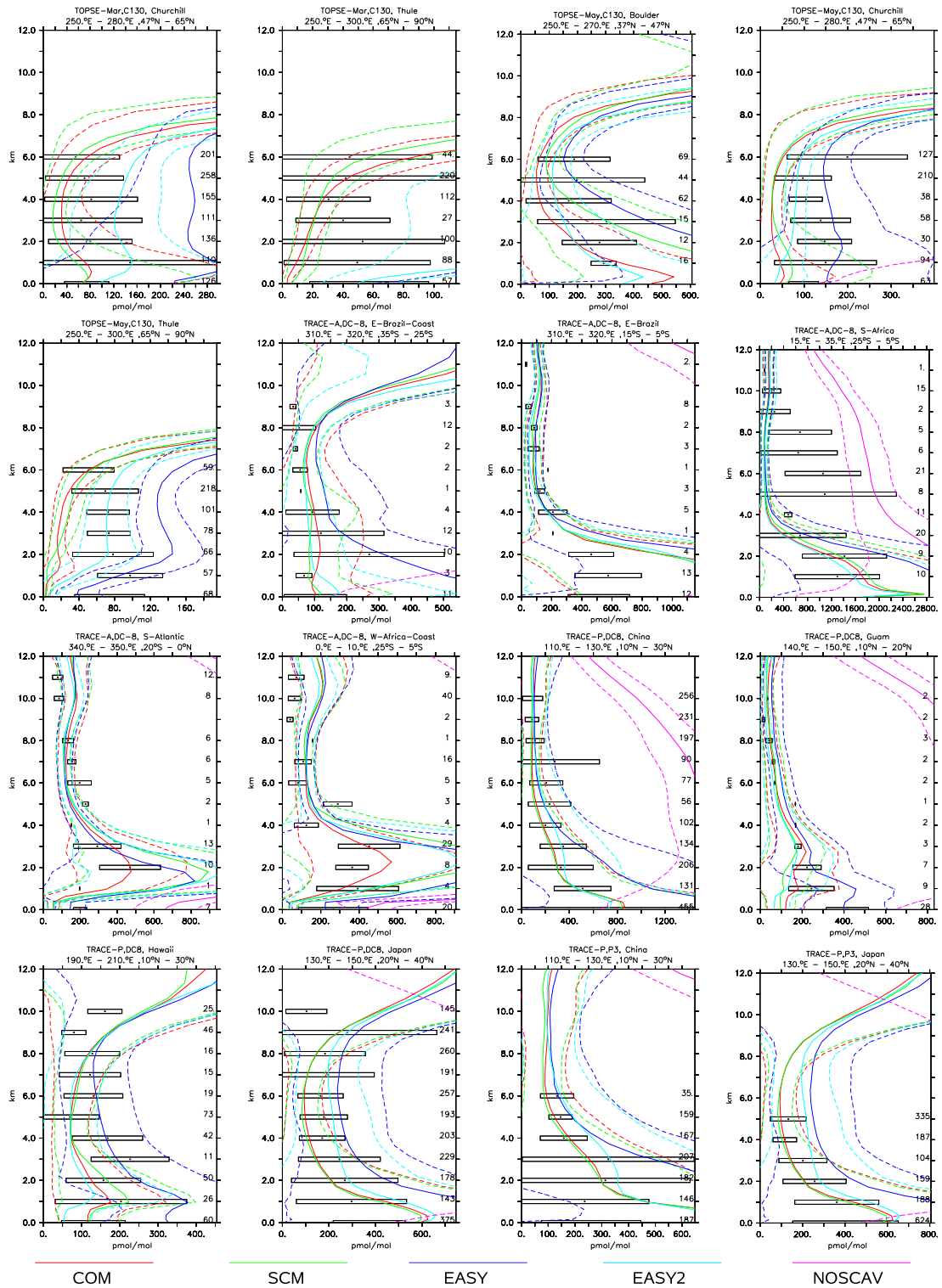




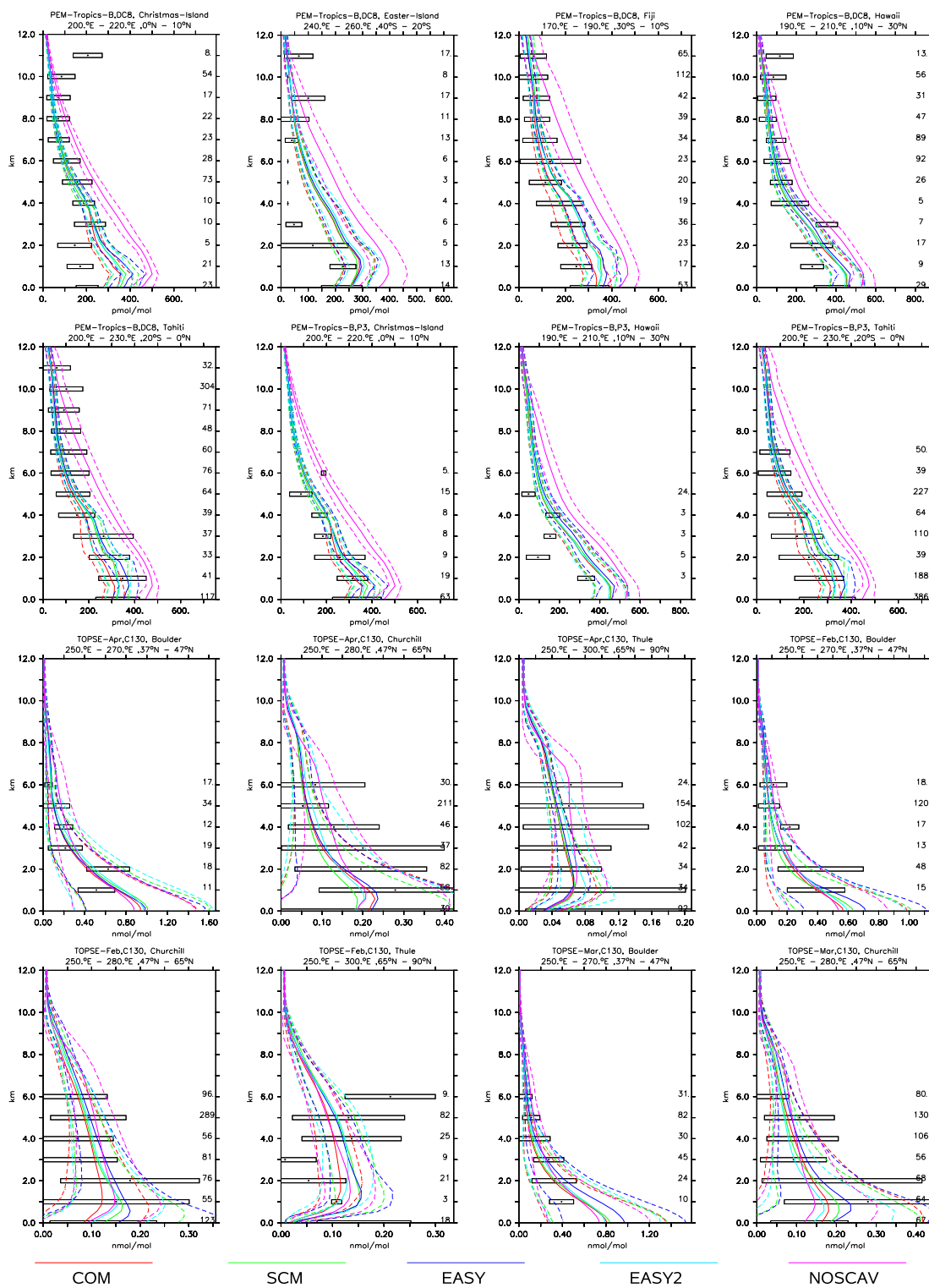
6.3 Nitric Acid (HNO₃)

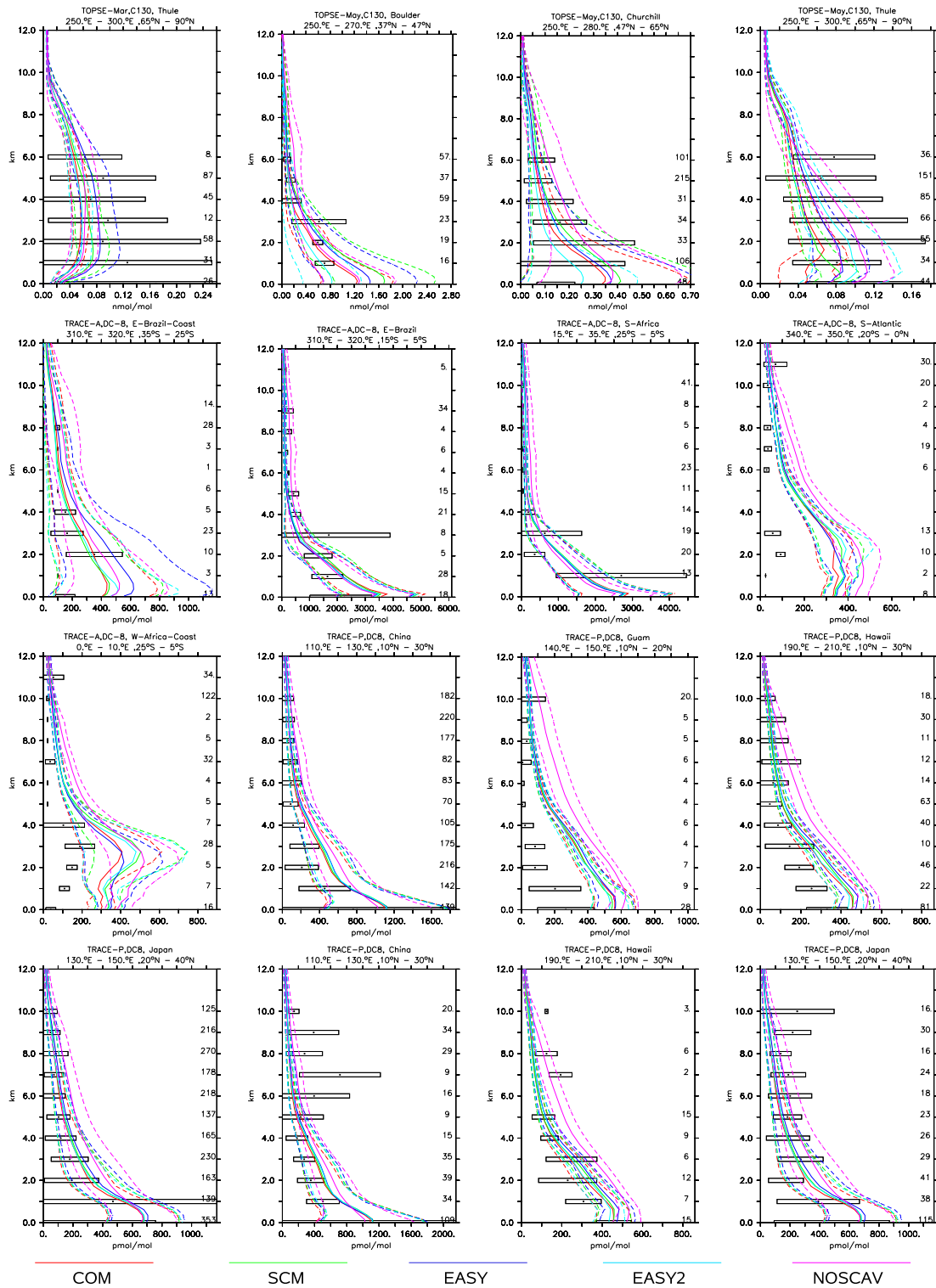




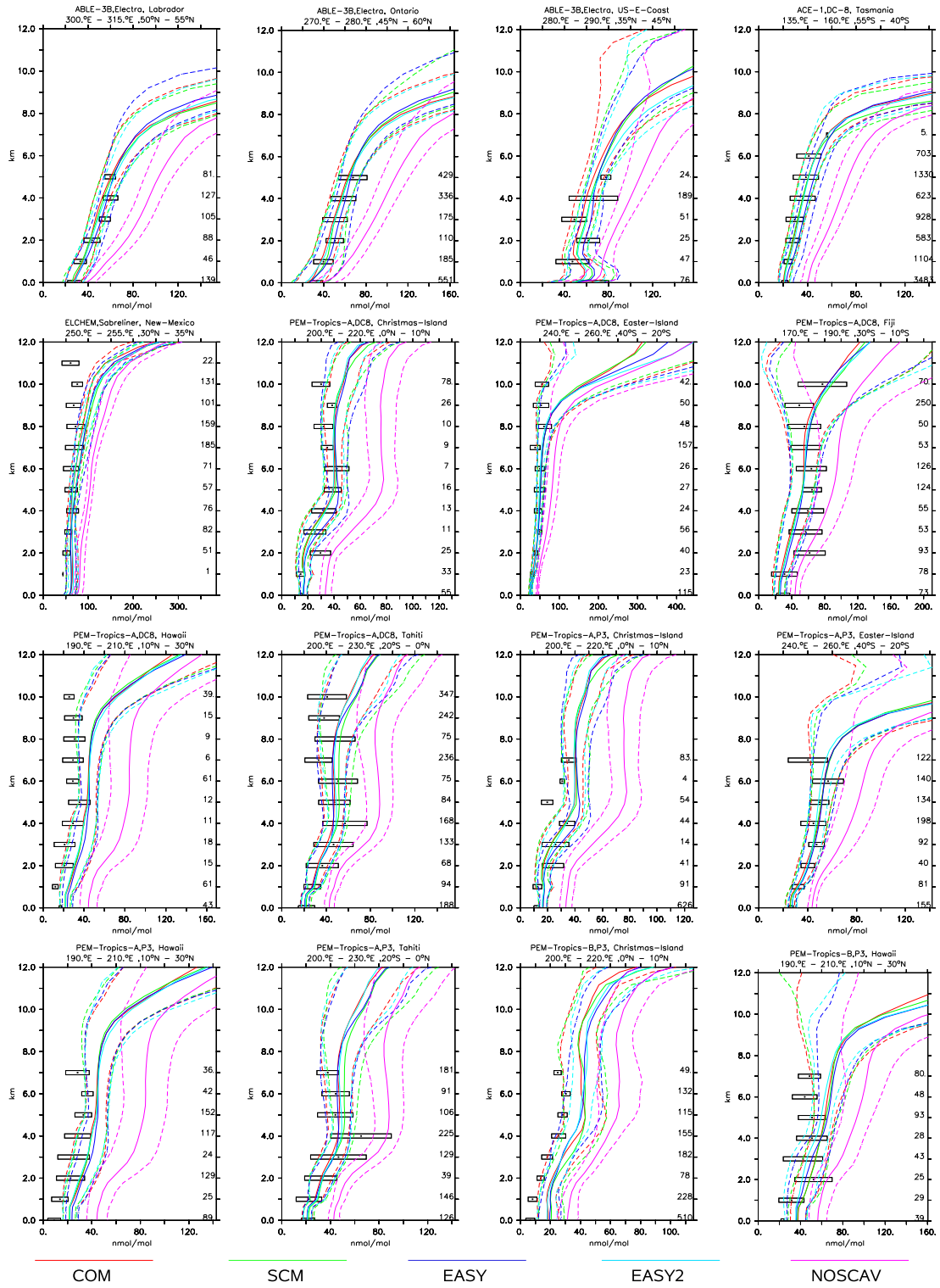


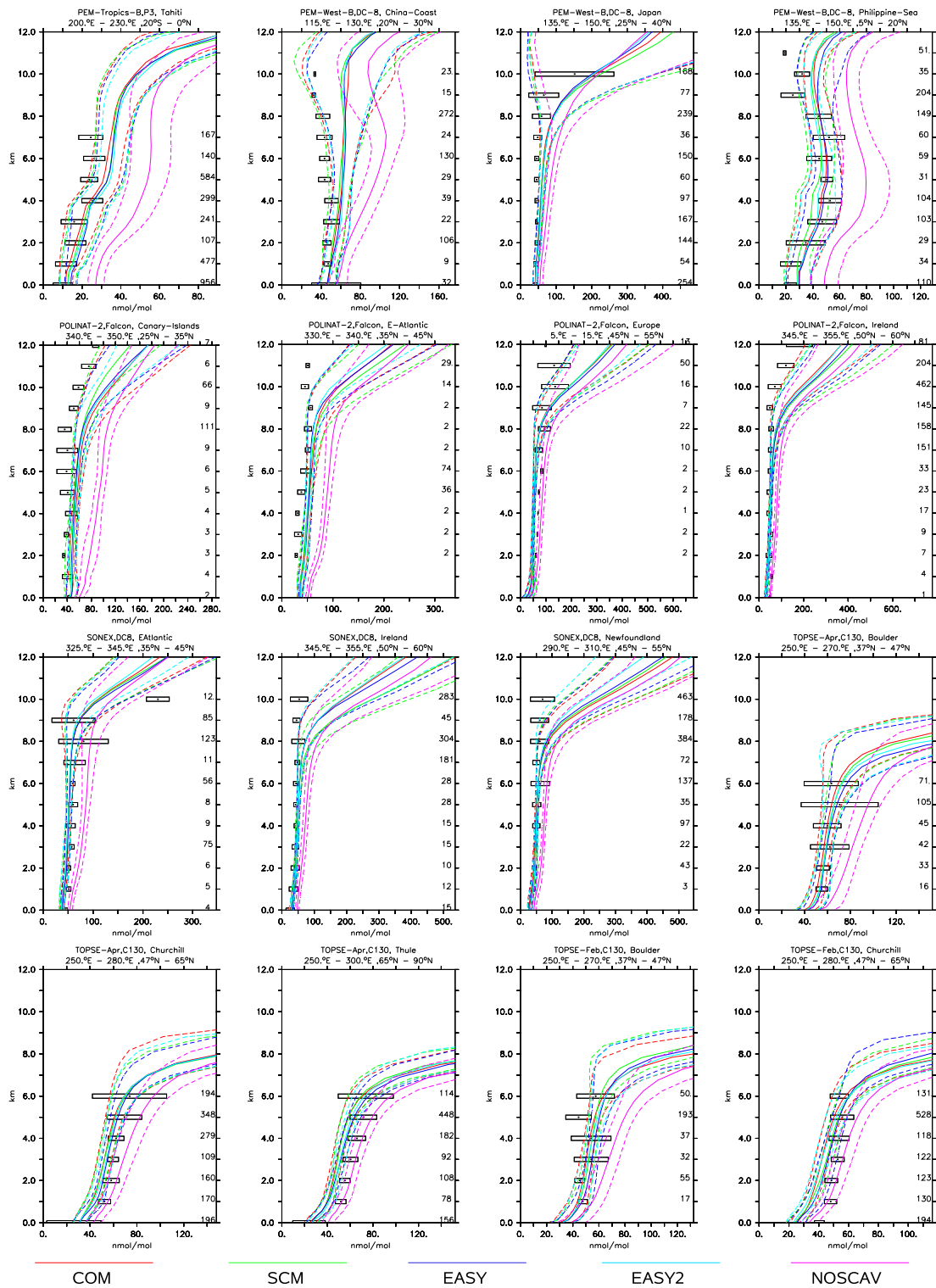
6.4 Formaldehyde (HCHO)

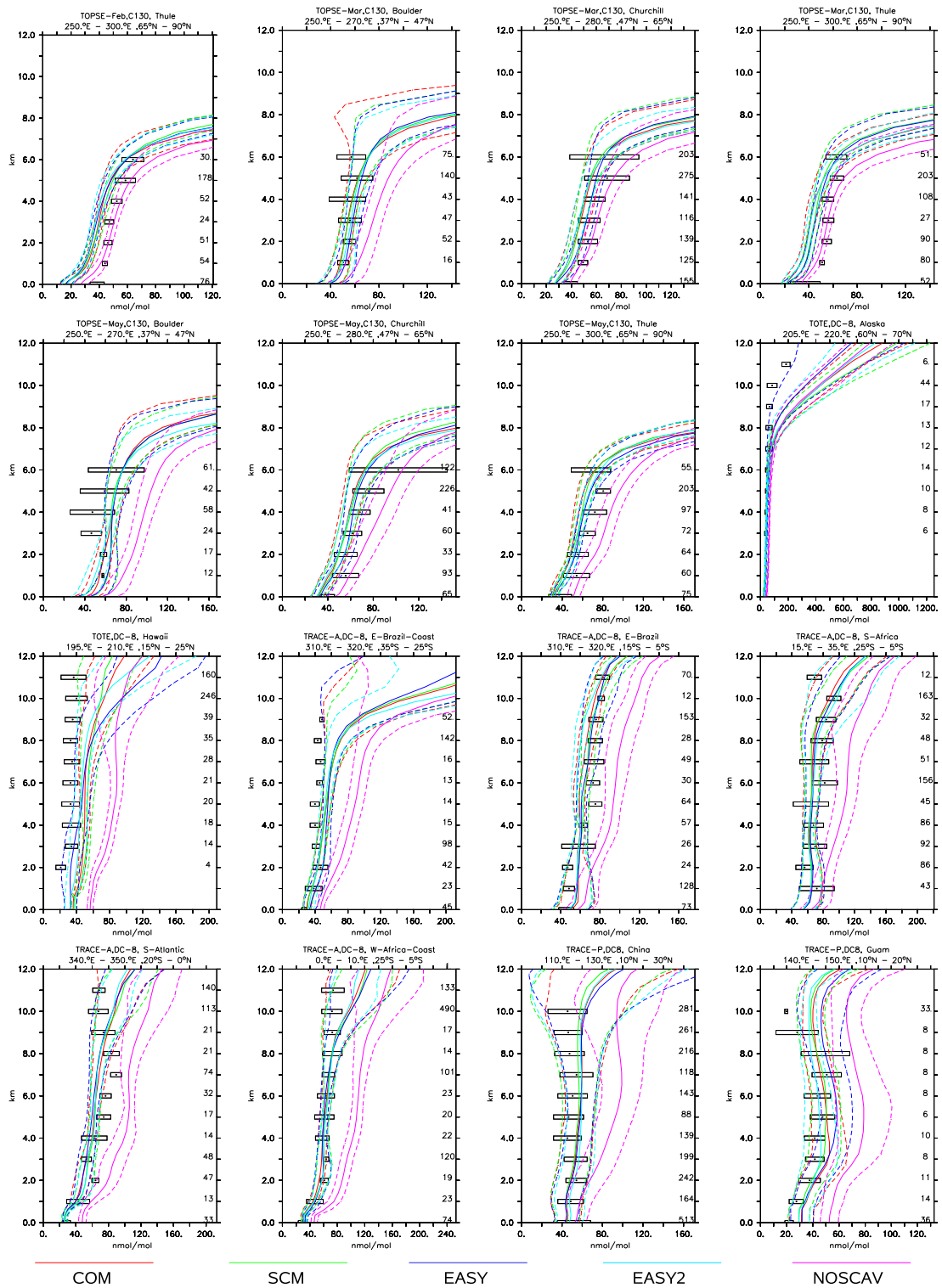


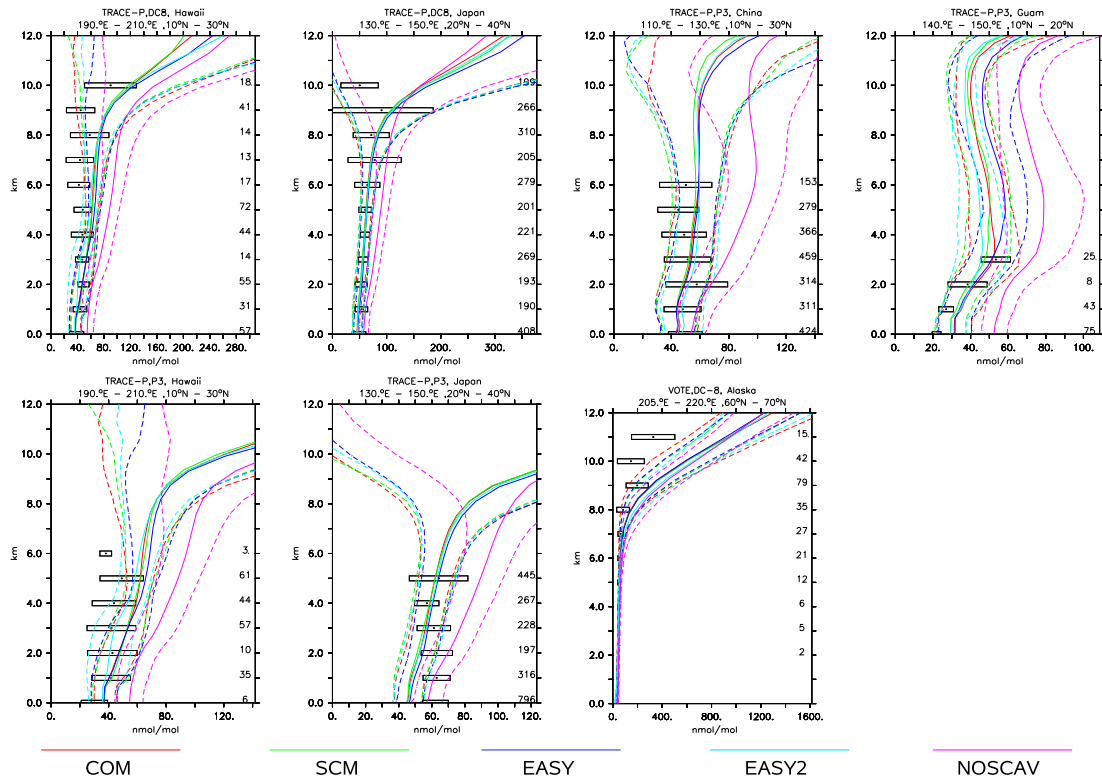


6.5 Ozone (O_3)









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