

Supplementary Material for the paper

The influence of natural and anthropogenic secondary sources on the glyoxal global distribution

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Table 1. Photolysis reactions in TM4-ECPL and related references

#	reaction		refs.
*	$O_3 + hv$	$\rightarrow O(^3P) + O_2$	1
j1	$O_3 + hv$	$\rightarrow O(^1D) + O_2$	1
j2	$H_2O_2 + hv$	$\rightarrow 2OH$	1
j3	$NO_2 + hv$	$\rightarrow NO + O$	1
j4	$NO_3 + hv$	$\rightarrow NO_2 + O$	1
j5	$NO_3 + hv$	$\rightarrow NO + O_2$	1
j6	$HONO_2 + hv$	$\rightarrow NO_2 + OH$	1
j7	$HO_2NO_2 + hv$	$\rightarrow NO_2 + HO_2$	1
j8	$N_2O_5 + hv$	$\rightarrow NO_2 + NO_3$	1
j9	$CH_3OOH + hv + O_2$	$\rightarrow HCHO + HO_2 + OH$	1
j10	$CH_3ONO_2 + hv + O_2$	$\rightarrow HCHO + HO_2 + NO_2$	1
j11	$HCHO + hv$	$\rightarrow CO + H_2$	1
j12	$HCHO + hv + 2O_2$	$\rightarrow CO + 2HO_2$	1
j13	$C_2H_5OOH + hv + O_2$	$\rightarrow CH_3CHO + HO_2 + OH$	2
j14	$C_2H_5ONO_2 + hv + O_2$	$\rightarrow CH_3CHO + HO_2 + NO_2$	1
j15	$CH_3CHO + hv + 2O_2$	$\rightarrow CH_3O_2 + CO + HO_2$	1
j16	$CH_3C(O)O_2NO_2 + hv$	$\rightarrow CH_3COO_2 + NO_2$	1
j17	$CH_3COO_2H + hv + O_2$	$\rightarrow CH_3O_2 + CO_2 + OH$	2
j18	$C_3H_7O_2prim + hv + O_2$	$\rightarrow 1-C_2H_5CHO + HO_2 + OH$	2
j19	$C_3H_7ONO_2prim + hv$	$\rightarrow 1-C_2H_5CHO + HO_2 + NO_2$	4
j19	$C_2H_5CHOprim + hv + O_2$	$\rightarrow C_2H_5O_2 + CO + HO_2$	7
j20	$C_3H_7O_2sec + hv + O_2$	$\rightarrow CH_3COCH_3 + HO_2 + OH$	2
j21	$C_3H_7ONO_2sec + hv$	$\rightarrow CH_3COCH_3 + HO_2 + NO_2$	4
j22	$CH_3COCH_3 + hv + 2O_2$	$\rightarrow CH_3COO_2 + CH_3O_2$	5
j23	$CH_3COCHO + hv + 2O_2$	$\rightarrow 0.3*(CH_3O_2 + 2CO + HO_2) + 0.7*(CH_3COO_2 + CO + HO_2)$	1
j24	$CH_3COCH_2OOH + hv + O_2$	$\rightarrow CH_3COCHO + OH + HO_2$	2
j25	$HOCH_2CH_2OOH + hv + O_2$	$\rightarrow OH + e(2HCHO + HO_2) + f(HOCH_2CHO + HO_2)$	2, 8
j26	$HOCH_2CH_2ONO_2 + hv + O_2$	$\rightarrow NO_2 + e(HCHO + HO_2) + f(HOCH_2CHO + HO_2)$	1, 8
j27	$HOCH_2CHO + hv + 2O_2$	$\rightarrow HCHO + CO + 2HO_2$	1
j28	$CHOCHO + hv$	$\rightarrow 2CO + 2HO_2$	1
j29	$C_4H_9ONO_2 + hv + O_2$	$\rightarrow NO_2 + 0.67(CH_3CH_2COCH_3 + HO_2) + 0.33(C_2H_5O_2 + CH_3CHO)$	4
j30	$C_4H_9OOH + hv + O_2$	$\rightarrow OH + 0.67(CH_3CH_2COCH_3 + HO_2) + 0.33(C_2H_5O_2 + CH_3CHO)$	2
j31	$CH_3CH_2COCH_3 + hv + 2O_2$	$\rightarrow CH_3COO_2 + C_2H_5O_2$	5
j32	$CH_3CHONO_2COCH_3 + hv + O_2$	$\rightarrow CH_3CHO + CH_3COO_2 + NO_2$	4
j33	$CH_3CHOOHCOCH_3 + hv + O_2$	$\rightarrow CH_3CHO + CH_3COO_2 + OH$	2
j34	$CH_3COCOCH_3 + hv + 2O_2$	$\rightarrow 2CH_3COO_2$	6
j35	$ISOOH + hv + O_2$	$\rightarrow HCHO + OH + HO_2 + 0.64MVK + 0.36MACR$	2
j36	$NITRATES + hv + O_2$	$\rightarrow HCHO + HO_2 + NO_2 + 0.64MVK + 0.36MACR$	4
j37	$MVKOOH + hv + O_2$	$\rightarrow CH_3COO_2 + HOCH_2CHO + OH$	2
j38	$MACROOH + hv + O_2$	$\rightarrow CH_3COCH_2OH + CO + OH + HO_2$	2
j39	$CH_2ONO_2CH_2OOH + hv$	$\rightarrow OH + NO_2 + 2HCHO$	2
j40	$CH_2ONO_2CH_2OOH + hv$	$\rightarrow CH_3CHO + HCHO + NO_2 + OH$	2
j41	$CH_3COCOOH + hv$	$\rightarrow CH_3CHO + CO_2$	2
j43	$MACR + hv$	$\rightarrow 0.67HO_2 + 0.33MACRO_2 + 0.67CH_2O + 0.67CH_3COO_2 + 0.33OH$	1
j44	$MVK + hv$	$\rightarrow 0.3CH_3CO_3 + 0.7C_3H_6 + 0.7CO + 0.3CH_3O_2$	1

* not explicitly accounted in the model; it is solved in the EBI code.

References

1. IUPAC Subcommittee on Gas Kinetic Data Evaluation for Atmospheric Chemistry, Summary of Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry, Web Version February, http://www.iupac-kinetic.ch.cam.ac.uk/summary/IUPACsumm_web_Feb2006.pdf, 2006
2. $j = j_{13}$
3. $j = 1.7 \times j_{22}$
4. $j = j_{10}$
5. $j = 3 \times 10^{-4} \times j_3$
6. $j = 0.285 \times j_3$
7. $j = (2.58 \times 10^{-4} + 1.2 \times 10^{-5}) \times j_3$
8. $R1 = 2.7 \times 10^{14} \exp(-6350/T)$
 $R2 = 6.3 \times 10^{-14} \exp(-550/T)$
 $e = R1/(R1 + R2 \times [O_2])$, $f = 1 - e$
T= temperature, lumping as in
Poisson, N., Kanakidou, M., and Crutzen, P. J.: Impact of Non Methane Hydrocarbons on tropospheric chemistry and particular the oxidizing power of the global troposphere: 3-Dimensional Modelling results, J. Atmos. Chem., 36, 157-230, 2000.

Table 2. Thermal reactions in TM4-ECPL as related references.

#	reaction	rate coefficient	Refs
*	$O(^1D) + M \rightarrow O(^3P) + M$	4×10^{-11}	1
*	$O(^3P) + O_2 + M \rightarrow O_3 + M$	$6.0 \times 10^{-34} (T/300)^{-2.6} (O_2)$ $5.6 \times 10^{-34} (T/300)^{-2.6} (N_2)$	1
*	$O(^1D) + H_2O \rightarrow 2 OH$	2.2×10^{-10}	1
k1	$O_3 + OH \rightarrow HO_2 + O_2$	$1.7 \times 10^{-12} \exp(-940/T)$	1
k2	$HO_2 + O_3 \rightarrow OH + O_2$	$2.03 \times 10^{-16} (T/300)^{4.57} \exp(693/T)$	1
k3	$HO_2 + OH \rightarrow H_2O + O_2$	$4.8 \times 10^{-11} \exp(250/T)$	1
k4	$HO_2 + HO_2 \rightarrow H_2O_2 + O_2$	$1.9 \times 10^{-33} [N_2] \exp(980/T)$	1
k5	$H_2O_2 + OH \rightarrow H_2O + HO_2$	$2.9 \times 10^{-12} \exp(-160/T)$	1
k6	$HO_2 + NO \rightarrow NO_2 + HO$	$3.6 \times 10^{-12} \exp(270/T)$	1
k7	$NO + O_3 \rightarrow NO_2 + O_2$	$1.4 \times 10^{-12} \exp(-1310/T)$	1
k8	$NO + NO_3 \rightarrow 2NO_2$	$1.8 \times 10^{-11} \exp(110/T)$	1
k9	$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.4 \times 10^{-13} \exp(-2470/T)$	1
k10	$NO_2 + OH + M \rightarrow HONO_2 + M$	$3.3 \times 10^{-30} (T/300)^{-3.0} [N_2]$ 4.1×10^{-11} $F_c = 0.4$ $3.6 \times 10^{-30} (T/300)^{-4.1} [N_2]$	1
k11	$NO_2 + NO_3 + M \rightarrow N_2O_5 + M$	$1.9 \times 10^{-12} (T/300)^{0.2}$ $F_c = 0.35$ $1.8 \times 10^{-31} (T/300)^{-3.2} [N_2]$	1
k12	$NO_2 + HO_2 + M \rightarrow HO_2NO_2 + M$	4.7×10^{-12} $F_c = 0.6$	1
k13	$HO_2 + NO_3 \rightarrow OH + NO_2 + O_2$	4.0×10^{-12}	1
k14	$HONO_2 + OH \rightarrow H_2O + NO_3$	1.5×10^{-13}	1
k15	$HO_2NO_2 + HO \rightarrow H_2O + O_2 + NO_2$	$3.2 \times 10^{-13} \exp(690/T)$ $4.1 \times 10^{-5} \exp(-10650/T) [N_2]$	1
k16	$HO_2NO_2 + M \rightarrow HO_2 + NO_2 + M$	$4.8 \times 10^{15} \exp(-11170/T)$ $F_c = 0.6$ $1.3 \times 10^{-3} (T/300)^{-3.5} \exp(-11000/T) [N_2]$	1
k17	$N_2O_5 + M \rightarrow NO_2 + NO_3 + M$	$9.7 \times 10^{14} (T/300)^{0.1} \exp(-11080/T)$ $F_c = 0.35$	1
k18	$CH_4 + OH \rightarrow H_2O + CH_3O_2$	$1.85 \times 10^{-12} \exp(-1690/T)$	1
k19	$CH_3O_2 + NO \rightarrow HCHO + HO_2 + NO_2$	$2.3 \times 10^{-12} \exp(360/T)$	1
k10	$CH_3O_2 + NO_3 \rightarrow HCHO + HO_2 + NO_2$	1.3×10^{-12}	1
k21	$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	$3.8 \times 10^{-13} \exp(780/T)$	1
k22	$CH_3O_2 + CH_3O_2 \rightarrow k22a(2HCHO + 2HO_2 + O_2) + (1-k22a)(CH_3OH + HCHO + O_2)$	$k22 = 7.4 \times 10^{-13} \exp(-520/T)$ $k22a = 5.4 \exp(0.870/T)$	1
k23	$CH_3OOH + OH \rightarrow CH_3O_2 + H_2O$	1.9×10^{-12}	1
k24	$CH_3OOH + OH \rightarrow H_2O + HCHO + OH$	3.6×10^{-12}	1
k25	$CH_3ONO_2 + OH \rightarrow HCHO + NO_2 + H_2O$	$4.0 \times 10^{-13} \exp(-845/T)$	1
k26	$HCHO + OH \rightarrow H_2O + CO + HO_2$	$5.4 \times 10^{-12} \exp(135/T)$	1
k27	$CH_3OH + OH \rightarrow H_2O + HCHO + HO_2$	$2.85 \times 10^{-12} \exp(-345/T)$	1
k28	$CO + OH \rightarrow HO_2 + CO_2$	$1.44 \times 10^{-13} (1 + [N_2]) / 4 \times 10^{19}$	1
k29	$C_2H_6 + OH + O_2 \rightarrow H_2O + C_2H_5O_2$	$6.9 \times 10^{-12} \exp(-1000/T)$	1
k30	$C_2H_5O_2 + NO + O_2 \rightarrow (1 - RTC2) \times [CH_3CHO + HO_2 + NO_2] + RTC2 \times C_2H_5ONO_2$	$k30 = 2.6 \times 10^{-12} \exp(380/T)$ $R1 = 1.94 \times 10^{-22} [AIR] \exp(0.972)$ $R2 = 0.826 (T/300)^{-8.1}$	2

				$A = 1/(1+\log(R1/R2)^2)$	
				$RTC2 = 0.4R1/(1+R1/R2)0.411^A$	
k31	$C_2H_5O_2 + HO_2$	\rightarrow	$C_2H_5OOH + O_2$	$3.8 \times 10^{-13} \exp(900/T)$	1
k32	$C_2H_5O_2 + CH_3O_2$	\rightarrow	$(1 - k32a)(CH_3CHO + HCHO + 2HO_2 - O_2) + k32a(CH_3CHO + CH_3OH + O_2)$	$R1=0.45$ $k32a = 0.5((1-k22a)+(1-R1))$	2
k33	$C_2H_5OOH + OH$	\rightarrow	$C_2H_5O_2 + H_2O$	$k33 = 2.6 \times 10^{-12} \exp(190/T)$	2
k34	$C_2H_5OOH + OH$	\rightarrow	$CH_3CHO + OH + H_2O$	$k34 = 4.5 \times 10^{-18} T^2 \exp(1069/T)$	2
k35	$C_2H_5ONO_2 + OH$	\rightarrow	$CH_3CHO + NO_2 + H_2O$	$k35 = 6.7 \times 10^{-13} \exp(-395/T)$	1
k36	$CH_3CHO + HO + O_2$	\rightarrow	$CH_3COO_2 + HO_2$	$4.4 \times 10^{-12} \exp(365/T)$	1
k37	$CH_3COO_2 + HO_2$	\rightarrow	$CH_3COOOH + O_2$	$5.2 \times 10^{-13} \exp(980/T)$	1
k38	$CH_3COO_2 + HO_2$	\rightarrow	$CH_3COOH + O_3$	$1.04 \times 10^{-13} \exp(983/T)$	2
k39	$CH_3COO_2 + NO + O_2$	\rightarrow	$CH_3O_2 + CO_2 + NO_2$	$7.5 \times 10^{-12} \exp(290/T)$	1
				$2.7 \times 10^{-28} (T/300)^{-7.1} [N_2]$	
k40	$CH_3COO_2 + NO_2 + M$	\rightarrow	$CH_3CO_3NO_2 + M$	$1.2 \times 10^{-11} (T/300)^{-0.9}$	1
				$Fc = 0.3$	
k41	$CH_3COO_2 + CH_3O_2$	\rightarrow	$HCHO + HO_2 + CH_3O_2 + CO_2$	9.9×10^{-12}	1
k42	$CH_3COO_2 + CH_3O_2$	\rightarrow	$CH_3COOH + HCHO + O_2$	1.1×10^{-12}	1
k43	$CH_3COO_2 + CH_3COO_2 + O_2$	\rightarrow	$2(CH_3O_2 + CO_2)$	$2.9 \times 10^{-12} \exp(500/T)$	1
k44	$CH_3COO_2NO_2 + OH$	\rightarrow	$HCHO + CO_2 + NO_2 + H_2O$	3×10^{-14}	1
				$4.9 \times 10^{-3} \exp(-12100/T) [N_2]$	
k45	$CH_3COO_2NO_2$	\rightarrow	$CH_3COO_2 + NO_2$	$5.4 \times 10^{16} \exp(-13830/T)$	1
				$Fc = 0.3$	
k46	$CH_3COO_2NO_2$	\rightarrow	$CH_3ONO_2 + CO_2$	$2.1 \times 10^{12} \exp(-12525/T)$	2
k47	$CH_3COO_2H + OH$	\rightarrow	$CH_3COO_2 + H_2O$	like k36	2
k48	$CH_3COOH + OH + O_2$	\rightarrow	$CH_3O_2 + CO_2 + H_2O$	$4.2 \times 10^{-14} \exp(855/T)$	1
k49	$C_3H_8 + OH + O_2$	\rightarrow	$(0.3)C_3H_7O_2prim + (0.7) C_3H_7O_2sec + H_2O$	$7.6 \times 10^{-12} \exp(-585/T)$	1
k50	$C_3H_7O_2prim + NO + O_2$	\rightarrow	$(1 - RTC3P) \times [C_2H_5CHO + HO_2 + NO_2] + RTC3P \times C_3H_7ONO_2prim$	$2.9 \times 10^{-12} \exp(350/T)$	1
k51	$C_3H_7O_2sec + NO + O_2$	\rightarrow	$(1 - RTC3S) \times [CH_3COCH_3 + HO_2 + NO_2] + RTC3S \times C_3H_7ONO_2sec$	$2.7 \times 10^{-12} \exp(360/T)$	1
k52	$C_3H_7O_2prim + HO_2$	\rightarrow	$C_3H_7OOHprim + O_2$	$k52 = 3.4 \times 10^{-15} \exp(100/T)$	1
k53	$C_3H_7O_2prim + CH_3O_2$	\rightarrow	$(1 - k32a)(C_2H_5CHO + HCHO + 2HO_2 + O_2) + k32a(C_2H_5CHOprim + CH_3OH + O_2)$	$R1=2.5 \times 10^{-13}$ $k56 = 2(R1*k25)^{0.5}$	2
k54	$C_3H_7OOHprim + OH$	\rightarrow	$C_3H_7O_2prim + H_2O$	like k33	
k55	$C_3H_7OOHprim + OH$	\rightarrow	$C_2H_5CHO prim + OH + H_2O$	like k34	
k56	$C_3H_7ONO_2prim + OH$	\rightarrow	$C_2H_5CHO prim + NO_2 + H_2O$	5.8×10^{-13}	1
k57	$C_2H_5CHO + OH$	\rightarrow	$1/2 (3CH_3COO_2 + H_2O + HO_2)$	$k57 = 5.1 \times 10^{-12} \exp(405/T)$	1
k58	$C_2H_5CHO + NO_3 + O_2$	\rightarrow	$HNO_3 + CH_3CH_2O_2 + CO$	6.5×10^{-15}	1
k59	$C_3H_7O_2sec + HO_2$	\rightarrow	$C_3H_7OOHsec + O_2$	$6.2 \times 10^{-13} \exp(-230/T)$	1
				$R1 = 5 \times 10^{-15}$	
k60	$C_3H_7O_2sec + CH_3O_2$	\rightarrow	$(1 - k60a)(CH_3COCH_3 + HCHO + 2HO_2 + O_2) + k60a(CH_3COCH_3 + CH_3OH + O_2)$	$k60a = 0.5((1-k22a) + (1-0.45))$ $k60 = 2((R1k25)^{0.5})$	2
k61	$C_3H_7OOHsec + OH$	\rightarrow	$C_3H_7O_2sec + H_2O$	like k33	2
k62	$C_3H_7OOHsec + OH$	\rightarrow	$CH_3COCH_3 + OH + H_2O$	$2.12 \times 10^{-18} * T^2 \exp(688/T)$	2
k63	$C_3H_7ONO_2sec + OH$	\rightarrow	$CH_3COCH_3 + NO_2 + H_2O$	$6.2 \times 10^{-13} \exp(-230/T)$	1
k64	$CH_3COCH_3 + OH + O_2$	\rightarrow	$CH_3COCH_2O_2 + H_2O$	$\{8.8 \times 10^{-12} \exp(-1320/T) + 1.7 \times 10^{-14} \exp(420/T)\}$	1
k65	$CH_3COCH_2O_2 + NO + O_2$	\rightarrow	$CH_3COCHO + NO_2 + HO_2$	like k50	2

k66	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{HO}_2$	\rightarrow	$\text{CH}_3\text{COCH}_2\text{OOH} + \text{O}_2$	like k52	2
k67	$\text{CH}_3\text{COCHO} + \text{OH} + \text{O}_2$	\rightarrow	$\text{CH}_3\text{COO}_2 + \text{CO} + \text{H}_2\text{O}$	1.5×10^{-11}	1
k68	$\text{CH}_3\text{COCH}_2\text{OOH} + \text{OH}$	\rightarrow	$\text{CH}_3\text{COCH}_2\text{O}_2 + \text{H}_2\text{O}$	like k33	2
k69	$\text{C}_2\text{H}_4 + \text{OH} + \text{O}_2 + \text{M}$	\rightarrow	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{M}$	$k_0=8.6 \times 10^{-29}(T/300)^{-3.1}[\text{N}_2]$ $k_\infty=9 \times 10^{-12}(T/300)^{-0.85}$ $Fc = 0.48$	1
k70	$\text{C}_2\text{H}_4 + \text{O}_3 + 2\text{O}_2$	\rightarrow	$(0.0044)\text{CHOCHO} + (1.37)\text{HCHO} + (0.43)\text{CO}$ $+ (0.26)\text{HO}_2 + (0.12)\text{OH} + (0.002)\text{H}_2\text{O}_2$ $+ (0.13)\text{H}_2 + (0.31)\text{H}_2\text{O} + (0.2)\text{CO}_2$	$9.1 \times 10^{-15}\text{exp}(-2580/T)$	1
k71	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{NO} + \text{O}_2$	\rightarrow	$(1-\text{RTC}2) \times [\text{NO}_2 + e(2\text{HCHO} + \text{HO}_2)]$ $+ f(\text{HOCH}_2\text{CHO} + \text{HO}_2) + \text{RTC}2 \times$ $\text{HOCH}_2\text{CH}_2\text{ONO}_2$	$\text{R}1 = 2.7 \times 10^{14}\text{exp}(-6350/T)$ $\text{R}2 = 6.3 \times 10^{-14}\text{exp}(-550/T)$ $e = \text{R}1/(\text{R}1 + \text{R}2 \times [\text{O}_2]), f = 1 - e$ $k71 = 9 \times 10^{-12}$	1
k72	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{HO}_2$	\rightarrow	$\text{HOCH}_2\text{CH}_2\text{OOH} + \text{O}_2$	1.2×10^{-11}	1
k73	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{CH}_3\text{O}_2$	\rightarrow	$(1 - k32a)(\text{HOCH}_2\text{CHO} + \text{HCHO} + 2\text{HO}_2 + \text{O}_2)$ $+ k32a(\text{HOCH}_2\text{CHO} + \text{CH}_3\text{OH} + \text{O}_2)$	like k32	2
k74	$\text{HOCH}_2\text{CH}_2\text{OOH} + \text{OH}$	\rightarrow	$\text{HOCH}_2\text{CH}_2\text{O}_2 + \text{H}_2\text{O}$	like k33	2
k75	$\text{HOCH}_2\text{CH}_2\text{OOH} + \text{OH}$	\rightarrow	$\text{HOCH}_2\text{CHO} + \text{OH} + \text{H}_2\text{O}$	like k34	2
k76	$\text{HOCH}_2\text{CH}_2\text{ONO}_2 + \text{OH}$	\rightarrow	$\text{HOCH}_2\text{CHO} + \text{NO}_2 + \text{H}_2\text{O}$	like k35	2
k77	$\text{HOCH}_2\text{CHO} + \text{OH}$	\rightarrow	$\text{CO}_2 + \text{HCHO}$	8.8×10^{-12}	1
k79	$\text{HOCH}_2\text{CHO} + \text{OH} + \text{O}_2$	\rightarrow	$\text{CHOCHO} + \text{HO}_2 + \text{H}_2\text{O}$	2.2×10^{-12}	1
k80	$\text{CHOCHO} + \text{OH} + \text{O}_2$	\rightarrow	$2\text{CO} + \text{HO}_2 + \text{H}_2\text{O}$	$2.8 \times 10^{-12}\text{exp}(340/T)$	3
k81	$\text{CHOCHO} + \text{NO}_3 + \text{O}_2$	\rightarrow	$\text{HNO}_3 + \text{HO}_2 + 2\text{CO}$	$1. \times 10^{-15}$	4
k82	$\text{C}_3\text{H}_6 + \text{OH} + \text{O}_2$	\rightarrow	$\text{HOC}_3\text{H}_6\text{O}_2$	$8 \times 10^{-27}(T/300)^{-3.5}[\text{N}_2]$ $3.0 \times 10^{-11}(T/300)^{-1.0}$ $Fc = 0.5$	1
k83	$\text{C}_3\text{H}_6 + \text{O}_3 + 2\text{O}_2$	\rightarrow	$0.5(\text{HCHO} + 0.15\text{CH}_3\text{COOH})$ $+ 0.71\text{CH}_3\text{O}_2 + 0.68\text{CO}$ $+ 0.54\text{OH} + 0.17\text{HO}_2) +$ $(1 - 0.35\text{RTC}3\text{P} - 0.65\text{RTC}3\text{S})$	$5.5 \times 10^{-15}\text{exp}(-1880/T)$	1
k84	$\text{HOC}_3\text{H}_6\text{O}_2 + \text{NO}$	\rightarrow	$x [\text{CH}_3\text{CHO} + \text{HCHO} + \text{HO}_2 + \text{NO}_2 + \text{O}_2] +$ $0.35\text{RTC}3\text{P} \times \text{C}_3\text{H}_7\text{ONO}_2\text{prim} + 0.65\text{RTC}3\text{S} \times$ $\text{C}_3\text{H}_7\text{ONO}_2\text{sec}$	like k30	2
k85	$\text{HOC}_3\text{H}_6\text{O}_2 + \text{HO}_2$	\rightarrow	$\text{HOC}_3\text{H}_6\text{OOH} + \text{O}_2$	like k52	2
k86	$\text{HOC}_3\text{H}_6\text{O}_2 + \text{CH}_3\text{O}_2$	\rightarrow	$(1 - k60a)(\text{CH}_3\text{CHO} + 2\text{HCHO} + 2\text{HO}_2 + \text{O}_2) +$ $k60a(\text{CH}_3\text{COCH}_2\text{OH} + \text{CH}_3\text{OH} + \text{O}_2)$	like k53	2
k87	$\text{HOC}_3\text{H}_6\text{OOH} + \text{OH}$	\rightarrow	$\text{HOC}_3\text{H}_6\text{O}_2 + \text{H}_2\text{O}$	2×10^{-11}	2
k88	$\text{C}_4\text{H}_{10} + \text{OH} + \text{O}_2$	\rightarrow	$\text{C}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	$9.1 \times 10^{-12}\text{exp}(-405/T)$ like k30	2
k89	$\text{C}_4\text{H}_9\text{O}_2 + \text{NO}$	\rightarrow	$(1 - \text{RTC}4\text{S}) \times [\text{NO}_2 + 0.67(\text{CH}_3\text{CH}_2\text{COCH}_3 +$ $\text{HO}_2) + 0.33(\text{C}_2\text{H}_5\text{O}_2 + \text{CH}_3\text{CHO} + \text{O}_2)]$ $+ \text{RTC}4\text{S} \times \text{C}_4\text{H}_9\text{ONO}_2)$	$\text{R}1=1.94 \times 10^{-22} [\text{AIR}] \text{exp}(0.9740)$ $\text{R}2=0.826(T/300)^{-8.1}$ $A=1/(1 + \log(\text{R}1/\text{R}2)^2)$ $\text{RTC}4\text{P}=0.4\text{R}1/(1+\text{R}1/\text{R}2)0.411^A$ $\text{RTC}4\text{S}=0.45*k33*R1/(1+\text{R}1/\text{R}2)0.411^A$	1
k90	$\text{C}_4\text{H}_9\text{O}_2 + \text{HO}_2$	\rightarrow	$\text{C}_4\text{H}_9\text{OOH} + \text{O}_2$	like k52	2
k91	$\text{C}_4\text{H}_9\text{O}_2 + \text{CH}_3\text{O}_2$	\rightarrow	$(1 - k60a)[\text{HCHO} + \text{HO}_2]$ $+ 0.67(\text{CH}_3\text{CH}_2\text{C}(\text{O})\text{CH}_3 + \text{HO}_2 + \text{O}_2) +$ $0.33(\text{CH}_3\text{CHO} + \text{CH}_3\text{CH}_2\text{O}_2 + \text{O}_2)]$ $+ k60a(\text{CH}_3\text{CH}_2\text{COCH}_3 + \text{CH}_3\text{OH} + \text{O}_2)$	like k60	2
k92	$\text{C}_4\text{H}_9\text{ONO}_2\text{sec} + \text{OH}$	\rightarrow	$\text{CH}_3\text{CH}_2\text{COCH}_3 + \text{NO}_2 + \text{H}_2\text{O}$	1.71×10^{-12}	2
k93	$\text{C}_4\text{H}_9\text{OOH} + \text{OH}$	\rightarrow	$\text{C}_4\text{H}_9\text{O}_2 + \text{H}_2\text{O}$	like k33	2

k94	$C_4H_9OOH + OH$	\rightarrow	$CH_3CH_2COCH_3 + OH + H_2O$	$2.12 \times 10^{-18} * T^2 \exp(1131/T)$	2
k95	$CH_3CH_2COCH_3 + OH + 0.5O_2$	\rightarrow	$CH_3CHO_2COCH_3$	$1.3 \times 10^{-12} \exp(-25/T)$	1
k96	$CH_3CHO_2COCH_3 + NO + O_2$	\rightarrow	$(1 - RTC4S) \times [CH_3CHO + CH_3COO_2 + NO_2] + RTC4S \times CH_3CHONO_2COCH_3$	like k30	2
k97	$CH_3CHO_2COCH_3 + HO_2$	\rightarrow	$CH_3CHOOHCOCH_3 + O_2$	like k52	2
k98	$CH_3CHONO_2COCH_3 + OH$	\rightarrow	$CH_3COCOCH_3 + NO_2 + H_2O$	9.20×10^{-13}	2
k99	$CH_3CHOOHCOCH_3 + OH$	\rightarrow	$CH_3CHO_2COCH_3 + H_2O$	like k33	2
k100	$CH_3CHOOHCOCH_3 + OH$	\rightarrow	$CH_3COCOCH_3 + OH + H_2O$	$2.12 * 10^{-18} * T^2 \exp(983/T)$	2
k101	$ISOPRENE + OH \rightarrow$	\rightarrow	$0.99 ISOPO_2 + 0.03 CHOCHO$	$2.7 \times 10^{-11} \exp(390/T)$ k102 = 0.45 * k30 R1 = 1.94 x 10 ⁻²² [AIR] exp(0.95*5)	1
k102	$ISOPO_2 + NO + O_2$	\rightarrow	$(1 - RTC5S) \times [HCHO + HO_2 + NO_2 + 0.64 MVK + 0.36 MACR] + RTC5S \times NITRATES$	R2 = 0.826(T/300) ^{-8.1} A = 1/(1 + log(R1/R2) ²) RTC5P = 0.4R1/(1+R1/R2)0.411 ^A RTC5S = 0.45*k30*R1/(1+R1/R2)0.411 ^A	2
k103	$ISOPO_2 + HO_2$	\rightarrow	$ISOOH + O_2$	like k52	2
k104	$ISOPO_2 + CH_3O_2 + O_2$	\rightarrow	$(1 - k60a)(2(HCHO + HO_2) + 0.64 MVK + 0.36 MACR) + k60a(0.64 MVK + 0.36 MACR + 2O_2 + HCHO + CH_3OH)$	like k60	2
k105	$ISOOH + OH$	\rightarrow	$RO_2 + H_2O$	like k85	2
k106	$ISOOH + OH + 2O_2$	\rightarrow	$ISOPO_2 + H_2O$	2×10^{-11}	2
k107	$RO_2 + NO$	\rightarrow	$HOCH_2CHO + CH_3COCHO + HO_2 + NO_2$	like k30	2
k108	$RO_2 + HO_2$	\rightarrow	$CH_3COCHO + HOCH_2CHO + H_2O$	like k52	2
k109	$NITRATES + OH + O_2$	\rightarrow	$CH_3COCHO + HOCH_2CHO + H_2O + NO_2$	R1 = 1.9 x 10 ⁻¹¹ exp(450/T) R2 = 9.5 x 10 ⁻¹² exp(504/T) k = 0.49k80 + 0.28R2 + 0.23R1	2
k110	$MVK + O_3$	\rightarrow	$0.38 CH_3COCHO + 0.2088 CH_3COO_2 + 0.26 CH_3COCO_2 + 0.26 CO + 0.0432 CH_3COOH + 0.108 CH_3CHO + 0.62 HCHO + 0.048 CO_2 + 0.54 HO_2 + 0.1008 OH + 0.048 H_2 + 0.116 H_2O$	$8.5 \times 10^{-16} \exp(-1520/T)$	2
k111	$MVK + OH$	\rightarrow	$MVKO_2$	$2.6 \times 10^{-12} \exp(610/T)$	1
k112	$MVKO_2 + NO + O_2$	\rightarrow	$CH_3COO_2 + HOCH_2CHO + NO_2$	like k30	1
k113	$MVKO_2 + HO_2$	\rightarrow	$MVKOOH + O_2$	like k52	2
k114	$MVKOOH + OH$	\rightarrow	$MVKO_2 + H_2O$	like k106	2
k115	$MVKOOH + OH + 3O_2$	\rightarrow	$CH_3COO_2 + 2CO + OH + 2HO_2 + H_2O$	R1 = 2.12 x 10 ⁻¹⁸ T ² exp(1045/T) R2 = 4.5 x 10 ⁻¹⁸ T ² exp(1032/T) k115 = R1 + R2	2
k116	$MACR + O_3 + 1.476O_2$	\rightarrow	$0.2 CH_3COCHO + 1.6 HCHO + 1.658 CO + 0.142 CO_2 + 1.116 HO_2 + 0.72 OH + 0.058 H_2O + 0.024 H_2$	$1.4 \times 10^{-15} \exp(-2100/T)$	1
k117	$MACR + OH$	\rightarrow	$MACRO_2$	$8.0 \times 10^{-12} \exp(380/T)$	1
k118	$MACRO_2 + NO + O_2$	\rightarrow	$CH_3COCH_2OH + CO + NO_2 + HO_2$	like k30	2
k119	$MACRO_2 + HO_2$	\rightarrow	$MACROOH + O_2$	like k52	2
k120	$MACROOH + OH$	\rightarrow	$MACRO_2$	like k33	2
k121	$MACROOH + OH + O_2$	\rightarrow	$CH_3COCHO + CO + 2HO_2 + OH + H_2O$	$4.5 * 10^{-18} * T^2 \exp(1032/T)$	2
k122	$MACROOH + OH$	\rightarrow	$CH_3COCH_2OH + CO + OH + H_2O$	like k57	2

k123	CH ₃ COCH ₂ OH + OH	→	CH ₃ COCHO + HO ₂ + H ₂ O 0.425 MACR + 0.18 MVK + 0.12	3.0 x 10 ⁻¹²	1
k124	ISOPRENE + O ₃	→	CH ₂ CCH ₃ COOH + 0.12 CH ₃ COCOOH + 0.84 HCHO + 0.3 CO + 0.24 CO ₂ + 0.24 HCOOH + 0.04C ₃ H ₆ + 0.34OH + 0.025H ₂ + 0.19H ₂ O	1.03 x 10 ⁻¹⁴ exp(-1995/T)	1
k125	HCOOH + OH + O ₂	→	CO ₂ + HO ₂ + H ₂ O	4.5 x 10 ⁻¹³	2
k126	C ₄ H ₁₀ + NO ₃ + O ₂	→	C ₄ H ₉ O ₂ + HNO ₃	2.8 x 10 ⁻¹² exp(-3280/T)	1
k127	HCHO + NO ₃ + O ₂	→	HNO ₃ + HO ₂ + CO	5.6 x 10 ⁻¹⁶	1
k128	CH ₃ CHO + NO ₃ + O ₂	→	HNO ₃ + CH ₃ O ₂ + CO	1.4 x 10 ⁻¹² exp(-1860/T)	1
k129	CH ₃ OH + NO ₃ + O ₂	→	HNO ₃ + HCHO + HO ₂	9.4 x 10 ⁻¹³ exp(-2650/T)	1
k130	C ₂ H ₄ + NO ₃	→	CH ₂ ONOCH ₂ OO	3.3 x 10 ⁻¹² exp(-2880/T)	1
k131	CH ₂ ONO ₂ CH ₂ OO + NO	→	2NO ₂ + 2HCHO	like k30	1
k132	CH ₂ ONO ₂ CH ₂ OO + NO	→	2NO ₂ + CH ₃ CHO + HCHO	like k30	
k133	CH ₂ ONO ₂ CH ₂ OO + HO ₂	→	CH ₂ ONO ₂ CH ₂ O ₂ H + O ₂	0.4 *3.5 x 10 ⁻¹⁵ exp(1000/T)	
k134	CH ₂ ONO ₂ CH ₂ OO + HO ₂	→	CH ₂ ONO ₂ CH ₂ O ₂ H + O ₂	0.6 *3.5 x 10 ⁻¹⁵ exp(1000/T)	
k135	CH ₂ ONO ₂ CH ₂ O ₂ H + OH	→	NO ₂ + HCHO + CO + 2HO ₂ + OH	like k34	
k136	CH ₂ ONO ₂ CH ₂ O ₂ H + OH	→	CH ₂ ONO ₂ CH ₂ OO + H ₂ O	like k33	
K137	C ₃ H ₆ + NO ₃	→	CH ₃ CHONO ₂ CH ₂ OO	4.6 x 10 ⁻¹³ exp(-1155/T)	1
k138	ISOPRENE + NO ₃	→	NITRATES	3.15 x 10 ⁻¹² exp(-450/T)	1
k139	MACR + NO ₃	→	HNO ₃ + MACRO ₂	3.4 x 10 ⁻¹⁵	1
k140	CH ₃ O ₂ + HO ₂	→	0.5CH ₂ O + 0.5CH ₃ O ₂ H	3.8 x 10 ⁻¹³ exp(780/T)	1
k141	CH ₃ COCOOH + OH	→	CH ₃ C(O)OO + CO ₂ + H ₂ O	4.9 x 10 ⁻¹⁴ exp(276/T)	7
k142	DMS + OH	→	0.995CH ₃ O ₂ + HCHO + 0.995SO ₂ + 0.005MSAg	1.13 x 10 ⁻¹¹ exp(-253/T)	1
k144	DMS + OH	→	DMSO	1.0 x 10 ⁻³⁹ [O ₂] exp(5820/T) / {1 + 5.0 x 10 ⁻³⁰ [O ₂] exp(6280/T)}	1
k144	DMS + NO ₃	→	CH ₃ O ₂ + HNO ₃ + HCHO + SO ₂	1.9 x 10 ⁻¹³ exp(520/T)	1
k145	DMSO + OH	→	MSIA	8.7 x 10 ⁻¹¹	11
k146	MSIA + OH	→	CH ₃ O ₂ + SO ₂	1. x 10 ⁻¹⁰	11
k147	DMSO	→	MSAp	1. x 10 ⁻¹⁰	11
k148	MSIA	→	MSAp	1. x 10 ⁻¹⁰	11
k149	MSAg	→	MSAp	4.5 x 10 ⁻⁵	11
k150	SO ₂ + OH	→	HO ₂ + SO ₃ + 2ACID	4.5 x 10 ⁻³¹ (T/300) ^{-3.9} [N ₂] 1.3 x 10 ⁻¹² (T/300) ^{-0.7} Fc = 0.525	1
k151	ACID + NH ₃	→	NH ₄		9
k152	NH ₃ + OH	→	NH ₂	3.5 x 10 ⁻¹² exp(-925/T)	1
k153	NH ₂ + NO	→	Products	1.6 x 10 ⁻¹¹ (T/298) ^{-1.4}	1
k154	NH ₂ + NO ₂	→	Products	2.0 x 10 ⁻¹¹ (T/298) ^{-1.3}	1
k155	NH ₂ + HO ₂	→	Products	3.4 x 10 ⁻¹¹	10
k156	NH ₂ + O ₂	→	Products	6 x 10 ⁻²¹	1
k157	NH ₂ + O ₃	→	Products	4.3 x 10 ⁻¹² exp(-930/T)	10
k158	a-PINENE + O ₃	→	TERO ₂	6.3 x 10 ⁻¹⁶ exp(-580/T)	1
k159	a-PINENE + OH	→	TERO ₂	1.2 x 10 ⁻¹¹ exp(440/T)	1
k160	a-PINENE + NO ₃	→	TERO ₂ + HNO ₃	1.2 x 10 ⁻¹² exp(490/T)	1

k161	b-PINENE + O ₃	→	TERO2 +b1*HCHO + b2*HCHO	1.5 x 10 ⁻¹⁷	5
k162	b-PINENE + OH	→	TERO ₂	2.38 x 10 ⁻¹¹ exp(357/T)	5
k163	b-PINENE + NO ₃	→	TERO ₂ + HNO ₃	1.6 x 10 ⁻¹⁰ exp(-1248/T)	5
k164	BENZENE + OH	→	0.64*(6/8)AROO ₂ + 0.36CHOCHO	2.47 x 10 ⁻¹² exp(-207/T)	6
k165	TOLUENE + O ₃	→	(7/8)*AROO ₂ + c2*MGLY	2.34 x 10 ⁻¹² exp(-6694/T)	5
k166	TOLUENE + OH	→	0.65* (7/8)AROO ₂ + 0.36CHOCHO+ c2*MGLY	5.69 x 10 ⁻¹²	5
k167	TOLUENE + NO ₃	→	(7/8)*AROO ₂ + HNO ₃	6.8 x 10 ⁻¹⁷	5
k168	XYLENE + O ₃	→	AROO2 + d2 (MGLY + 1/4C ₄ H ₉ O ₂)	(2.4 x 10 ⁻¹³ exp(-5586/T)+5.37 x 10 ⁻¹³ exp(-6039/T)+1.91 x 10 ⁻¹³ exp(-5586/T))/3	5
k169	XYLENE + OH	→	0.68AROO2 + 0.32CHOCHO + d2 (MGLY + 1/4C ₄ H ₉ O ₂)	1.72 x 10 ⁻¹¹	5
k170	XYLENE + NO ₃	→	AROO2 + HNO ₃	3.54 x 10 ⁻¹⁶	5
k171	TERO ₂ + NO + O ₂	→	[(X-a1-a2) +(X-b1-b2)]*(1 - RTC5S) *(HCHO + HO ₂ + NO ₂ + 0.64 MVK + 0.36MACR] + RTC5S * NITRATES]	like k30	
k172	TERO ₂ + HO ₂	→	[(X-a1-a2) +(X-b1-b2)]*[ISOOH + O ₂]	like k31	
k173	TERO ₂ + CH ₃ O ₂ + O ₂	→	[(X-a1-a2) +(X-b1-b2)]*(1 - k60a) (2(HCHO + HO ₂) +	like k60	
k174	TERO ₂ +TERO ₂	→	Products	like k53	
k175	AROO ₂ + NO	→	[(X-c1-c2) +(X-d1-d2)]*(1-RTC4S) *[NO ₂ + 0.67(CH ₃ CH ₂ COCH ₃ + HO ₂) + 0.33(C ₂ H ₅ O ₂ + CH ₃ CHO + O ₂) + RTC4S *C ₄ H ₉ ONO ₂)	like 30	
k176	AROO ₂ + HO ₂	→	[(X-c1-c2) +(X-d1-d2)]*[C ₄ H ₉ OOH+O ₂]	like 52	
k177	AROO ₂ + CH ₃ O ₂	→	[(X-c1-c2) +(X-d1-d2)]*(1 - k60a) [HCHO+HO ₂ +0.67(CH ₃ CH ₂ C(O)CH ₃ +HO ₂ +O ₂)	like 60	
k178	AROO ₂ + AROO ₂	→	Products	like 53	
k179	C ₂ H ₂ + OH	→	0.635(CHOCHO + OH) + 0.365(HCOOH + CO + HO ₂)	5 x 10 ⁻³⁰ (T/300) ^{-1.5} [N ₂] 1 x 10 ⁻¹² Fc=0.37	1
k180	CH ₃ COO ₂ + CH ₃ COCH ₂ O ₂	→	CH ₃ COOH + CH ₃ COCHO + O ₂	2.5 x 10 ⁻¹²	1
k181	CH ₃ COO ₂ + CH ₃ COCH ₂ O ₂	→	CH ₃ O ₂ + CH ₃ COCH ₂ OH + CO ₂	2.5 x 10 ⁻¹²	1
k182	C ₂ H ₅ O ₂ + CH ₃ COO ₂	→	C ₂ H ₅ O(CH ₃ CHO+HO ₂) + CH ₃ O ₂ + CO ₂	0.5 * 4.4 x 10 ⁻¹³ exp(1070/T)	1
k183	C ₂ H ₅ O ₂ + CH ₃ COO ₂	→	CH ₃ CHO + CH ₃ COOH + O ₂	0.5 * 4.4 x 10 ⁻¹³ exp(1070/T)	1
k184	ISOPO ₂ + NO ₃	→	HO ₂ + NO ₂ + HCHO + 0.36MACR + 0.64MVK	2.3 10 ⁻¹²	7
k185	RO ₂ + NO ₃	→	HO ₂ + HOCH ₂ CHO + CH ₃ COCHO + NO ₂	2.3 10 ⁻¹²	7
k186	TERO ₂ + NO ₃	→	HO ₂ + NO ₂ + 2(HCHO +0.36MACR + 0.64MVK)	2.3 10 ⁻¹²	7

* not explicitly accounted in the model; it is solved in the EBI code.

For three bodies reactions:

$$k = \frac{kO}{1 + \frac{kO}{k\infty}} xFc \frac{1}{1 + \log\left(\frac{kO}{k\infty}\right)^2}$$

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Table 3. Emissions used in TM4. Units are Tg(Species) y⁻¹. NOx and NH₃ are in Tg(N) y⁻¹. DMS, SO₂ and SO₄ is in Tg(S) y⁻¹

<i>Species</i>	<i>Tg y⁻¹</i>	<i>Reference</i>
NOx	53	POET 2000
NH ₃	52	EDGAR v2.0
SO ₂	90	EDGAR v2.0
SO ₄	2	EDGAR v2.0
DMS	19	Spiro. et al. (1992)
CO	1111	POET 2000
HCHO	4	POET 2000
CH ₃ OH	243	POET 2000
HCOOH	20.4 ⁽¹⁾	Kesselmeier and Staudt (1999); Keene and Galloway (1988)
C ₂ H ₆	12	POET 2000
C ₂ H ₄	17	POET 2000
C ₂ H ₂	7	EDGAR v2.0
CH ₃ COOH	9 ⁽¹⁾	Kesselmeier and Staudt (1999); Keene and Galloway (1988)
CH ₃ CHO	8	POET 2000
Carboxylic Acids (as 50% HCOOH + 50% CH ₃ COOH)	19 ⁽²⁾	EDGAR v2.0
C ₃ H ₈	12	POET 2000
CH ₃ C(O)CH ₃	27	POET 2000
C ₃ H ₆	7	POET 2000
C ₄ H ₁₀	75 ⁽³⁾	POET 2000
CH ₃ C(O)CH ₂ CH ₃	14	POET 2000
Isoprene	506 ⁽⁴⁾	POET 2000
Benzene	7	POET 2000
Toluene	14	POET 2000
Xylene	12	POET 2000
Monoterpenes (as 50% a-Pinene + 50% b- Pinene)	238	POET 2000

- (1) Natural emissions
- (2) Anthropogenic emissions
- (3) including higher alkanes
- (4) including 1Tg y⁻¹ from oceans

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