The Chemical Mechanism of MECCA

KPP version: 2.2.1_rs3

MECCA version: 2.5h

Date: November 11, 2009.

Selected reactions:

"((Tr && (G || Het) && !Cl && !Br && !I) || St) && !Hg"

Number of aerosol phases: 0

Number of species in selected mechanism:

Gas phase:	75
Aqueous phase:	0
All species:	75

Number of reactions in selected mechanism:

Gas phase (Gnnn):	136
Aqueous phase (Annn):	0
Henry (Hnnn):	0
Photolysis (Jnnn):	44
Heterogeneous (HETnnn):	13
Equilibria (EQnn):	0
Dummy (Dnn):	0
All equations:	193

Table 1: Gas phase reactions

#	labels	reaction	rate coefficient	reference
G1000	StTrG	$O_2 + O(^1D) \rightarrow O(^3P) + O_2$	3.3E-11*EXP(55./temp)	Sander et al. (2006)
G1001	StTrG	$O_2 + O(^3P) \rightarrow O_3$	6.E-34*((temp/300.)**(-2.4))*cair	Sander et al. (2006)
G1002	StG	$O_3 + O(^1D) \rightarrow 2\,O_2$	1.2E-10	Sander et al. (2006)*
G1003	StG	$O_3 + O(^3P) \rightarrow 2\,O_2$	8.E-12*EXP(-2060./temp)	Sander et al. (2006)
G2100	StTrG	$H + O_2 \rightarrow HO_2$	k_3rd(temp,cair,4.4E-32,1.3,4.7E-11, 0.2,0.6)	Sander et al. (2006)
G2101	StG	$H + O_3 \rightarrow OH + O_2$	1.4E-10*EXP(-470./temp)	Sander et al. (2006)
G2102	StG	$H_2 + O(^1D) \rightarrow H + OH$	1.1E-10	Sander et al. (2006)
G2103	StG	$OH + O(^3P) \rightarrow H + O_2$	2.2E-11*EXP(120./temp)	Sander et al. (2006)
G2104	StTrG	$OH + O_3 \rightarrow HO_2 + O_2$	1.7E-12*EXP(-940./temp)	Sander et al. (2006)
G2105	StTrG	$OH + H_2 \rightarrow H_2O + H$	2.8E-12*EXP(-1800./temp)	Sander et al. (2006)
G2106	StG	$HO_2 + O(^3P) \rightarrow OH + O_2$	3.E-11*EXP(200./temp)	Sander et al. (2006)
G2107	StTrG	$HO_2 + O_3 \rightarrow OH + 2\,O_2$	1.E-14*EXP(-490./temp)	Sander et al. (2006)
G2108a	StG	$HO_2 + H \rightarrow 2\,OH$	7.2E-11	Sander et al. (2006)
G2108b	StG	$HO_2 + H \rightarrow H_2 + O_2$	6.9E-12	Sander et al. (2006)
G2108c	StG	$HO_2 + H \rightarrow O(^3P) + H_2O$	1.6E-12	Sander et al. (2006)
G2109	StTrG	$HO_2 + OH \rightarrow H_2O + O_2$	4.8E-11*EXP(250./temp)	Sander et al. (2006)
G2110	StTrG	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	k_HO2_HO2	Christensen et al. (2002), Kircher and Sander (1984)*
G2111	StTrG	$H_2O + O(^1D) \rightarrow 2\,OH$	1.63E-10*EXP(60./temp)	Sander et al. (2006)
G2112	StTrG	$H_2O_2 + OH \rightarrow H_2O + HO_2$	1.8E-12	Sander et al. (2006)
G3100	StGN	$N + O_2 \rightarrow NO + O(^3P)$	1.5E-11*EXP(-3600./temp)	Sander et al. (2006)
G3101	StTrG	$N_2 + O(^1D) \rightarrow O(^3P) + N_2$	2.15E-11*EXP(110./temp)	Sander et al. (2006)
G3102a	StGN	$N_2O + O(^1D) \rightarrow 2\,NO$	6.7E-11*EXP(20./temp)	Sander et al. (2006)
G3102b	StGN	$N_2O + O(^1D) \rightarrow N_2 + O_2$	4.7E-11*EXP(20./temp)	Sander et al. (2006)
G3103	StTrGN	$NO + O_3 \rightarrow NO_2 + O_2$	3.E-12*EXP(-1500./temp)	Sander et al. (2006)
G3104	StGN	$NO + N \rightarrow O(^3P) + N_2$	2.1E-11*EXP(100./temp)	Sander et al. (2006)
G3105	StGN	$NO_2 + O(^3P) \rightarrow NO + O_2$	5.1E-12*EXP(210./temp)	Sander et al. (2006)
G3106	StTrGN	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*EXP(-2450./temp)	Sander et al. (2006)
G3107a	StGN	$NO_2 + N \rightarrow N_2O + O(^3P)$	0.5 *5.8E-12*EXP(220./temp)	Sander et al. (2006), Funke et al. (2008)
G3107b	StGN	$NO_2 + N \rightarrow NO + NO$	0.25 *5.8E-12*EXP(220./temp)	Funke et al. (2008)
G3107c	StGN	$NO_2 + N \rightarrow N_2 + O_2$	0.25 *5.8E-12*EXP(220./temp)	Funke et al. (2008)
G3108	StTrGN	$NO_3 + NO \rightarrow 2\,NO_2$	1.5E-11*EXP(170./temp)	Sander et al. (2006)

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

#	labels	reaction	rate coefficient	reference
G3109	StTrGN	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2	Sander et al. (2006)*
G3110	StTrGN	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(2.7E-27*EXP(11000./temp))	Sander et al. (2006)*
G3200	TrG	$NO + OH \rightarrow HONO$	k_3rd(temp,cair,7.0E-31,2.6,3.6E-11, 0.1,0.6)	Sander et al. (2006)
G3201	StTrGN	$NO + HO_2 \rightarrow NO_2 + OH$	3.5E-12*EXP(250./temp)	Sander et al. (2006)
G3202	StTrGN	$NO_2 + OH \rightarrow HNO_3$	k_3rd(temp,cair,1.8E-30,3.0,2.8E-11,0., 0.6)	Sander et al. (2006)
G3203	StTrGN	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2	Sander et al. (2006)*
G3204	TrGN	$NO_3 + HO_2 \rightarrow NO_2 + OH + O_2$	3.5E-12	Sander et al. (2006)
G3205	TrG	$HONO + OH \rightarrow NO_2 + H_2O$	1.8E-11*EXP(-390./temp)	Sander et al. (2006)
G3206	StTrGN	$HNO_3 + OH \rightarrow H_2O + NO_3$	k_HNO3_OH	Sander et al. (2006)*
G3207	StTrGN	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*EXP(10900./temp))	Sander et al. (2006)*
G3208	StTrGN	$HNO_4 + OH \rightarrow NO_2 + H_2O$	1.3E-12*EXP(380./temp)	Sander et al. (2006)
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. (2006)
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	$CH_3OH + OH \rightarrow HCHO + HO_2$	2.9E-12*EXP(-345./temp)	Sander et al. (2006)
G4103	StTrG	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	4.1E-13*EXP(750./temp)	Sander et al. (2006)*
G4104	StTrGN	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	2.8E-12*EXP(300./temp)	Sander et al. (2006)
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. (2006)
G4106b	StTrG	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH + O_2$	9.5E-14*EXP(390./temp)/(1.+ 26.2*EXP(-1130./temp))	Sander et al. (2006)
G4107	StTrG	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	k_CH3OOH_OH	Sander et al. (2006)*
G4108	StTrG	$HCHO + OH \rightarrow CO + H_2O + HO_2$	9.52E-18*EXP(2.03*log(temp)+636./temp)	Sivakumaran et al. (2003)
G4109	TrGN	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	3.4E-13*EXP(-1900./temp)	Sander et al. (2006)*
G4110	StTrG	$CO + OH \rightarrow H + CO_2$	1.57E-13 + cair*3.54E-33	McCabe et al. (2001)
G4111	TrG	$HCOOH + OH \rightarrow HO_2$	4.0E-13	Sander et al. (2006)
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. (2006)
G4204	TrGNC	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	2.6E-12*EXP(365./temp)	Sander et al. (2006)
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

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

#	labels	reaction	rate coefficient	reference
G4207	TrGC	$C_2H_5OOH + OH \rightarrow .3\ C_2H_5O_2 + .7\ CH_3CHO + .7\ OH$	`k_CH3OOH_OH`	see note
G4208	TrGC	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	`4.4E-12*EXP(365./temp)`	Atkinson et al. (2006)
G4209	TrGNC	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	`1.4E-12*EXP(-1900./temp)`	Sander et al. (2006)
G4210	TrGC	$CH_3COOH + OH \rightarrow CH_3O_2 + CO_2 + H_2O$	`4.2E-14*EXP(855./temp)`	Atkinson et al. (2006)
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`	Sander et al. (2006)
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. (2006)
G4215b	TrGC	$CH_3C(O)OO + CH_3O_2 \rightarrow CH_3COOH + HCHO$	`0.1*2.E-12*EXP(500./temp)`	Sander et al. (2006)
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. (2006)*
G4222	TrGC	$C_2H_2 + OH \rightarrow CH_3O_2$	`k_3rd(temp,cair,5.5e-30,0.0,8.3e-13,` `-2.,0.6)`	Sander et al. (2006)
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. (2006)
G4312a	TrGC	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3C(O)OO$	`8.6E-13*EXP(700./temp)`	Tyndall et al. (2001)
G4313	TrGNC	$CH_3COCH_2O_2 + NO \rightarrow NO_2 + CH_3C(O)OO + HCHO$	`2.9E-12*EXP(300./temp)`	Sander et al. (2006)
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	$Cl + O_3 \rightarrow ClO + O_2$	`2.8E-11*EXP(-250./temp)`	Atkinson et al. (2007)
G6101	StGCl	$ClO + O(^3P) \rightarrow Cl + O_2$	`2.5E-11*EXP(110./temp)`	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G6102a	StTrGCl	$ClO + ClO \rightarrow Cl_2 + O_2$	1.0E-12*EXP(-1590./temp)	Atkinson et al. (2007)
G6102b	StTrGCl	$ClO + ClO \rightarrow 2\ Cl + O_2$	3.0E-11*EXP(-2450./temp)	Atkinson et al. (2007)
G6102c	StTrGCl	$ClO + ClO \rightarrow Cl + OClO$	3.5E-13*EXP(-1370./temp)	Atkinson et al. (2007)
G6102d	StTrGCl	$ClO + ClO \rightarrow Cl_2O_2$	k_ClO_ClO	Atkinson et al. (2007)
G6103	StTrGCl	$Cl_2O_2 \rightarrow ClO + ClO$	k_ClO_ClO/(9.3E-28*EXP(8835./temp))	Atkinson et al. (2007), Sander et al. (2006)*
G6200	StGCl	$Cl + H_2 \rightarrow HCl + H$	3.9E-11*EXP(-2310./temp)	Atkinson et al. (2007)
G6201a	StGCl	$Cl + HO_2 \rightarrow HCl + O_2$	4.4E-11-7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6201b	StGCl	$Cl + HO_2 \rightarrow ClO + OH$	7.5E-11*EXP(-620./temp)	Atkinson et al. (2007)
G6202	StTrGCl	$Cl + H_2O_2 \rightarrow HCl + HO_2$	1.1E-11*EXP(-980./temp)	Atkinson et al. (2007)
G6203	StGCl	$ClO + OH \rightarrow .94\ Cl + .94\ HO_2 + .06\ HCl + .06\ O_2$	7.3E-12*EXP(300./temp)	Atkinson et al. (2007)
G6204	StTrGCl	$ClO + HO_2 \rightarrow HOCl$	2.2E-12*EXP(340./temp)	Atkinson et al. (2007)
G6205	StTrGCl	$HCl + OH \rightarrow Cl + H_2O$	1.7E-12*EXP(-230./temp)	Atkinson et al. (2007)
G6206	StGCl	$HOCl + OH \rightarrow ClO + H_2O$	3.0E-12*EXP(-500./temp)	Sander et al. (2006)
G6300	StTrGNCl	$ClO + NO \rightarrow NO_2 + Cl$	6.2E-12*EXP(295./temp)	Atkinson et al. (2007)
G6301	StTrGNCl	$ClO + NO_2 \rightarrow ClNO_3$	k_3rd_iupac(temp,cair,1.6E-31,3.4, 7.E-11,0.,0.4)	Atkinson et al. (2007)
G6303	StGNCl	$ClNO_3 + O(^3P) \rightarrow ClO + NO_3$	4.5E-12*EXP(-900./temp)	Atkinson et al. (2007)
G6304	StTrGNCl	$ClNO_3 + Cl \rightarrow Cl_2 + NO_3$	6.2E-12*EXP(145./temp)	Atkinson et al. (2007)
G6400	StTrGCl	$Cl + CH_4 \rightarrow HCl + CH_3O_2$	6.6E-12*EXP(-1240./temp)	Atkinson et al. (2006)
G6401	StTrGCl	$Cl + HCHO \rightarrow HCl + CO + HO_2$	8.1E-11*EXP(-34./temp)	Atkinson et al. (2006)
G6402	StTrGCl	$Cl + CH_3OOH \rightarrow HCHO + HCl + OH$	5.9E-11	Atkinson et al. (2006)*
G6403	StTrGCl	$ClO + CH_3O_2 \rightarrow HO_2 + Cl + HCHO$	3.3E-12*EXP(-115./temp)	Sander et al. (2006)
G6404	StGCl	$CCl_4 + O(^1D) \rightarrow ClO + 3\ Cl$	3.3E-10	Sander et al. (2006)
G6405	StGCl	$CH_3Cl + O(^1D) \rightarrow OH + Cl$	1.65E-10	see note
G6406	StGCl	$CH_3Cl + OH \rightarrow H_2O + Cl$	2.4E-12*EXP(-1250./temp)	Sander et al. (2006)
G6407	StGCCl	$CH_3CCl_3 + O(^1D) \rightarrow OH + 3\ Cl$	3.E-10	see note
G6408	StTrGCCl	$CH_3CCl_3 + OH \rightarrow H_2O + 3\ Cl$	1.64E-12*EXP(-1520./temp)	Sander et al. (2006)
G6500	StGFCl	$CF_2Cl_2 + O(^1D) \rightarrow ClO + Cl$	1.4E-10	Sander et al. (2006)
G6501	StGFCl	$CFCl_3 + O(^1D) \rightarrow ClO + 2\ Cl$	2.3E-10	Sander et al. (2006)
G7100	StTrGBr	$Br + O_3 \rightarrow BrO + O_2$	1.7E-11*EXP(-800./temp)	Atkinson et al. (2007)
G7101	StGBr	$BrO + O(^3P) \rightarrow Br + O_2$	1.9E-11*EXP(230./temp)	Atkinson et al. (2007)
G7200	StTrGBr	$Br + HO_2 \rightarrow HBr + O_2$	7.7E-12*EXP(-450./temp)	Atkinson et al. (2007)
G7201	StTrGBr	$BrO + HO_2 \rightarrow HOBr + O_2$	4.5E-12*EXP(500./temp)	Atkinson et al. (2007)
G7202	StTrGBr	$HBr + OH \rightarrow Br + H_2O$	6.7E-12*EXP(155./temp)	Atkinson et al. (2007)

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

#	labels	reaction	rate coefficient	reference
G7203	StGBr	$HOBr + O(^3P) \rightarrow OH + BrO$	1.2E-10*EXP(-430./temp)	Atkinson et al. (2007)
G7204	StTrGBr	$Br_2 + OH \rightarrow HOBr + Br$	2.0E-11*EXP(240./temp)	Atkinson et al. (2007)
G7301	StTrGNBr	$BrO + NO \rightarrow Br + NO_2$	8.7E-12*EXP(260./temp)	Atkinson et al. (2007)
G7302	StTrGNBr	$BrO + NO_2 \rightarrow BrNO_3$	k_BrO_NO2	Atkinson et al. (2007)*
G7400	StTrGBr	$Br + HCHO \rightarrow HBr + CO + HO_2$	7.7E-12*EXP(-580./temp)	Atkinson et al. (2006)
G7403	StTrGBr	$CH_3Br + OH \rightarrow H_2O + Br$	2.35E-12*EXP(-1300./temp)	Sander et al. (2006)
G7603a	StTrGClBr	$BrO + ClO \rightarrow Br + OClO$	1.6E-12*EXP(430./temp)	Atkinson et al. (2007)
G7603b	StTrGClBr	$BrO + ClO \rightarrow Br + Cl + O_2$	2.9E-12*EXP(220./temp)	Atkinson et al. (2007)
G7603c	StTrGClBr	$BrO + ClO \rightarrow BrCl + O_2$	5.8E-13*EXP(170./temp)	Atkinson et al. (2007)
G9200	StTrGS	$SO_2 + OH \rightarrow H_2SO_4 + HO_2$	k_3rd(temp,cair,3.3E-31,4.3,1.6E-12,0.,0.6)	Sander et al. (2006)
G9400a	TrGS	$DMS + OH \rightarrow CH_3SO_2 + HCHO$	1.13E-11*EXP(-253./temp)	Atkinson et al. (2004)*
G9400b	TrGS	$DMS + OH \rightarrow DMSO + HO_2$	k_DMS_OH	Atkinson et al. (2004)*
G9401	TrGNS	$DMS + NO_3 \rightarrow CH_3SO_2 + HNO_3 + HCHO$	1.9E-13*EXP(520./temp)	Atkinson et al. (2004)
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`$(T, M, k_0^{300}, n, k_{\inf}^{300}, m, f_c)$. In the code, the temperature T is called `temp` and the concentration of "air molecules" M is called `cair`. Using the auxiliary variables $k_0(T)$, $k_{\inf}(T)$, and k_{ratio}, `k_3rd` is defined as:

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

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

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

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

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

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

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

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

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

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

G1002: The path leading to 2 O(^{3}P) + O_2 results in a null cycle regarding odd oxygen and is neglected.

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(ind_ 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: Sander et al. (2006) recommend a zero product yield for HCHO.

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

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

G4206: The rate coefficient was 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.

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

G4218: Same value as for G4107: $CH_3OOH+OH$ assumed.

G4220: This is 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: The product distribution is for terminal olefin carbons from Zaveri and Peters (1999).

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

G6402: The initial products are probably HCl and CH_2OOH (Atkinson et al., 2006). It is assumed that CH_2OOH dissociates into HCHO and OH.

G6405: Average of reactions with CH_3Br and CH_3F from Sander et al. (2006) (B. Steil, pers. comm.).

G6407: Rough extrapolation from reactions with CH_3CF_3, CH_3CClF_2, and CH_3CCl_2F from Sander et al. (2006).

G7302: The rate coefficient is: `k_BrO_NO2 = k_ 3rd(temp,cair,5.2E-31,3.2,6.9E-12,2.9,0.6)`.

G9400: Addition path. The rate coefficient is: `k_DMS_OH = 1.0E-39*EXP(5820./temp)*C(ind_O2) / (1.+5.0E-30*EXP(6280./temp)*C(ind_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	$PAN + h\nu \rightarrow .6\ CH_3C(O)OO + .6\ NO_2 + .4\ CH_3O_2 + .4\ NO_3 + .4\ CO_2$	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

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Table 2: Photolysis reactions (... continued)

#	labels	reaction	rate coefficient	reference
J6401	StGClJ	$CCl_4 + h\nu \rightarrow 4\ Cl$	jx(ip_CCl4)	see note
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	$BrNO_3 + h\nu \rightarrow 0.29\ Br + 0.29\ NO_3 + 0.71\ BrO + 0.71\ NO_2$	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	StGFBrJ	$CF_2ClBr + h\nu \rightarrow Br + Cl$	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 MECCA 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.

J7301: The quantum yields are from Sander et al. (2003).

Table 3: Henry's law coefficients

substance	$\dfrac{k_H^{\ominus}}{\text{M/atm}}$	$\dfrac{-\Delta_{\text{soln}}H/R}{\text{K}}$	reference
O_2	1.3×10^{-3}	1500.	Wilhelm et al. (1977)
O_3	1.2×10^{-2}	2560.	Chameides (1984)
OH	3.0×10^{1}	4300.	Hanson et al. (1992)
HO_2	3.9×10^{3}	5900.	Hanson et al. (1992)
H_2O_2	$1. \times 10^{5}$	6338.	Lind and Kok (1994)
NO	1.9×10^{-3}	1480.	Schwartz and White (1981)
NO_2	7.0×10^{-3}	2500.	Lee and Schwartz (1981)*
NO_3	2.	2000.	Thomas et al. (1993)
HONO	4.9×10^{1}	4780.	Schwartz and White (1981)
HNO_3	$2.45 \times 10^{6}/1.5 \times 10^{1}$	8694.	Brimblecombe and Clegg (1989)*
HNO_4	1.2×10^{4}	6900.	Régimbal and Mozurkewich (1997)
CH_3O_2	6.	5600.	Jacob (1986)*
CH_3OOH	3.0×10^{2}	5322.	Lind and Kok (1994)
HCHO	7.0×10^{3}	6425.	Chameides (1984)
HCOOH	3.7×10^{3}	5700.	Chameides (1984)
CO_2	3.1×10^{-2}	2423.	Chameides (1984)
Cl_2	9.2×10^{-2}	2081.	Bartlett and Margerum (1999)
HCl	2./1.7	9001.	Brimblecombe and Clegg (1989)
HOCl	6.7×10^{2}	5862.	Huthwelker et al. (1995)
Br_2	7.7×10^{-1}	3837.	Bartlett and Margerum (1999)
HBr	1.3	10239.	Brimblecombe and Clegg (1989)*
HOBr	9.3×10^{1}	5862.	Vogt et al. (1996)*
BrCl	9.4×10^{-1}	5600.	Bartlett and Margerum (1999)
SO_2	1.2	3120.	Chameides (1984)
H_2SO_4	$1. \times 10^{11}$	0.	see note
DMSO	$5. \times 10^{4}$	6425.	De Bruyn et al. (1994)*

*Notes:

The temperature dependence of the Henry constants is:

$$K_H = K_H^{\ominus} \times \exp\left(\frac{-\Delta_{\text{soln}}H}{R} \left(\frac{1}{T} - \frac{1}{T^{\ominus}} \right) \right)$$

where $\Delta_{\text{soln}}H$ = molar enthalpy of dissolution [J/mol] and $R = 8.314$ J/(mol K).

NO_2: The temperature dependence is from Chameides (1969).

HNO_3: Calculated using the acidity constant from Davis and de Bruin (1964).

CH_3O_2: This value was estimated by Jacob (1986).

HBr: Calculated using the acidity constant from Lax

HOBr: This value was estimated by Vogt et al. (1996).

H_2SO_4: To account for the very high Henry's law coefficient of H_2SO_4, a very high value was chosen arbitrarily.

DMSO: Lower limit cited from another reference.

Table 4: Accommodation coefficients

substance	$\alpha^{\ominus}$	$\dfrac{-\Delta_{\mathrm{obs}}H/R}{\mathrm{K}}$	reference
O_2	0.01	2000.	see note
O_3	0.002	0.	DeMore et al. (1997)*
OH	0.01	0.	Takami et al. (1998)*
HO_2	0.5	0.	Thornton and Abbatt (2005)
H_2O_2	0.077	3127.	Worsnop et al. (1989)
NO	5.0×10^{-5}	0.	Saastad et al. (1993)*
NO_2	0.0015	0.	Ponche et al. (1993)*
NO_3	0.04	0.	Rudich et al. (1996)*
N_2O_5	0.1	0.	DeMore et al. (1997)*
HONO	0.04	0.	DeMore et al. (1997)*
HNO_3	0.5	0.	Abbatt and Waschewsky (1998)*
HNO_4	0.1	0.	DeMore et al. (1997)*
CH_3O_2	0.01	2000.	see note
CH_3OOH	0.0046	3273.	Magi et al. (1997)
HCHO	0.04	0.	DeMore et al. (1997)*
HCOOH	0.014	3978.	DeMore et al. (1997)
CO_2	0.01	2000.	see note
Cl_2	0.038	6546.	Hu et al. (1995)
HCl	0.074	3072.	Schweitzer et al. (2000)*
HOCl	0.5	0.	see note
$ClNO_3$	0.108	0.	Deiber et al. (2004)*
Br_2	0.038	6546.	Hu et al. (1995)
HBr	0.032	3940.	Schweitzer et al. (2000)*
HOBr	0.5	0.	Abbatt and Waschewsky (1998)*
$BrNO_3$	0.063	0.	Deiber et al. (2004)*
BrCl	0.38	6546.	see note
SO_2	0.11	0.	DeMore et al. (1997)
H_2SO_4	0.65	0.	Pöschl et al. (1998)*
CH_3SO_3H	0.076	1762.	De Bruyn et al. (1994)
DMSO	0.048	2578.	De Bruyn et al. (1994)

*Notes:

The temperature dependence of the accommodation coefficients is given by (Jayne et al., 1991):

$$\frac{\alpha}{1-\alpha} = \exp\left(\frac{-\Delta_{\mathrm{obs}}G}{RT}\right)$$

$$= \exp\left(\frac{-\Delta_{\mathrm{obs}}H}{RT} + \frac{\Delta_{\mathrm{obs}}S}{R}\right)$$

where $\Delta_{\mathrm{obs}}G$ is the Gibbs free energy barrier of the transition state toward solution (Jayne et al., 1991), and $\Delta_{\mathrm{obs}}H$ and $\Delta_{\mathrm{obs}}S$ are the corresponding enthalpy and entropy, respectively. The equation can be rearranged to:

$$\ln\left(\frac{\alpha}{1-\alpha}\right) = \frac{-\Delta_{\mathrm{obs}}H}{R} \times \frac{1}{T} + \frac{-\Delta_{\mathrm{obs}}S}{R}$$

and further:

$$\mathrm{d}\ln\left(\frac{\alpha}{1-\alpha}\right)\bigg/\mathrm{d}\left(\frac{1}{T}\right) = \frac{-\Delta_{\mathrm{obs}}H}{R}$$

If no data were available, a value of $\alpha = 0.01$, $\alpha = 0.1$, or $\alpha = 0.5$, and a temperature dependence of $-\Delta_{\mathrm{obs}}H/R = 2000$ K has been assumed.

O_2: Estimate.

O_3: Value measured at 292 K.

OH: Value measured at 293 K.

NO: Value measured between 193 and 243 K.

NO_2: Value measured at 298 K.

NO_3: Value is a lower limit, measured at 273 K.

N_2O_5: Value for sulfuric acid, measured between 195 and 300 K.

HONO: Value measured between 247 and 297 K.

HNO_3: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

HNO_4: Value measured at 200 K for water ice.

CH_3O_2: Estimate.

HCHO: Value measured between 260 and 270 K.

CO_2: Estimate.

HCl: Temperature dependence derived from published data at 2 different temperatures

HOCl: Assumed to be the same as $\alpha(\mathrm{HOBr})$.

$ClNO_3$: Value measured at 274.5 K.

HBr: Temperature dependence derived from published data at 2 different temperatures

HOBr: Value measured at room temperature. Abbatt and Waschewsky (1998) say $\gamma > 0.2$. Here $\alpha = 0.5$ is used.

$BrNO_3$: Value measured at 273 K.

BrCl: Assumed to be the same as $\alpha(\mathrm{Cl}_2)$.

H_2SO_4: Value measured at 303 K.

Table 5: Henry's law equilibria

#	labels	reaction	rate coefficient	reference

*Notes:

The forward (`k_exf`) and backward (`k_exb`) rate coefficients are calculated in the file `messy_mecca_aero.f90` using the accommodation coefficients in subroutine `mecca_aero_alpha` and Henry's law constants in subroutine `mecca_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 $k_{exf}(X) = k_{mt}(X) \times lwc/([H_2O] + 5.0E2[Cl^-] + 3.0E5[Br^-])$.

H6301, H6302, H7601: The total uptake is determined by $k_{mt}(ClNO_3)$. 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 $k_{mt}(BrNO_3)$. The relative rates are assumed to be the same as for N_2O_5 (H3201, H6300, H7300).

Table 6: Heterogeneous reactions

#	labels	reaction	rate coefficient	reference
HET200	StHetN	$N_2O_5 + H_2O \rightarrow 2\ HNO_3$	`khet_St(ihs_N2O5_H2O)`	see note
HET201	TrHetN	$N_2O_5 \rightarrow 2\ NO_3^-(aq) + 2\ H^+(aq)$	`khet_Tr(iht_N2O5)`	see note
HET202	TrHetN	$HNO_3 \rightarrow NO_3^-(aq) + H^+(aq)$	`khet_Tr(iht_HNO3)`	see note
HET410	StHetCl	$HOCl + HCl \rightarrow Cl_2 + H_2O$	`khet_St(ihs_HOCl_HCl)`	see note
HET420	StHetNCl	$ClNO_3 + HCl \rightarrow Cl_2 + HNO_3$	`khet_St(ihs_ClNO3_HCl)`	see note
HET421	StHetNCl	$ClNO_3 + H_2O \rightarrow HOCl + HNO_3$	`khet_St(ihs_ClNO3_H2O)`	see note
HET422	StHetNCl	$N_2O_5 + HCl \rightarrow ClNO_2 + HNO_3$	`khet_St(ihs_N2O5_HCl)`	see note
HET510	StHetBr	$HOBr + HBr \rightarrow Br_2 + H_2O$	`khet_St(ihs_HOBr_HBr)`	see note
HET520	StHetNBr	$BrNO_3 + H_2O \rightarrow HOBr + HNO_3$	`khet_St(ihs_BrNO3_H2O)`	see note
HET540	StHetNClBr	$ClNO_3 + HBr \rightarrow BrCl + HNO_3$	`khet_St(ihs_ClNO3_HBr)`	see note
HET541	StHetNClBr	$BrNO_3 + HCl \rightarrow BrCl + HNO_3$	`khet_St(ihs_BrNO3_HCl)`	see note
HET542	StHetClBr	$HOCl + HBr \rightarrow BrCl + H_2O$	`khet_St(ihs_HOCl_HBr)`	see note
HET543	StHetClBr	$HOBr + HCl \rightarrow BrCl + H_2O$	`khet_St(ihs_HOBr_HCl)`	see note

*Notes:

Heterogeneous reaction rates are calculated with an external module and then supplied to the MECCA chemistry (see `www.messy-interface.org` for details)

Table 7: Acid-base and other eqilibria

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

*Notes:

Table 8: Aqueous phase reactions

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

*Notes:

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