The Chemical Mechanism of MECCA1

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Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	`3.2E-11*EXP(70./temp)`	Sander et al. (2003)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	`6.E-34*((temp/300.)**(-2.4))*cair`	Sander et al. (2003)
G1002	StG	$O_3 + O(^1D) \rightarrow 2\ O_2$	`1.2E-10`	Sander et al. (2003)*
G1003	StG	$O_3 + O(^3P) \rightarrow 2\ O_2$	`8.E-12*EXP(-2060./temp)`	Sander et al. (2003)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	`k_3rd(temp,cair,5.7E-32,1.6,7.5E-11,0.,0.6)`	Sander et al. (2003)
G2101	StG	$H + O_3 \rightarrow OH$	`1.4E-10*EXP(-470./temp)`	Sander et al. (2003)
G2102	StG	$H_2 + O(^1D) \rightarrow H + OH$	`1.1E-10`	Sander et al. (2003)
G2103	StG	$OH + O(^3P) \rightarrow H$	`2.2E-11*EXP(120./temp)`	Sander et al. (2003)
G2104	StTrG	$OH + O_3 \rightarrow HO_2$	`1.7E-12*EXP(-940./temp)`	Sander et al. (2003)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	`5.5E-12*EXP(-2000./temp)`	Sander et al. (2003)
G2106	StG	$HO_2 + O(^3P) \rightarrow OH$	`3.E-11*EXP(200./temp)`	Sander et al. (2003)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH$	`1.E-14*EXP(-490./temp)`	Sander et al. (2003)
G2108a	StG	$HO_2 + H \rightarrow 2\ OH$	`0.69*8.1E-11`	Sander et al. (2003)*
G2108b	StG	$HO_2 + H \rightarrow H_2$	`0.29*8.1E-11`	Sander et al. (2003)*
G2108c	StG	$HO_2 + H \rightarrow O(^3P) + H_2O$	`0.02*8.1E-11`	Sander et al. (2003)*
G2109	StTrG	$HO_2 + OH \rightarrow H_2O$	`4.8E-11*EXP(250./temp)`	Sander et al. (2003)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2$	`k_HO2_HO2`	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\ OH$	`2.2E-10`	Sander et al. (2003)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	`2.9E-12*EXP(-160./temp)`	Sander et al. (2003)
G3100	StGN	$N + O_2 \rightarrow NO + O(^3P)$	`1.5E-11*EXP(-3600./temp)`	Sander et al. (2003)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	`1.8E-11*EXP(110./temp)`	Sander et al. (2003)
G3102a	StGN	$N_2O + O(^1D) \rightarrow 2\ NO$	`6.7E-11`	Sander et al. (2003)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	`4.9E-11`	Sander et al. (2003)

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

#	labels	reaction	rate coefficient	reference
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	`3.E-12*EXP(-1500./temp)`	Sander et al. (2003)
G3104	StGN	$NO + N \rightarrow O(^3P) + N_2$	`2.1E-11*EXP(100./temp)`	Sander et al. (2003)
G3105	StGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	`5.6E-12*EXP(180./temp)`	Sander et al. (2003)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	`1.2E-13*EXP(-2450./temp)`	Sander et al. (2003)
G3107	StGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	`5.8E-12*EXP(220./temp)`	Sander et al. (2003)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\ NO_2$	`1.5E-11*EXP(170./temp)`	Sander et al. (2003)
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	`k_NO3_NO2`	Sander et al. (2003)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	`k_NO3_NO2/(3.E-27*EXP(10990./temp))`	Sander et al. (2003)*
G3200	TrG	$NO + OH \rightarrow HONO$	`k_3rd(temp,cair,7.E-31,2.6,3.6E-11,0.1,0.6)`	Sander et al. (2003)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	`3.5E-12*EXP(250./temp)`	Sander et al. (2003)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	`k_3rd(temp,cair,2.E-30,3.,2.5E-11,0.,0.6)`	Sander et al. (2003)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	`k_NO2_HO2`	Sander et al. (2003)
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	`3.5E-12`	Sander et al. (2003)
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	`1.8E-11*EXP(-390./temp)`	Sander et al. (2003)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	`k_HNO3_OH`	Sander et al. (2003)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	`k_NO2_HO2/(2.1E-27*EXP(10900./temp))`	Sander et al. (2003)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	`1.3E-12*EXP(380./temp)`	Sander et al. (2003)
G4100	StG	$CH_4 + O(^1D) \rightarrow .75\ CH_3O_2 + .75\ OH + .25\ HCHO + .4\ H + .05\ H_2$	`1.5E-10`	Sander et al. (2003)
G4101	StTrG	$CH_4 + OH \rightarrow CH_3O_2 + H_2O$	`1.85E-20*EXP(2.82*log(temp)-987./temp)`	Atkinson (2003)*
G4102	TrG	$CH_3OH + OH \rightarrow HCHO + HO_2$	`7.3E-12*EXP(-620./temp)`	Sander et al. (2003)
G4103a	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH$	`4.1E-13*EXP(750./temp)/(1.+1./497.7*EXP(1160./temp))`	Sander et al. (2003)*
G4103b	StTrG	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	`4.1E-13*EXP(750./temp)/(1.+497.7*EXP(-1160./temp))`	Sander et al. (2003)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	`2.8E-12*EXP(300./temp)`	Sander et al. (2003)
G4105	TrGN	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	`1.3E-12`	Atkinson et al. (1999)
G4106a	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow 2\ HCHO + 2\ HO_2$	`9.5E-14*EXP(390./temp)/(1.+1./26.2*EXP(1130./temp))`	Sander et al. (2003)
G4106b	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH$	`9.5E-14*EXP(390./temp)/(1.+26.2*EXP(-1130./temp))`	Sander et al. (2003)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	`k_CH3OOH_OH`	Sander et al. (2003)*
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	`9.52E-18*EXP(2.03*log(temp)+636./temp)`	Sivakumaran et al. (2003)

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

#	labels	reaction	rate coefficient	reference
G4109	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	`3.4E-13*EXP(-1900./temp)`	Sander et al. (2003)*
G4110	StTrG	$CO + OH \rightarrow H + CO_2$	`1.57E-13 + cair*3.54E-33`	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow HO_2$	`4.E-13`	Sander et al. (2003)
G4200	TrGC	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$	`1.49E-17*temp*temp*EXP(-499./temp)`	Atkinson (2003)
G4203	TrGC	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	`7.5E-13*EXP(700./temp)`	Sander et al. (2003)
G4204	TrGNC	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	`2.6E-12*EXP(365./temp)`	Sander et al. (2003)
G4205	TrGNC	$C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$	`2.3E-12`	Atkinson et al. (1999)
G4206	TrGC	$C_2H_5O_2 + CH_3O_2 \rightarrow .75\ HCHO + HO_2 + .75\ CH_3CHO + .25\ CH_3OH$	`1.6E-13*EXP(195./temp)`	see note
G4207	TrGC	$C_2H_5OOH + OH \rightarrow .3\ C_2H_5O_2 + .7\ CH_3CHO + .7\ OH$	`k_CH3OOH_OH`	see note
G4208	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	`5.6E-12*EXP(270./temp)`	Sander et al. (2003)
G4209	TrGNC	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	`1.4E-12*EXP(-1900./temp)`	Sander et al. (2003)
G4210	TrGC	$CH_3COOH + OH \rightarrow CH_3O_2$	`4.E-13*EXP(200./temp)`	Sander et al. (2003)
G4211a	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	`4.3E-13*EXP(1040./temp)/(1.+1./37.*EXP(660./temp))`	Tyndall et al. (2001)
G4211b	TrGC	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	`4.3E-13*EXP(1040./temp)/(1.+37.*EXP(-660./temp))`	Tyndall et al. (2001)
G4212	TrGNC	$CH_3C(O)OO + NO \rightarrow CH_3O_2 + NO_2$	`8.1E-12*EXP(270./temp)`	Tyndall et al. (2001)
G4213	TrGNC	$CH_3C(O)OO + NO_2 \rightarrow PAN$	`k_PA_NO2`	Tyndall et al. (2001)
G4214	TrGNC	$CH_3C(O)OO + NO_3 \rightarrow CH_3O_2 + NO_2$	`4.E-12`	Canosa-Mas et al. (1996)
G4215a	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow HCHO + HO_2 + CH_3O_2 + CO_2$	`0.9*2.E-12*EXP(500./temp)`	Sander et al. (2003)
G4215b	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow CH_3COOH + HCHO + CO_2$	`0.1*2.E-12*EXP(500./temp)`	Sander et al. (2003)
G4216	TrGC	$CH_3C(O)OO + C_2H_5O_2 \rightarrow .82\ CH_3O_2 + CH_3CHO + .82\ HO_2 + .18\ CH_3COOH$	`4.9E-12*EXP(211./temp)`	Atkinson et al. (1999), Kirchner and Stockwell (1996)*
G4217	TrGC	$CH_3C(O)OO + CH_3C(O)OO \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	`2.5E-12*EXP(500./temp)`	Tyndall et al. (2001)
G4218	TrGC	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO$	`k_CH3OOH_OH`	see note
G4220	TrGNC	$PAN + OH \rightarrow HCHO + NO_2$	`2.E-14`	see note
G4221	TrGNC	$PAN \rightarrow CH_3C(O)OO + NO_2$	`k_PAN_M`	Sander et al. (2003)*
G4301a	TrGC	$C_3H_6 + O_3 \rightarrow .57\ HCHO + .47\ CH_3CHO + .33\ OH + .26\ HO_2 + .07\ CH_3O_2 + .06\ C_2H_5O_2 + .23\ CH_3C(O)OO + .06\ CH_4 + .31\ CO + .22\ HCOOH + .03\ CH_3OH$	`6.5E-15*EXP(-1900./temp)`	Sander et al. (2003)*
G4302a	TrGC	$C_3H_6 + OH \rightarrow .98\ CH_3CHO + .98\ HCHO$	`k_3rd(temp,cair,8.E-27,3.5,3.E-11,0.,0.5)`	Atkinson et al. (1999)
G4311	TrGC	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2 + H_2O$	`1.33E-13+3.82E-11*EXP(-2000./temp)`	Sander et al. (2003)
G4312a	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3C(O)OO$	`8.6E-13*EXP(700./temp)`	Tyndall et al. (2001)

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

#	labels	reaction	rate coefficient	reference
G4313	TrGNC	$CH_3COCH_2O_2 + NO \rightarrow NO_2 + CH_3C(O)OO + HCHO$	2.9E-12*EXP(300./temp)	Sander et al. (2003)
G4314a	TrGC	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow .5\ CH_3OH + CH_3C(O)OO + .8\ HCHO + .3\ HO_2$	7.5E-13*EXP(500./temp)	Tyndall et al. (2001)
G4400a	TrGC	$C_4H_{10} + OH \rightarrow 0.8\ CH_3C(O)OO + .85\ CH_3CHO + .1\ HCHO$	1.81E-17*temp*temp*EXP(114./temp)	Atkinson (2003)
G6100	StTrGCl	$Cl + O_3 \rightarrow ClO$	2.3E-11*EXP(-200./temp)	Sander et al. (2003)
G6101	StGCl	$ClO + O(^3P) \rightarrow Cl$	3.E-11*EXP(70./temp)	Sander et al. (2003)
G6102	StTrGCl	$ClO + ClO \rightarrow Cl_2O_2$	k_ClO_ClO	Atkinson et al. (2005)
G6103	StTrGCl	$Cl_2O_2 \rightarrow ClO + ClO$	k_ClO_ClO/(1.27E-27*EXP(8744./temp))	Sander et al. (2003)*
G6200	StGCl	$Cl + H_2 \rightarrow HCl + H$	3.7E-11*EXP(-2300./temp)	Sander et al. (2003)
G6201a	StGCl	$Cl + HO_2 \rightarrow HCl$	1.8E-11*EXP(170./temp)	Sander et al. (2003)
G6201b	StGCl	$Cl + HO_2 \rightarrow ClO + OH$	4.1E-11*EXP(-450./temp)	Sander et al. (2003)
G6202	StTrGCl	$Cl + H_2O_2 \rightarrow HCl + HO_2$	1.1E-11*EXP(-980./temp)	Sander et al. (2003)
G6203a	StGCl	$ClO + OH \rightarrow Cl + HO_2$	7.4E-12*EXP(270./temp)	Sander et al. (2003)
G6203b	StGCl	$ClO + OH \rightarrow HCl$	6.E-13*EXP(230./temp)	Sander et al. (2003)
G6204	StTrGCl	$ClO + HO_2 \rightarrow HOCl$	2.7E-12*EXP(220./temp)	Sander et al. (2003)
G6205	StTrGCl	$HCl + OH \rightarrow Cl + H_2O$	2.6E-12*EXP(-350./temp)	Sander et al. (2003)
G6206	StGCl	$HOCl + OH \rightarrow ClO + H_2O$	3.E-12*EXP(-500./temp)	Sander et al. (2003)
G6300	StTrGNCl	$ClO + NO \rightarrow NO_2 + Cl$	6.4E-12*EXP(290./temp)	Sander et al. (2003)
G6301	StTrGNCl	$ClO + NO_2 \rightarrow ClNO_3$	k_3rd(temp,cair,1.8E-31,3.4,1.5E-11, 1.9,0.6)	Sander et al. (2003)
G6303	StGNCl	$ClNO_3 + O(^3P) \rightarrow ClO + NO_3$	2.9E-12*EXP(-800./temp)	Sander et al. (2003)
G6304	StTrGNCl	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	6.5E-12*EXP(135./temp)	Sander et al. (2003)
G6400	StTrGCl	$Cl + CH_4 \rightarrow HCl + CH_3O_2$	9.6E-12*EXP(-1360./temp)	Sander et al. (2003)
G6401	StTrGCl	$Cl + HCHO \rightarrow HCl + CO + HO_2$	8.1E-11*EXP(-30./temp)	Sander et al. (2003)
G6402	StTrGCl	$Cl + CH_3OOH \rightarrow CH_3O_2 + HCl$	5.7E-11	Sander et al. (2003)
G6403	StTrGCl	$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	3.3E-12*EXP(-115./temp)	Sander et al. (2003)
G6404	StGCl	$CCl_4 + O(^1D) \rightarrow ClO + 3\ Cl$	3.3E-10	Sander et al. (2003)
G6405	StGCl	$CH_3Cl + O(^1D) \rightarrow OH + Cl$	1.65E-10	Sander et al. (2003)*
G6406	StGCl	$CH_3Cl + OH \rightarrow H_2O + Cl$	2.4E-12*EXP(-1250./temp)	Sander et al. (2003)
G6407	StGCCl	$CH_3CCl_3 + O(^1D) \rightarrow OH + 3\ Cl$	3.E-10	Sander et al. (2003)*
G6408	StTrGCCl	$CH_3CCl_3 + OH \rightarrow H_2O + 3\ Cl$	1.6E-12*EXP(-1520./temp)	Sander et al. (2003)
G6500	StGFCl	$CF_2Cl_2 + O(^1D) \rightarrow ClO + Cl$	1.4E-10	Sander et al. (2003)
G6501	StGFCl	$CFCl_3 + O(^1D) \rightarrow ClO + 2\ Cl$	2.3E-10	Sander et al. (2003)
G7100	StTrGBr	$Br + O_3 \rightarrow BrO$	1.7E-11*EXP(-800./temp)	Sander et al. (2003)

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

#	labels	reaction	rate coefficient	reference
G7101	StGBr	$BrO + O(^3P) \rightarrow Br + O_2$	`1.9E-11*EXP(230./temp)`	Sander et al. (2003)
G7200	StTrGBr	$Br + HO_2 \rightarrow HBr$	`1.5E-11*EXP(-600./temp)`	Sander et al. (2003)
G7201	StTrGBr	$BrO + HO_2 \rightarrow HOBr$	`3.4E-12*EXP(540./temp)`	Sander et al. (2003)
G7202	StTrGBr	$HBr + OH \rightarrow Br + H_2O$	`1.1E-11`	Sander et al. (2003)
G7203	StGBr	$HOBr + O(^3P) \rightarrow OH + BrO$	`1.2E-10*EXP(-430./temp)`	Sander et al. (2003)
G7301	StTrGNBr	$BrO + NO \rightarrow Br + NO_2$	`8.8E-12*EXP(260./temp)`	Sander et al. (2003)
G7302	StTrGNBr	$BrO + NO_2 \rightarrow BrNO_3$	`k_BrO_NO2`	Sander et al. (2003)*
G7400	StTrGBr	$Br + HCHO \rightarrow HBr + CO + HO_2$	`1.7E-11*EXP(-800./temp)`	Sander et al. (2003)
G7403	StTrGBr	$CH_3Br + OH \rightarrow H_2O + Br$	`2.35E-12*EXP(-1300./temp)`	Sander et al. (2003)
G7603a	StTrGClBr	$BrO + ClO \rightarrow Br + OClO$	`9.5E-13*EXP(550./temp)`	Sander et al. (2003)
G7603b	StTrGClBr	$BrO + ClO \rightarrow Br + Cl$	`2.3E-12*EXP(260./temp)`	Sander et al. (2003)
G7603c	StTrGClBr	$BrO + ClO \rightarrow BrCl$	`4.1E-13*EXP(290./temp)`	Sander et al. (2003)
G9200	TrStGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	`k_3rd(temp,cair,3.E-31,3.3,1.5E-12,0.,0.6)`	Sander et al. (2003)
G9400a	TrGS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	`1.13E-11*EXP(-253./temp)`	Atkinson et al. (2003)*
G9400b	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	`k_DMS_OH`	Atkinson et al. (2003)*
G9401	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	`1.9E-13*EXP(520./temp)`	Atkinson et al. (2003)
G9402	TrGS	$DMSO + OH \rightarrow .6\ SO_2 + HCHO + .6\ CH_3O_2 + .4\ HO_2 + .4\ CH_3SO_3H$	`1.E-10`	Hynes and Wine (1996)
G9403	TrGS	$CH_3SO_2 \rightarrow SO_2 + CH_3O_2$	`1.9E13*EXP(-8661./temp)`	Barone et al. (1995)
G9404	TrGS	$CH_3SO_2 + O_3 \rightarrow CH_3SO_3$	`3.E-13`	Barone et al. (1995)
G9405	TrGS	$CH_3SO_3 + HO_2 \rightarrow CH_3SO_3H$	`5.E-11`	Barone et al. (1995)

*Notes:

Rate coefficients for three-body reactions are defined via the function `k_3rd`(T, M, k_0^{300}, n, $k_{\rm inf}^{300}$, m, $f_{\rm c}$). 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:

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

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

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

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

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:

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

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

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

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

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

G1002: path leading to 2 $O(^3P)$ + O_2 neglected

G01Diag: `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))

G2108: branching ratio from Hack et al., see note B5 of Sander et al. (2003)

G2110: 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)

G3109: The rate coefficient is: k_NO3_NO2 = k_3rd(temp,cair,2.E-30,4.4,1.4E-12,0.7,0.6).

G3110: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G3203: The rate coefficient is: k_NO2_HO2 = k_3rd(temp,cair,1.8E-31,3.2,4.7E-12,1.4,0.6).

G3206: 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: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G4103: product distribution is from Elrod et al. (2001)

G4107: The rate coefficient is: k_CH3OOH_OH = 3.8E-12*EXP(200./temp)

G4109: same temperature dependence assumed as for $CH_3CHO+NO_3$

G4201: product distribution is from von Kuhlmann (2001) (see also Neeb et al. (1998))

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

G4213: The rate coefficient is: k_PA_NO2 = k_3rd(temp,cair,8.5E-29,6.5,1.1E-11,1.,0.6).

G4216: 1.0E-11 from Atkinson et al. (1999), temperature dependence from Kirchner and Stockwell (1996)

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: 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.

G4301: product distribution is for terminal olefin carbons from Zaveri and Peters (1999)

G4304: 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: The rate coefficient is: k_PrO2_NO = 2.7E-12*EXP(360./temp)

G4306: 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

G4309: products are from von Kuhlmann (2001)

G4315: same value as for G4107: $CH_3OOH+OH$ assumed

G4319: same value as for PAN assumed

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

G4409: The factor 0.25 was recommended by Uli Poeschl (pers. comm. 2004).

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: value for $C_4H_9ONO_2$ used here

G4503: same temperature dependence assumed as for other RO_2+HO_2 reactions

G4504: Yield of 12 % $RONO_2$ assumed as suggested in Table 2 of Sprengnether et al. (2002).

G6102: The rate coefficient is: k_ClO_ClO = k_3rd_iupac(temp,cair,2.E-32,4.,1.E-11,0.,0.45).

G6103: The rate coefficient is defined as backward reaction divided by equilibrium constant.

G6204: 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.

G6405: average of reactions with CH_3Br and CH_3F (B. Steil, pers. comm., see also note A15 in Sander et al. (2003)).

G6407: 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)).

G7302: The rate coefficient is: `k_BrO_NO2 = k_3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)`.

G7303: The rate coefficient is defined as backward reaction (Sander et al., 2003) divided by equilibrium constant (Orlando and Tyndall, 1996).

G8101: This value was assumed by Jimenez et al. (2003).

G8102: The product as well as the reaction were assumed by von Glasow et al. (2002). An alternative pathway is the formation of new particles. This reaction needs to be updated when laboratory measurements become available.

G8103: product distribution is from Bloss et al. (2001)

G8203: assumed (J. Crowley, pers. comm. 2004)

G8300: The rate coefficient is: `k_I_NO2` = `k_3rd(temp,cair,3.E-31,1.,6.6E-11,0.,0.6)`.

G8304: J. Moldanova and J. Plane, pers. comm.

G8305: The rate coefficient is defined as backward reaction (Sander et al., 2003) divided by equilibrium constant (van den Bergh and Troe, 1976).

G8306: Note that in an earlier study by Jenkin et al. (1985), a value of 5E-3 s^{-1} was assumed.

G8600: Turnipseed et al. (1997) found a branching ratio of 14% for the sum of channels which do not produce `I` atoms. We assume that `OIO` and `Cl` are produced in this case.

G8701: Gilles et al. (1997) found an upper limit of 35% for I atom production. We assume 35% I and 65% OIO as products. See also Rowley et al. (2001) for info about products.

G9400a: Abstraction path. The assumed reaction sequence (omitting H_2O and O_2 as products) according to Yin et al. (1990) is:

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

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

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

G9400b: 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))`.

Table 2: Photolysis reactions

#	labels	reaction	rate coefficient	reference
J1000	StTrGJ	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	`JX(ip_O2)`	see note
J1001a	StTrGJ	$O_3 + h\nu \rightarrow O(^1D)$	`JX(ip_O1D)`	see note
J1001b	StTrGJ	$O_3 + h\nu \rightarrow O(^3P)$	`JX(ip_O3P)`	see note
J2100	StGJ	$H_2O + h\nu \rightarrow H + OH$	`JX(ip_H2O)`	see note
J2101	StTrGJ	$H_2O_2 + h\nu \rightarrow 2\ OH$	`JX(ip_H2O2)`	see note
J3100	StGNJ	$N_2O + h\nu \rightarrow O(^1D)$	`JX(ip_N2O)`	see note
J3101	StTrGNJ	$NO_2 + h\nu \rightarrow NO + O(^3P)$	`JX(ip_NO2)`	see note
J3102	StGNJ	$NO + h\nu \rightarrow N + O(^3P)$	`JX(ip_NO)`	see note
J3103a	StTrGNJ	$NO_3 + h\nu \rightarrow NO_2 + O(^3P)$	`JX(ip_NO2O)`	see note
J3103b	StTrGNJ	$NO_3 + h\nu \rightarrow NO$	`JX(ip_NOO2)`	see note
J3104a	StTrGNJ	$N_2O_5 + h\nu \rightarrow NO_2 + NO_3$	`JX(ip_N2O5)`	see note
J3104b	StGNJ	$N_2O_5 + h\nu \rightarrow NO + O(^3P) + NO_3$	`JX(ip_NO3NOO)`	see note
J3200	TrGJ	$HONO + h\nu \rightarrow NO + OH$	`JX(ip_HONO)`	see note
J3201	StTrGNJ	$HNO_3 + h\nu \rightarrow NO_2 + OH$	`JX(ip_HNO3)`	see note
J3202	StTrGNJ	$HNO_4 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$	`JX(ip_HNO4)`	see note
J4100	StTrGJ	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	`JX(ip_CH3OOH)`	see note
J4101a	StTrGJ	$HCHO + h\nu \rightarrow H_2 + CO$	`JX(ip_COH2)`	see note
J4101b	StTrGJ	$HCHO + h\nu \rightarrow H + CO + HO_2$	`JX(ip_CHOH)`	see note
J4102	StGJ	$CO_2 + h\nu \rightarrow CO + O(^3P)$	`JX(ip_CO2)`	see note
J4103	StGJ	$CH_4 + h\nu \rightarrow CO + 0.31\ H + 0.69\ H_2 + 1.155\ H_2O$	`JX(ip_CH4)`	see note
J4200	TrGCJ	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	`JX(ip_CH3OOH)`	see note
J4201	TrGCJ	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	`JX(ip_CH3CHO)`	see note
J4202	TrGCJ	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	`JX(ip_PAA)`	see note
J4204	TrGNCJ	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	`JX(ip_PAN)`	see note
J4301	TrGCJ	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	`JX(ip_CH3COCH3)`	see note
J6000	StTrGClJ	$Cl_2 + h\nu \rightarrow Cl + Cl$	`JX(ip_Cl2)`	see note
J6100	StTrGClJ	$Cl_2O_2 + h\nu \rightarrow 2\ Cl$	`1.4*JX(ip_Cl2O2)`	see note
J6101	StTrGClJ	$OClO + h\nu \rightarrow ClO + O(^3P)$	`JX(ip_OClO)`	see note
J6200	StGClJ	$HCl + h\nu \rightarrow Cl + H$	`JX(ip_HCl)`	see note
J6201	StTrGClJ	$HOCl + h\nu \rightarrow OH + Cl$	`JX(ip_HOCl)`	see note
J6301a	StTrGNClJ	$ClNO_3 + h\nu \rightarrow Cl + NO_3$	`JX(ip_ClNO3)`	see note
J6301b	StTrGNClJ	$ClNO_3 + h\nu \rightarrow ClO + NO_2$	`JX(ip_ClONO2)`	see note
J6400	StGClJ	$CH_3Cl + h\nu \rightarrow Cl + CH_3O_2$	`JX(ip_CH3Cl)`	see note
J6401	StGClJ	$CCl_4 + h\nu \rightarrow 4\ Cl$	`JX(ip_CCl4)`	see note

Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J6402	StGCClJ	$CH_3CCl_3 + h\nu \rightarrow 3\ Cl$	`JX(ip_CH3CCl3)`	see note
J6500	StGFClJ	$CFCl_3 + h\nu \rightarrow 3\ Cl$	`JX(ip_CFCl3)`	see note
J6501	StGFClJ	$CF_2Cl_2 + h\nu \rightarrow 2\ Cl$	`JX(ip_CF2Cl2)`	see note
J7200	StTrGBrJ	$HOBr + h\nu \rightarrow Br + OH$	`JX(ip_HOBr)`	see note
J7301	StTrGNBrJ	$BrNO_3 + h\nu \rightarrow Br + NO_3$	`JX(ip_BrNO3)`	see note
J7400	StGBrJ	$CH_3Br + h\nu \rightarrow Br + CH_3O_2$	`JX(ip_CH3Br)`	see note
J7500	StGFBrJ	$CF_3Br + h\nu \rightarrow Br$	`JX(ip_CF3Br)`	see note
J7600	StTrGClBrJ	$BrCl + h\nu \rightarrow Br + Cl$	`JX(ip_BrCl)`	see note
J7601	StGFClBrJ	$CF_2ClBr + h\nu \rightarrow Br + Cl$	`JX(ip_CF2ClBr)`	see note
J9002	StGSJ	$SF_6 + h\nu \rightarrow$ products	`JX(ip_SF6)`	see note

*Notes: J-values are calculated with an external module and then supplied to the MECCA1 chemistry

J6100: Stimpfle et al. (2004) claim 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

#	labels	reaction	rate coefficient	reference

*Notes:

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_mecca1_aero.f90` using the accommodation coefficients in subroutine `mecca1_aero_alpha` and Henry's law constants in subroutine `mecca1_aero_henry`.

k_{mt} = mass transfer coefficient

lwc = liquid water content of aerosol mode

H3201, H6300, H6301, H6302, H7300, H7301, H7302, H7601, H7602: For uptake of X (= N_2O_5, $ClNO_3$, $BrNO_3$) and subsequent reaction with H_2O, Cl^-, and Br^-, we define $k_{\mathrm{exf}}(X) = k_{\mathrm{mt}}(X) \times lwc/([H_2O] + 5.0E2[Cl^-] + 3.0E5[Br^-])$.

H6301, H6302, H7601: The total uptake is determined by $k_{\mathrm{mt}}(ClNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

H7301, H7302, H7602: The total uptake is determined by $k_{\mathrm{mt}}(BrNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

Table 4: PSC reactions

#	labels	reaction	rate coefficient	reference
PSC200	StPscN	$N_2O_5 + H_2O \rightarrow HNO_3 + HNO_3$	`khet_N2O5_H2O`	see note
PSC410	StPscCl	$HOCl + HCl \rightarrow Cl_2 + H_2O$	`khet_HOCl_HCl`	see note
PSC420	StPscNCl	$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	`khet_ClNO3_HCl`	see note
PSC421	StPscNCl	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	`khet_ClNO3_H2O`	see note
PSC520	StPscNBr	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	`khet_BrNO3_H2O`	see note
PSC541	StPscNClBr	$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	`khet_BrNO3_HCl`	see note
PSC543	StPscClBr	$HOBr + HCl \rightarrow BrCl + H_2O$	`khet_HOBr_HCl`	see note

*Notes: PSC reaction rates are calculated with an external module and then supplied to the MECCA1 chemistry (see `http://www.messy-interface.org` for details)

Table 5: Acid-base and other eqilibria

#	labels	reaction	$K_0[M^{m-n}]$	-$\Delta H/R[K]$	reference

*Notes:

EQ82 and EQ83: Thermodynamic calculations on the IBr/ICl equilibrium according to the data tables from Wagman et al. (1982):

ICl	+	Br^-	$\rightleftharpoons$	IBr	+	Cl^-
-17.1		-103.96	=	-4.2		-131.228

$$\frac{\Delta G}{[\text{kJ/mol}]} = -4.2 - 131.228 - (-17.1 - 103.96) = -14.368$$

$$K = \frac{[\text{IBr}] \times [\text{Cl}^-]}{[\text{ICl}] \times [\text{Br}^-]} = \exp\left(\frac{-\Delta G}{RT}\right) = \exp\left(\frac{14368}{8.314 \times 298}\right) = 330$$

This means we have equal amounts of IBr and ICl when the $[Cl^-]/[Br^-]$ ratio equals 330.

Table 6: Aqueous phase reactions

#	labels	reaction	k_0 $[M^{1-n}s^{-1}]$	$-E_a/R[K]$	reference

A6102: Jacobi (1996) found an upper limit of `6E9` and cite an upper limit from another study of `2E9`. Here, we set the rate coefficient to `1E9`.

A6301: There is also an earlier study by Exner et al. (1992) which found a smaller rate coefficient but did not consider the back reaction.

A7400: assumed to be the same as for Br_2^- + H_2O_2.

A9205: D. Sedlak, pers. comm. (1993)

A9106: see also: (Huie and Neta, 1987; Warneck, 1991). If this reaction produces a lot of SO_4^-, it will have an effect. However, we currently assume only the stable $S_2O_8^{2-}$ as product. Since $S_2O_8^{2-}$ is not treated explicitly in the mechanism, we use SO_4^{2-} as a proxy. Note that this destroys the mass consistency for sulfur species.

A9208: D. Sedlak, pers. comm. (1993)

A9105: The rate coefficient for the sum of the paths (leading to either HSO_5^- or SO_4^{2-}) is from Huie and Neta (1987), the ratio 0.28/0.72 is from Deister and Warneck (1990).

A9605: assumed to be the same as for SO_3^{2-} + HOCl.

A9705: assumed to be the same as for SO_3^{2-} + HOBr.

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