Supplementary material for Manuscript ***von Kuhlmann and Lawrence*****, The impact of ice uptake of HNO_3 on atmospheric chemistry. Manuscript-Number: acpd-2005-0201**

A Table of reactions

Table 1: Gas phase reactions used in MATCH-MPIC.

No.	Reaction	Rate constant	Reference (* = see notes)
1	O_3 + h$\nu \rightarrow O(^1D)$	J_O1D	Landgraf and Crutzen (1998)
2	$O(^1D) + N_2 \rightarrow O_3$	2.1E-11*exp(115/T)	Ravishankara et al. (2002)
3	$O(^1D) + O_2 \rightarrow O_3$	1.8E-11*exp(70/T)	Sander et al. (2003)
4	$O(^1D) + H_2O \rightarrow$ 2 OH	2.2E-10	Sander et al. (2003)
5	O_2 + h$\nu \rightarrow$ 2 O_3	J_O2	Landgraf and Crutzen (1998)
6	OH + $O_3 \rightarrow HO_2$	1.7E-12*exp(-940/T)	Sander et al. (2003)
7	OH + $H_2 \rightarrow H_2O + HO_2$	5.5E-12*exp(-2000/T)	Sander et al. (2003)*
8	$HO_2 + O_3 \rightarrow$ OH	1.E-14*exp(-490/T)	Sander et al. (2003)
9	HO_2 + OH $\rightarrow H_2O$	4.8E-11*exp(250/T)	Sander et al. (2003)
10	$HO_2 + HO_2 \rightarrow H_2O_2$	complex	Sander et al. (2003); Christensen et al. (2002)*
11	H_2O_2 + h$\nu \rightarrow$ 2 OH	J_H2O2	Landgraf and Crutzen (1998)
12	H_2O_2 + OH $\rightarrow H_2O + HO_2$	2.9E-12*exp(-160/T)	Sander et al. (2003)
13	NO + $O_3 \rightarrow NO_2 + O_2$	3.E-12*exp(-1500/T)	Sander et al. (2003)
14	NO + $HO_2 \rightarrow NO_2$ + OH	3.5E-12*exp(250/T)	Sander et al. (2003)
15	NO_2 + h$\nu \rightarrow$ NO + O_3	J_NO2	Landgraf and Crutzen (1998)
16	$NO_2 + O_3 \rightarrow NO_3 + O_2$	1.2E-13*exp(-2450/T)	Sander et al. (2003)
17	NO_2 + OH $\rightarrow HNO_3$	complex	Sander et al. (2003)
18	$NO_2 + HO_2 \rightarrow HNO_4$	k_NO2_HO2, complex	Sander et al. (2003)
19	NO_3 + h$\nu \rightarrow NO_2 + O_3$	J_NO2O	Landgraf and Crutzen (1998)
20	NO_3 + h$\nu \rightarrow$ NO	J_NOO2	Landgraf and Crutzen (1998)
21	NO_3 + NO $\rightarrow$ 2 NO_2	1.5E-11*exp(170/T)	Sander et al. (2003)
22	$NO_3 + NO_2 \rightarrow N_2O_5$	k_NO3_NO2, complex	Sander et al. (2003)
23	$NO_3 + HO_2 \rightarrow NO_2$ + OH + O_2	3.5E-12	Sander et al. (2003)
24	N_2O_5 + h$\nu \rightarrow NO_2 + NO_3$	J_N2O5	Landgraf and Crutzen (1998)
25	$N_2O_5 \rightarrow NO_2 + NO_3$	k_NO3_NO2/(3.E-27*exp(10990/T))	Sander et al. (2003)
26	$N_2O_5 + H_2O \rightarrow$ 2 HNO_3	2.5E-22+[H2O]*1.8E-39	Wahner et al. (1998)
27	HNO_3 + h$\nu \rightarrow NO_2$ + OH	J_HNO3	Landgraf and Crutzen (1998)
28	HNO_3 + OH $\rightarrow H_2O + NO_3$	complex	Dransfield et al. (1999)
29	$HNO_4 \rightarrow NO_2 + HO_2$	k_NO2_HO2/(2.1E-27*exp(10900/T))	Sander et al. (2003)
30	HNO_4 + h$\nu \rightarrow$ .61 NO_2 + .61 HO_2 + .39 NO_3 + .39 OH	J_HNO4	Landgraf and Crutzen (1998); Atkinson et al. (1997)*
31	HNO_4 + OH $\rightarrow NO_2 + H_2O$	1.3E-12*exp(380/T)	Sander et al. (2003)
32	CO + OH $\rightarrow HO_2 + CO_2$	1.57E-13+[M]*3.54E-33	McCabe et al. (2001)
33	CH_4 + OH $\rightarrow CH_3O_2 + H_2O$	1.85E-20*exp(2.82*log(T)-987/T)	Atkinson (2003)
34	$CH_4 + O(^1D) \rightarrow$ .75 CH_3O_2 + .75 OH + .25 HCHO + .4 HO_2	1.5E-10	Sander et al. (2003)

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

No.	Reaction	Rate constant	Reference
35	$CH_3O_2 + HO_2 \rightarrow CH_3OOH$	4.1E-13*exp(750/T)/(1.+1./497.7*exp(1160/T))	Sander et al. (2003); Elrod et al. (2001)
36	$CH_3O_2 + HO_2 \rightarrow HCHO + H_2O + O_2$	4.1E-13*exp(750/T)/(1.+497.7*exp(-1160/T))	Sander et al. (2003); Elrod et al. (2001)
37	$CH_3O_2 + NO \rightarrow HCHO + NO_2 + HO_2$	2.8E-12*exp(300/T)	Sander et al. (2003)
38	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	1.3E-12	Atkinson et al. (1999)
39	$CH_3O_2 + CH_3O_2 \rightarrow 2\ HCHO + 2\ HO_2$	9.5E-14*exp(390/T)/(1.+1./26.2*exp(1130/T))	Sander et al. (2003)
40	$CH_3O_2 + CH_3O_2 \rightarrow HCHO + CH_3OH$	9.5E-14*exp(390/T)/(1.+26.2*exp(-1130/T))	Sander et al. (2003)
41	$CH_3OOH + OH \rightarrow .7\ CH_3O_2 + .3\ HCHO + .3\ OH + H_2O$	k_CH3OOH_OH= 3.8E-12*exp(200/T)	Sander et al. (2003)
42	$CH_3OOH + h\nu \rightarrow HCHO + OH + HO_2$	J_CH3OOH	Landgraf and Crutzen (1998)
43	$HCHO + OH \rightarrow CO + H_2O + HO_2$	9.52E-18*exp(2.03*log(T)+636/T)	Sivakumaran et al. (2003)
44	$HCHO + NO_3 \rightarrow HNO_3 + CO + HO_2$	3.4E-13*exp(-1900/T)	Sander et al. (2003)
45	$HCHO + h\nu \rightarrow CO + H_2$	J_COH2	Landgraf and Crutzen (1998)
46	$HCHO + h\nu \rightarrow CO + HO_2$	J_CHOH	Landgraf and Crutzen (1998)
47	$CH_3OH + OH \rightarrow HCHO + HO_2$	7.3E-12*exp(-620/T)	Sander et al. (2003)
48	$HCOOH + OH \rightarrow HO_2$	4.E-13	Sander et al. (2003)
49	$CH_3O_2 + NO_2 \rightarrow CH_3O_2NO_2$	complex	Sander et al. (2003)
50	$CH_3O_2NO_2 \rightarrow NO_2 + CH_3O_2$	k_NO2_HO2/(2.1E-27*exp(10900/T))	Sander et al. (2003)
51	$CH_3O_2NO_2 + h\nu \rightarrow .667\ NO_2 + .667\ HO_2 + .333\ NO_3 + .333\ OH$	J_HNO4	this work*
52	$C_2H_6 + OH \rightarrow C_2H_5O_2 + H_2O$	1.49E-17*T*T*exp(-499/T)	Atkinson (2003)
53	$C_2H_5O_2 + HO_2 \rightarrow C_2H_5OOH$	7.5E-13*exp(700/T)	Sander et al. (2003)
54	$C_2H_5O_2 + NO \rightarrow CH_3CHO + HO_2 + NO_2$	2.6E-12*exp(365/T)	Tyndall et al. (2001)
55	$C_2H_5O_2 + NO_3 \rightarrow CH_3CHO + HO_2 + NO_2$	2.3E-12	Atkinson et al. (1999)
56	$C_2H_5O_2 + CH_3O_2 \rightarrow .75\ HCHO + HO_2 + .75\ CH_3CHO + .25\ CH_3OH$	1.6E-13*exp(195/T)	Kirchner and Stockwell (1996); Sander et al. (2003)*
57	$C_2H_5OOH + OH \rightarrow .3\ C_2H_5O_2 + .7\ CH_3CHO + .7\ OH$	=k_CH3OOH_OH	see note
58	$C_2H_5OOH + h\nu \rightarrow CH_3CHO + HO_2 + OH$	=J_CH3OOH	see note
59	$CH_3CHO + OH \rightarrow CH_3C(O)OO + H_2O$	5.6E-12*exp(270/T)	Sander et al. (2003)
60	$CH_3CHO + NO_3 \rightarrow CH_3C(O)OO + HNO_3$	1.4E-12*exp(-1900/T)	Sander et al. (2003)
61	$CH_3CHO + h\nu \rightarrow CH_3O_2 + HO_2 + CO$	=0.19*J_CHOH	von Kuhlmann et al. (2003)
62	$CH_3COOH + OH \rightarrow CH_3O_2$	4.E-13*exp(200/T)	Sander et al. (2003)
63	$CH_3C(O)OO + HO_2 \rightarrow CH_3C(O)OOH$	4.3E-13*exp(1040/T)/(1+1/37*exp(660/T))	Sander et al. (2003)
64	$CH_3C(O)OO + HO_2 \rightarrow CH_3COOH + O_3$	4.3E-13*exp(1040/T)/(1+37*exp(-660/T))	Sander et al. (2003)
65	$CH_3C(O)OO + NO \rightarrow CH_3O_2 + NO_2$	8.1E-12*exp(270/T)	Sander et al. (2003)
66	$CH_3C(O)OO + NO_2 \rightarrow PAN$	k_PA_NO2, complex	Sander et al. (2003)

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

No.	Reaction	Rate constant	Reference
67	$CH_3C(O)OO + NO_3 \rightarrow CH_3O_2 + NO_2$	4.E-12	Canosa-Mas et al. (1996)
68	$CH_3C(O)OO + CH_3O_2 \rightarrow HCHO + HO_2 + CH_3O_2 + CO_2$	2.E-12*exp(500/T)/(1+1/2.2E6*exp(3820/T))	Sander et al. (2000, 2003)
69	$CH_3C(O)OO + CH_3O_2 \rightarrow CH_3COOH + HCHO + CO_2$	2.E-12*exp(500/T)/(1+2.2E6*exp(3820/T)	Sander et al. (2000, 2003)
70	$CH_3C(O)OO + C_2H_5O_2 \rightarrow .82\ CH_3O_2 + CH_3CHO + .82\ HO_2 + .18\ CH_3COOH$	4.9E-12*exp(211/T)	Atkinson et al. (1999); Kirchner and Stockwell (1996)*
71	$CH_3C(O)OO + CH_3C(O)OO \rightarrow 2\ CH_3O_2 + 2\ CO_2 + O_2$	2.5E-12*exp(500/T)	Tyndall et al. (2001)
72	$CH_3C(O)OOH + OH \rightarrow CH_3C(O)OO$	=k_CH3OOH_OH	see note
73	$CH_3C(O)OOH + h\nu \rightarrow CH_3O_2 + OH$	=0.025*J_CHOH	von Kuhlmann et al. (2003)
74	$NACA + OH \rightarrow NO_2 + HCHO + CO$	5.6E-12*exp(270/T)	see note
75	$NACA + h\nu \rightarrow NO_2 + HCHO + CO$	=0.19*J_CHOH	von Kuhlmann et al. (2003)
76	$PAN + OH \rightarrow HCHO + NO_2$	2.E-14	Sander et al. (2003)*
77	$PAN \rightarrow CH_3C(O)OO + NO_2$	k_PAN_M=k_PA_NO2/(9.E-29*exp(14000/T)	Sander et al. (2003)
78	$PAN + h\nu \rightarrow CH_3C(O)OO + NO_2$	J_PAN	von Kuhlmann et al. (2003)
79	$C_3H_8 + OH \rightarrow .82\ C_3H_7O_2 + .18\ C_2H_5O_2 + H_2O$	1.65E-17*T*T*exp(-87/T)	Atkinson (2003)*
80	$C_3H_7O_2 + HO_2 \rightarrow C_3H_7OOH$	k_PrO2_HO2=1.9E-13*exp(1300/T)	Atkinson (1997)*
81	$C_3H_7O_2 + NO \rightarrow .96\ CH_3COCH_3 + .96\ HO_2 + .96\ NO_2 + .04\ C_3H_7ONO_2$	k_PrO2_NO	Atkinson et al. (1999)*
82	$C_3H_7O_2 + CH_3O_2 \rightarrow CH_3COCH_3 + .8\ HCHO + .8\ HO_2 + .2\ CH_3OH$	k_PrO2_CH3O2	Kirchner and Stockwell (1996)
83	$C_3H_7OOH + OH \rightarrow .3\ C_3H_7O_2 + .7\ CH_3COCH_3 + .7\ OH$	=k_CH3OOH_OH	see note
84	$C_3H_7OOH + h\nu \rightarrow CH_3COCH_3 + HO_2 + OH$	=J_CH3OOH	see note
85	$CH_3COCH_3 + OH \rightarrow CH_3COCH_2O_2 + H_2O$	1.33E-13+3.82E-11*exp(-2000/T)	Sander et al. (2003)
86	$CH_3COCH_3 + h\nu \rightarrow CH_3C(O)OO + CH_3O_2$	J_CH3COCH3	von Kuhlmann et al. (2003)
87	$CH_3COCH_2O_2 + HO_2 \rightarrow CH_3COCH_2O_2H$	8.6E-13*exp(700/T)	Tyndall et al. (2001)
88	$CH_3COCH_2O_2 + NO \rightarrow NO_2 + CH_3C(O)OO + HCHO$	2.9E-12*exp(300/T)	Sander et al. (2003)
89	$CH_3COCH_2O_2 + CH_3O_2 \rightarrow .5\ CH_3COCHO + .5\ CH_3OH + .3\ CH_3C(O)OO + .8\ HCHO + .3\ HO_2 + .2\ CH_3COCH_2OH$	7.5E-13*exp(500/T)	Tyndall et al. (2001)
90	$CH_3COCH_2O_2H + OH \rightarrow .3\ CH_3COCH_2O_2 + .7\ CH_3COCHO + .7\ OH$	=k_CH3OOH_OH	see note
91	$CH_3COCH_2O_2H + h\nu \rightarrow CH_3C(O)OO + HO_2 + OH$	=J_CH3OOH	von Kuhlmann et al. (2003)
92	$CH_3COCH_2OH + OH \rightarrow CH_3COCHO + HO_2$	3.E-12	Atkinson et al. (1999)
93	$CH_3COCH_2OH + h\nu \rightarrow CH_3C(O)OO + HCHO + HO_2$	=0.074*J_CHOH	von Kuhlmann et al. (2003)*
94	$CH_3COCHO + OH \rightarrow CH_3C(O)OO + CO$	8.4E-13*exp(830/T)	Tyndall et al. (1995)
95	$CH_3COCHO + h\nu \rightarrow CH_3C(O)OO + CO + HO_2$	J_CH3COCHO	von Kuhlmann et al. (2003)
96	$C_3H_7ONO_2 + OH \rightarrow CH_3COCH_3 + NO_2$	6.2E-13*exp(-230/T)	Atkinson et al. (1999)
97	$C_3H_7ONO_2 + h\nu \rightarrow CH_3COCH_3 + NO_2 + HO_2$	=3.7*J_PAN	von Kuhlmann et al. (2003)
98	$C_2H_4 + O_3 \rightarrow HCHO + .22\ HO_2 + .12\ OH + .23\ CO + .54\ HCOOH + .1\ H_2$	1.2E-14*exp(-2630./T)	Sander et al. (2003); Neeb et al. (1998)

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

No.	Reaction	Rate constant	Reference
99	C_2H_4 + OH → 2/3 $CH_3CH(O_2)CH_2OH$	complex	Sander et al. (2003); Müller and Brasseur (1995)
100	C_3H_6 + O_3 → .57 HCHO + .47 CH_3CHO + .33 OH + .26 HO_2 + .07 CH_3O_2 + .06 $C_2H_5O_2$ + .23 $CH_3C(O)OO$ + .04 CH_3COCHO + .06 CH_4 + .31 CO + .22 HCOOH + .03 CH_3OH	`6.5E-15*exp(-1900/T)`	Sander et al. (2003); Zaveri and Peters (1999)
101	C_3H_6 + OH → $CH_3CH(O_2)CH_2OH$	complex	Atkinson et al. (1999)
102	C_3H_6 + NO_3 → ONIT	`4.6E-13*exp(-1155/T)`	Atkinson et al. (1999)
103	$CH_3CH(O_2)CH_2OH$ + HO_2 → C_3H_6OOH	`6.5E-13*exp(650/T)`	Müller and Brasseur (1995)
104	$CH_3CH(O_2)CH_2OH$ + NO → .98 CH_3CHO + .98 HCHO + .98 HO_2 + .98 NO_2 + .02 ONIT	`4.2E-12*exp(180/T)`	Müller and Brasseur (1995)*
105	C_3H_6OOH + OH → .5 $CH_3CH(O_2)CH_2OH$ + .5 CH_3COCH_2OH + .5 OH + H_2O	`3.8E-12*exp(200./T)`	Müller and Brasseur (1995)
106	C_4H_{10} + OH → $C_4H_9O_2$ + H_2O	`1.81E-17*T*T*exp(114/T)`	Atkinson (2003)
107	$C_4H_9O_2$ + CH_3O_2 → .88 $CH_3COC_2H_5$ + .68 HCHO + 1.23 HO_2 + .12 CH_3CHO + .12 $C_2H_5O_2$ + .18 CH_3OH	`k_PrO2_CH3O2`	Poisson et al. (2000)*
108	$C_4H_9O_2$ + HO_2 → C_4H_9OOH	`k_PrO2_HO2`	Poisson et al. (2000)*
109	$C_4H_9O_2$ + NO → .84 NO_2 + .56 $CH_3COC_2H_5$ + .56 HO_2 + .28 $C_2H_5O_2$ + .84 CH_3CHO + .16 ONIT	`k_PrO2_NO`	Poisson et al. (2000); Zaveri and Peters (1999)*
110	C_4H_9OOH + OH → .15 $C_4H_9O_2$ + .85 $CH_3COC_2H_5$ + .85 OH + .85 H_2O	`k_CH3OOH_OH`	Poisson et al. (2000)*
111	C_4H_9OOH + hν → OH + .67 $CH_3COC_2H_5$ + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	`=J_CH3OOH`	Poisson et al. (2000)*
112	$CH_3COC_2H_5$ + OH → MEKO2	`1.3E-12*exp(-25/T)`	Atkinson et al. (1999)
113	$CH_3COC_2H_5$ + hν → $CH_3C(O)OO$ + $C_2H_5O_2$	`=0.42*J_CHOH`	von Kuhlmann et al. (2003)
114	MEKO2 + HO_2 → MEKOOH	`k_PrO2_HO2`	Poisson et al. (2000)*
115	MEKO2 + NO → .985 CH_3CHO + .985 $CH_3C(O)OO$ + .985 NO_2 + .015 ONIT	`k_PrO2_NO`	Poisson et al. (2000)*
116	MEKOOH + OH → .8 MeCOCO + .8 OH + .2 MEKO2	`k_CH3OOH_OH`	Poisson et al. (2000)*
117	MEKOOH + hν → $CH_3C(O)OO$ + CH_3CHO + OH	`=J_CH3OOH`	see note
118	MeCOCO + hν → 2 $CH_3C(O)OO$	`=2.15*J_CH3COCHO`	von Kuhlmann et al. (2003)*
119	ONIT + OH → $CH_3COC_2H_5$ + NO_2 + H_2O	`1.7E-12`	Atkinson et al. (1999)*
120	ONIT + hν → NO_2 + .67 $CH_3COC_2H_5$ + .67 HO_2 + .33 $C_2H_5O_2$ + .33 CH_3CHO	`=3.7*J_PAN`	von Kuhlmann et al. (2003)*
121	ISOP + O_3 → .28 HCOOH + .65 MVK + .1 MVKO2 + .1 $CH_3C(O)OO$ + .14 CO + .58 HCHO + .09 H_2O_2 + .08 CH_3O_2 + .25 OH + .25 HO_2	`7.86E-15*exp(-1913/T)`	Pöschl et al. (2000)
122	ISOP + OH → ISO2	`2.54E-11*exp(410/T)`	Pöschl et al. (2000)
123	ISOP + NO_3 → ISON	`3.03E-12*exp(-446/T)`	Pöschl et al. (2000)
124	ISO2 + HO_2 → ISOOH	`2.22E-13*exp(1300/T)`	Boyd et al. (2003)
125	ISO2 + NO → .88 NO_2 + .88 MVK + .88 HCHO + .88 HO_2 + .12 ISON	`2.54E-12*exp(360/T)`	Pöschl et al. (2000); Sprengnether et al. (2002)*
126	ISO2 + CH_3O_2 → .5 MVK + 1.25 HCHO + HO_2 + .25 CH_3COCHO + .25 CH_3COCH_2OH + .25 CH_3OH	`2.E-12`	von Kuhlmann (2001)
127	ISO2 + ISO2 → 2 MVK + HCHO + HO_2	`2.E-12`	Pöschl et al. (2000)
128	ISOOH + OH → MVK + OH	`1.E-10`	Pöschl et al. (2000)

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

No.	Reaction	Rate constant	Reference
129	ISOOH + hν $\rightarrow$ MVK + HCHO + HO_2 + OH	=J_CH3OOH	Pöschl et al. (2000)*
130	ISON + OH $\rightarrow$ CH_3COCH_2OH + NACA	1.3E-11	Pöschl et al. (2000)
131	ISON + hν $\rightarrow$ MVK + HCHO + NO_2 + HO_2	=3.7*J_PAN	von Kuhlmann et al. (2003)
132	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./T) +7.51E-16*exp(-1521/T))	Pöschl et al. (2000)
133	MVK + OH $\rightarrow$ MVKO2	.5*(4.1E-12*exp(452./T) +1.9E-11*exp(175./T))	Pöschl et al. (2000)
134	MVK + hν $\rightarrow$ $CH_3C(O)OO$ + HCHO + CO + HO_2	=0.019*J_COH2+ .015*J_CH3COCHO	von Kuhlmann et al. (2003)*
135	MVKO2 + HO_2 $\rightarrow$ MVKOOH	1.82E-13*exp(1300./T)	Pöschl et al. (2000)
136	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./T)	Pöschl et al. (2000)
137	MVKO2 + NO_2 $\rightarrow$ MPAN	.25*k_PA_NO2	Pöschl et al. (2000)*
138	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	von Kuhlmann (2001)
139	MVKO2 + MVKO2 $\rightarrow$ CH_3COCH_2OH + CH_3COCHO + .5 CO + .5 HCHO + HO_2	2.E-12	Pöschl et al. (2000)
140	MVKOOH + OH $\rightarrow$ MVKO2	3.E-11	Pöschl et al. (2000)
141	MVKOOH + hν $\rightarrow$ OH + .5 CH_3COCHO + .25 CH_3COCH_2OH + .75 HCHO + .75 HO_2 + .25 $CH_3C(O)OO$ + .25 CO	=J_CH3OOH	see note
142	MPAN + OH $\rightarrow$ CH_3COCH_2OH + NO_2	3.2E-11	Orlando et al. (2002)
143	MPAN $\rightarrow$ MVKO2 + NO_2	=k_PAN_M	Pöschl et al. (2000)
144	MPAN + hν $\rightarrow$ CH_3COCH_2OH + NO_2	=J_PAN	Pöschl et al. (2000)

Notes:

7: H_2 is kept constant at 531 nmol/mol (Novelli et al., 1999).

10: The pressure independent term has been updated to Christensen et al. (2002).

31: Photolysis of HNO_4 in the near-IR is included based on Roehl et al. (2002), constraint to levels above 400 hPa and neglecting cloud effects.

35+36: Branching ratio is base on Elrod et al. (2001).

44: The same temperature dependence as for CH_3CHO + NO_3 has been assumed.

51: Same photolysis rate as for HNO_4 + hν, but without near-IR part has been assumed.

56: Rate coefficient calculated 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 and branching is calculated based on Villenave and Lesclaux (1996) and Tyndall et al. (2001).

57: The same rate as for CH_3OOH + OH has been asssumed.

58: The same photolysis rate as for CH_3OOH + hν has been asssumed.

70: Room temperature value is from Atkinson et al. (1999), temperature dependence and products are based on Kirchner and Stockwell (1996)

72: The same rate as for CH_3OOH + OH has been asssumed.

74: The same rate as for CH_3CHO + OH has been asssumed.

76: One half of the upper limit in Sander et al. (2003) is used.

79: Only formation of secondary peroxy-radicals is taken into account. Primary peroxy-radicals are channeled into ethylperoxy-radical instead.

80: The generic rate for RO2 + HO2 from Atkinson et al. (1997) has been used.

83: The same rate as for CH_3OOH + OH has been asssumed.

84: The same photolysis rate as for $CH_3OOH + h\nu$ has been asssumed.

90: The same rate as for CH_3OOH + OH has been asssumed.

91: The same photolysis rate as for $CH_3OOH + h\nu$ has been asssumed.

93: A constant quantum yield of 0.65 from Orlando et al. (1999) has been applied in this work.

104: Nitrate yield adopted from the Master Chemical Mechanism (MCM) (Carter and Atkinson, 1996; Saunders et al., 1997).

107-109, 114, 115: Same rates as for the corresponding propyl group are assumed.

109: An overall nitrate yield of 16% as for higher alkanes in Zaveri and Peters (1999) is used.

110: The same rate as for CH_3OOH + OH has been assumed.

111: The same photolysis rate as for $CH_3OOH + h\nu$ has been asssumed.

115: Nitrate yield adopted from the Master Chemical Mechanism (MCM) (Carter and Atkinson, 1996; Saunders et al., 1997).

117: The same photolysis rate as for $CH_3OOH + h\nu$ has been asssumed.

118: Based on ration in the Master Chemical Mechanism (MCM) (Carter and Atkinson, 1996; Saunders et al., 1997).

119+120: The value for $C_4H_9ONO_2$ used here.

125: Nitrate yield based on Sprengnether et al. (2002) is used.

133+134: The mean value for methylvinylketone and methacrolein is used.

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

141: The same photolysis rate as for $CH_3OOH + h\nu$ has been asssumed.

B Full set of model versus observation comparisons for HNO_3

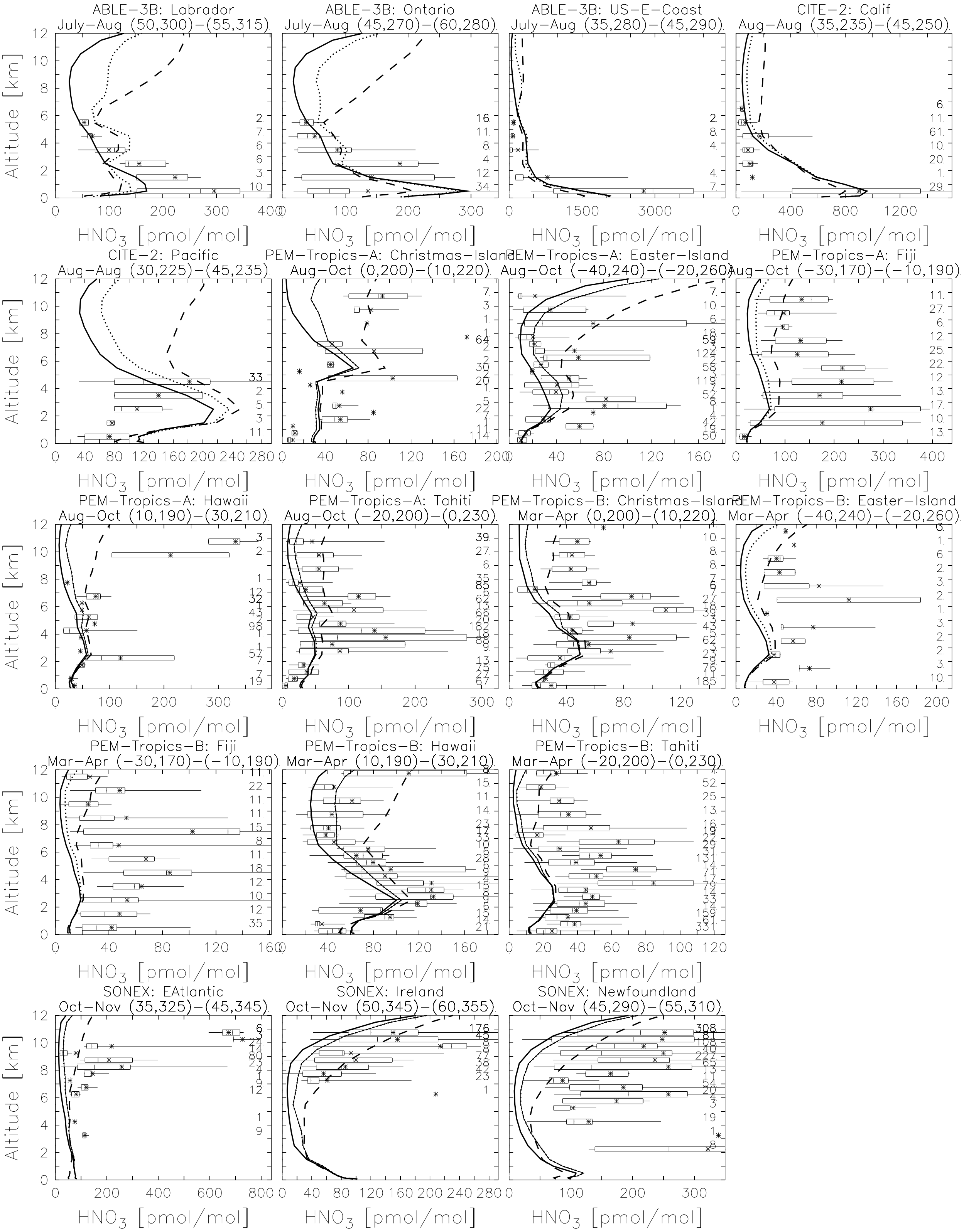

Figure 1: Comparison of regional vertical profiles of HNO_3 to model output. Solid, dotted and dashed lines are for the HIGHUP, LANGM, and NOUP simulations, respectively. Boxes, whiskers, horizontal line and asterix mark the central 50 and 90%, median and mean of the observations, respectively.

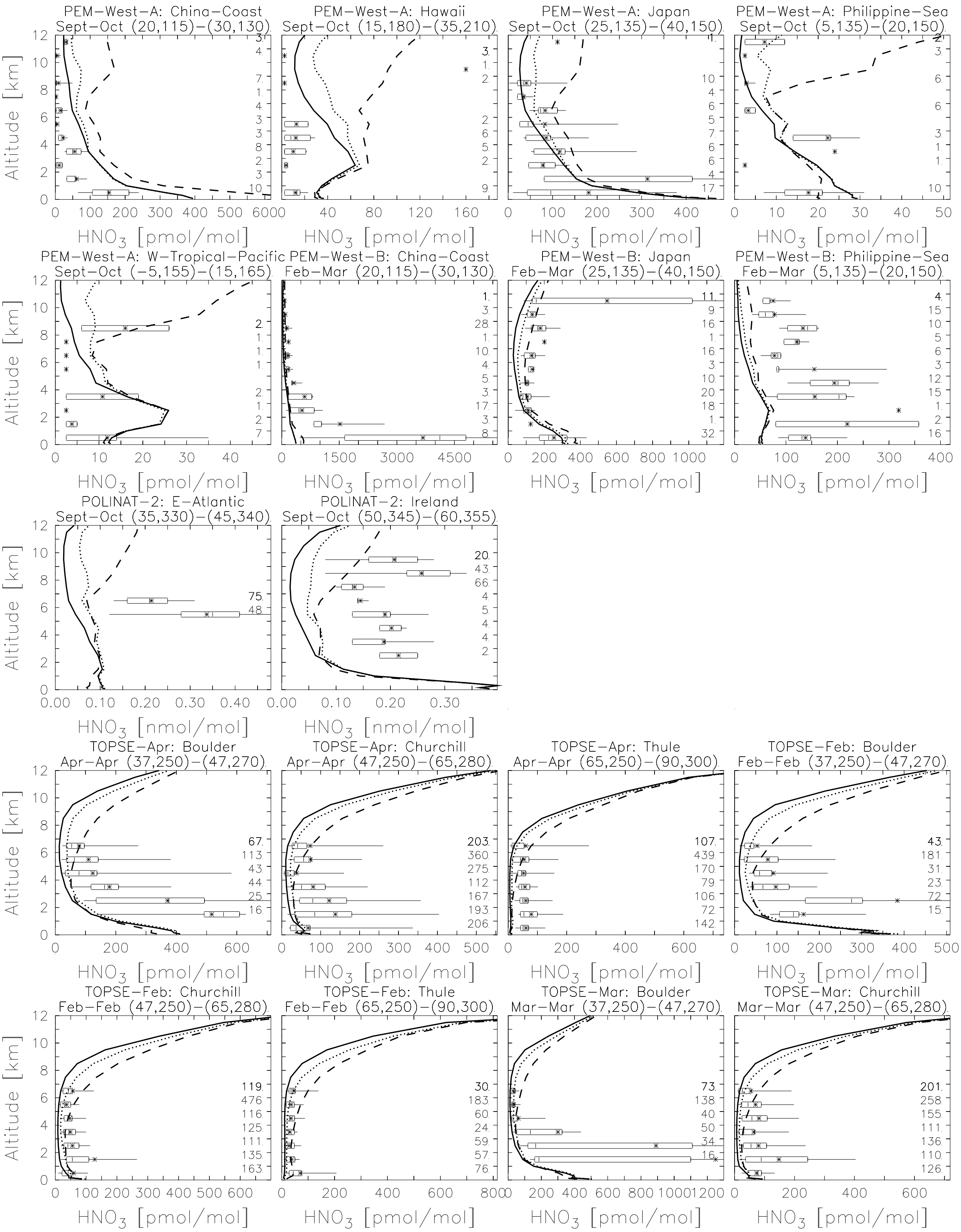

Figure 1: (continued).

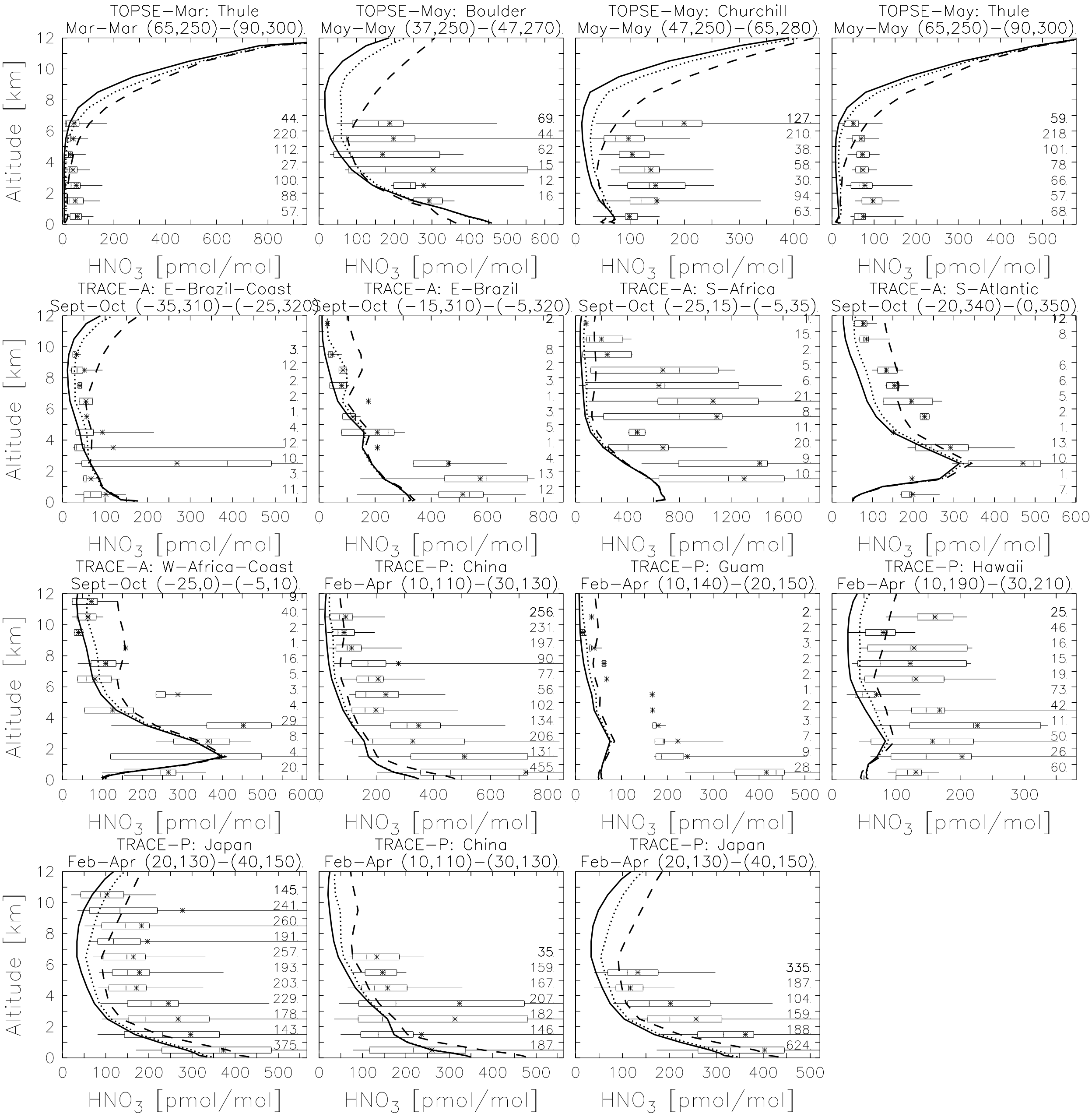

Figure 1: (continued).

References

Atkinson, R.: Gas-Phase Tropospheric Chemistry of Volatile Organic Compounds: 1. Alkanes and Alkenes, J. Phys. Chem. Ref. Data, 26, 215–290, 1997.

Atkinson, R.: Kinetics of the gas-phase reactions of OH radicals with alkanes and cycloalkanes, Atmos. Chem. Phys. Discuss., 3, 4183–4358, 2003.

Atkinson, R., Baulch, D. L., Cox, R. A., Hampson, Jr, R. F., Kerr, J. A., Rossi, M. J., and Troe, J.: Evaluated Kinetic and Heterogeneous Data for Atmospheric Chemistry: Supplement V, J. Phys. Chem. Ref. Data, 26, 521–1011, 1997.

Atkinson, R., Baulch, D. L., Cox, R. A., Hampson, Jr, R. F., Kerr, J. A., Rossi, M. J., and Troe, J.: Evaluated kinetic and photochemical data for atmospheric chemistry, Organic species: Supplement VII, J. Phys. Chem. Ref. Data, 28, 191–393, http://www.iupac–kinetic.ch.cm.ac.uk, http://www.iupac-kinetic.ch.cm.ac.uk, 1999.

Boyd, A. A., Flaud, P.-M., Daugey, N., and Lesclaux, R.: Rate constants for RO_2 + HO_2 reactions measured under a large excess of HO_2, J. Phys. Chem. A, 107, 818–821, 2003.

Canosa-Mas, C. E., King, M. D., Lopez, R., Percival, C. J., Wayne, R. P., Shallcross, D. E., Pyle, J. A., and Daell, V.: Is the reaction between $CH_3(O)O_2$ and NO_3 important in the nigh-time troposphere?, J. Chem. Soc., Faraday Trans., 92, 2211–2222, 1996.

Carter, W. P. L. and Atkinson, R.: Development and Evaluation of a Detailed Mechanism for the Atmospheric Reactions of Isoprene and NO_x, Int. J. Chem. Kinet., 28, 497–530, 1996.

Christensen, L. E., Okumura, M., Sander, S. P., Salawitch, R. J., Toon, G. C., Sen, B., Blavier, J.-F., and Jucks, K. W.: Kinetics of $HO_2 + HO_2 \longrightarrow H_2O_2 + O_2$: Implications for for Stratospheric H_2O_2, Geophys. Res. Lett., 29, 1299, doi:10.1029/2001GL014 525, 2002.

Dransfield, T. J., Perkins, K. K., Donahue, N. M., Anderson, J. G., Sprengnether, M. M., and Demerjian, K. L.: Temperature and Pressure Dependent Kinetics of the Gas-Phase Reaction of the Hydroxy Radicals with Nitrogen Dioxide, Geophys. Res. Lett., 26, 687– 690, 1999.

Elrod, M. J., Ranschaert, D. L., and Schneider, N. J.: Direct kinetics study of the temperature dependence of the CH_2O branching channel for the CH_3O_2 + HO_2 reaction, Int. J. Chem. Kinet., 33, 363–376, 2001.

Kirchner, F. and Stockwell, W. R.: Effect of peroxy radical reactions on the predicted concentration of ozone, nitrogenous compounds, and radicals, J. Geophys. Res., 101, 21 007–21 022, 1996.

Landgraf, J. and Crutzen, P. J.: An Efficient Method for Online Calculations of Photolysis and Heating Rates, J. Atmos. Chem., 25, 863–878, 1998.

Madronich, S. and Calvert, J. G.: Permutation reactions of organic peroxy radicals in the troposphere, J. Geophys. Res., 95D, 5697–5715, 1990.

McCabe, D. C., Gierczak, T., Talukdar, R. K., and Ravishankara, A. R.: Kinetics of the reaction OH + CO under atmospheric conditions, Geophys. Res. Lett., 28, 3135–3138, 2001.

Müller, J.-F. and Brasseur, G.: IMAGES: A three-dimensional chemical transport model of the global troposphere, J. Geophys. Res., 100, 16 445–16 490, 1995.

Neeb, P., Horie, O., and Moortgat, G. K.: The Ethene-Ozone Reaction in the Gas Phase, J. Phys. Chem. A, 102, 6778–6785, 1998.

Novelli, P. C., Lang, P. M., Masarie, K. A., Hurst, D. F., Myers, R., and Elkins, J. W.: Molecular hydrogen in the troposphere: Global distribution and budget, J. Geophys. Res., 104, 30 427–30 444, 1999.

Orlando, J. J., Tyndall, G. S., Frachebroud, J.-M., Estupinan, E. G., Haberkorn, S., and Zimmer, A.: The rate and mechanism of the gas phase oxidation of hydroxyacetone, Atmos. Environ., 33, 1621–1629, 1999.

Orlando, J. J., Tyndall, G. S., Bertman, S. B., Chen, W., and Burkholder, J. B.: Rate coefficient for the reaction of OH with CH2=C(CH3)C(O)OONO2 (MPAN), Atmos. Environ., 36, 1895–1900, 2002.

Poisson, N., Kanakidou, M., and Crutzen, P. J.: Impact of non-methane hydrocarbons on tropospheric chemistry and the oxidizing power of the global troposphere: 3-dimensional modelling results, J. Atmos. Chem., 36, 157–230, 2000.

Pöschl, U., von Kuhlmann, R., Poisson, N., and Crutzen, P. J.: Development and Intercomparison of Condensed Isoprene Oxidation Mechanisms for Global Atmospheric Modeling, J. Atmos. Chem., 37, 29–52, 2000.

Ravishankara, A. R., Dunlea, E. J., Blitz, M. A., Dillon, T. J., Heard, D. E., Pilling, M. J., a nd J. M. Nicovich, R. S. S., and Wine, P. H.: Redetermination of the rate coefficient for the reaction of $O(^1D)$ with N_2, Geophys. Res. Lett., 29, 1745, doi:10.1029/2002GL014 850, 2002.

Roehl, C. M., Nizkorodov, S. A., Zhang, H., Blake, G. A., and Wennberg, P. O.: Photodissociation of Peroxynitric Acid in the Near-IR, J. Phys. Chem. A, 106, 3766–3772, 2002.

Sander, S. P., Friedl, R. R., DeMore, W. B., Ravishankara, A. R., Golden, D. M., Kolb, C. E., Kurylo, M. J., Hampson, R. F., Huie, R. E., Molina, M. J., and Moortgat, G. K.: Chemical Kinetics and Photochemical Data for Use in Stratospheric Modeling — Supplement to Evaluation 12: Update of Key Reactions, Evaluation 13, 00-3, Jet Propulsion Laboratory, Pasadena, California, 2000.

Sander, S. P., Friedl, R. R., Ravishankara, A. R., Golden, D. M., Kolb, C. E., Kurylo, M. J., Huie, R. E., Orkin, V. L., Molina, M. J., Moortgat, G. K., and Finlayson-Pitts, B. J.: Chemical Kinetics and Photochemical Data for Use in Atmospheric Studies, Evaluation Number 14, 02-25, Jet Propulsion Laboratory, Pasadena, California, 2003.

Saunders, S. M., Jenkin, M. E., Derwent, R. G., and Pilling, M. J.: World Wide Web site of a Master Chemical Mechanism (MCM) for use in tropospheric chemistry models, Atmos. Environ., 31, 1249, http://www.chem.leeds.ac.uk/Atmospheric/MCM/-mcmproj.html, 1997.

Sivakumaran, V., Hölscher, D., Dillon, T. J., and Crowley, J. N.: Reaction between OH and HCHO: Temperature dependent rate coefficients (202 - 399 K) and product pathways (298 K), Phys. Chem. Chem. Phys., 5, 4821–4827, 2003.

Sprengnether, M., Demerjian, K. L., Donahue, N. M., and Anderson, J. G.: Product analysis of the OH oxidation of isoprene and 1,3-butadiene in the presence of NO, J. Geophys. Res., 107, 4268, doi:10.1029/2001JD000 716, 2002.

Tyndall, G. S., Staffelbach, T. A., Orlando, J. J., and Calvert, J. G.: Rate coefficients for the reactions of OH radicals with methylglyoxal and acetaldehyde, Int. J. Chem. Kinet., 27, 1009–1020, 1995.

Tyndall, G. S., Cox, R. A., Granier, C., Lesclaux, R., Moortgat, G. K., Pilling, M. J., Ravishankara, A. R., and Wallington, T. J.: The atmospheric chemistry of small organic peroxy radicals, J. Geophys. Res., 106, 12 157–12 182, 2001.

Villenave, E. and Lesclaux, R.: Kinetic of the cross reaction of CH_3O_2 and $C_2H_5O_2$ radicals with selected peroxy radicals, J. Phys. Chem., 100, 14 372–14 382, 1996.

von Kuhlmann, R.: Tropospheric Photochemistry of Ozone, its Precursors and the Hydroxyl Radical: A 3D-Modeling Study Considering Non-Methane Hydrocarbons, Ph.D. thesis, Johannes Gutenberg-Universität Mainz, Mainz, Germany, http://www.mpch-mainz.mpg.de/˜kuhlmann/rvkdisshtml, 2001.

von Kuhlmann, R., Lawrence, M. G., Crutzen, P. J., and Rasch, P. J.: A model for studies of tropospheric ozone and nonmethane hydrocarbons: Model description and ozone results, J. Geophys. Res., 108, 4294, doi:10.1029/2002JD002 893, http://www.mpch-mainz.mpg.de/˜kuhlmann/matcheval, 2003.

Wahner, A., Mentel, T. F., and Sohn, M.: Gas-phase reaction of N_2O_5 with water vapor: Importance of heterogeneous hydrolysis of N_2O_5 and surface desorption of HNO_3 in a large teflon chamber, Geophys. Res. Lett., 25, 2169–217, 1998.

Zaveri, R. A. and Peters, L. K.: A new lumped structure photochemical mechanism for large-scale applications, J. Geophys. Res., 104, 30 387–30 415, 1999.