Supplementary Online Material

Air quality modelling using the Met Office Unified Model: model description and initial evaluation

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Table S1. Chemical species present in the RAQ gas phase chemistry scheme of the model.

Item	Tracer name	Species name	Advected	Dry dep.	Wetdep.	Emitted
1	O(3P)	$O(^3P)$	-	-	-	-
2	O(1D)	$O(^1D)$	-	-	-	-
3	OH	OH	-	-	-	-
4	O3	O_3	Yes	Yes	-	-
5	NO	NO	Yes	-	-	Yes
6	NO3	NO_3	Yes	-	Yes	-
7	NO2	NO_2	Yes	Yes	-	-
8	N2O5	N_2O_5	Yes	-	Yes	-
9	HO2NO2	HO_2NO_2	Yes	-	Yes	-
10	HONO2	HNO_3	Yes	Yes	Yes	-
11	H2O2	H_2O_2	Yes	Yes	Yes	-
12	CH4	CH_4	Yes	Yes	-	Yes
13	CO	CO	Yes	Yes	-	Yes
14	HCHO	HCHO (formaldehyde)	Yes	-	Yes	Yes
15	HO2	HO_2	-	-	Yes	-
16	MeOO	CH_3OO	-	-	Yes	-
17	MeOOH	CH_3OOH	Yes	Yes	Yes	-
18	EtOO	C_2H_5OO	-	-	-	-
19	C2H6	C_2H_6 (ethane)	Yes	-	-	Yes
20	MeCO3	CH_3COO_2	-	-	-	-
21	EtOOH	C_2H_5OOH	Yes	Yes	Yes	-
22	MeCHO	CH_3CHO (acetaldehyde)	Yes	-	-	Yes
23	PAN	$CH_3COO_2NO_2$ (peroxyacetyl nitrate)	Yes	Yes	-	-
24	s-BuOO	s-C_4H_9OO	-	-	-	-
25	C3H8	C_3H_8 (propane)	Yes	-	-	Yes

26	i-PrOOH	i-C_3H_7OOH	Yes	Yes	Yes	-
27	Me2CO	CH_3COCH_3 (acetone)	Yes	-	-	Yes
28	O3S	O_3 (stratospheric tracer)	Yes	Yes	-	-
29	C5H8	C_5H_8 (isoprene)	Yes	-	-	Yes
30	i-PrOO	i-C_3H_7OO	-	-	-	-
31	ISOOH	HOC_5H_8OOH	Yes	Yes	Yes	-
32	ISON	$(NO_3)C_4H_6CHO$	Yes	-	Yes	-
33	MGLY	CH_3COCHO (methyl glyoxal)	Yes	-	Yes	-
34	MVK	$CH_2CHCOCH_3$ (methyl vinyl ketone and other species lumped)	Yes	-	-	-
35	MVKOOH	$CH_3COCH(OH)CH_2OH$	Yes	Yes	Yes	-
36	MeCOCH2OO	$CH_3COCH_2O_2$	-	-	-	-
37	MEKO2	$CH_3COCH(O_2)CH_3$	-	-	-	-
38	HOC2H4O2	$HOC_2H_4O_2$	-	-	-	-
39	ORGNIT	Lumped organic nitrates	Yes	Yes	Yes	-
40	HOC3H6O2	$CH_3CHO_2CH_2OH$	-	-	-	-
41	CH3OH	CH_3OH (methanol)	Yes	-	Yes	Yes
42	OXYL1	$HOC_6H_4(CH_3)_2O_2$	-	-	-	-
43	H2	H_2	Yes	Yes	-	Yes
44	MEMALD1	$CHOCH(OH)CO_2CH_3CHO$	-	-	-	-
45	RNC2H4	$CH_2(NO_3)CHO$	Yes	-	-	-
46	HOIPO2	$HOC_5H_8O_2$	-	-	-	-
47	RNC3H6	$CH_3CH(NO_3)CHO$	Yes	-	-	-
48	HOMVKO2	$CH_3COCH(OH)CH_2O_2$	-	-	-	-
49	C2H4	C_2H_4 (ethene)	Yes	-	-	Yes
50	C3H6	C_3H_6 (propene)	Yes	-	-	Yes
51	C4H10	C_4H_{10} (butane)	Yes	-	-	Yes

52	s-BuOOH	s-C_4H_9OOH	Yes	Yes	Yes	-
53	MEK	$CH_3COC_2H_5$	Yes	-	-	-
54	TOLUENE	toluene	Yes	-	-	Yes
55	TOLP1	$HOC_6H_5CH_3O_2$	-	-	-	-
56	MEMALD	$CH_3COCHCHCHO$ (methyl maleic dialdehyde)	Yes	-	-	-
57	GLY	CHOCHO (glyoxal)	Yes	-	Yes	-
58	oXYLENE	o-xylene	Yes	-	-	Yes

Table S2. Bimolecular reactions in the RAQ mechanism.

Reaction	K (cm^3 $molecule^{-1}$ s^{-1})	Notes
$O(^1D) + H_2O \rightarrow 2\ OH$	$2.2 \cdot 10^{-10}$	Atk1
$NO + O_3 \rightarrow NO_2 + O_2$	$1.4 \cdot 10^{-12} \cdot \exp(-1310/T)$	Atk1
$NO_2 + O_3 \rightarrow NO_3 + O_2$	$1.4 \cdot 10^{-13} \cdot \exp(-2470/T)$	Atk1
$OH + O_3 \rightarrow HO_2 + O_2$	$1.7 \cdot 10^{-12} \cdot \exp(-940/T)$	Atk1
$HO_2 + O_3 \rightarrow OH + 2O_2$	$2.03 \cdot 10^{-16} \cdot (T/300)^{4.57} \cdot \exp(693/T)$	Atk1
$NO + NO_3 \rightarrow 2\ NO_2$	$1.8 \cdot 10^{-11} \cdot \exp(110/T)$	Atk1
$NO_2 + O(^3P) \rightarrow NO + O_2$	$5.5 \cdot 10^{-12} \cdot \exp(188/T)$	Atk1
$NO + HO_2 \rightarrow OH + NO_2$	$3.6 \cdot 10^{-12} \cdot \exp(270/T)$	Atk1
$NO_2 + NO_3 \rightarrow NO + NO_2 + O_2$	$4.5 \cdot 10^{-14} \cdot \exp(-1260/T)$	C97
$HO_2NO_2 + OH \rightarrow NO_2 + H_2O + O_2$	$3.2 \cdot 10^{-13} \cdot \exp(690/T)$	IUP1
$NO_3 + NO_3 \rightarrow 2\ NO_2 + O_2$	$8.5 \cdot 10^{-13} \cdot \exp(-2450/T)$	NIST
$HO_2 + OH \rightarrow H_2O + O_2$	$4.8 \cdot 10^{-11} \cdot \exp(250/T)$	Atk1
$OH + H_2O_2 \rightarrow HO_2 + H_2O$	$2.9 \cdot 10^{-12} \cdot \exp(-160/T)$	C97
$OH + H_2 + O_2 \rightarrow HO_2 + H_2O$	$5.5 \cdot 10^{-12} \cdot \exp(-2000/T)$	C97
$NO_3 + HO_2 \rightarrow HNO_3 + O_2$	$4.2 \cdot 10^{-12}$	NIST
$NO_3 + HO_2 \rightarrow OH + NO_2 + O_2$	$3.5 \cdot 10^{-12}$	NIST
$OH + CH_3OOH \rightarrow CH_3O_2 + H_2O$	$2.66 \cdot 10^{-12} \cdot \exp(200/T)$	NIST (*)
$OH + CH_3OOH \rightarrow HCHO + OH$	$1.14 \cdot 10^{-12} \cdot \exp(200/T)$	NIST
$OH + C_2H_5OOH \rightarrow C_2H_5O_2 + H_2O$	$2.66 \cdot 10^{-12} \cdot \exp(200/T)$	assumed as *
$OH + i\text{-}C_3H_7OOH \rightarrow i\text{-}C_3H_7O_2 + H_2O$	$2.66 \cdot 10^{-12} \cdot \exp(200/T)$	assumed as *
$OH + s\text{-}C_4H_9OOH \rightarrow s\text{-}C_4H_9O_2 + H_2O$	$2.66 \cdot 10^{-12} \cdot \exp(200/T)$	assumed as *
$OH + CH_4 + O_2 \rightarrow CH_3O_2 + H_2O$	$1.85 \cdot 10^{-12} \cdot \exp(-1690/T)$	Atk2
$NO + CH_3O_2 + O_2 \rightarrow HCHO + NO_2 + HO_2$	$2.3 \cdot 10^{-12} \cdot \exp(360/T)$	Atk2
$CH_3OH + OH + O_2 \rightarrow HCHO + HO_2 + H_2O$	$7.3 \cdot 10^{-12} \cdot \exp(-620/T)$	NIST
$CH_3O_2 + HO_2 \rightarrow CH_3OOH + O_2$	$4.1 \cdot 10^{-13} \cdot \exp(750/T)$	C97
$OH + HCHO + O_2 \rightarrow HO_2 + CO + H_2O$	$5.4 \cdot 10^{-12} \cdot \exp(135/T)$	Atk2
$NO_3 + HCHO \rightarrow HO_2 + CO + HNO_3$	$5.8 \cdot 10^{-16}$	C97
$OH + C_2H_6 \rightarrow C_2H_5O_2$	$6.9 \cdot 10^{-12} \cdot \exp(-1000/T)$	Atk2
$C_2H_5O_2 + NO \rightarrow CH_3CHO + NO_2 + HO_2$	$2.6 \cdot 10^{-12}$	NIST
$C_2H_5O_2 + CH_3O_2 + O_2 \rightarrow CH_3CHO + HCHO + 2\ HO_2$	$2.0 \cdot 10^{-13}$	NIST
$OH + CH_3CHO + O_2 \rightarrow CH_3COO_2 + H_2O$	$4.4 \cdot 10^{-12} \cdot \exp(365/T)$	Atk2
$CH_3COO_2 + NO + O_2 \rightarrow CH_3O_2 + NO_2 + CO_2$	$2.0 \cdot 10^{-11}$	C97
$OH + n\text{-}C_4H_{10} + O_2 \rightarrow s\text{-}C_4H_9O_2 + H_2O$	$7.9 \cdot 10^{-13} \cdot (T/300)^2 \cdot \exp(300/T)$	based on C97
$s\text{-}C_4H_9O_2 + NO \rightarrow CH_3COC_2H_5 + NO_2 + HO_2$	$2.54 \cdot 10^{-12} \cdot \exp(360/T)$	based on C97

$s\text{-}C_4H_9O_2 + CH_3O_2 + O_2 \rightarrow CH_3COC_2H_5 + 2\ HO_2 + HCHO$	$2.5 \cdot 10^{-13}$	based on C97 & NIST
$OH + CH_3COC_2H_5 + O_2 \rightarrow CH_3COCH(O_2)CH_3 + H_2O$	$1.3 \cdot 10^{-12} \cdot \exp(-25/T)$	IUP2
$C_2H_5O_2 + C_2H_5O_2 \rightarrow 2\ CH_3CHO + 2\ HO_2$	$6.4 \cdot 10^{-14}$	IUP2
$CH_3COO_2 + CH_3COO_2 + O_2 \rightarrow 2CH_3O_2 + 2\ CO_2$	$2.9 \cdot 10^{-12} \cdot \exp(500/T)$	IUP2
$OH + C_3H_8 \rightarrow i\text{-}C_3H_7O_2 + H_2O$	$7.6 \cdot 10^{-12} \cdot \exp(-585/T)$	IUP2
$i\text{-}C_3H_7O_2 + NO \rightarrow NO_2 + HO_2 + CH_3COCH_3$	$2.7 \cdot 10^{-12} \cdot \exp(360/T)$	IUP2
$CH_3COCH_2O_2 + NO \rightarrow NO_2 + HCHO + CH_3COO_2$	$2.45 \cdot 10^{-12} \cdot \exp(360/T)$	based on C99 & NIST
$CH_3COCH_2O_2 + CH_3O_2 \rightarrow HO_2 + 2\ HCHO + CH_3COO_2$	$3.8 \cdot 10^{-12}$	NIST
$i\text{-}C_3H_7O_2 + CH_3O_2 \rightarrow 2HO_2 + HCHO + CH_3COCH_3$	$4.0 \cdot 10^{-14}$	C99
$OH + PAN \rightarrow NO_3 + HCHO$	$9.5 \cdot 10^{-13} \cdot \exp(-650/T)$	NIST
$HO_2 + C_2H_5O_2 \rightarrow C_2H_5OOH + O_2$	$3.8 \cdot 10^{-13} \cdot \exp(900/T)$	IUP2
$OH + C_2H_5OOH \rightarrow CH_3CHO + OH + H_2O$	$8.0 \cdot 10^{-12}$	based on C99
$HO_2 + i\text{-}C_3H_7O_2 \rightarrow i\text{-}C_3H_7OOH + O_2$	$1.51 \cdot 10^{-13} \cdot \exp(1300/T)$	based on C99
$OH + i\text{-}C_3H_7OOH \rightarrow CH_3COCH_3 + OH + H_2O$	$1.66 \cdot 10^{-11}$	based on C99
$HO_2 + s\text{-}C_4H_9O_2 \rightarrow s\text{-}C_4H_9OOH + O_2$	$1.82 \cdot 10^{-13} \cdot \exp(1300/T)$	based on C99
$OH + s\text{-}C_4H_9OOH \rightarrow CH_3COC_2H_5 + OH + H_2O$	$2.15 \cdot 10^{-11}$	based on C99 & NIST
$NO + CH_3COCH(O_2)CH_3 \rightarrow CH_3COO_2 + NO_2 + CH_3CHO$	$2.54 \cdot 10^{-12} \cdot \exp(360/T)$	based on C97 & NIST
$CH_3O_2 + CH_3COCH(O_2)CH_3 + O_2 \rightarrow HCHO + HO_2 + CH_3CHO + CH_3COO_2$	$8.8 \cdot 10^{-13}$	based on C99
$CH_2O_2CH_2OH + NO \rightarrow 2HCHO + HO_2 + NO_2$	$9.0 \cdot 10^{-12}$	C97
$CH_3O_2 + CH_2O_2CH_2OH + O_2 \rightarrow 3HCHO + 2\ HO_2$	$2.0 \cdot 10^{-12}$	based on C97
$O_3 + C_2H_4 \rightarrow HCHO + 0.31\ CO + 0.13\ H_2 + 0.2\ HO_2 + 0.47\ HCHO$	$1.2 \cdot 10^{-14} \cdot \exp(-2630/T)$	C97
$O_3 + C_3H_6 \rightarrow HCHO + 0.3\ CH_4 + 0.4\ CO + 0.28\ OH + 0.3HO_2 + 0.58CH_3O_2 + 0.12CH_3OH + 0.6CO_2$	$2.75 \cdot 10^{-15} \cdot \exp(-1878/T)$	MCM
$O_3 + C_3H_6 \rightarrow CH_3CHO + 0.24\ H_2 + 0.58\ CO + 0.18\ HO_2$	$2.75 \cdot 10^{-15} \cdot \exp(-1878)$	MCM
$CH_3CHO_2CH_2OH + NO \rightarrow HCHO + HO_2 + CH_3CHO + NO_2$	$2.54 \cdot 10^{-12} \cdot \exp(360/T)$	based on C97
$CH_3O_2 + CH_3CHO_2CH_2OH + O_2 \rightarrow 2\ HCHO + 2\ HO_2 + CH_3CHO$	$6.0 \cdot 10^{-13}$	based on C97
$O_3 + C_5H_8 \rightarrow CH_2CHCOCH_3 + 0.78\ CO + 0.22\ HCHO + 0.27\ HO_2 + 0.27\ OH$	$7.86 \cdot 10^{-15} \cdot \exp(-1913/T)$	C99, MCM
$O_3 + CH_2CHCOCH_3 \rightarrow CH_3COCHO + 0.76\ CO + 0.24\ HCHO + 0.36\ HO_2 + 0.36\ OH$	$7.56 \cdot 10^{-16} \cdot \exp(-1521/T)$	C99
$CH_3COO_2 + HO_2 \rightarrow 0.3\ O3 + 0.8\ CH_3O_2 + 0.2\ CH_3COO_2$	$5.2 \cdot 10^{-13} \cdot \exp(980/T)$	IUP2

$HOC_5H_8O_2 + CH_3O_2 \rightarrow CH_2CHCOCH_3 + HCHO + 2\ HO_2$	$5.0 \cdot 10^{-13}$	based on C97 & MIM
$CH_3COCH(OH)CH_2O_2 + CH_3O_2 \rightarrow CH_3COCHO + HCHO + 2\ HO_2$	$2.0 \cdot 10^{-12}$	MIM
$HOC_5H_8O_2 + HO_2 \rightarrow HOC_5H_8OOH + O_2$	$2.45 \cdot 10^{-13} \cdot \exp(1250/T)$	C99
$HOC_5H_8OOH + OH \rightarrow CH_2CHCOCH_3 + HCHO + OH$	$4.2 \cdot 10^{-11}$	C99
$CH_3COCH(OH)CH_2O_2 + HO_2 \rightarrow CH_3COCH(OH)CH_2OH$	$2.23 \cdot 10^{-13} \cdot \exp(1250/T)$	C99
$CH_3COCH(OH)CH_2OH + OH \rightarrow CH_3COCHO + HCHO + OH$	$5.77 \cdot 10^{-11}$	C99
$CH_3COCHO + OH \rightarrow CH_3COO_2 + CO$	$1.72 \cdot 10^{-11}$	C99
$CHOCHO + OH \rightarrow HO_2 + 2\ CO$	$1.14 \cdot 10^{-11}$	C99
$OH + C_5H_8 + O_2 \rightarrow HOC_5H_8O_2$	$2.54 \cdot 10^{-11} \cdot \exp(410/T)$	C97, MCM
$HOC_5H_8O_2 + NO \rightarrow CH_2CHCOCH_3 + NO_2 + HCHO + HO_2$	$2.08 \cdot 10^{-12} \cdot \exp(180/T)$	based on MIM
$OH + CH_2CHCOCH_3 + O_2 \rightarrow CH_3COCH(OH)CH_2O_2$	$4.13 \cdot 10^{-12} \cdot \exp(452/T)$	based on MIM
$CH_3COCH(OH)CH_2O_2 + NO \rightarrow NO_2 + HO_2 + HCHO + CH_3COCHO$	$2.5 \cdot 10^{-12} \cdot \exp(360/T)$	MIM
$NO_3 + C_2H_6 \rightarrow C_2H_5O_2 + HNO_3$	$5.7 \cdot 10^{-12} \cdot \exp(-4426/T)$	NIST
$NO_3 + n\text{-}C_4H_{10} \rightarrow s\text{-}C_4H_9O_2 + HNO_3$	$2.8 \cdot 10^{-12} \cdot \exp(-3280/T)$	NIST
$NO_3 + C_2H_4 \rightarrow CH_2(NO_3)CHO + HO_2$	$3.3 \cdot 10^{-12} \cdot (T/300)^2 \cdot \exp(-2880/T)$	based on C97, IUP2, Atk2
$CH_2(NO_3)CHO + OH \rightarrow HCHO + NO_2 + CO_2$	$4.95 \cdot 10^{-12}$	estimated
$NO_3 + C_3H_6 \rightarrow CH_3CH(NO_3)CHO + HO_2$	$4.59 \cdot 10^{-13} \cdot \exp(-1156/T)$	Atk2, NIST
$CH_3CH(NO_3)CHO + OH \rightarrow CH_3CHO + NO_2$	$5.25 \cdot 10^{-12}$	estimated
$NO_3 + CH_3CHO \rightarrow CH_3COO_2 + HNO_3$	$1.4 \cdot 10^{-12} \cdot \exp(-1860/T)$	Atk2
$NO_3 + C_5H_8 \rightarrow (NO_3)C_4H_6CHO + HO_2$	$3.03 \cdot 10^{-12} \cdot \exp(-446/T)$	MIM, MCM
$(NO_3)C_4H_6CHO + OH \rightarrow CH_2CHCOCH_3 + NO_2$	$4.16 \cdot 10^{-11}$	based on MIM
$OH + \text{o-xylene} \rightarrow HO_2 + 0.8\ CH_3COCHCHCHO + 0.8\ CH_3COCHO$	$1.36 \cdot 10^{-11}$	MCM
$NO_2 + HOC_6H_4(CH_3)_2O_2 \rightarrow ORGNIT$	$1.0 \cdot 10^{-11}$	estimated
$OH + CH_3COCHCHCHO \rightarrow CHOCH(OH)CO_2CH_3CHO$	$5.6 \cdot 10^{-11}$	C97
$CHOCH(OH)CO_2CH_3CHO + NO \rightarrow HO_2 + NO_2 + CHOCHO + CH_3COCHO$	$2.54 \cdot 10^{-12} \cdot \exp(360/T)$	based on C97 & MIM
$OH + \text{toluene} \rightarrow HO_2 + CH_3COCHCHCHO + CHOCHO$	$1.18 \cdot 10^{-12} \cdot \exp(338/T)$	based on MCM
$OH + \text{toluene} \rightarrow HOC_6H_5CH_3O_2$	$3.6 \cdot 10^{-13}$	based on MCM
$OH + \text{o-xylene} \rightarrow HOC_6H_4(CH_3)_2O_2$	$1.36 \cdot 10^{-11}$	MCM
$OH + ORGNIT \rightarrow CH_3COCHCHCHO +$	$2.7 \cdot 10^{-12}$	estimated

$CHOCHO + NO_2$		
$NO_3 + ORGNIT \rightarrow CH_3COCHCHCHO + CHOCHO + 2\ NO_2$	$7.0 \cdot 10^{-14}$	estimated
$HOC_6H_4(CH_3)_2O_2 + HO_2 \rightarrow CH_3COCHCHCHO + CH_3COCHO$	$2.5 \cdot 10^{-13} \cdot \exp(1300/T)$	MCM
$CHOCH(OH)CO_2CH_3CHO + CH_3O_2 \rightarrow 2HO_2 + HCHO + CHOCHO + CH_3COCHO$	$1.0 \cdot 10^{-13}$	C97
$HO_2 + HOC_6H_5CH_3O_2 \rightarrow CH_3COCHCHCHO + CHOCHO + OH$	$1.0 \cdot 10^{-11}$	estimated
$NO_2 + HOC_6H_5CH_3O_2 \rightarrow ORGNIT$	$1.0 \cdot 10^{-11}$	estimated

Values of the reaction rates are based on the following references:

C97: Collins et al., 1997.

C99: Collins et al., 1999.

Atk1: Atkinson et al., ACP, 2004.

Atk2: Atkinson et al., ACP, 2006a.

IUP1: Atkinson et al., IUPAC web – O_x, HO_x, NO_x and SO_x reactions, 2006b.

IUP2: Atkinson et al., IUPAC web – Organic reactions, 2006c.

NIST: http://kinetics.nist.gov/kinetics, 2007.

MCM: http://mcm.leeds.ac.uk/MCMv3.1, 2008.

MIM (Mainz Isoprene Mechanism): von Kuhlmann and Lawrence, 2006.

For organic reactions where different product routes are possible, we used branching ratios from the Master Chemical Mechanism (MCMv3.1).

Table S3. Termolecular reactions in RAQ mechanism.

	Termolecular reactions	$k = (k_0\ [M] / (1 + k_0 [M] / k_\infty)) \times F_c^{\,n}$ $n = \{1 + (\log_{10}(k_0\ [M] / k_\infty))^2\}^{-1}$	Notes
T1.	$O(^3P) + NO\ (+ M) \rightarrow NO_2\ (+ M)$	$k_0 = 1.0 \cdot 10^{-31} \cdot (T/300)^{-1.6}$ $k_\infty = 3.0 \cdot 10^{-11} \cdot (T/300)^{0.3}$ $F_c = 0.85$	Atk1
T2.	$NO_2 + NO_3\ (+ M) \rightarrow N_2O_5\ (+ M)$	$k_0 = 3.6 \cdot 10^{-30} \cdot (T/300)^{-4.1}$ $k_\infty = 1.9 \cdot 10^{-12} \cdot (T/300)^{0.2}$ $F_c = 0.35$	Atk1
T3.	$NO_2 + OH\ (+ M) \rightarrow HNO_3\ (+ M)$	$k_0 = 3.3 \cdot 10^{-30} \cdot (T/300)^{-3.0}$ $k_\infty = 4.1 \cdot 10^{-11}$ $F_c = 0.4$	Atk1
T4.	$NO_2 + HO_2\ (+ M) \rightarrow HO_2NO_2\ (+ M)$	$k_0 = 1.8 \cdot 10^{-31} \cdot (T/300)^{-3.2}$ $k_\infty = 4.7 \cdot 10^{-12}$ $F_c = 0.6$	Atk1
T5.	$HO_2NO_2\ (+ M) \rightarrow HO_2 + NO_2\ (+ M)$	$k_0 = 4.1 \cdot 10^{-5} \cdot \exp(-10650/T)$ $k_\infty = 4.8 \cdot 10^{15} \cdot \exp(-11170/T)$ $F_c = 0.6$	Atk1
T6.	$N_2O_5\ (+ M) \rightarrow NO_2 + NO_3\ (+ M)$	$k_0 = 1.3 \cdot 10^{-3} \cdot (T/300)^{-3.5} \cdot \exp(-11000/T)$ $k_\infty = 9.7 \cdot 10^{14} \cdot (T/300)^{0.1} \cdot \exp(-11080/T)$ $F_c = 0.35$	Atk1
T7.	$CH_3COO_2 + NO_2\ (+ M) \rightarrow PAN\ (+ M)$	$k_0 = 2.7 \cdot 10^{-28} \cdot (T/300)^{-7.1}$ $k_\infty = 1.2 \cdot 10^{-11} \cdot (T/300)^{-0.9}$ $F_c = 0.3$	Atk2
T8.	$PAN\ (+ M) \rightarrow CH_3COO_2 + NO_2\ (+ M)$	$k_0 = 4.9 \cdot 10^{-3} \cdot \exp(-12100/T)$ $k_\infty = 5.4 \cdot 10^{16} \cdot \exp(-13830/T)$ $F_c = 0.3$	Atk2
T9.	$OH + C_2H_4\ (+ M) \rightarrow CH_2O_2CH_2OH\ (+ M)$	$k_0 = 8.6 \cdot 10^{-29} \cdot (T/300)^{-3.1}$ $k_\infty = 9.0 \cdot 10^{-12} \cdot (T/300)^{-0.85}$ $F_c = 0.48$	IUP2
T10.	$OH + C_3H_6\ (+ M) \rightarrow CH_3CHO_2CH_2OH\ (+ M)$	$k_0 = 8.0 \cdot 10^{-27} \cdot (T/300)^{-3.5}$ $k_\infty = 3.0 \cdot 10^{-11} \cdot (T/300)^{-1.0}$ $F_c = 0.5$	IUP2

Atk1: Atkinson et al., ACP, 2004; Atk2: Atkinson et al., ACP, 2006a; IUP2: Atkinson et al., IUPAC web – Organic reactions, 2006c.

Table S4. Complex reactions in RAQ mechanism. The overall rate *k* is used in the model for each group of complex reactions unless otherwise indicated.

	Reaction	K (cm^3 $molecule^{-1}$ s^{-1})	Notes
R1.	$O(^3P) + O_2 + M \rightarrow O_3 + M$	$k_1 = 6.0 \cdot 10^{-34} \cdot (T/300)^{-2.6}$	Atk1
		$k = k_1 \cdot [M] \cdot [O_2]$	
R6.	$O(^1D) + M \rightarrow O(^3P) + M$	$k_6 = 3.2 \cdot 10^{-11} \cdot \exp(70/T)$	C97
R7.	$O(^1D) + M \rightarrow O(^3P) + M$	$k_7 = 1.8 \cdot 10^{-11} \cdot \exp(110/T)$	
		$k = k_6 \cdot [O_2] + k_7 \cdot [N_2]$	
R50.	$OH + HNO_3 \rightarrow NO_3 + H_2O$	$k_{50} = 2.7 \cdot 10^{-17} \cdot \exp(2199/T)$	C97
R51.	$OH + HNO_3 \rightarrow NO_3 + H_2O$	$k_{51} = 6.5 \cdot 10^{-34} \cdot \exp(1335/T)$	
R35.	$OH + HNO_3 \rightarrow NO_3 + H_2O$	$k_{35} = 2.4 \cdot 10^{-14} \cdot \exp(460/T)$	
		$k = k_{35} + k_{51} \cdot [M] / (1 + k_{51} \cdot [M] / k_{50})$	
R37.	$HO_2+HO_2(+M) \rightarrow H_2O_2+O_2(+M)$	$k_{37} = 1.9 \cdot 10^{-33} \cdot \exp(980/T)$	C97
R38.	$HO_2+HO_2(+H_2O) \rightarrow H_2O_2+O_2(+H_2O)$	$k_{38} = 1.4 \cdot 10^{-21} \cdot \exp(2200/T)$	
R36.	$HO_2+HO_2(+M) \rightarrow H_2O_2+O_2(+M)$	$k_{36} = 2.2 \cdot 10^{-13} \cdot \exp(600/T)$	
		$k = (k_{36} + k_{37} \cdot [M]) \cdot (1 + k_{38} \cdot [H_2O])$	
R61.	$CH_3O_2+CH_3O_2 \rightarrow 2HCHO+2\ HO_2$	$k_{61} = 7.4 \cdot 10^{-13} \cdot \exp(-520/T)$	C97
R62.	$CH_3O_2+CH_3O_2 \rightarrow HCHO+\ CH_3OH$	$k_{62,0} = 1.03 \cdot 10^{-13} \cdot \exp(365/T)$	
		$k_{62} = k_{62,0} - k_{61}$	
		(both branches considered, with rates k_{61} & k_{62})	
R69.	$OH + CO \rightarrow HO_2 + CO_2$	$k_{69} = 3.54 \cdot 10^{-33}$ (pressure dependent term)	C97
R70.	$OH + CO \rightarrow HO_2 + CO_2$	$k_{70} = 1.5 \cdot 10^{-13}$	
		$k = k_{70} + k_{69} \cdot [M]$	
R74.	$CH_3O_2 + CH_3COO_2 \rightarrow 2\ HCHO$	$k_{74,0} = 4.4 \cdot 10^{5} \cdot \exp(-3910/T)$	C97
R80.	$CH_3O_2 + CH_3COO_2 \rightarrow HCHO + HO_2 + CH_3O_2 + CO_2$	$k_{80,0} = 1.1 \cdot 10^{-11}$	
		$k_{74} = k_{80,0} \cdot \{1 - k_{74,0} / (1 + k_{74,0})\}$	
		$k_{80} = k_{80,0} \cdot \{k_{74,0} / (1 + k_{74,0})\}$	
		(both branches considered, with rates k_{74} & k_{80})	
R89.	$CH_3COCH_3+OH \rightarrow CH_3COCH_2O_2 + H_2O$	$k_{89} = 8.8 \cdot 10^{-12} \cdot \exp(-1320/T)$	IUP2
R94.	$CH_3COCH_3+OH \rightarrow CH_3COCH_2O_2 + H_2O$	$k_{94} = 1.7 \cdot 10^{-14} \cdot \exp(423/T)$	
		$k = k_{89} + k_{94}$	

[M], [O_2], [N_2]: molecular density (in cm^{-3}) of air, O_2 and N_2, respectively.

C97: Based on Collins et al. (1997); Atk1: Atkinson et al., ACP, 2004; IUP2: Atkinson et al., IUPAC web – Organic reactions, 2006c.

Table S5. Photochemical reactions in RAQ mechanism.

J1.	$O_3 + h\nu$	→	$O(^3P)$
J2.	$O_3 + h\nu$	→	$O(^1D)$
J3.	$NO_2 + h\nu$	→	$NO + O(^3P)$
J4.	$H_2O_2 + h\nu$	→	$OH + OH$
J5.	$HNO_3 + h\nu$	→	$NO_2 + OH$
J6.	$HCHO + h\nu$	→	$CO + HO_2 + HO_2$
J7.	$HCHO + h\nu$	→	$CO + H_2$
J8.	$CH_3CHO + h\nu$	→	$CH_3O_2 + HO2 + CO$
J9.	$CH_3COC_2H_5 + h\nu$	→	$C_2H_5O_2 + CH_3COO_2$
J10.	$CH_3COCH_3 + h\nu$	→	$CH_3COO_2 + CH_3O_2$
J11.	$HO_2NO_2 + h\nu$	→	$HO_2 + NO_2$
J12.	$CH_3COCHO + h\nu$	→	$CH_3COO2 + HO2 + CO$
J13.	$CHOCHO + h\nu$	→	$HO_2 + HO_2 + CO + CO$
J14.	$NO_3 + h\nu$	→	$NO + O_2$
J15.	$NO_3 + h\nu$	→	$NO_2 + O(^3P)$
J16.	$N_2O_5 + h\nu$	→	$NO_2 + NO_3$
J17.	$CH_3OOH + h\nu$	→	$HCHO + HO_2 + OH$
J18.	$PAN + h\nu$	→	$CH_3COO_2 + NO_2$
J19.	$C_2H_5OOH + h\nu$	→	$OH + HO_2 + CH_3CHO$
J20.	$i\text{-}C_3H_7OOH + h\nu$	→	$OH + HO_2 + CH_3COCH_3$
J21.	$s\text{-}C_4H_9OOH + h\nu$	→	$OH + HO_2 + CH_3COC_2H_5$
J22.	$HOC_5H_8OOH + h\nu$	→	$OH + CH_2CHCOCH_3 + HCHO + HO_2$
J23.	$CH_3COCH(OH)CH_2OH + h\nu$	→	$OH + CH_3COCHO + HCHO + HO_2$

Table S6. Henry's Law constants for the species which undergo wet deposition in the RAQ mechanism.

Species	k_1 (M atm^{-1})	c_1 (K)	k_2 (M atm^{-1})	c_2 (K)	Reference for k_1 and c_1
NO3	2.0	2000	--	--	Sander (1999)
N2O5	2.1 x 10^5	8700	0.2000 x 10^2	--	Assumed as HNO3
HO2NO2	1.3 x 10^4	6900	0.1000 x 10^{-4}	--	Sander (1999)
HONO2	2.1 x 10^5	8700	0.2000 x 10^2	--	Sander (1999)
H2O2	8.3 x 10^4	7400	0.2400 x 10^{-11}	-3730	Sander (1999)
HCHO	3.3 x 10^3	6500	--	--	Sander (1999)
MeOO	2.0 x 10^3	6600	--	--	Sander (1999)
HO2	4.0 x 10^3	5900	0.2000 x 10^{-4}	--	Sander (1999)
MeOOH	3.1 x 10^2	5000	--	--	Sander (1999)
EtOOH	3.4 x 10^2	5700	--	--	Sander (1999)
i-PrOOH	3.4 x 10^2	5700	--	--	Assumed as EtOOH
ISOOH	1.7 x 10^6	9700	--	--	Staudinger & Roberts (1996)
ISON	3.0 x 10^3	7400	--	--	Staudinger & Roberts (1996)
MGLY	3.5 x 10^3	7200	--	--	Sander (1999)
MVKOOH	1.7 x 10^6	9700	--	--	Assumed as ISOOH
ORGNIT	1.3 x 10^2	--	--	--	Average of values in Schwarzenbach et al. (1988)
CH3OH	2.2 x 10^2	5200	--	--	Sander (1999)
s-BuOOH	3.4 x 10^2	5700	--	--	Assumed as EtOOH
GLY	3.6 x 10^5	--	--	--	Sander (1999)

Temperature dependent Henry's law coefficients are calculated as:

$$k_h = k_1 \times \exp\left[c_1 \left(\frac{1}{T} - \frac{1}{T_0} \right) \right]$$

where

T_0 = 298.15 K
T = ambient temperature (K)

This equation only accounts for physical solubility. If the species dissociates in the aqueous phase then k_h is multiplied by a second term to calculate the effective Henry's law coefficient, which also considers the effects of complex formation:

$$k_{eff} = k_h \times k_2 \times \exp\left[c_2 \left(\frac{1}{T} - \frac{1}{T_0} \right) \right]$$

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