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Supplement of

FORest Canopy Atmosphere Transfer (FORCAsT) 1.0: a 1-D model of biosphere–atmosphere chemical exchange

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Contents

Model Description

Figure S1 shows a schematic overview of the separate components of the FORCAsT canopy model, which is still driven by the routines of its predecessor, CACHE (Forkel et al., 2006). While the RACM chemistry scheme is called directly from these routines, the CACM-MPMPO scheme (and any mechanism generated via KPP, that is included in FORCAsT in the future) is accessed via an interface through which canopy conditions, emission rates and deposition velocities are passed.

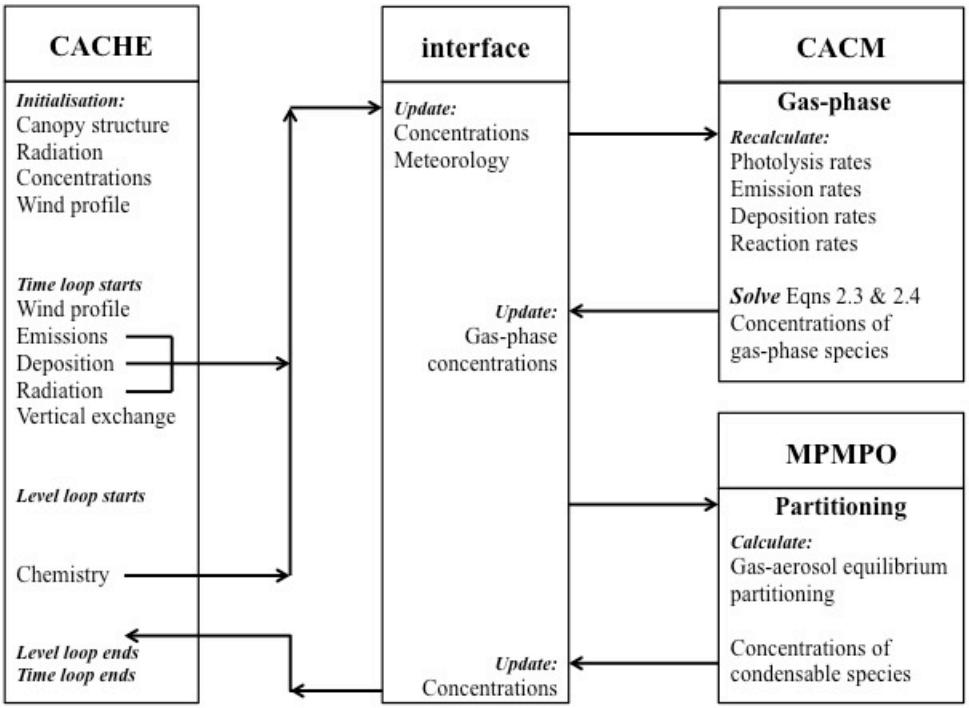

Figure S1. A schematic of the components of the FORCAsT program.

Parameter values, initial and boundary conditions for UMBS for the August 4-5, 2009 two-day simulation using 40 model layers are given below. The methodology and derivation of these are described in Bryan et al. (2012). The baseline conditions correspond to the MIM+MIX simulation in Bryan et al. (2012).

The contents and format of the output files from CACHE, RACM and CACM are also described briefly here. CACHE output files are common to all simulations and deal with canopy structure, vegetation, soil and atmospheric conditions, and energy fluxes. RACM or CACM output files are generated according to the chemistry scheme selected; only one set of these output files would be produced for a FORCAsT simulation.

The majority of the site-specific parameters and conditions required to run the FORCAsT model are set by the user via the input file, “inputn”. Some initial and boundary conditions, particularly gas-phase concentrations must be altered directly in program subroutines. Details of the user-required inputs in inputn are given first, followed by those that must be specified elsewhere in the code.

A brief overview of the CACM chemical mechanism is given in Appendix A, and the RACM mechanism in Appendix B.

Input file: inputn

Table S1 lists the variables that can be set by the user in the inputn file, and provides the values used for the two-day simulation period at UMBS described here and in Bryan et al. (2012) together with a brief description of the variable and any further relevant commentary that may aid the user.

Line	Variable Name	Value	Description and commentary
1	jday iyear	216 2009	Julian day and year at start of two-day simulation period
2	lat long std long	45.559 84.715 75.00	"std long" is solar longitude of the relevant time zone and needs to include correction for daylight saving time if applicable – here 60 for Eastern Standard Time plus 15 for daylight saving
3	ichem impmpo	0 1	Chemistry mechanism: 0=CACM, 1=RACM-MIM; MPMPO switch: 0=off, 1=on
4	hcpy htr levhtr levcpy del	22.5 6.0 8 18 0.28	Canopy height (m), trunk height (m), model level for top of trunk space, model level for top of canopy, delta setting to determine level spacings.[1]
5	tlai sizelf	3.80 0.08	Total projected LAI in canopy column (m^2 m^{-2})[2] and average length of leaf (default value 0.1)
6	df(j)	0.15 0.08 0.1 0.1 0.3 0.2 0.3 0.4 1.2 0.8	Fractional distribution of total LAI in canopy layers (default values for mixed deciduous forest: 0.15, 0.08, 0.1, 0.1, 0.3, 0.2, 0.3, 0.4, 1.2, 0.8)
7	stable	.true.	If true, it specifies a strongly stable atmospheric column in the calculation of K_H
8	vgday vgn	17. 10.	Daytime and night-time geostrophic wind speed (m s^{-1}; default value 10)
9	zrday zrn alphaday alphan	.4 .4 2. 2.	Daytime and night-time surface roughness and wind extinction coefficients (ditto) for wind profile calculation (Baldocchi, D., 1988)
10	itot clump kmax	9 1.0 3	Number of leaf angle classes, foliage clumping factor, number of radiation classes (visible, near-infrared, thermal)
11	inrad wpm2	1 0	Flag if incoming solar radiation read from file (inrad=1) or model default used (inrad=0); if radiation from file, flag whether it is in W m^{-2} (wpm2=1) or μmoles m^{-2} s^{-1} (wpm2=0)
12	ratiod ration	0.55 0.55	Daytime and night-time cloud coverage fraction (only used if inrad=0)
13	emis emisol	.95 .93	Thermal emissivity of leaves, and soil (default values .95, .93, .2)
14	rsoil(k) rleaf(k) tleaf(k)	.15 .2 .1 .2 .45 .1 .1 .3 .1	Reflectivity of soil and leaf surfaces, and transmissivity of leaf surface to each radiation type (default values for mixed deciduous forest: .2, .3, .1, .11, .37, .04, .08, .45, .0)
15	avisr bvisr cvisr anirr bnirr	0. 0. 8.16 0. 0. 41.18	Coefficients of parabola for hemispherical reflection of visible and near-infrared radiation
16	avist bvist cvist anirt bnirt	0. 0. 3.22 0. 0. 57.23	Coefficients of parabola for hemispherical transmission of visible and near-infrared radiation
17	ispher nalpha gr(i)	0 9 .07 .16 .29 .30 .18 .18 .18 .18 .18	Flag if leave angle distribution spherical (ispher=0) or other (ispher=1), number of leaf angle classes for calculation of distribution, user-specifed leaf area fraction distribution (only used if ispher=0, and imunu=0 – see below)

18	imunu xmeu xneu	1 1.101 1.930	Flag whether "xmeu" input is μ (imunu=1) or mean leaf angle (imunu=2) and "xneu" input is ν (imunu=1) or standard deviation (imunu=2) of leaf angle, μ (or mean) for leaf angle distribution calculation, ν (or s.d.) (default setting: 1; to use a specified leaf area fraction, imunu should be set to 0 – see above)
19	imunua xmeuaz xneuaz beta0 nbeta	0 180. 15. 37.62 50	As above for leaf azimuthal angle distribution calculation (imuna=0: μ and ν; imunua=2: mean and s.d.), mean, standard deviation, azimuthal angle calculation starting angle, number of angle classes for distribution
20	rcut20 rsmin anstom radn	3000. 90. 3. 100.	Response of stomatal conductance to variations in radiation: cuticular resistance, minimum stomatal conductance, …, response factor (default values for mixed deciduous forest: 3000., 120., 3., 100.)
21	trsopt trsmax trsmin rsexp rsm	30. 45. -2. 6. 5.	Response of stomatal conductance to variations in temperature: optimum, max and min temperatures, exponential response factor, …
22	psi1 psi2	-10.0 -25.0	Response of stomatal conductance to variations in leaf water potential: potential pressure at which stomata begin to close, and are fully closed (bar) (default values: -15.0, 20.0)
23	rastom d1 bkv	1. 0. 0.5	Coefficients for calculation of leaf photosynthesis: Ratio of stomatal resistance on top and bottom of leaf, vpd for start of stomatal closure (mbar), response factor for stomatal conductance to vpd variations
24	rroot	3.E6	Root resistance (m^4 kg^{-1} s^{-1})
25	aroot	2.4	Root depth coefficient
26	zs	-0.05 -0.1 -0.2 -0.4 -0.7 -1.0	Soil level depths (m)
27	rhosoil sandfc siltfc clayfc	1.14 0.32 0.35 0.33	Soil density, fractions of sand, silt and clay
28	eta	0.18 0.15 0.17 0.18 0.18 0.18 0.18 0.18 0.18 0.18 0.18 0.18 0.18 0.18 0.18	Initial volumetric soil moisture for each soil level (m^3 m^{-3})
29	temp	298.0 299.0 299.0 299.0 299.0 299.8 299.5 295.5 294.5 294.5 294.5 294.5 294.0 294.0 294.0	Initial soil temperature for each soil level (K)

Table S1. Model variables specified by the user in the "inputn" file. These variables are read into the "init" subroutine within the "main.f" source file, other than those in lines 15-19, which are read into the "cpstruct" subroutine within the "plant.f" source file. Both "init" and "cpstruct" are called solely to initialise the model settings.

[1] Not all combinations of trunk and canopy levels and spacing parameter are possible. A certain amount of trial and error is required from the user in order to reproduce the correct heights of the trunk space and crown top, as well as ensuring the top of the model domain is appropriate (i.e. between 3 and 5 km). As a last resort, the total number of model levels (nlev) could be altered to facilitate this fit.

[2] The total LAI will depend on the Julian day of the simulation and should be altered accordingly.

Emissions

FORCAsT provides the user with the opportunity to specify emission factors for isoprene, soil NO and up to 16 different individual mono- and sesquiterpenes, which can then be lumped as required for the chemistry scheme being used. The terpenoids that are currently included are: α-pinene, β-pinene, 3-Δ-carene, sabinene, myrcene, limonene, α-terpinene, β-terpinene, α-phellandrene, β-phellandrene, α-caryophellene, β-caryophellene, ocimene.

Foliar emissions calculated by FORCAsT for UMBS were limited to isoprene, cyclic monoterpenes with a single double bond (lumped as α-pinene) and cyclic diene monoterpenes (lumped as δ-limonene). This corresponds to the biogenic species included specifically in the RACM chemistry mechanism (Stockwell et al., 1997). Emission factors for each of these were calculated as described in Bryan et al. (2012) and are listed below in Table 2.

Soil emissions of nitrogen oxide were found to be high at UMBS. The emission factor for these emissions was based on measurements made at site during the CABINEX campaign (Bryan et al., 2012) and is also given in Table S2.

	ε (nmol m^{-2} s^{-1})	
Species	Synthesis	Pool
Isoprene	4.73	0.0
α-pinene	0.0	0.021
δ-limonene	0.0	0.017
NO (soil)	0.05	

Table S2. Emission factors for calculating biogenic emissions of terpenoids (Ortega et al., 2007; Ortega and Helmig, 2008) and NO (Alaghmand et al., 2011); based on flux measurement data from the PROPHET tower site at UMBS.

Site-specific pool and synthesis emission factors for isoprene and individual terpenes should be specified directly into the "sourcest" subroutine, in source file "sources.f". The lumping of these compounds into groups appropriate for the chemistry scheme being used with FORCAsT is also carried out within this subroutine, which may therefore require modification for a specific site or chemistry scheme.

Advection

It was observed during the CABINEX intensive measurement period that air masses from the south brought high levels of anthropogenic pollutants, resulting in elevated atmospheric concentrations of many species. The largest increases in mixing ratios were observed for NO_2, formaldehyde, the isoprene oxidation products methacrolein and methyl vinyl ketone (MACR-MVK), and a range of VOCs assumed to be of anthropogenic origin. The observed advection rates for the site during the simulation period are shown in Table S3. The heights within the boundary layer to which the pollutants were advected were determined by analysing HYSPLIT back-trajectories of the air masses arriving at UMBS on Aug 4^{th}-5^{th}, 2009 (Bryan et al., 2012). The model levels corresponding to these heights are also shown in Table S3.

Species	Wind direction	Advection rate (ppb h^{-1})	Model levels
NO_2	090° to 270°	0.05**U*	22 - 26
	135° to 225°	0.25**U*	22 - 26
Formaldehyde	135° to 225°	1.00**U*	22 - 26
MACR-MVK	135° to 225°	1.00**U*	22 - 26
other VOC[1]	135° to 225°	0.25**U**sf	22 - 26

Table S3. Advection rates and associated wind directions for the simulation period (Bryan et al., 2012). In each case, an effective concentration enhancement factor has been scaled by the observed wind speed (*U*, m s^{-1}) at the top of the PROPHET tower.

[1]Other VOC included in the advection scheme correspond to the RACM chemistry scheme species (Stockwell et al., 1997) HC3 (alkanes, etc with fast reaction rates with respect to the OH radical, sf=0.001), HC5 (alkanes, etc with intermediate reaction rates with respect to the OH radical, sf=1.0), OLT (alkenes with terminal double bonds, sf=0.5), OLI (alkenes with internal double bonds, sf=0.05), KET (ketones, sf=1.0) and HCHO (formaldehyde, sf=0.1).

Time and location-specific values of wind direction(s) and concentration enhancement factors should be set by the user directly into the "advect" subroutine, in source file "sources.f". The model levels to which these enhancements are applied are also specified in this routine.

Deposition

Variables required to calculate the cuticular and stomatal resistances to dry deposition are set by the user in the "inputn" input file, as described above. The boundary layer, mesophyllic and actual cuticular resistances are then calculated at each timestep and for each canopy layer based on the diffusivity, Henry's Law coefficient and the reactivity of the depositing species.

The Henry's Law coefficient (henry), ratio of molecular diffusivity relative to water (dfakt), and reactivity factor relative to ozone (f_0) for each of the chemical species included in the RACM-MIM mechanism (Stockwell et al., 1997; Geiger et al., 2003) are shown in Table S4 below.

Species	henry	dfakt	f_0
ACO3	11.4	2.0	1.0
ADDC	1.0e-22	2.3	0.0
ADDT	1.0e-22	2.2	0.0
ADDX	1.0e-22	2.3	0.0
ALD	11.4	1.6	0.0[a]
API	4.76e-3	2.6	0.0
APIP	4.76e-3	2.6	0.0
CH4	1.50E-3	0.9	0.0
CO	8.2e-3	1.2	0.0
CO2	1.86e-1	1.5	0.0
CSL	4.0e5	2.4	0.0
CSLP	1.0e-22	2.4	0.0
DCB	1.4e6	2.1	0.0
DIEN	4.76e-3	1.7	0.0
ETE	4.7e-3	1.9	0.0
ETEP	1.0e-22	1.9	0.0
ETH	2.0e-3	1.2	0.0
ETHP	1.0e-22	1.2	0.0
GLY	1.4e6	1.7	0.0
H2	1.0e-22	0.2	0.0
H2O	1.0e-22	1.0	0.0
H2O2	7.45e4	1.4	1.0
HC3	1.42e-3	1.5	0.0
HC3P	1.0e-22	1.5	0.0
HC5	1.13e-3	1.9	0.0
HC5P	1.0e-22	1.0	0.0
HC8	1.42e-3	2.4	0.0
HC8P	1.0e-22	2.5	0.0
HCHO	22970.	1.3	1.0[a]
HKET	7.80e3	2.0	0.0
HNO3	2.69e13	1.92	0.0
HNO4	2.0e13	2.14	0.0
HO	1.0e-22	1.0	1.0
HO2	1.0e-22	1.3	1.0
HONO	3.47e5	1.58	0.1
ISO	4.76e-3	1.9	0.0
ISOP	4.76e-3	1.9	0.0
KET	33.0	2.0	0.0[l]
KETP	33.0	1.9	0.0[a]
LIM	4.74e-3	2.6	0.0
LIMP	4.74e-3	2.6	0.0
MACR	11.4	1.9	1.0[a]

Species	henry	dfakt	f_0
MGLY	3.71e3	1.9	0.0
MO2	1.0e-22	1.0	0.0
N2	1.0e-22	0.9	0.0
N2O5	1.0e20	2.2	1.0
NO	1.9e-3	1.32	0.0
NO2	0.0064	1.646	0.1
NO3	15.0	1.8	1.0
O1D	1.0e-22	1.0	0.0
O2	1.0e-22	1.0	0.0
O3	0.0113	1.4	1.0
O3P	1.0e-22	1.0	0.0
OLI	1.35e-3	1.9	0.0
OLIP	1.35e-3	1.9	0.0
OLND	1.0e-22	1.5	0.0
OLNN	1.0e-22	1.5	0.0
OLT	4.76e-3	1.5	0.0
OLTP	4.76e-3	1.5	0.0
ONIT	1.13	2.5	0.0
OP1	221.	1.6	0.1
OP2	1.68e6	1.8	0.1
ORA1	9.85e6	1.6	0.0
ORA2	9.63e5	1.8	0.0
PAA	473.	2.0	0.1
PAN	2.97	2.66	0.1
PHO	1.0e-22	1.0	0.0
SO2	2.53e5	1.9	0.0
SULF	1.0e20	0.2	1.0
TCO3	1.0e-22	1.8	0.0
TOL	0.151	2.3	0.0
TOLP	1.0e-22	2.3	0.0
TPAN	2.97	2.8	0.1
UDD	1.40e6	2.5	0.0
XO2	1.0e-22	1.0	0.0
XYL	0.145	2.4	0.0
XYLP	1.0e-22	2.4	0.0
HACE[b]	1.0e-22	1.3	1.0
ISHP[b]	1.0e-22	0.0	0.0
ISON[b]	1.0e-22	0.0	0.0
MACP[b]	1.0e-22	0.0	0.0
MAHP[b]	1.0e-22	0.0	0.0
MPAN[b]	1.0e-22	0.0	0.0
NALD[b]	1.0e-22	0.0	0.0

Table S4. Values of parameters required for calculation of dry deposition rates for the 84 distinct chemical species or groups within the RACM-MIM scheme.

[a]The reactivity factors for reactive biogenic oxidation products were increased from the default values to 1.0 in line with the recommendations of Karl et al. (2010).

[b]A description of these species (introduced by Bryan et al. (2012) following the recommendation of Geiger et al. (2003) is given in Table SB1 of Appendix B).

Modifications to these values should be made by the user directly into the "sinks" subroutine, in source file "sources.f".

Turbulent exchange

Measurements of u^* and σ_w by sonic anemometers mounted at 20.6 and 36.94m, averaged from 10Hz raw data to half-hourly values by Reynolds' averaging, were used to constrain the modelled vertical profiles of eddy diffusivity within the canopy. The ratio of the transport lifetime to Lagrangian timescale (τ/T_L; TAU/TL within FORCAsT) was taken as 4.0, as adopted by Stroud et al. (2005).

Sedimentation velocity for aerosols

Effective settling velocities V_S of particles are calculated based on hourly particle size distribution data measured in the understory (VanReken et al., 2015). For each measured particle size bin i, settling velocity $V_{S,i}$ was calculated based on the midpoint particle diameter $d_{p,i}$ of each bin. Effective settling velocity is then calculated as the volume-weighted average:

$$V_s = \frac{\sum_i d_{p,i}^3 N_i V_{s,i}}{\sum_i d_{p,i}^3 N_i}$$

where N_i is the particle number concentration (m^{-3}) in size bin i.

Aerosol Liquid Water Content (ALWC)

Aerosol Liquid Water Content (ALWC) is an input to the MPMPO module and is needed to determined aerosol aqueous-phase concentrations. Hourly-mean hygroscopity parameter was κ estimated by comparing the measured CCN concentrations at 0.3% supersaturation to the particle size distribution following a method similar to Roberts et al. (2010). Wet aerosol volume was then calculated based on the particle size distribution, κ, and ambient relative humidity (VanReken et al., 2015).

Chemistry – gas-phase and aerosol initial concentrations

Initial conditions for gas-phase species are set in the cacm_Initialize.f90 file. For this UMBS case study, concentrations are based on measurements made at the PROPHET tower at UMBS at 00:00 EST on Aug 4th 2009, the start of the simulation period. The concentrations of reactive primary emissions and their oxidation products are assumed to decay exponentially with height through the boundary layer. Initial concentrations of CACM species (see Table SA1 in Appendix A for a description of the species) are calculated in cacm_Initialize.f90 for every model level, as shown in Table S5 below, and those of RACM species are similarly calculated in the chem_init subroutine within chem.f. The initial concentrations of species not listed in Table S5 are set to zero.

Species #	CACM Name	Level dependent initial concentration (ppm)[a]
1	SULF	2.8e5/(Patm/101325./((82.05746/6.0221e23)*Tair))*exp(-zlev*xx)
101	CO2	395.
103	HNO3	0.1e-3*exp(-zlev*xx)
106	CH4	1.76
112	AROH[b]	0.06e-3*exp(-zlev*xx)
113	PAN	1.0e-3*exp(-zlev*xx)
120	C2H4	1.5e-3*.1*exp(-zlev*xx)
130	N2O5	0.0e-3*.1*exp(-zlev*xx)
135	AROL[c]	0.2e-3*.1*exp(-zlev*xx)
147	SO2	154.2e-6 *exp(-zlev*xx)
155	ALKM	0.3e-3*exp(-zlev*xx)
168	H2O2	0.5e-3*exp(-zlev*xx*xx)
212	HNO3	0.1e-3*exp(-zlev*xx)
213	KETL[d]	2.5e-3*exp(-zlev*xx*xx)
251	ETOH	0.02e-3*.1*exp(-zlev*xx)
262	CO	100.0e-3

269	DLMN[e]	0.04e-3*exp(-zlev*xx)
270	HCHO	0.5e-3*exp(-zlev*xx)
271	ISO	0.2e-3*exp(-zlev*xx)
276	APIN[e]	0.04e-3*exp(-zlev*xx)
282	ALD1[f]	0.39e-3*exp(-zlev*xx)
286	MGLY	20.0e-6*exp(-zlev*xx)
287	MCR[g]	0.40e-3*exp(-zlev*xx)*0.5
292	NO2	0.834e-3*exp(-zlev*0.1*xx)
292	NO2	if(zlev.gt.20.) VAR(292)=1.048e-3*exp(-zlev*0.1*xx)
292	NO2	if(zlev.gt.34.) VAR(292)= 1.253e-3*exp(-zlev*0.1*xx)
292	NO2	if(zlev.gt.300.) VAR(292)=200.0e-6
292	NO2	if(zlev.gt.600.) VAR(292)=100.0e-6
292	NO2	if(zlev.gt.1500.) VAR(292)=50.0e-6
293	NO3	2.1e-6*exp(-zlev*xx)
295	NO	3.0e-6*exp(-zlev*0.1*xx)
297	O3	25.0e-3+zlev*.10e-3
297	O3	if(VAR(297).gt.60.e-3) VAR(297)=60.e-3
297	O3	if(zlev.gt.1150.) VAR(297)=60.e-3
300	MVK[g]	0.40e-3*exp(-zlev*xx)*0.5
Various[h]	Condensable species	4.9/MW*exp(-zlev*xx*0.125)

Table S5. Initial concentrations at midnight of August 4, 2009 at UMBS.

[a]Variable zlev indicates the mid-point height of the model layer, and xx, a height-dependent decay coefficient, is set to 0.01. Tair is the air temperature and Patm the atmospheric pressure for the model layer.
[b]The initial concentrations of AROH are based on an assumed advection rate of toluene to the site.
[c]The initial concentrations of AROL are based on an assumed advection rate of xylene to the site.
[d]The initial concentrations of KETL are based on the measured concentration of acetone at three heights within the canopy from the PROPHET tower at UMBS at the start of the simulation period.
[e]Initial concentrations of individual monoterpenes assume that the measured total monoterpene concentrations at three heights within the canopy from the PROPHET tower at UMBS at the start of the simulation period are split equally between δ-limonene and α- pinene.
[f]The initial concentrations of ALD1 are based on the measured concentration of acetaldehyde at three heights within the canopy from the PROPHET tower at UMBS at the start of the simulation period.
[g]Initial concentrations of methyl vinyl ketone and methacrolein assume an equal split of the measured MVK+MACR concentrations at three heights within the canopy from the PROPHET tower at UMBS at the start of the simulation period.
[h]List of species are given in Table S4; initial concentration profiles give total condensable of 2 μg m^{-3} at the lowest model layers.

FORCAsT output files:

Output data from all sections of the FORCAsT canopy exchange model are stored in space-delimited ASCII files. Data are output at half-hourly intervals for the entire two-day simulation period. Data represent values calculated at the mid-point height of every model level for which they are applicable. Tables S6-S8 below give a brief description of the variables stored in each output file, together with its format.

CACHE

Data from the CACHE vegetation, atmospheric dynamics and radiation calculations that are applicable to all model simulations regardless of the chosen chemistry mechanism are output directly from the FORCAsT driver via a call to the save.f subroutines. Time varying data are output at half-hourly intervals, resulting in 96 time steps for 48-hour simulations; level-dependent data are output for the appropriate model levels. CACHE output files are prefixed with "cache_". Data are written to these output files from the subroutines within save.f. Table S6 provides a description of the data contained in these output files.

Data concerning the model set-up and initial conditions are output directly to standard output (stdout), which provides a full description of the data it contains; this data can be re-directed to a run-time log file.

File name	Description of data	Format of data
cache_cpy.out[a]	Time, level, variable: leaf temperature[b], stomatal resistance[b], sunlit fraction[b], PAR extinction coefficient, sensible heat flux, latent heat flux.	2 header rows: variable, units of data; 1 row of data per canopy level for each output timestep (total: 1728 rows of 35 columns)
cache_met.out	Time, level, meteorological variable: photosynthetically active radiation (PAR), air temperature, wind speed, eddy diffusivity for heat, latent heat flux, pressure, air density, relative humidity, potential temperature.	2 header rows: variable, units of data; 1 row of data per level for each output timestep (total: 3840 rows of 11 columns)
cache_misc.out[c]	Time, solar, thermal, and net radiation at the canopy top; solar, thermal and net radiation at the soil surface, cosine zenith angle	3 header rows: level key, description, units of data; 1 row of data for each output timestep (total: 96 rows of 8 columns)

Table S6. CACHE calculated canopy and atmosphere variables output files.

[a]This output file contains only data for the crown space within the model, this currently corresponds to model levels 9-18.
[b]Values of these variables are given for each leaf angle class within each canopy level.
[c]Values of these variables are given for a single model level only.

CACM-MPMPO

Data from CACM gas-phase chemistry and MPMPO aerosol routines are output via a call to the subroutine SaveData in cacm_Util.f90 from subroutine cacm_driver in cacm_Main.f90. The gas-phase output files are pre-fixed by "cacm_"; aerosol output files are denoted by "mpmpo". These output files are all opened/created and the first of the header rows written from the FORCAsT initialisation subroutine init within main.f.

File name	Description of data	Format of data
cacm_aprd.out	Production/loss rates of condensable species (ppm s^{-1})[a] Time, level, key, budgets of 99 species	4 header rows: description, key, species number, species name; 1 row of data for each of production rate, loss rate, total budget, and gas-aerosol transfer rate[2] per level for each timestep (total: 15360 rows of 102 columns)
cacm_depn.out	Dry deposition rates of deposited species (ppm s^{-1}) Time, level, rates of 120 species	3 header rows: description, species number, species name; 1 row of data per level for each timestep (total: 3840 rows of 122 columns)
cacm_emis.out	Emission and/or advection rates of species (ppm s^{-1})	3 header rows: description, species number, species name;

	Time, level, source rates of 24 species	1 row of data per level for each timestep (total: 3840 rows of 26 columns)
cacm_gas.out	Concentration of gas-phase species (ppmv) Time, level, concentrations of 306 species	3 header rows: description, species number, species name; 1 row of data per level for each timestep (total: 3840 rows of 308 columns)
cacm_gprd.out	Production/loss rates of gas-phase species (ppm s^{-1}) Time, level, key, budgets of 34 species	4 header rows: description, key, species number, species name; 1 row of data for each of production rate, loss rate and total budget per level for each timestep (total: 11520 rows of 37 columns)
cacm_hchoprd.out	Production/loss rates of CH_2O from key species (ppm s^{-1}) Time, level, key, budgets of 21 species	4 header rows: description, key, species number, species name; 1 row of data for each of production rate, loss rate and total budget per level for each timestep (total: 11520 rows of 24 columns)
cacm_ho2prd.out	Ditto for HO_2 (ppm s^{-1}) Time, level, key, budgets of 22 species	4 header rows: description, key, species number, species name; 1 row of data for each of production rate, loss rate and total budget per level for each timestep (total: 11520 rows of 25 columns)
cacm_mvkmcrprd.out	Ditto for MVK-MCR (ppm s^{-1}) Time, level, key, budgets of 11 species	4 header rows: description, key, species number, species name; 1 row of data for each of production rate, loss rate and total budget per level for each timestep (total: 11520 rows of 24 columns)
cacm_noprd.out	Ditto for NO (ppm s^{-1}) Time, level, key, budgets of 22 species	4 header rows: description, key, species number, species name; 1 row of data for each of production rate, loss rate and total budget per level for each timestep (total: 11520 rows of 25 columns)
cacm_no2prd.out	Ditto for NO_2 (ppm s^{-1}) Time, level, key, budgets of 22 species	4 header rows: description, key, species number, species name; 1 row of data for each of production rate, loss rate and total budget per level for each timestep (total: 11520 rows of 25 columns)
cacm_ro2tprd.out	Ditto for total RO_2 (ppm s^{-1}) Time, level, key, budgets of 22 species	4 header rows: description, key, species number, species name; 1 row of data for each of production rate, loss rate and total budget per level for each timestep (total: 11520 rows of 25 columns)
cacm_no3r.out	Total reactivity of NO_3 (s^{-1}) against key co-reactants Time, level, loss rate of NO_3 against 31 species, total	3 header rows: description, co-reactant species number, species name; 1 row of data per level for each timestep (total: 3840 rows of 34 columns)
cacm_o3r.out	Total reactivity of O_3 (s^{-1}) against key co-reactants Time, level, loss rate of O_3 against 18 species, total	3 header rows: description, co-reactant species number, species name; 1 row of data per level for each timestep (total: 3840 rows of 21 columns)
cacm_ohr.out	Total reactivity of OH (s^{-1}) against key co-reactants Time, level, loss rate of OH against 77 species, total	3 header rows: description, co-reactant species number, species name; 1 row of data per level for each timestep (total: 3840 rows of 80 columns)
cacm_phot.out	Reaction rates of photolysis reactions (s^{-1}) Time, level, rates of 26 reactions	3 header rows: description, photolysed species number, species name; 1 row of data per level for each timestep (total: 3840 rows of 26 columns)
mpmpo_gas.out	Gas concentration of condensable surrogates (μg m^{-3}) Time, level, concentrations of 12 surrogates and total SOA	3 header rows: description, key, surrogate group number or name; 1 row of data for each level and timestep (total: 3840 rows of 15 columns)
mpmpo_aer.out	Aerosol concentration of condensable surrogates (μg m^{-3}) Time, level, concentrations of 12 surrogates and total SOA	3 header rows: description, key, surrogate group number or name; 1 row of data for each level and timestep (total: 3840 rows of 15 columns)
mpmpo_diff.out	Gas-to-aerosol rate of condensable surrogates (μg m^{-3} min^{-1}) Time, level, rates of 12 surrogates and total SOA	3 header rows: description, key, surrogate group number or name; 1 row of data for each gas-aerosol transfer rate[b] per level for each timestep (total: 3840 rows of 15 columns)

Table S7. CACM-MPMPO gas-phase and aerosol scheme output files.

[a]These are gas-phase production and loss rates for the chemical species later treated as condensable in the MPMPO aerosol routines.
[b]These are the variable "diff" calculated in the call_mpmpo subroutine in box_model.f90.
Note that all production and loss rates are instantaneous rates calcuated at the time of output.

RACM

Data from RACM gas-phase chemistry routines are either output directly from subroutines within chem.f or via the output routines in the FORCAsT save.f. The output files are named fort.xyy, where yy is the number designated to each species in the RACM-MIM scheme and x denotes the type of data in the file. See Table S8 below for further details of this naming convention. These output files are all opened/created as required; header rows are written via the subroutines in save.f.

File name	Description of data	Format of data
fort.1yy	Concentration of species (mole fraction) Time, concentration at each model level	1 header row: mid-point height for each model level; 1 row of data for all levels at each timestep (total: 96 rows of 41 columns)
fort.3yy	Time, budget, production rate, loss rate of species (ppm min^{-1})	1 row of data per level for each timestep (total: 3840 rows of 4 columns)
fort.6zz[a]	Reaction rate of photolysis reaction (s^{-1}) Time, rate at each model level	1 header row: mid-point height for each model level; 1 row of data for all levels at each timestep (total: 96 rows of 41 columns)
fort.933	Total reactivity of OH (ppm min^{-1}) against key co-reactants Time, total loss rate of OH	1 row of data per level for each timestep (total: 3840 rows of 2 columns)

Table S8. RACM chemistry scheme output files.

[a]These are rates for the photolysis reactions and are numbered according to reaction number (Stockwell et al., 1997) rather than species.

Code structure of FORCAsT:

The subroutines and modules within the CACHE, interface and CACM-MPMPO programs are outlined below.

CACHE: The driving program is named racmb and is located in the main.f source code file.

racmb (*main.f*)

1. **init** (*main.f*)

initialisation subroutine

Parameters read from "inputn" file;

1.1. **cpstruct** (*plant.f*)

sets up the physical canopy structure

1.1.1. **lad** (*radia.f*)

calculates leaf angle distribution

1.2. **declin** (*radia.f*)

calculates sun declination and time equation

1.3. **wprofil** (*transp.f*)

computes vertical wind profile i.e. horizontal wind speed at each level (Baldocchi)

T, p and θ profiles for each level computed;

1.4. **chem_init** (*chem.f*)

concentrations of chemical species initialized for each level

[called only if RACM chemistry selected]

parameters read from "inputn" file;

T_{leaf} and T_{soil} initialised;

soil properties for loam read in from ***f2dat*** directory;

1.5. **icsevu** (*soil.f*)

sets soil initial conditions

2a.**print-header** (*save.f*)

writes header rows to output files (.out for CACM, fort.*** for RACM)*

2b.**print-data** (*save.f*)

writes initial data as required to output files

Time loop starts

Top-of-canopy radiation (PAR) read in from fort.500 input file

3. **declin** (*radia.f*)

calculates solar time and sun declination angle for each leaf angle class

4. **zenith** (*radia.f*)

calculates sun zenith and azimuth angles for each leaf angle class

5. **dstlit** (*radia.f*)

calculates distribution of leaf-normal angle for each leaf angle class

6. **radin4** (*radia.f*) for coszen > 0.01

calculates fraction of diffuse/direct PAR and NIR from total solar radiation

[called only during daylight hours, i.e. if coszen > 0.01]

7. **difint** (*radia.f*)

calculates interception factors for diffuse radiation in each canopy layer

8. **skyir** (*radia.f*)

calculates incoming thermal radiation

9. **radiat** (*radia.f*)

calculates back-scattered, up-welling and down-welling radiation in each canopy layer

calculates sunlit and shaded fractions of leaf area for each leaf angle class

10. **stoma** (*plant.f*)
calculates combined stomatal and cuticular resistance for each leaf angle class for each canopy layer
11. **lfebal** (*plant.f*)
performs an energy balance for each leaf angle class for each canopy layer
calculates evaporation, transpiration and leaf temperature
12. **rootex** (*plant.f*)
calculates the potential water extraction for each soil layer
13. **stress** (*plant.f*)
calculates leaf water potential for each leaf angle class for each canopy layer

Wind speed (U) read in from fort.5034 input file

Friction velocity (u^*) read in from fort.5081 and fort.5082 input files

Vertical wind deviation (σ_w) read in from fort.5091 and fort.5092 input files

14. **wprofil** (*transp.f*)
computes vertical wind profile i.e. horizontal wind speed at each level (Baldocchi,1988)
15. **atk** (*transp.f*)
calculates vertical exchange coefficients K_H and K_M
16. **sourcest** (*sources.f*)
calculates biogenic VOC and soil emission rates for each canopy level (Steinbrecher et al.,)
17. **sinks** (*sources.f*)
calculates sink rates due to dry deposition for all RACM species (Baldocchi, et al., Gao et al., 1993)
18. **advection** (*sources.f*)
calculates species advection rates to/from the site due to long-range transport of air mass

Sedimentation velocity (V_s) read in from fort.5093 input file

19. **newc** (*transp.f*)
calculates new concentrations of all chemical species at all levels due to vertical mixing
uses an implicit method to solve the partial differential equations required in calculation of mixing
20. **newt** (*transp.f*)
calculates new air temperature at all levels due to vertical mixing
uses an implicit method to solve the partial differential equations required in calculation of mixing

Level loop starts

21. **CHEMISTRY** – user can select the scheme to be used

A. CACM

21A **boxmodel** (*box_model.f90*)
the CACHE-*CACM interface module*

21A.1 **CACM_driver** *(cacm_Main.f90)*
simulates gas-phase chemistry, emission, deposition, and advection using Rosenbrock solver;
interfaces to subroutines generated by KPP.

21A.1.1 **Initialize** (*cacm_Initialize.f90*)
initialises concentrations of main gas-phase species

Start of iteration time loop for solver

21A.1.2 **GetMass** (*cacm_Initialize.f90*)
calculates mass of atoms selected for tracking (currently none are selected)

21A.1.3 **Update_SUN** (*cacm_Rates.f90*)
updates photolysis solar time correction factor

21A.1.4 **Update_RCONST** (*cacm_Rates.f90*)
updates reaction rate coefficients for all chemical reactions for current conditions

21A.1.5 **Integrate** (*cacm_Integrator.f90*)
iterative solution of mass balance equations for all variable gas-phase species

21A.1.5.1 **Rosenbrock** (*cacm_Integrator.f90*)

driver for the solution of mass balance equations using selected method

21A.1.5.1.1 **Rosx** (*cacm_Integrator.f90*)

initializes coefficients required by the selected Rosenbrock method (x)

21A.1.5.1.2 **ros_Integrator** (*cacm_Integrator.f90*)

solution of mass balance equations

21A.1.5.1.2.1 **FunTemplate** (*cacm_Integrator.f90*)

template to call ODE function

21A.1.5.1.2.1.1 **Update_SUN** (*cacm_Rates.f90*)

updates photolysis solar time correction factor

21A.1.5.1.2.1.2 **Update_RCONST** (*cacm_Rates.f90*)

updates reaction rate coefficients

21A.1.5.1.2.1.3 **Fun** (*cacm_Function.f90*)

updates reaction rates and time derivatives of gas-phase concentrations

21A.1.5.1.2.2 **ros_FunTimeDerivative** (*cacm_Integrator.f90*)

driver to calculate partial derivatives of concentrations

21A.1.5.1.2.2.1 **FunTemplate** (*cacm_Rates.f90*)

see above

21A.1.5.1.2.3 **JacTemplate** (*cacm_Integrator.f90*)

driver to call ODE Jacobian function

21A.1.5.1.2.1.1 **Update_SUN** (*cacm_Rates.f90*)

updates photolysis solar time correction factor

21A.1.5.1.2.1.2 **Update_RCONST** (*cacm_Rates.f90*)

updates reaction rate coefficients

21A.1.5.1.2.1.3 **JacSP** (*cacm_Jacobian.f90*)

creates sparse matrix formulation of Jacobian variables

21A.1.5.1.2.4 **ros_PrepareMatrix** (*cacm_Integrator.f90*)

prepares the triangular matrix of linear equations

21A.1.5.1.2.4.1 **ros_Decomp** (cacm_Rates.f90)

21A.1.5.1.2.5 **ros_Solve** (*cacm_Integrator.f90*)

solves the resulting matrix by back and forward substitution

End of iteration time loop for solver

21A.1.6 **GetMass** (*cacm_Util.f90*)

updates mass of atoms selected for tracking (currently none are selected)

21A.1.7 **InitSaveData** (*cacm_Initialize.f90*)

writes header rows to cacm_*.out gas-phase output files
writes header rows to mpmpo_*.out aerosol-phase output files
[only called on first call to CACM_driver]

21A.1.8 **SaveData** (*cacm_Util.f90*)

writes data to cacm_*.out gas-phase output files

21A.2 **call_mpmpo** *(box_model.f90)*

maps 99 condensible species to 12 surrogate groups

21A.2.1 **MAIN_MPMPO** *(soa_main_mpmpo.f)*

calculate initial UNIFAC and ZSR parameters

21A.2.1.1 **MPMPO** (*mode_oamain.f*)

calculates gas-aerosol partitining

21A.2.1.1.1 **VP_GET** (*mode_soatinit.f*)

calculates T-dependent saturation vapor pressure for surrogate groups

21A.2.1.1.2 **AQCONST_GET** (*mode_soatinit.f*)

calculates T-dependent Henry's Law and dissociation constants for surrogate groups

21A.2.1.1.3 **SI_GET** (*mode_soatinit.f*)

calculates T-dependent term in UNIFAC parameterization

21A.2.1.1.4 **SOAEQL** (*mode_soaeql.f*)

calculate gas- and aerosol-phase equilibrim concentrations for surrogate groups

21A.2.1.1.5 **ZSRPUN** (*mode_zsrpun.f*)

calculates water content in organic aerosol phase using ZSR

writes data to mpmpo_*.out aerosol-phase output files

B. RACM

21B.1 **photrat** (*chem.f*)

updates photolysis frequencies based on current zenith angle

21B.2 **racmh** (*chem.f*)

calculates the atmospheric concentrations of all chemical species

21B.2.1. **chem** (*chem.f*)

calculates chemical (thermal) reaction rate constants for each chemical reaction

21B.2.2. **crjk** (*chem.f*)

calculates updated photolysis and thermal reaction rates for each reaction for each iteration

21B.2.3. **newrap_noxox** (*chem.f*)

explicit solution (using Newton-Raphson iteration following Hertel) of mass balance equations for the strongly coupled NO_x and O_x species grouped in Hertel: NO, NO_2, O_3, O^3P and O^1D

21B.2.5.1. **noxox** (*chem.f*)

calculates production and loss rates of the NO_x and O_x species

21B.2.5.2. **ludcmp** (*chem.f*)

applies LU decomposition to the matrix of mass balance equations

21B.2.5.3. **lubksb** (*chem.f*)

applies back-substitution of the resulting triangular matrix to solve the mass balance equations

21B.2.4. **newrap_hoxhnox** (*chem.f*)

explicit solution (using Newton-Raphson iteration following Hertel) of mass balance equations for the strongly coupled HO_x and HO_xNO_x species grouped in Hertel: HO, HO_2, HONO and HNO_4

21B.2.6.1. **hoxhnox** (*chem.f*)

calculates production and loss rates of the HO_x and HO_xNO_x species

21B.2.6.2. **ludcmp** (*chem.f*)

applies LU decomposition to the matrix of mass balance equations

21B.2.6.3. **lubksb** (*chem.f*)

applies back-substitution of the resulting triangular matrix to solve the mass balance equations

21B.2.5. **prodloss** (*chem.f*)

calculates production and loss rates of the remaining species

Level loop ends

22. **erdbod** (*soil.f*)

calculates temperature and water content in each soil layer

22.1. **wert** (*soil.f*)

calculates soil properties at each soil level boundary

22.1.1. **icsevu** (*soil.f*)

iterative calls to cubic spline interpolation

22.1.2. **dcsevu** (*soil.f*)

iterative calls to cubic spline interpolation

22.2. **solveb** (*soil.f*)

solves tridiagonal system of equations through simplified Gaussian elimination

23. **grenzn** (*soil.f*)

calculates fluxes of energy and water from the soil surface to the lowest model level

23.1. **icsevu** (*soil.f*)

cubic spline interpolation

23.2. **dcsevu** (*soil.f*)

cubic spline interpolation

24.**print-data** (*save.f*)

called from main.f

writes CACHE and RACM data as required to output files

Time loop ends

Appendix A

CACM chemistry mechanism

Table SA1 lists the 300 gas-phase species included in the CACM chemistry scheme by the species number, name by which they are referred to in the model code, a full name (or brief description for lumped species) and the name by which they were previously identified by Griffin et al. (2002) and Chen et al. (2005). In addition to the 300 variable species, CACM treats oxygen (species number 302) and water vapour (species number 303) as species with fixed concentrations.

Table SA1. The gas-phase variable species included in the CACM mechanism. The third column of the table gives the name assigned to the species in the original description of the CACM model (Griffin et al., 2002).

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
1	H2SO4	H2SO4	sulfuric acid
2	NH3	NH3	ammonia
3	AP1401	AP3	3-methyl-4-heptylnitrate
4	AP1402	AP2	2-methyl-2-hydroxy-5-heptylnitrate
5	UR1401	UR16	2-methyl-2-hydroxy-5-heptanone
6	AP1501	AP11	8-hexadecylnitrate
7	AP1502	AP12	8-hydroxy-11-hexadecylnitrate
8	UR1501	UR20	11-hydroxy-8-hexadecanone
9	UR2301	UR1	3-methyl-heptanoic acid
10	ACID	ACID	lumped organic acids < C6
11	UR6201	UR21	keto-propanoic acid
12	UR6301	UR28	oxalic acid
13	AP7101	AP4	1, 2-dimethyl-3-nitrooxymethyl-benzene
14	UR7101	UR12	1, 2, 3-trimethyl-5-nitro-benzene
15	UR7102	UR26	4,5-dimethyl-6-keto-2,4-heptadienoic acid
16	UR7103	UR24	maleic anhydride
17	UR7104	UR25	3H-furan-2-one
18	UR7201	UR13	3-n-propyl-4-nitro-toluene
19	AP7301	AP1	2-nitrooxymethyl-6-methyl-phenol
20	UR7301	UR22	2,6-dimethyl-3,4-dinitro-phenol
21	UR7302	UR2	3-hydroxy-4-methyl-benzoic acid
22	UR7303	UR29	4-hydroxy-3, 5-dimethyl-2, 4-hexadiendioic acid
23	UR7401	UR14	2-nitro-4-methyl-benzoic acid
24	UR7402	UR30	2-methyl-5-carboxy-2, 4-hexadiendioic acid
25	AP7401	AP5	4-nitrooxymethyl-benzaldehyde
26	AP7501	AP6	4-nitrooxymethyl-benzoic acid
27	UR7601	UR11	1, 2-dimethyl-3-hydroxy-naphthalene
28	UR7602	UR15	1, 2-dimethyl-3-nitro-naphthalene
29	UR7603	UR19	1-methyl-2-formyl-naphthalene
30	UR7604	UR27	2-carboxy-acetophenone
31	UR7605	UR31	2-(dimethyl-propenoic acid)-benzoic acid
32	AP7601	AP10	1-methyl-2-nitrooxymethyl-naphthalene

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
33	AP8101	AP101[b]	2-nitrato-3-hydroxy-pinane
34	AP8102	AP102[b]	2-nitrato-3-oxo-pinane
35	AP8103	AP103[b]	2,2-dimethyl-3-acetyl-cyclobutyl-methyl-nitrate
36	AP8104	AP104[b]	2,2-dimethyl-3-acetyl-cyclobutyl-nitrate
37	UR8103	UR103[b]	2,3-pinane-epoxide
38	UR8107	UR107[b]	2,3-dihydroxy-pinane
39	UR8108	UR108[b]	2-(2,2-dimethyl-3-formylmethyl-cyclobutyl)-2-keto-acetaldehyde
40	AERS12[c]	-	phthalic acid
41	UR8101	UR101[b]	pinonic acid
42	UR8102	UR102[b]	norpinonic acid
43	UR8104	UR104[b]	pinic acid
44	UR8105	UR105[b]	10-hydroxy-pinonic acid
45	UR8106	UR106[b]	1-hydroxy-pinonic acid
46	AP8201	AP201[b]	2-nitrato-10-hydroxy-pinane
47	AP8202	AP202[b]	2-formyl-2-nitrato-6-dimethyl-norpinane
48	UR8201	UR201[b]	2,10-pinane-epoxide
49	UR8202	UR202[b]	2,10-hydroxy-pinane
50	UR8203	UR203[b]	2,10-dinitrato-pinane
51	UR8204	UR204[b]	3-hydroxy-nopinone
52	UR8205	UR205[b]	3-oxo-nopinone
53	AP8305	AP305[b]	2-isopropenyl-5-keto-hexylnitrate
54	AP8306	AP306[b]	1-hydroxy-2-methyl-2-nitrato-3-formylmethyl-6-keto-heptane
55	AP8307	AP307[b]	2-methyl-2-nitrato-3-formylmethyl-6-keto-heptanal
56	AP8308	AP308[b]	1-methyl-1-nitrato-2-hydroxy-4-acetyl-cyclohexane
57	AP8309	AP309[b]	1-methyl-1-nitrato-2-keto-4-acetyl-cyclohexane
58	AP8310	AP310[b]	2-acetyl-5-keto-hexylnitrate
59	UR8301	UR301[b]	limononic acid
60	UR8302	UR302[b]	1-methyl-4-isopropenyl-1,2-cyclohexane-epoxide
61	UR8303	UR303[b]	3-isopropenyl-6-methyl-cyclohexanone
62	UR8304	UR304[b]	keto-limononic acid
63	UR8305	UR305[b]	1-methyl-4-acetyl-1,2-cyclohexane-epoxide
64	UR8306	UR306[b]	3-acetyl-6-methyl-cyclohexanone
65	UR8307	UR307[b]	7-hydroxy-limononic acid
66	UR8308	UR308[b]	limonalic acid
67	UR8309	UR309[b]	limonic acid
68	UR8310	UR310[b]	7-hydroxy-keto-limononic acid
69	UR8311	UR311[b]	keto-limonalic acid
70	UR8312	UR312[b]	keto-limonic acid
71	UR8313	UR313[b]	1-methyl-1,2-dihydroxy-4-isopropenyl-cyclohexane
72	UR8314	UR314[b]	1-methyl-4-(1-methyl-1,2-dihydroxy-ethyl)-cyclohexene
73	UR8315	UR315[b]	5-keto-limonaldehyde
74	UR8316	UR316[b]	5-hydroxy-limonaldehyde
75	UR8317	UR317[b]	3-(1-methyl-1,2-dihydroxy-ethyl)-6-keto-heptanal

Table SA1. *Continued*

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
76	UR8318	UR318[b]	3-acetyl-3-hydroxy-6-keto-heptanal
77	UR8319	UR319[b]	3-acetyl-5-hydroxy-6-keto-heptanal
78	UR8320	UR320[b]	1-methyl-1,2-dihydroxy-4-acetyl-cyclohexane
79	UR8321	UR321[b]	3-hydroxymethyl-2,6-heptanedione
80	UR8322	UR322[b]	3-formyl-2,6-heptanedione
81	UR8323	UR323[b]	3-acetyl-5,6-dioxo-heptanal
82	UR8324	UR324[b]	3-acetyl-4-formyl-butanoic acid
83	AP6101	-	isoprene nitrate formed from OH+isoprene-derived peroxy radical
84	UR8401	UR3	2-hydroxy-3-isopropyl-6-keto-heptanoic acid
85	UR8402	UR4	2-isopropyl-5-keto-hexanal
86	UR8403	UR5	1-methyl-3-hydroxy-4-isopropyl-1, 2-cyclohexane epoxide
87	UR8404	UR6	2-hydroxy-3-isopropyl-6-methyl-cyclohexanone
88	UR8405	UR17	2-hydroxy-3-isopropyl-hexadial
89	UR8501	UR7	3, 7-dimethyl-6-keto-3-octenal
90	UR8502	UR8	3-isopropyl-6-keto-3-heptenoic acid
91	UR8503	UR9	1-methyl-4-isopropyl-1, 2-cyclo-4-hexene epoxide
92	UR8504	UR10	3-isopropyl-6-methyl-3-cyclohexenone
93	UR8505	UR18	3-isopropyl-2-pentendial
94	UR8506	UR23	3-isopropyl-4-hydroxy-2-butenoic acid
95	AP6102	-	isoprene nitrate formed from isoprene-derived peroxy radical cross reactions
96	AP8502	AP9	5-isopropyl-6-nitrato-4-hexen-2-one
97	AS3PD	S3PD	3-hydroxy-2, 4-dimethyl-2, 4-hexadienalic acid
98	AS5PD	S5PD	2-hydroxyl-3-isopropyl-6-keto-heptanoic acid
99	AS7PD	S7PD	3, 5-dimethyl-1, 4-dibenzoic acid
100	AS10PD	S10PD	1-methyl-1-hydroxy-2-nitrato-3-oxo-4-isopropyl-cyclohexane
101	CO2	CO2	CO_2
102	ADAC	ADAC	lumped aromatic diacids (terephthalic acid)
103	SO2	SO2	SO_2
104	OSD	OSD	O^1D
105	RAD7303	RAD8	radical from NO_3 oxidation of RPR7301
106	CH4	CH4	methane
107	C2H6[c]	-	ethane
108	MTBE	MTBE	methyl-tert-butyl ether
109	ALKH	ALKH	lumped alkanes > C12 (n-hexadecane)
110	MEOH	MEOH	methanol
111	ALCH	ALCH	lumped higher alcohols (2-hexanol)
112	AROH	AROH	lumped high SOA yield aromatic species (3-n-propyl-toluene)
113	PAN2301	PAN7	peroxy 3-methyl-heptionyl nitrate
114	PAN3201	PAN2	peroxy acetyl nitrate (PAN)
115	PAN8301	PAN301[b]	peroxy 5-formyl-4-isopropenyl-pentionyl nitrate
116	PAN8302	PAN302[b]	peroxy 5-formyl-4-acetyl-pentionyl nitrate
117	PAN3301	PAN1	peroxy pentionyl nitrate

Table SA1. *Continued*

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
118	PAN8401	PAN8	peroxy 2-hydroxy-3-isopropyl-6-keto-heptionyl nitrate
119	PAH	PAH	lumped gas-phase polycyclic aromatic hydrocarbons (1,2-dimethyl-naphthalene)
120	ETOH	ETOH	ethanol
121	RP7304	RP17	4-hydroxy-3, 5-dimethyl-2, 4-hexadienalic acid
122	RAD7301	RAD1	radical from NO_3 oxidation of AROO
123	RP7406	RP18	2-methyl-5-formyl-2, 4-hexadiendioic acid
124	RAD7201	RAD4	hexadienyl radical from OH oxidation of AROH
125	RAD7601	RAD7	hexadienyl radical from OH oxidation of PAH
126	RP7603	RP19	2-(dimethyl-propenal)-benzoic acid
127	PAN8101	PAN101[b]	peroxy 2,2-dimethyl-3-acetyl-cyclobutyl-acetyl-nitrate
128	PAN8102	PAN102[b]	peroxy 2,2-dimethyl-3-acetyl-cyclobutyl-formyl-nitrate
129	PAN8103	PAN103[b]	peroxy 2,2-dimethyl-3-formylmethyl-cyclobutyl-formyl-nitrate
130	N2O5	N2O5	nitrogen pentoxide
131	PAN6101	PAN3	unsaturated peroxy propionyl nitrate (PPN)
132	PAN6301	PAN5	methylene-PPN
133	PAN6302	PAN6	peroxy nitrate derived from glyoxal
134	PAN6303	PN10	peroxy nitrate derived from glyoxalic acid
135	AROL	AROL	lumped low SOA yield aromatic species (1,2,3-trimethyl-benzene)
136	RAD7101	RAD3	hexadienyl radical from OH oxidation of AROL
137	PAN8501	PAN9	peroxy 3-isopropyl-4-hydroxy-2-butenionyl nitrate
138	PAN7101	PAN4	keto-PPN
139	AP8301	AP301[b]	1-methyl-1-nitrato-2-hydroxy-4-isopropenyl-cyclohexane
140	AP8304	AP304[b]	2-methyl-2-nitrato-2-(4-methyl-4-cyclohexenyl)-acetaldehyde
141	RAD7501	RAD6	hexadienyl radical from OH oxidation of ARAC
142	HNO4	HNO4	pernitric acid
143	RP8101	RP101[b]	pinalic-3-acid
144	RP8102	RP102[b]	1-hydroxy-pinonaldehyde
145	RP8103	RP103[b]	10-hydroxy-pinonaldehyde
146	RPR7401	RPR5	2-nitro-4-methyl-benzaldehyde
147	HONO	HONO	nitrous acid
148	RAD7302	RAD2	hexadienyl radical from OH oxidation of AROO
149	AP8302	AP302[b]	1-methyl-4-(1-methyl-1-nitrato-2-hydroxy-ethyl)-cyclohexene
150	AP8303	AP303[b]	1-methyl-1-nitrato-2-keto-4-isopropenyl-cyclohexane
151	RPR7301	RPR4	2,6-dimethyl-4-nitro-phenol
152	RP7601	RP14	2-(dimethyl-propenal)-benzaldehyde
153	RP7602	RP15	2-formyl-acetophenone
154	RPR7303	RPR9	4-hydroxy-3, 5-dimethyl-2, 4-hexadiendial
155	ALKM	ALKM	lumped alkanes C7-C12 (3,5-dimethyl-heptane)
156	RO27601	RO231	aromatic peroxy radical from side chain oxidation of PAH
157	RO21502	RO241	hydroxy alkyl peroxy radical from oxidation of ALKH (8-hydroxy, 11-peroxy)

Table SA1. *Continued*

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
158	AROO	AROO	lumped phenolic species (2,6-dimethyl-phenol)
159	RAD7401	RAD5	hexadienyl radical from OH oxidation of ARAL
160	ARAC	ARAC	lumped aromatic monoacids (p-toluic acid)
161	RPR7302	RPR2	3-hydroxy-4-methyl-benzaldehyde
162	RPR7404	RPR7	4-formyl-benzoic acid
163	RPR7402	RPR6	benzene-1, 4-dialdehyde
164	RP7405	RP13	2-carboxyl-5-methyl-2, 4-hexadiendial
165	RP7403	RP12	2-methyl-5-formyl-2, 4-hexadiendial
166	RP7101	RP11	4, 5-dimethyl-6-keto-2, 4-heptadienal
167	RP7102	RP10	2-methyl-butenalic acid
168	H2O2	H2O2	H_2O_2
169	RO28501	RO227	cyclic hydroxy alkenyl peroxy radical from oxidation of BIOH (C6 cycle, 1-methyl, 1-ene, 4-peroxy, 4-isopropyl, 5-hydroxy)
170	RO28502	RO228	cyclic nitrato alkenyl peroxy radical from oxidation of BIOH
171	RO27101	RO221	aromatic peroxy radical from side chain oxidation of AROL
172	RO21201[c]	-	ethyl peroxy radical from oxidation of C_2H_6
173	RO21402	RO218	branched hydroxy alkyl peroxy radical > C6 from oxidation of OLEH and ALKM (C7 chain, 2-methyl, 2-hydroxy, 5-peroxy)
174	RO27303	RO242	bicyclic peroxy radical from the O_2 bridging in RO7302
175	RO27202	RO244	bicyclic peroxy radical from the O_2 bridging in RO27201
176	RO27403	RO245	bicyclic peroxy radical from the O_2 bridging in RO27402
177	RO27103	RO243	bicyclic peroxy radical from the O_2 bridging in RO27102
178	RO27503	RO246	bicyclic peroxy radical from the O_2 bridging in RO27502
179	RO21501	RO232	alkyl peroxy radical from oxidation of ALKH (8-peroxy)
180	RP8302	RP302[b]	3,6-dioxo-heptanal
181	RP8303	RP303[b]	3-acetyl-pentadial
182	RO28301	RO2301[b]	cyclic hydroxy alkenyl peroxy radical from oxidation of δ-limonene (C6 cycle, 1-methyl, 1-peroxy, 2-hydroxy, 4-isopropenyl)
183	RO28309	RO2309[b]	acyl radical from decomposition of RO28306
184	RO28313	RO2313[b]	cyclic hydroxy alkyl peroxy radical from oxidation of limona ketone (C6 cycle, 1-methyl, 1-peroxy, 2-hydroxy, 4-acetyl)
185	RO28318	RO2318[b]	acyl radical from decomposition of RO28317
186	RO28401	RO224	cyclic dihydroxy alkyl peroxy radical from OH oxidation of BIOL (C6 cycle, 1-methyl, 1-peroxy, 2, 3-dihydroxy, 4-isopropyl)
187	RO28402	RO225	cyclic hydroxy nitrato alkyl peroxy radical from NO_3 oxidation of BIOL (C6 cycle, 1-methyl, 1-peroxy, 2-nitrato, 3-hydroxy, 4-isopropyl)
188	RO22102	RO23	nitrato alkyl peroxy radical < C6 from oxidation of ETHE and OLEL (C4, 1-nitrato, 2-peroxy)
189	ALKL	ALKL	lumped alkanes C2-C6 (2-methyl-butane)
190	RO28404	RO256	acyl radical from aldehydic H abstraction of RPR8401
191	RO27603	RO247	bicyclic peroxy radical from the O_2 bridging in RO27602

Table SA1. *Continued*

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
192	RO28505	RO240	branched hydroxy keto alkenyl peroxy radical from oxidation of BIOH (C6 chain, 1-hydroxy, 2-isopropyl, 2-ene, 4-peroxy, 5-keto)
193	RP6301	RP16	glyoxalic acid
194	NOPI	NOPI[b]	nopinone
195	RO22301	RO219	branched nitrato alkyl peroxy radical from oxidation of OLEH (C8 chain, 4-methyl, 1-nitrato, 2-peroxy)
196	RO22202	RO23	nitrato alkyl peroxy radical < C6 from oxidation of ETHE and OLEL (C4, 1-nitrato, 2-peroxy)
197	RO27301	RO217	aromatic peroxy radical from side chain oxidation of AROO
198	RO26102	RO210	branched hydroxy alkenyl peroxy radical from oxidation of ISOP (C4 chain, 2-methyl, 3-peroxy, 4-hydroxy)
199	RO26103	RO211	branched nitrato alkenyl peroxy radical from oxidation of ISOP (C4 chain, 1-nitrato, 2-methyl, 2-peroxy)
200	RO26104	RO212	branched nitrato alkenyl peroxy radical from oxidation of ISOP (C4 chain, 2-methyl, 3-peroxy, 4-nitrato)
201	RO26201	RO249	peroxy radical formed from OH oxidation of MVK
202	RO26302	RO251	peroxy radical from OH addition to double bond in MCR
203	RO26303	RO252	peroxy radical from NO3 addition to double bond in MCR
204	RO28302	RO2302[b]	cyclic hydoxy alkenyl peroxy radical from oxidation of δ-limonene (C6 cycle, 1-methyl, 1-ene, 4-(1-methyl-2-hydroxy-1-ethyl peroxy))
205	RO28310	RO2310[b]	keto hydroxy alkyl peroxy radical from oxidation of limonaldehyde (C7 chain, 1-hydroxy, 2-peroxy, 2-methyl,3-formylmethyl, 6-keto)
206	RO28314	RO2314[b]	cyclic nitrato alkyl peroxy radical from oxidation of limona ketone (65% C6 cycle, 1-methyl, 1-peroxy, 2-nitrato, 4-acetyl; 35% C6 cycle, 1-methyl, 1-nitrato, 2-peroxy, 4-acetyl)
207	RO28403	RO226	branched keto hydroxy aldehydic peroxy radical from oxidation of BIOL (C7 chain, 2-hydroxy, 3-isopropyl, 5-peroxy, 6-keto)
208	RO27401	RO222	aromatic peroxy radical from side chain oxidation of ARAL
209	RO28504	RO230	branched keto aldehydic peroxy radical from oxidation of BIOH (C7 chain, 3-isopropyl, 3-ene, 5-peroxy, 6-keto)
210	RO22101	RO22	hydroxy alkyl peroxy radical <C6 from oxidation of ETHE, ETOH, and ALCH (C4, 1-peroxy, 2-hydroxy)
211	RO22201	RO22	hydroxy alkyl peroxy radical from oxidation of OLEL
212	HNO3	HNO3	nitric acid
213	KETL	KETL	lumped ketones C3-C6 (2-pentanone)
214	KETH	KETH	lumped ketones > C6 (2-heptanone)
215	RO26105	RO213	keto alkenyl peroxy radical from oxidation of ISOP (C4, 3-keto, 4-peroxy)
216	OOH2[c]	-	HO_2 radical generated by RO_2+HO_2 reaction
217	RO28304	RO2304[b]	cyclic nitrato alkenyl peroxy radical from oxidation of δ-limonene (80% is C6 cycle, 1-methyl, 1-ene, 4-(1-methyl-2-nitrato-1-ethyl peroxy); 20% is C6 cycle, 1-methyl, 1-ene, 4-(1-methyl-1-nitrato-2-ethyl peroxy))
218	RO28306	RO2306[b]	keto alkenyl aldehydic peroxy radical from oxidation of d-limonene (C7 chain, 3-isopropenyl, 6-keto, 7-peroxy)

Table SA1. *Continued*

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
219	RO28308	RO2308[b]	cyclic alkenyl peroxy radical from oxidation of δ-limonene (C6 cycle, 1-methyl, 1-ene, 4-peroxy, 4-acetyl)
220	RO28311	RO2311[b]	keto nitrato alkyl peroxy radical from oxidation of limonaldehyde (80% C7 chain, 1-nitrato, 2-peroxy, 2-methyl, 3-formylmethyl, 6-keto 20% C7 chain, 1-peroxy, 2-nitrato, 2-methyl, 3-formylmethyl, 6-keto)
221	RO28312	RO2312[b]	keto aldehydic peroxy radical from oxidation of limonaldehyde (C7 chain, 3-peroxy, 3-acetyl, 6-keto)
222	RO28317	RO2317[b]	keto aldehydic peroxy radical from oxidation of limona ketone (C7 chain, 3-acetyl, 6-keto, 7-peroxy)
223	RO28103	RO2103[b]	cyclic keto alkyl peroxy radical from oxidation of a-pinene (C4 cycle, 1-methyl peroxy, 2,2-dimethyl, 3-acetyl)
224	RO26304	RO253	dicarbonyl peroxy radical from MCR+O_3 reaction (C3 chain, 1-peroxy, 2-keto, 3-aldehydic)
225	RO28503	RO229	branched keto alkenyl peroxy radical from oxidation of BIOH (C6 chain, 1-peroxy, 2-isopropyl, 2-ene, 5-keto)
226	RO28315	RO2315[b]	keto alkyl peroxy radical from oxidation of limona ketone (C6 chain, 1-peroxy, 2-acetyl, 5-keto)
227	RO27501	RO223	aromatic peroxy radical from side chain oxidation of ARAC
228	RO28201	RO2201[b]	hydroxy alkyl peroxy radical from oxidation of β-pinene (2-peroxy-10-hydroxy-pinane)
229	RO28202	RO2202[b]	nitrato alkyl peroxy radical from oxidation of β-pinene (80% is 2-peroxy-10-nitrato-pinane; 20% is 2-nitrato-10-peroxy-pinane)
230	RO28303	RO2303[b]	cyclic nitrato alkenyl peroxy radical from oxidation of δ-limonene (65% is C6 cycle, 1-methyl, 1-peroxy, 2-nitrato, 4-isopropenyl; 35% is C6 cycle, 1-methyl, 1-nitrato, 2-peroxy, 4-isopropenyl)
231	RP8301	RP301[b]	keto-limonaldehyde (3-acetyl-6-keto-heptanal)
232	RO28105	RO2105[b]	cyclic keto alkyl peroxy radical from oxidation of α-pinene (C4 cycle, 1-(1-keto-ethyl peroxy), 2,2-dimethyl, 3-formylmethyl)
233	RO27602	RO238	peroxy radical from addition of O_2 to RAD7601
234	RO27102	RO234	peroxy radical from addition of O_2 to RAD7101
235	RO27201	RO235	peroxy radical from addition of O_2 to RAD7201
236	RO21101	RO21	methyl peroxy radical from oxidation of CH4
237	RO26107	RO239	unsaturated acyl peroxy radical from oxidation of ISOP (C3)
238	RO23301	RO26	acyl radical from aldehydic H abstraction of ALD2
239	RO28305	RO2305[b]	keto alkenyl aldehydic peroxy radical from oxidation of δ-limonene (C7 chain, 3-isopropenyl, 5-peroxy, 6-keto)
240	RO22302	RO255	acyl radical from aldehydic H abstraction of RPR2301
241	RO28316	RO2316[b]	keto aldehydic peroxy radical from oxidation of limona ketone (C7 chain, 3-acetyl, 5-peroxy, 6-keto)
242	RO28107	RO2107[b]	acyl peroxy radical from aldehydic H abstraction of norpinonaldehyde
243	RO28506	RO257	acyl radical from aldehydic H abstraction of RPR8501
244	RO27104	RO248	acyl radical from aldehydic H abstraction of MGLY
245	RO27701	RO215	ether alkyl peroxy radical from oxidation of MTBE (C5, accounts for attack on both sides of the ether bond))

Table SA1. *Continued*

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
246	RO27302	RO233	peroxy radical from addition of O_2 to RAD7302
247	BIOL	BIOL	lumped low SOA yield monoterpene species (α-terpineol)
248	BIOH	BIOH	lumped high SOA yield monoterpene species (γ-terpinene)
249	RO27402	RO236	peroxy radical from addition of O2 to RAD7401
250	RO22103	RO24	aldehydic alkyl peroxy radical from oxidation of ISOP and ETHE (C2)
251	ETHE	ETHE	ethene
252	RO28109	RO2109[b]	acyl peroxy radical from oxidation of α-pinene and β-pinene (C4 cycle, 1-formyl peroxy, 2,2-dimethyl, 3-formylmethyl)
253	RO26306	RO258	acyl acid peroxy radical from aldehydic H abstraction of glyoxalic acid
254	RO26305	RO254	acyl radical from decomposition of RO26304
255	RO28106	RO2106[b]	acyl peroxy radical from aldehydic H abstraction of pinonaldehyde
256	RO25201	RO216	keto alkyl peroxy radical from oxidation of KETH (C7, 2-keto, 3-peroxy)
257	RO26106	RO214	alkenyl peroxy radical from oxidation of ISOP (C2)
258	ARAL	ARAL	lumped aromatic monoaldehydes (p-tolualdehyde)
259	RO27502	RO237	peroxy radical from addition of O_2 to RAD7501
260	OLEH	OLEH	lumped alkenes > C6 (4-methyl-1-octene)
261	BPIN	BPIN	β-pinene
262	CO	CO	CO
263	RPR8401	RPR3	2-hydroxy-3-isopropyl-6-keto-heptanal
264	OOH1[c]	-	HO_2 radical generated by RO_2+NO reaction
265	RO21401	RO220	branched alkyl peroxy radical > C6 from oxidation of OLEH and ALKM (C7 chain, 3-methyl, 4-peroxy)
266	RPR2301	RPR1	3-methyl-heptanal
267	RO28101	RO2101[b]	hydroxy alkyl peroxy radical from oxidation of α-pinene (2-peroxy-3-hydroxy-pinane)
268	RO28102	RO2102[b]	nitrato alkyl peroxy radical from oxidation of α-pinene (65% is 2-peroxy-3-nitrato-pinane, 35% is 2-nitrato-3-peroxy-pinane)
269	DLMN	DLMN	δ-limonene
270	HCHO	HCHO	formaldehyde
271	ISOP	ISOP	isoprene
272	RO28203	RO2203[b]	keto alkyl peroxy radical from oxidation of nopinone (3-peroxy-2-norpinone) (3-peroxy-2-norpinone)
273	RO26301	RO250	acyl radical from aldehydic H abstraction of MCR
274	RPR8501	RPR8	3-isopropyl-4-hydroxy-2-butenal
275	RO26101	RO29	branched hydroxy alkenyl peroxy radical from oxidation of ISOP (C4 chain, 1-hydroxy, 2-methyl, 2-peroxy)
276	APIN	APIN	α-pinene
277	PINA	PINA[b]	pinonaldehyde
278	LMKT	LMKT[b]	limona ketone (1-methyl-4-acetyl-hexene)
279	RO28307	RO2307[b]	keto alkenyl peroxy radical from oxidation of δ-limonene (C6 chain, 1-peroxy, 2-isopropenyl, 5-keto)

Table SA1. *Continued*

Species No.	Species Code	Previous Name[a]	Species Name or Description[a]
280	RO28104	RO2104[b]	cic keto aldehydic peroxy radical from oxidaion of α-pinene (C4 cycle, 1-peroxy, 1-acetyl, 2,2-dimethyl, 3-formylmethyl)
281	EDLM	EDLM[b]	limonaldehyde (3-isopropenyl-6-keto-heptanal)
282	ALD1[c]	-	acetaldehyde
283	RO25101	RO27	keto alkyl peroxy radical < C6 from oxidation of ISOP and KETL (C4, 2-keto, 3-peroxy)
284	NRPA	NRPA[b]	norpinonaldehyde
285	RO28108	RO2108[b]	cyclic keto alkyl peroxy radical from oxidation of α-pinene and β-pinene (C4 cycle, 1-peroxy, 2,2-dimethyl, 3-acetyl)
286	MGLY	MGLY	methyl glyoxal
287	MCR	MCR	methacrolein
288	RO23201	RO28	acetyl peroxy radical for oxidation of ALD1, KETL, KETH
289	RO21301	RO25	alkyl peroxy radical < C6 from oxidation of KETL, ISOP, ALKL, BIOH, and OLEL (C3, 1-peroxy)
290	ALD2	ALD2[b]	lumped higher aldehydes (n-pentanal)
291	OLEL	OLEL	lumped alkenes C3-C6 (1-pentene)
292	NO2	NO2	NO_2
293	NO3	NO3	NO_3
294	RO2T	RO2T	total peroxy radical
295	NO	NO	NO
296	HO2	HO2	HO_2
297	O3	O3	O_3
298	O	O	O^3P
299	OH	OH	OH
300	MVK	MVK	methyl vinyl ketone

Table SA1. *Continued*

[a] Unless otherwise noted, nomenclature and description of the species are taken from Table 1 in Griffin et al. (2002) description of the gas-phase CACM reactions.

[b] Species nomenclature and description introduced or updated in Tables S2, S4 and S6 in Chen et al. (2005).

[c] Species introduced in Chen et al. (2005)

Table SA2. The gas-phase reactions included in the CACM mechanism. The second column shows the number assigned in the original description of the CACM model (Griffin et al., 2002; or where noted Chen et al., 2005). The nomenclature used in the table reflects the current species code (see Table SA1 above). Reaction rates are only given in the final column where they have changed since those given in the original descriptions of the mechanism.

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
1	1	NO2 + UV	→	NO + O	
2	2	O	→	O3	7.5454 x $T^{-3.8}$
3	3	NO2 + O	→	NO + O2	
4	4	NO2 + O	→	NO3	
5	5	NO + O3	→	NO2 + O2	
6	6	NO2 + O3	→	NO3 + O2	
7	7	NO3 + NO	→	2 NO2	
8	8	2 NO	→	2 NO2	
9	9	NO2 + NO3	→	N2O5	
10	10	N2O5	→	NO2 + NO3	
11	11	N2O5 + H2O	→	2 HNO3	
12	12	NO2 + NO3	→	NO2 + NO	
13	13	NO3 + UV	→	NO	
14	14	NO3 + UV	→	NO2 + O	
15	15	O3 + UV	→	O + O2	
16	16	O3 + UV	→	OSD + O2	
17	17	OSD + H2O	→	2 OH	
18	18	OSD	→	O	
19	19	NO + OH	→	HONO	
20	20	HONO + UV	→	0.1 NO2 + 0.9 NO + 0.1 HO2 + 0.9 OH	
21	21	NO2 + H2O	→	HONO + HNO3 - NO2	
22	22	NO2 + OH	→	HNO3	
23	23	HNO3 + OH	→	NO3 + H2O	
24	24	CO + OH	→	CO2 + HO2	
25	25	O3 + OH	→	HO2 + O2	
26	26	NO + HO2	→	NO2 + OH	
27	27	NO2 + HO2	→	HNO4	
28	28	HNO4	→	NO2 + HO2	
29	29	HNO4 + OH	→	NO2 + O2 + H2O	
30	30	HO2 + O3	→	OH + 2 O2	
31	31	2 HO2	→	H2O2	
32	32	2 HO2 + H2O	→	H2O2 + O2 + H2O	
33	33	NO3 + HO2	→	0.2 HNO3 + 0.8 NO2 + 0.8 OH	
34	34	O3 + O	→	2 O2	
35	35	SO2 + OH	→	H2SO4 + HO2	
36	36	H2O2 + UV	→	2 OH	
37	37	H2O2 + OH	→	HO2 + H2O	
38	38	NO + O	→	NO2	

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
39	39	HONO + OH	→	NO2 + H2O	
40	40	NO3 + OH	→	NO2 + HO2	
41	41	2 NO3	→	2 NO2 + O2	
42	42	HO2 + OH	→	O2 + H2O	
43	-[b]	OOH1 + UV	→	HO2 + OH +HCHO	5.42x10^{-06} [g]
44	-[b]	OOH1 + OH	→	HO2	1.90x10^{-12} x e$^{(190.0/T)}$
45	-[b]	OOH1 + OH	→	OH	1.0x10^{-12} x e$^{(190.0/T)}$
46	-[b]	OOH2 + UV	→	OH + HCHO	k_{43}
47	-[b]	OOH2 + OH	→	DUMMY[e]	k_{44}
48	-[b]	OOH2 + OH	→	OH	k_{45}
49	95	RO2T + NO	→	NO	
50	96	2 RO2T	→	RO2T	1.00x10^{-12} [h]
51	94	RO2T + HO2	→	HO2	1.50x10^{-12} x e$^{(800.2/T)}$ [i]
52	43	CH4 + OH	→	RO21101 + RO2T + H2O	
53	110	RO21101 + NO	→	HCHO + NO2 + HO2	
54	111	RO21101 + RO2T	→	HCHO + RO2T + HO2 + O2	k_{50}
55	112[a]	RO21101 + HO2	→	OOH1	k_{51}
56	-[b]	C2H6 + OH	→	RO21201 + RO2T + H2O	1.52x10^{-17} x e$^{(-498.0/T)}$
57	-[b]	RO21201 + NO	→	ALD1 + NO2 + HO2	4.09x10^{-12} x e$^{(180.2/T)}$
58	-[b]	RO21201 + RO2T	→	ALD1 + RO2T + HO2 + O2	k_{50}
59	-[b]	RO21201 + HO2	→	OOH1 + ALD1	k_{51}
60	58	ALKL + OH	→	RO21301 + RO2T + H2O	
61	122[a]	RO21301 + NO	→	AP1401	
62	122[a]	RO21301 + NO	→	ALD1 + NO2 + HO2	
63	123[a]	RO21301 + RO2T	→	ALD1 + RO2T + HO2 + O2	k_{50}
64	124[a]	RO21301 + HO2	→	OOH1 + ALD1	k_{51}
65	78	ALKM + OH	→	RO21401 + RO2T + H2O	
66	176	RO21401 + NO	→	AP1401	
67	176	RO21401 + NO	→	RO21402 + NO2 + RO2T	
68	177	RO21401 + RO2T	→	RO21402 + 2 RO2T + O2	k_{50}
69	178[a]	RO21401 + HO2	→	RO21402 + OOH2 + RO2T	k_{51}
70	170	RO21402 + NO	→	AP1402	
71	170	RO21402 + NO	→	UR1401 + NO2 + HO2	
72	171	RO21402 + RO2T	→	UR1401 + RO2T + HO2 + O2	k_{50}
73	172[a]	RO21402 + HO2	→	UR1401 + OOH1	k_{51}
74	-[b]	AP1401	→	DUMMY2[e]	
75	-[b]	AP1402	→	DUMMY2[e]	
76	-[b]	UR1401	→	DUMMY[e]	1.67x10^{-06}
77	93	ALKH + OH	→	RO21501 + RO2T + H2O	See Table 6 in Griffin et al. (2002)[j]
78	215	RO21501 + NO	→	AP1501	
79	215	RO21501 + NO	→	RO21502 + NO2 + RO2T	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
80	216	RO21501 + RO2T	→	RO21502 + 2 RO2T + O2	k_{50}
81	217[a]	RO21501 + HO2	→	RO21502 + OOH2 + RO2T	k_{51}
82	218	RO21502 + NO	→	AP1502	
83	218	RO21502 + NO	→	UR1501 + NO2 + HO2	
84	219	RO21502 + RO2T	→	UR1501 + RO2T + HO2 + O2	k_{50}
85	220	RO21502 + HO2	→	UR1501 + OOH1	k_{51}
86	-[b]	AP1501	→	DUMMY2[e]	
87	-[b]	AP1502	→	DUMMY2[e]	
88	-[b]	UR1501	→	DUMMY[e]	k_{76}
89	49	ETHE + OH	→	RO22101 + RO2T	
90	50	ETHE + NO3	→	RO22102 + RO2T	
91	51[a]	ETHE + O3	→	0.37 ACID + 0.63 CO + HCHO + 0.12 HO2 + 0.12 OH + 0.14 H2O	
92	52	ETHE + O	→	0.6 RO21101 + 0.4 RO22103 + 0.6 CO + RO2T + HO2	
93	113[a]	RO22101 + NO	→	1.61 HCHO + 0.195 ALD1 + NO2 + HO2	$4.10 \times 10^{-12} \times e^{(180.2/T)}$
94	114[a]	RO22101 + RO2T	→	1.61 HCHO + 0.195 ALD1 + RO2T + HO2 + O2	k_{50}
95	115[a]	RO22101 + HO2	→	OOH1 + 0.195 ALD1	k_{51}
96	116[a]	RO22102 + NO	→	2 HCHO + 2 NO2	k_{93}
97	117[a]	RO22102 + RO2T	→	2 HCHO + NO2 + RO2T + O2	k_{50}
98	118[a]	RO22102 + HO2	→	OOH2 + NO2	k_{51}
99	119	RO22103 + NO	→	CO + HCHO + NO2 + HO2	
100	120	RO22103 + RO2T	→	CO + HCHO + RO2T + HO2 + O2	k_{50}
101	121[a]	RO22103 + HO2	→	CO + OOH1	k_{51}
102	54	OLEL + OH	→	RO22201 + RO2T	
103	55	OLEL + NO3	→	RO22202 + RO2T	
104	56	OLEL + O3	→	0.24 ACID + 0.2 CO2 + 0.1 ALKL + 0.56 CO + 0.5 HCHO + 0.36 OH + 0.28 HO2 + 0.5 ALD1 + 0.28 RO21301 + 0.28 RO2T	
105	57	OLEL + O	→	0.5 ALKL + 0.1 RO22103 + 0.1 RO21301 + 0.4 ALD2 + 0.2 RO2T	
106	113	RO22201 + NO	→	HCHO + ALD2 + NO2 + HO2	
107	114	RO22201 + RO2T	→	HCHO + ALD2 + RO2T + HO2 + O2	k_{50}
108	115[a]	RO22201 + HO2	→	OOH1 + ALD2	k_{51}
109	116	RO22202 + NO	→	HCHO + ALD2 + 2 NO2	
110	117	RO22202 + RO2T	→	HCHO + ALD2 + NO2 + RO2T + HO2 + O2	k_{50}
111	118[a]	RO22202 + HO2	→	OOH1 + ALD2 + NO2	k_{51}
112	74	OLEH + OH	→	RO21402 + RO2T	
113	75	OLEH + NO3	→	RO22301 + RO2T	
114	76	OLEH + O3	→	0.56 CO + 0.2 CO2 + 0.36 OH + 0.28 HO2 + 0.5 HCHO + 0.5 RPR2301 + 0.12 ACID + 0.12 UR2301 + 0.1 ALKM + 0.28 RO21401 + 0.28 RO2T	
115	77	OLEH + O	→	0.5 ALKM + 0.1 RO22103 + 0.1 RO21401 + 0.4 RPR2301 + 0.2 RO2T	
116	173	RO22301 + NO	→	RPR2301 + HCHO + 2 NO2	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
117	174	RO22301 + RO2T	→	RPR2301 + HCHO + NO2 + RO2T + O2	k_{50}
118	175[a]	RO22301 + HO2	→	OOH2 + RPR2301 + NO2	k_{51}
119	300	RPR2301 + OH	→	RO22302 + RO2T + H2O	
120	301	RPR2301 + NO3	→	HNO3 + RO22302 + RO2T	
121	302	RPR2301 + UV	→	CO + RO21401 + RO2T + HO2	
122	303	RO22302 + NO	→	CO2 + RO21401 + NO2 + RO2T	
123	304	RO22302 + NO2	→	PAN2301	
124	305[a]	PAN2301	→	RO22302 + NO2	
125	306[a]	RO22302 + HO2	→	UR1401 + O3	
126	307[a]	RO22302 + RO2T	→	CO2 + RO21401 + 1 RO2T + O2	1.00×10^{-11} [k]
127	-[b]	UR2301	→	DUMMY[e]	k_{76}
128	44	HCHO + UV	→	CO + 2 HO2	
129	45	HCHO + UV	→	CO	
130	46	HCHO + OH	→	CO + HO2 + H2O	
131	47	HCHO + NO3	→	HNO3 + CO + HO2	
132	59[a]	ALD1 + UV	→	RO21101 + CO + RO2T + HO2	4.87×10^{-06}
133	60[a]	ALD1 + OH	→	RO23201 + RO2T + H2O	$5.60 \times 10^{-12} \times e^{(312.0/T)}$
134	61[a]	ALD1 + NO3	→	HNO3 + RO23201 + RO2T	$1.40 \times 10^{-12} \times e^{(-1862.0/T)}$
135	133	RO23201 + NO	→	CO2 + RO21101 + NO2 + RO2T	
136	134	RO23201 + NO2	→	PAN3201	
137	135[a]	PAN3201	→	RO23201 + NO2	
138	136	RO23201 + HO2	→	ACID + O3	
139	137	RO23201 + RO2T	→	CO2 + RO21101 + 2 RO2T + O2	k_{126}
140	59	ALD2 + UV	→	CO + RO21301 + RO2T + HO2	
141	60	ALD2 + OH	→	RO23301 + RO2T + H2O	
142	61	ALD2 + NO3	→	HNO3 + RO23301 + RO2T	
143	125	RO23301 + NO	→	CO2 + RO21301 + NO2	
144	126	RO23301 + NO2	→	PAN3301	
145	127[a]	PAN3301	→	RO23301 + NO2	
146	128	RO23301 + HO2	→	ACID + O3	
147	129	RO23301 + RO2T	→	CO2 + RO21301 + 2 RO2T + O2	k_{126}
148	48	MEOH + OH	→	HCHO + HO2 + H2O	
149	53	ETOH + OH	→	ALD1 + HO2 + H2O	
150	53	ETOH + OH	→	RO22101 + RO2T + H2O	
151	69	ALCH + OH	→	RO22201 + RO2T + H2O	
152	62	KETL + OH	→	RO25101 + RO2T	
153	63	KETL + UV	→	RO23201 + RO21301 + 2 RO2T	
154	130	RO25101 + NO	→	RO23201 + ALD2 + NO2 + RO2T	
155	131[a]	RO25101 + RO2T	→	RO23201 + ALD2 + 1 RO2T + O2	k_{50}
156	132[a]	RO25101 + HO2	→	OOH2 + RO23201 + ALD2 + RO2T	k_{51}
157	70	KETH + OH	→	RO25201 + RO2T	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
158	71	KETH + UV	➔	RO23201 + RO21301 + 2 RO2T	
159	164	RO25201 + NO	➔	RO23201 + ALD2 + NO2 + RO2T	
160	165[a]	RO25201 + RO2T	➔	RO23201 + ALD2 + 1 RO2T + O2	k_{50}
161	166[a]	RO25201 + HO2	➔	OOH2 + RO23201 + ALD2 + RO2T	k_{51}
162	64	ISOP + OH	➔	0.34 RO26102 + 0.66 RO26101 + RO2T	
163	65	ISOP + NO3	➔	0.66 RO26103 + 0.34 RO26104 + RO2T	
164	66	ISOP + O3	➔	0.068 CO2 + 0.461 CO + 0.5 HCHO + 0.664 OH + 0.366 HO2 + 0.054 OLEL + 0.121 ACID + 0.389 MVK + 0.17 MCR + 0.271 RO26105 + 0.095 RO26106 + 0.366 RO2T	
165	67	ISOP + O	➔	0.075 ALD2 + 0.925 OLEL	
166	138[a]	RO26101 + NO	➔	AP6101	
167	138	RO26101 + NO	➔	HCHO + NO2 + HO2 + MVK	
168	139	RO26101 + RO2T	➔	HCHO + RO2T + HO2 + MVK + O2	k_{50}
169	140[a]	RO26101 + HO2	➔	OOH1 + MVK	k_{51}
170	141	RO26102 + NO	➔	HCHO + MCR + NO2 + HO2	
171	142	RO26102 + RO2T	➔	HCHO + MCR + RO2T + HO2 + O2	k_{50}
172	143[a]	RO26102 + HO2	➔	OOH1 + MCR	k_{51}
173	144	RO26103 + NO	➔	HCHO + 2 NO2 + MVK	
174	145	RO26103 + RO2T	➔	HCHO + NO2 + RO2T + MVK + O2	k_{50}
175	146[a]	RO26103 + HO2	➔	OOH2 + NO2 + MVK	k_{51}
176	147	RO26104 + NO	➔	HCHO + MCR + 2 NO2	
177	148	RO26104 + RO2T	➔	HCHO + MCR + NO2 + RO2T + O2	k_{50}
178	149[a]	RO26104 + HO2	➔	OOH2 + MCR + NO2	k_{51}
179	150	RO26105 + NO	➔	RO26107 + HCHO + NO2 + RO2T	
180	151	RO26105 + RO2T	➔	RO26107 + HCHO + 2 RO2T + O2	k_{50}
181	152[a]	RO26105 + HO2	➔	OOH2 + RO26107 + RO2T	k_{51}
182	158[a]	RO26106 + NO	➔	AP6102	
183	158	RO26106 + NO	➔	RO25101 + NO2 + RO2T	
184	159	RO26106 + RO2T	➔	RO25101 + 2 RO2T + O2	k_{50}
185	160[a]	RO26106 + HO2	➔	OOH2 + RO25101 + RO2T	k_{51}
86	153	RO26107 + NO	➔	CO2 + RO26106 + NO2 + RO2T	
187	154	RO26107 + NO2	➔	PAN6101	
188	155	PAN6101	➔	RO26107 + NO2 + RO2T	
189	156	RO26107 + HO2	➔	0.5 ACID + 0.5 OLEL + O3	
190	157	RO26107 + RO2T	➔	CO2 + RO26106 + 2 RO2T + O2	k_{126}
191	271	OH + MVK	➔	RO26201 + RO2T	
192	272[a]	O3 + MVK	➔	0.56 CO + 0.2 CO2 + 0.28 HO2 + 0.36 OH + 0.5 MGLY + 0.5 HCHO + 0.12 ACID + 0.1 ALD1 + 0.12 UR6201 + 0.2 H2O	
193	273	O + MVK	➔	0.85 KETL + 0.15 RO22103 + 0.15 RO23201 + 0.3 RO2T	
194	274	RO26201 + NO	➔	MGLY + NO2 + HO2	
195	275	RO26201 + RO2T	➔	HCHO + MGLY + RO2T + HO2 + O2	k_{50}

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
196	276[a]	RO26201 + HO2	→	OOH1 + HCHO + MGLY	k_{51}
197	-[b]	UR6201	→	DUMMY[e]	k_{76}
198	277[a]	MCR + OH	→	0.7 RO26302 + 0.3 RO26301 + RO2T + 0.3 H2O	
199	278[a]	MCR + NO3	→	0.7 RO26303 + 0.3 HNO3 + 0.3 RO26301 + RO2T	
200	279	MCR + O3	→	0.41 CO + 0.41 HO2 + 0.82 OH + 0.5 HCHO + 0.59 MGLY + 0.09 ACID + 0.41 RO26304 + 0.41 RO2T	
201	280[a]	MCR + O	→	0.15 CO + 0.15 HO2 + 0.85 ALD2 + 0.15 RO25101 + 0.15 RO2T	
202	281	RO26301 + NO	→	CO2 + RO26106 + NO2 + RO2T	$1.11x10^{-11}$ x $e^{(182.2/T)}$
203	282	RO26301 + NO2	→	PAN6301	
204	283	PAN6301	→	RO26301 + NO2 + RO2T	
205	284	RO26301 + HO2	→	0.5 ACID + 0.5 OLEL + O3	
206	285	RO26301 + RO2T	→	CO2 + RO26106 + 2 RO2T + O2	k_{126}
207	286	RO26302 + NO	→	HCHO + MGLY + NO2 + HO2	
208	287	RO26302 + RO2T	→	HCHO + MGLY + RO2T + HO2 + O2	k_{50}
209	288[a]	RO26302 + HO2	→	OOH1 + MGLY	k_{51}
210	289	RO26303 + NO	→	HCHO + MGLY + 2 NO2	
211	290	RO26303 + RO2T	→	HCHO + MGLY + NO2 + RO2T + O2	k_{50}
212	291[a]	RO26303 + HO2	→	OOH2 + MGLY + NO2	k_{51}
213	292	RO26304 + NO	→	RO26305 + HCHO + NO2 + RO2T	
214	294[a]	RO26304 + RO2T	→	RO26305 + HCHO + 2 RO2T + O2	k_{50}
215	293[a]	RO26304 + HO2	→	OOH2 + RO26305 + RO2T	k_{51}
216	295	RO26305 + NO	→	CO2 + CO + NO2 + HO2	k_{202}
217	296	RO26305 + NO2	→	PAN6302	
218	297[a]	PAN6302	→	RO26305 + NO2 + RO2T	
219	298	RO26305 + HO2	→	RP6301 + O3	
220	299	RO26305 + RO2T	→	CO2 + CO + RO2T + HO2 + O2	k_{126}
221	339	RP6301 + OH	→	RO26306 + RO2T + H2O	
222	340	RP6301 + NO3	→	HNO3 + RO26306 + RO2T	
223	341	RP6301 + UV	→	2 CO + HO2 + OH	
224	342	RO26306 + NO	→	CO2 + CO + NO2 + OH	k_{202}
225	343	RO26306 + NO2	→	PAN6303	
226	344	PAN6303	→	RO26306 + NO2 + RO2T	
227	345	RO26306 + HO2	→	UR6301 + O3	
228	346	RO26306 + RO2T	→	CO2 + CO + RO2T + OH + O2	k_{126}
229	-[b]	UR6301	→	DUMMY[e]	k_{76}
230	79	AROL + OH	→	0.74 RAD7101 + 0.16 AROO + 0.1 RO27101 + 0.06 RO2T + 0.16 HO2 + 0.06 H2O	
231	98	RAD7101	→	RO27102 + RO2T	
232	105	RAD7101 + NO2	→	UR7101 + H2O	
233	179	RO27101 + NO	→	AP7101	
234	179	RO27101 + NO	→	ARAL + NO2 + HO2	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
235	180	RO27101 + RO2T	→	ARAL + RO2T + HO2 + O2	k_{50}
236	181[a]	RO27101 + HO2	→	ARAL + OOH1	k_{51}
237	228	RO27102	→	RO27103 + RO2T	
238	229[a]	RO27102 + NO	→	0.3 RP7101 + 0.7 UR7103 + NO2 + HO2	
239	230[a]	RO27102 + RO2T	→	0.3 RP7101 + 0.7 UR7103 + RO2T + HO2 + O2	k_{50}
240	231[a]	RO27102 + HO2	→	0.3 RP7101 + 0.7 UR7103 + OOH1	k_{51}
241	232	RO27103 + NO	→	RP7102 + MGLY + NO2 + HO2	
242	233	RO27103 + RO2T	→	RP7102 + MGLY + RO2T + HO2 + O2	k_{50}
243	234[a]	RO27103 + HO2	→	RP7102 + OOH1 + MGLY	k_{51}
245	332	RP7102 + OH	→	UR7103 + HO2 + H2O	
246	333	RP7102 + UV	→	UR7104	
247	263	MGLY + OH	→	RO27104 + RO2T + H2O	
248	264	MGLY + NO3	→	HNO3 + RO27104 + RO2T	
249	265	MGLY + UV	→	CO + RO23201 + RO2T + HO2	
250	266	RO27104 + NO	→	CO2 + RO23201 + NO2 + RO2T	
251	267	RO27104 + NO2	→	PAN7101	
252	268	PAN7101	→	RO27104 + NO2 + RO2T	
253	269	RO27104 + HO2	→	UR6201 + O3	
254	270	RO27104 + RO2T	→	CO2 + RO23201 + 2 RO2T + O2	k_{126}
255	-[b]	AP7101	→	DUMMY[e]	k_{76}
256	-[b]	UR7101	→	DUMMY[e]	k_{76}
257	-[b]	UR7102	→	DUMMY[e]	k_{76}
258	-[b]	UR7103	→	DUMMY[e]	k_{76}
259	-[b]	UR7104	→	DUMMY[e]	k_{76}
260	80	AROH + OH	→	0.84 RAD7201 + 0.16 AROO + 0.16 HO2	
261	99	RAD7201	→	RO27201 + RO2T	
262	106	RAD7201 + NO2	→	UR7201 + H2O	
263	235	RO27201	→	RO27202 + RO2T	
264	236[a]	RO27201 + NO	→	0.5 RP7101 + 0.5 UR7103 + NO2 + HO2	
265	237[a]	RO27201 + RO2T	→	0.5 RP7101 + 0.5 UR7103 + RO2T + HO2 + O2	k_{50}
266	238[a]	RO27201 + HO2	→	0.5 RP7101 + 0.5 UR7103 + OOH1	k_{51}
267	239	RO27202 + NO	→	RP7102 + MGLY + NO2 + HO2	
268	240	RO27202 + RO2T	→	RP7102 + MGLY + RO2T + HO2 + O2	k_{50}
269	241[a]	RO27202 + HO2	→	RP7102 + OOH1 + MGLY	k_{51}
270	-[b]	UR7201	→	DUMMY[e]	k_{76}
271	72	AROO + NO3	→	RAD7301 + HNO3	
272	73	AROO + OH	→	0.74 RAD7302 + 0.16 AROO + 0.1 RO27301 + 0.1 RO2T + 0.16 HO2 + 0.10 H2O	
273	103	RAD7301 + NO2	→	RPR7301	
274	97	RAD7302	→	RO27302 + RO2T	
275	104	RAD7302 + NO2	→	RPR7301 + H2O	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
276	167	RO27301 + NO	→	AP7301	
277	167	RO27301 + NO	→	RPR7302 + NO2 + HO2	
278	168	RO27301 + RO2T	→	RPR7302 + RO2T + HO2 + O2	k_{50}
279	169[a]	RO27301 + HO2	→	RPR7302 + OOH1	k_{51}
280	221	RO27302	→	RO27303 + RO2T	
281	222[a]	RO27302 + NO	→	0.3 RPR7303 + 0.7 UR7103 + NO2 + HO2	
282	223[a]	RO27302 + RO2T	→	0.3 RPR7303 + 0.7 UR7103 + RO2T + HO2 + O2	k_{50}
283	224[a]	RO27302 + HO2	→	0.3 RPR7303 + 0.7 UR7103 + OOH1	k_{51}
284	225	RO27303 + NO	→	RP7102 + MGLY + NO2 + HO2	
285	226	RO27303 + RO2T	→	RP7102 + MGLY + RO2T + HO2 + O2	k_{50}
286	227[a]	RO27303 + HO2	→	RP7102 + OOH1 + MGLY	k_{51}
287	317	RPR7301 + NO3	→	RAD7303 + HNO3	
288	318	RAD7303 + NO2	→	UR7301 + H2O	
289	308	RPR7302 + OH	→	UR7302 - HO2 + O3 + H2O	
290	331	RPR7303 + OH	→	RP7304 - HO2 + O3 + H2O	
291	347	RP7304 + OH	→	UR7303 - HO2 + O3 + H2O	
292	-[b]	AP7301	→	DUMMY[e]	k_{76}
293	-[b]	UR7301	→	DUMMY[e]	k_{76}
294	-[b]	UR7302	→	DUMMY[e]	k_{76}
295	-[b]	UR7303	→	DUMMY[e]	k_{76}
296	81	ARAL + NO3	→	ARAC + HNO3 - HO2 + O3	
297	82	ARAL + OH	→	RPR7302 + HO2	
298	82	ARAL + OH	→	ARAC - HO2 + O3 + H2O	
299	82	ARAL + OH	→	RAD7401	
300	82	ARAL + OH	→	RO27401 + RO2T + H2O	
301	100	RAD7401	→	RO27402 + RO2T	
302	107	RAD7401 + NO2	→	RPR7401 + H2O	
303	182	RO27401 + NO	→	AP7401	
304	182	RO27401 + NO	→	RPR7402 + NO2 + HO2	
305	183	RO27401 + RO2T	→	RPR7402 + RO2T + HO2 + O2	k_{50}
306	184[a]	RO27401 + HO2	→	RPR7402 + OOH1	k_{51}
307	242	RO27402	→	RO27403 + RO2T	
308	243[a]	RO27402 + NO	→	0.3 RP7403 + 0.7 UR7103 + NO2 + HO2	
309	244[a]	RO27402 + RO2T	→	0.3 RP7403 + 0.7 UR7103 + RO2T + HO2 + O2	k_{50}
310	245[a]	RO27402 + HO2	→	0.3 RP7403 + 0.7 UR7103 + OOH1	k_{51}
311	246	RO27403 + NO	→	RP7102 + MGLY + NO2 + HO2	
312	247	RO27403 + RO2T	→	RP7102 + MGLY + RO2T + HO2 + O2	k_{50}
313	248[a]	RO27403 + HO2	→	RP7102 + OOH1 + MGLY	k_{51}
314	319	RPR7401 + OH	→	UR7401 - HO2 + O3 + H2O	
315	320	RPR7402 + OH	→	RPR7404 - HO2 + O3 + H2O	
316	335	RP7403 + OH	→	RP7405 - HO2 + O3 + H2O	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
317	321	RPR7404 + OH	→	ADAC - HO2 + O3 + H2O	
318	336	RP7405 + OH	→	RP7406 - HO2 + O3 + H2O	
319	348	RP7406 + OH	→	UR7402 - HO2 + O3 + H2O	
320	-[b]	AP7401	→	DUMMY[e]	k_{76}
321	-[b]	UR7401	→	DUMMY[e]	k_{76}
322	-[b]	UR7402	→	DUMMY[e]	k_{76}
323	83	ARAC + OH	→	0.16 UR7302 + 0.74 RAD7501 + 0.1 RO27501 + 0.1 RO2T + 0.16 HO2 + 0.1 H2O	1.05×10^{-12}
324	101	RAD7501	→	RO27502 + RO2T	
325	108	RAD7501 + NO2	→	UR7401 + H2O	
326	185	RO27501 + NO	→	AP7501	
327	185	RO27501 + NO	→	RPR7404 + NO2 + HO2	
328	186	RO27501 + RO2T	→	RPR7404 + RO2T + HO2 + O2	k_{50}
329	187[a]	RO27501 + HO2	→	RPR7404 + OOH1	k_{51}
330	249	RO27502	→	RO27503 + RO2T	
331	250[a]	RO27502 + NO	→	0.3 RP7405 + 0.7 UR7103 + NO2 + HO2	
332	251[a]	RO27502 + RO2T	→	0.3 RP7405 + 0.7 UR7103 + RO2T + HO2 + O2	k_{50}
333	252[a]	RO27502 + HO2	→	0.3 RP7405 + 0.7 UR7103 + OOH1	k_{51}
334	253	RO27503 + NO	→	RP7102 + MGLY + NO2 + HO2	
335	254	RO27503 + RO2T	→	RP7102 + MGLY + RO2T + HO2 + O2	k_{50}
336	255[a]	RO27503 + HO2	→	RP7102 + OOH1 + MGLY	k_{51}
337	-[b]	AP7501	→	DUMMY[e]	k_{76}
338	92	PAH + OH	→	0.16 HO2 + 0.16 UR7601 + 0.1 RO27601 + 0.74 RAD7601 + 0.1 RO2T + 0.1 H2O	
339	102	RAD7601	→	RO27602 + RO2T	
340	109	RAD7601 + NO2	→	UR7602	
341	212	RO27601 + NO	→	AP7601	
342	212	RO27601 + NO	→	UR7603 + NO2 + HO2	
343	213	RO27601 + RO2T	→	UR7603 + RO2T + HO2 + O2	k_{50}
344	214[a]	RO27601 + HO2	→	UR7603 + OOH1	k_{51}
345	256	RO27602	→	RO27603 + RO2T	
346	257	RO27602 + NO	→	RP7601 + NO2 + HO2	
347	258	RO27602 + RO2T	→	RP7601 + RO2T + HO2 + O2	k_{50}
348	259[a]	RO27602 + HO2	→	RP7601 + OOH1	k_{51}
349	260	RO27603 + NO	→	RP7602 + MGLY + NO2 + HO2	
350	261	RO27603 + RO2T	→	RP7602 + MGLY + RO2T + HO2 + O2	k_{50}
351	262[a]	RO27603 + HO2	→	RP7602 + OOH1 + MGLY	k_{51}
352	337	RP7601 + OH	→	RP7603 - HO2 + O3 + H2O	
353	338	RP7602 + OH	→	UR7604 - HO2 + O3 + H2O	
354	349	RP7603 + OH	→	UR7605 - HO2 + O3	
355	-[b]	AP7601	→	DUMMY[e]	k_{76}

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
356	-[b]	UR7601	→	DUMMY[e]	k_{76}
357	-[b]	UR7602	→	DUMMY[e]	k_{76}
358	-[b]	UR7603	→	DUMMY[e]	k_{76}
359	-[b]	UR7604	→	DUMMY[e]	k_{76}
360	-[b]	UR7605	→	DUMMY[e]	k_{76}
361	68	MTBE + OH	→	RO27701 + RO2T + H2O	
362	161[a]	RO27701 + NO	→	0.2 ALKL + 0.2 KETL + 0.4 HCHO + 0.2 ALD2 + NO2 + HO2 [f]	
363	162[a]	RO27701 + RO2T	→	0.2 ALKL + 0.2 KETL + 0.4 HCHO + 0.2 ALD2 + RO2T + HO2 + O2 [f]	k_{50}
364	163[a]	RO27701 + HO2	→	0.2 ALKL + 0.2 KETL + OOH1 + 0.2 ALD2 [f]	k_{51}
365	1A[c]	APIN + OH	→	RO28101 + RO2T	
366	2A[c]	APIN + NO3	→	RO28102 + RO2T	
367	3A[c]	APIN + O3	→	0.2 RO28103 + 0.2 CO + 0.8 OH + 0.05 UR8101 + 0.15 PINA + 0.15 H2O2 + 0.33 RO28104 + 0.27 RO28105 + 0.8 RO2T	
368	4A[c]	APIN + O	→	0.75 UR8103 + 0.25 NOPI	
369	5A[c]	RO28101 + NO	→	0.2 AP8101 + 0.2 KETH + 0.2 HCHO + 0.6 PINA + 0.8 NO2 + 0.8 HO2	
370	6A[c]	RO28101 + RO2T	→	0.3 UR8107 + 0.7 PINA + RO2T + HO2	
371	7A[c]	RO28101 + HO2	→	0.2 KETH + OOH1 + 0.8 PINA	
372	8A[c]	RO28102 + NO	→	0.175 AP8102 + 0.225 KETH + 0.225 HCHO + 0.6 PINA + 1.825 NO2+ 0.4 HO2	
373	9A[c]	RO28102 + RO2T	→	0.135 AP8101 + 0.07 AP8102 + 0.795 PINA + 0.795 NO2 + RO2T	
374	10A[c]	RO28102 + HO2	→	0.175 AP8102 + 0.225 KETH + 0.825 OOH2 + 0.175 OOH1 + 0.6 PINA + 0.825 NO2 + 0.225 HO2	
375	11A[c]	RO28103 + NO	→	AP8103	
376	11A[c]	RO28103 + NO	→	NRPA + NO2 + HO2	
377	12A[c]	RO28103 + RO2T	→	NRPA + RO2T + HO2	
378	13A[c]	RO28103 + HO2	→	OOH1 + NRPA	
379	14A[c]	RO28104 + NO	→	RO28108 + RO23201 + NO2 + 2 RO2T	
380	15A[c]	RO28104 + RO2T	→	0.3 RP8102 + 0.7 RO28108 + 0.7 RO23201 + 2.4 RO2T	
381	16A[c]	RO28104 + HO2	→	OOH2 + RO28108 + RO23201 + 2 RO2T	
382	17A[c]	RO28105 + NO	→	RO28109 + HCHO + NO2 + RO2T	
383	18A[c]	RO28105 + RO2T	→	0.05 UR8108 + 0.1 UR8105 + 0.05 RP8103 + 0.8 RO28109 + 0.8HCHO + 1.8 RO2T	
384	19A[c]	RO28105 + HO2	→	OOH2 + RO28109 + RO2T	
385	20A[c]	PINA + UV	→	RO28103 + CO + HO2	
386	21A[c]	PINA + OH	→	0.8 RO28106 + 0.2 RO28104 + RO2T	
387	22A[c]	PINA + NO3	→	HNO3 + RO28106 + RO2T	
388	23A[c]	RO28106 + NO	→	CO2 + RO28103 + NO2 + RO2T	
389	24A[c]	RO28106 + NO2	→	PAN8101	
390	25A[c]	PAN8101	→	RO28106 + NO2 + RO2T	
391	26A[c]	RO28106 + RO2T	→	0.2 UR8101 + 0.8 CO2 + 0.8 RO28103 + 1.8 RO2T	
392	27A[c]	RO28106 + HO2	→	UR8101 + O3	
393	28A[c]	NRPA + UV	→	CO + RO28108 + RO2T + HO2	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
394	29A[c]	NRPA + OH	→	0.8 RO28107 + 0.2 RO28104 + RO2T	
395	30A[c]	NRPA + NO3	→	HNO3 + RO28107 + RO2T	
396	31A[c]	RO28107 + NO	→	CO2 + RO28108 + NO2 + RO2T	
397	32A[c]	RO28107 + NO2	→	PAN8102	
398	33A[c]	PAN8102	→	RO28107 + NO2 + RO2T	
399	34A[c]	RO28107 + RO2T	→	0.2 UR8102 + 0.8 CO2 + 0.8 RO28108 + 1.8 RO2T	
400	35A[c]	RO28107 + HO2	→	UR8102 + O3	
401	36A[c]	RO28108 + NO	→	AP8104	
402	36A[c]	RO28108 + NO	→	KETH + NO2 + HO2	
403	37A[c]	RO28108 + RO2T	→	KETH + RO2T + HO2	
404	38A[c]	RO28108 + HO2	→	KETH + OOH1	
405	39A[c]	RO28109 + NO	→	CO2 + RO28108 + NO2 + RO2T	
406	40A[c]	RO28109 + NO2	→	PAN8103	
407	41A[c]	PAN8103	→	RO28109 + NO2 + RO2T	
408	42A[c]	RO28109 + RO2T	→	0.1 UR8104 + 0.6 CO2 + 0.3 RP8101 + 0.6 RO28108 + 1.6 RO2T	
409	43A[c]	RO28109 + HO2	→	UR8104	
410	48A[c]	RP8101 + OH	→	UR8104 - HO2 + O3	
411	49A[c]	RP8102 + OH	→	UR8106 - HO2 + O3	
412	50A[c]	RP8103 + OH	→	UR8105 - HO2 + O3	
413	-[b]	RP8101	→	AERS12	$1.5x10^{-35}$ x $e^{(14770.0/T)}$
414	-[b]	UR8101	→	AERS12	k_{413}
415	-[b]	UR8102	→	AERS12	k_{413}
416	-[b]	UR8104	→	AERS12	k_{413}
417	-[b]	UR8105	→	AERS12	k_{413}
418	-[b]	UR8106	→	AERS12	k_{413}
419	-[b]	AP8101	→	DUMMY2[e]	
420	-[b]	AP8102	→	DUMMY2[e]	
421	-[b]	AP8103	→	DUMMY2[e]	
422	-[b]	AP8104	→	DUMMY2[e]	
423	-[b]	UR8103	→	DUMMY[e]	k_{76}
424	-[b]	UR8107	→	DUMMY[e]	k_{76}
425	-[b]	UR8108	→	DUMMY[e]	k_{76}
426	1B[c]	BPIN + OH	→	RO28201 + RO2T	
427	2B[c]	BPIN + NO3	→	RO28202 + RO2T	
428	3B[c]	BPIN + O3	→	0.51 NOPI + 0.11 ACID + 0.03 CO + 0.84 HCHO + 0.35 H2O2 + 0.33 RO28203 + 0.33 OH + 0.16 ALKM + 0.16 CO2 + 0.33 RO2T	
429	4B[c]	BPIN + O	→	0.75 UR8201 + 0.25 NOPI	
430	5B[c]	RO28201 + NO	→	0.35 AP8201 + 0.65 NOPI + 0.65 HCHO + 0.65 NO2 + 0.65 HO2	
431	6B[c]	RO28201 + RO2T	→	0.3 UR8202 + 0.7 NOPI + 0.7 HCHO + RO2T + 0.7 HO2	
432	7B[c]	RO28201 + HO2	→	NOPI + OOH1	
433	8B[c]	RO28202 + NO	→	0.1 AP8202 + 0.4 UR8203 + 0.5 NOPI + 0.5 HCHO + 1.1 NO2 + 0.1 HO2	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
434	9B[c]	RO28202 + RO2T	→	0.318 NOPI + 0.058 NO2 + 0.318 HCHO + 0.28 AP8201 + 0.142 AP8202 + 0.26 UR8203 + 0.102 HO2 + RO2T	
435	10B[c]	RO28202 + HO2	→	0.17 AP8202 + 0.83 NOPI + 0.83 OOH2 + 0.17 OOH1 + 0.83 NO2	
436	11B[c]	NOPI + OH	→	RO28203 + RO2T	
437	12B[c]	RO28203 + NO	→	RO28109 + NO2 + RO2T	
438	13B[c]	RO28203 + RO2T	→	0.35 UR8204 + 0.3 UR8205 + 0.35 RO28109 + 1.35 RO2T	
439	14B[c]	RO28203 + HO2	→	OOH2 + RO28109 + RO2T	
440	-[b]	AP8201	→	DUMMY2[e]	
441	-[b]	AP8202	→	DUMMY2[e]	
442	-[b]	UR8201	→	DUMMY[e]	k_{76}
443	-[b]	UR8202	→	DUMMY[e]	k_{76}
444	-[b]	UR8203	→	DUMMY[e]	k_{76}
445	-[b]	UR8204	→	DUMMY[e]	k_{76}
446	-[b]	UR8205	→	DUMMY[e]	k_{76}
447	1L[c]	DLMN + OH	→	0.6 RO28301 + 0.4 RO28302 + RO2T	
448	2L[c]	DLMN + NO3	→	0.4 RO28304 + 0.6 RO28303 + RO2T	
449	3L[c]	DLMN + O3	→	0.033 EDLM + 0.069 H2O2 + 0.134 RO28305 + 0.133 RO28306 + 0.033 UR8301 + 0.698 OH + 0.267 RO28307 + 0.431 CO + 0.236 LMKT + 0.036 ACID + 0.2 HCHO + 0.164 RO28308 + 0.698 RO2T	
450	4L[c]	DLMN + O	→	0.75 UR8302 + 0.25 UR8303	
451	5L[c]	RO28301 + NO	→	0.36 AP8301 + 0.64 EDLM + 0.64 NO2 + 0.64 HO2	
452	6L[c]	RO28301 + RO2T	→	0.3 UR8313 + 0.7 EDLM + RO2T + 0.7 HO2	
453	7L[c]	RO28301 + HO2	→	OOH1 + EDLM	
454	8L[c]	RO28302 + NO	→	0.36 AP8302 + 0.64 HCHO + 0.64 LMKT + 0.64 NO2 + 0.64 HO2	
455	9L[c]	RO28302 + RO2T	→	0.3 UR8314 + 0.7 HCHO + 0.7 LMKT + RO2T + 0.7 HO2	
456	10L[c]	RO28302 + HO2	→	OOH1 + LMKT	
457	11L[c]	RO28303 + NO	→	0.175 AP8303 + 0.825 EDLM + 1.825 NO2 + 0.175 HO2	
458	12L[c]	RO28303 + RO2T	→	0.265 AP8301 + 0.175 AP8303 + 0.56 EDLM + 0.56 NO2 + 0.105 HO2 + RO2T	
459	13L[c]	RO28303 + HO2	→	0.175 AP8303 + 0.825 OOH2 + 0.175 OOH1 + 0.825 EDLM + 0.825 NO2	
460	14L[c]	RO28304 + NO	→	0.17 AP8304 + 0.83 HCHO + 0.83 LMKT + 1.83 NO2 + 0.17 HO2	
461	15L[c]	RO28304 + RO2T	→	0.142 AP8304 + 0.28 AP8302 + 0.578 HCHO + 0.578 LMKT + 0.578 NO2 + 0.102 HO2 + RO2T	
462	16L[c]	RO28304 + HO2	→	0.17 AP8304 + 0.83 OOH2 + 0.17 OOH1 + 0.83 LMKT + 0.83 NO2	
463	17L[c]	RO28305 + NO	→	0.8 EDLM + RO23201 + NO2 + RO2T	
464	18L[c]	RO28305 + RO2T	→	0.2 UR8315 + 0.2 UR8316 + 0.48 EDLM + 0.6 RO23201 + 1.6 RO2T	
465	19L[c]	RO28305 + HO2	→	OOH2 + 0.8 EDLM + RO23201 + RO2T	
466	20L[c]	RO28306 + NO	→	RO28309 + HCHO + NO2 + RO2T	
467	21L[c]	RO28306 + RO2T	→	0.1 UR8307 + 0.1 UR8315 + 0.1 UR8316 + 0.7 RO28309 + 0.7 HCHO + 1.7 RO2T	
468	22L[c]	RO28306 + HO2	→	RO28309 + OOH2 + RO2T	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
469	23L[c]	RO28307 + NO	→	0.12 AP8305 + 0.79 RO28305 + 0.88 NO2 + 0.79 RO2T	
470	24L[c]	RO28307 + RO2T	→	0.9 RO28305 + 1.9 RO2T	
471	25L[c]	RO28307 + HO2	→	OOH2 + 0.9 RO28305 + 0.9 RO2T	
472	26L[c]	RO28308 + NO	→	0.77 LMKT + RO23201 + NO2 + RO2T	
473	27L[c]	RO28308 + RO2T	→	0.77 LMKT + RO23201 + 2 RO2T	
474	28L[c]	RO28308 + HO2	→	OOH2 + 0.77 LMKT + RO23201 + RO2T	
475	29L[c]	RO28309 + NO	→	CO2 + 0.88 RO28307 + NO2 + 0.88 RO2T	
476	30L[c]	RO28309 + NO2	→	PAN8301	
477	31L[c]	PAN8301	→	RO28309 + NO2	
478	32L[c]	RO28309 + RO2T	→	0.3 UR8308 + 0.2 UR8309 + 0.5 CO2 + 0.44 RO28307 + 1.44 RO2T	
479	33L[c]	RO28309 + HO2	→	UR8309	
480	34L[c]	EDLM + OH	→	RO28310 + RO2T	
481	35L[c]	EDLM + NO3	→	RO28311 + RO2T	
482	36L[c]	EDLM + O3	→	0.59 RP8301 + 0.09 ACID + 0.41 CO + 0.5 HCHO + 0.09 H2O2 + 0.41 OH + 0.41 RO28312 + 0.41 RO2T	
483	37L[c]	EDLM + UV	→	CO + RO28307 + RO2T + HO2	
484	38L[c]	RO28310 + NO	→	0.36 AP8306 + 0.64 RP8301 + 0.64 HCHO + 0.64 NO2 + 0.64 HO2	
485	39L[c]	RO28310 + RO2T	→	0.3 UR8317 + 0.7 RP8301 + 0.7 HCHO + RO2T + 0.7 HO2	
486	40L[c]	RO28310 + HO2	→	RP8301 + OOH1	
487	41L[c]	RO28311 + NO	→	0.17 AP8307 + 0.83 RP8301 + 0.83 HCHO + 1.83 NO2 + 0.17 HO2	
488	42L[c]	RO28311 + RO2T	→	0.28 AP8306 + 0.142 AP8307 + 0.578 RP8301 + 0.578 HCHO + 0.578 NO2 +0.102 HO2 + RO2T	
489	43L[c]	RO28311 + HO2	→	0.17 AP8307 + 0.83 OOH2 + 0.83 RP8301 + 0.17 OOH1 + 0.83 NO2	
490	44L[c]	RO28312 + NO	→	RP8302 + RO23201 + NO2 + RO2T	
491	45L[c]	RO28312 + RO2T	→	0.3 UR8318 + 0.7 RP8302 + 0.7 RO23201 + 1.7 RO2T	
492	46L[c]	RO28312 + HO2	→	RP8302 + OOH2 + RO23201 + RO2T	
493	47L[c]	LMKT + UV	→	0.77 LMKT + RO23201 + RO2T	
494	48L[c]	LMKT + OH	→	RO28313 + RO2T	
495	49L[c]	LMKT + NO3	→	RO28314 + RO2T	
496	50L[c]	LMKT + O3	→	0.445 RO28315 + 0.445 CO +0.89 OH + 0.055 UR8304 + 0.055 H2O2 + 0.055 RP8301 + 0.223 RO28316 + 0.222 RO28317 + 0.89 RO2T	
497	51L[c]	LMKT + O	→	0.75 UR8305 + 0.25 UR8306	5.43×10^{-11}
498	52L[c]	RO28313 + NO	→	0.35 AP8308 + 0.65 RP8301 + 0.65 NO2 + 0.65 HO2	
499	53L[c]	RO28313 + RO2T	→	0.3 UR8320 + 0.7 RP8301 + RO2T + 0.7 HO2	
500	54L[c]	RO28313 + HO2	→	RP8301 + OOH1	
501	55L[c]	RO28314 + NO	→	0.175 AP8309 + 0.825 RP8301 + 1.825 NO2 + 0.175 HO2	
502	56L[c]	RO28314 + RO2T	→	0.265 AP8308 + 0.175 AP8309 + 0.56 RP8301 + 0.56 NO2 + 0.105 HO2 + RO2T	
503	57L[c]	RO28314 + HO2	→	0.175 AP8309 + 0.825 OOH2 + 0.825 RP8301 + 0.175 OOH1 + 0.825 NO2	
504	58L[c]	RO28315 + NO	→	0.1 AP8310 + 0.9 RO28316 + 0.9 NO2 + 0.9 RO2T	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
505	59L[c]	RO28315 + RO2T	→	0.2 UR8321 + 0.2 UR8322 + 0.53 RO28316 + 1.53 RO2T	
506	60L[c]	RO28315 + HO2	→	OOH2 + 0.88 RO28316 + 0.88 RO2T	
507	61L[c]	RO28316 + NO	→	RP8303 + RO23201 + NO2 + RO2T	
508	62L[c]	RO28316 + RO2T	→	0.2 UR8319 + 0.2 UR8323 + 0.6 RP8303 + 0.6 RO23201 + 1.6 RO2T	
509	63L[c]	RO28316 + HO2	→	RP8303 + OOH2 + RO23201 + RO2T	
510	64L[c]	RO28317 + NO	→	RO28318 + HCHO + NO2 + RO2T	
511	65L[c]	RO28317 + RO2T	→	0.1 UR8310 + 0.1 UR8319 + 0.1 UR8323 + 0.7 RO28318 + 0.7 HCHO + 1.7 RO2T	
512	66L[c]	RO28317 + HO2	→	RO28318 + OOH2 + RO2T	
513	67L[c]	RO28318 + NO	→	CO2 + 0.875 RO28315 + NO2 + 0.875 RO2T	
514	68L[c]	RO28318 + NO2	→	PAN8302	
515	69L[c]	PAN8302	→	RO28318 + NO2	
516	70L[c]	RO28318 + RO2T	→	0.3 UR8311 + 0.2 UR8312 + 0.5 CO2 + 0.4375 RO28315 + 1.4375 RO2T	
517	71L[c]	RO28318 + HO2	→	UR8312	
518	82L[c]	RP8301 + OH	→	0.1 UR8304 + 0.1 O3 + 0.8 HO2 + 0.8 RP8301 + 0.9 CO2 + NO2 - NO	
519	83L[c]	RP8302 + OH	→	0.1 UR8324 + 0.1 O3 + 0.8 HO2 + 0.77 RP8302 + 0.9 CO2 + NO2 - NO	
520	84L[c]	RP8303 + OH	→	0.1 UR8324 + 0.1 O3 + 0.8 HO2 + 0.77 RP8303 + 0.9 CO2 + NO2 - NO	
521	72L[a,c]	AP8301	→	EDLM + NO2	
522	73L[a,c]	AP8302	→	HCHO + LMKT + NO2	
523	74L[a,c]	AP8303	→	RO28307 + NO2 + RO2T	
524	75L[a,c]	AP8304	→	LMKT + NO2	
525	-[b]	UR8301	→	AERS12	k_{413}
526	-[b]	UR8304	→	AERS12	k_{413}
527	-[b]	UR8307	→	AERS12	k_{413}
528	-[b]	UR8308	→	AERS12	k_{413}
529	-[b]	UR8309	→	AERS12	k_{413}
530	-[b]	UR8310	→	AERS12	k_{413}
531	-[b]	UR8311	→	AERS12	k_{413}
532	-[b]	UR8312	→	AERS12	k_{413}
533	-[b]	UR8324	→	AERS12	k_{413}
534	-[b]	AP8305	→	DUMMY2[e]	
535	-[b]	AP8306	→	DUMMY2[e]	
536	-[b]	AP8307	→	DUMMY2[e]	
537	-[b]	AP8308	→	DUMMY2[e]	
538	-[b]	AP8309	→	DUMMY2[e]	
539	-[b]	AP8310	→	DUMMY2[e]	
540	-[b]	UR8302	→	DUMMY[e]	k_{76}
541	-[b]	UR8303	→	DUMMY[e]	k_{76}
542	-[b]	UR8305	→	DUMMY[e]	k_{76}
543	-[b]	UR8306	→	DUMMY[e]	k_{76}
544	-[b]	UR8313	→	DUMMY[e]	k_{76}

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
545	-[b]	UR8314	→	DUMMY[e]	k_{76}
546	-[b]	UR8315	→	DUMMY[e]	k_{76}
547	-[b]	UR8316	→	DUMMY[e]	k_{76}
548	-[b]	UR8317	→	DUMMY[e]	k_{76}
549	-[b]	UR8318	→	DUMMY[e]	k_{76}
550	-[b]	UR8319	→	DUMMY[e]	k_{76}
551	-[b]	UR8320	→	DUMMY[e]	k_{76}
552	-[b]	UR8321	→	DUMMY[e]	k_{76}
553	-[b]	UR8322	→	DUMMY[e]	k_{76}
554	-[b]	UR8323	→	DUMMY[e]	k_{76}
555	84	BIOL + OH	→	RO28401 + RO2T	
556	85	BIOL + NO3	→	RO28402 + RO2T	
557	86	BIOL + O3	→	0.445 CO + 0.055 H2O2 + 0.445 HO2 + 0.89 OH + 0.055 UR8401 + 0.445 UR8402 + 0.055 RPR8401 + 0.445 RO28403 + 0.445 RO2T	
558	87	BIOL + O	→	0.75 UR8403 + 0.25 UR8404	$1.35 \times 10^{-10} \times e^{(-500.3/T)}$
559	188[a]	RO28401 + NO	→	AP8101	
560	188	RO28401 + NO	→	RPR8401 + NO2 + HO2	
561	189	RO28401 + RO2T	→	RPR8401 + RO2T + HO2 + O2	k_{50}
562	190[a]	RO28401 + HO2	→	RPR8401 + OOH1	k_{51}
563	191	RO28402 + NO	→	RPR8401 + 2 NO2	
564	192	RO28402 + RO2T	→	RPR8401 + NO2 + RO2T + O2	k_{50}
565	193[a]	RO28402 + HO2	→	OOH2 + RPR8401 + NO2	k_{51}
566	194[a]	RO28403 + NO	→	UR8405 + RO23201 + NO2 +0 RO2T	
567	195	RO28403 + RO2T	→	UR8405 + RO23201 + 2 RO2T + O2	k_{50}
568	196[a]	RO28403 + HO2	→	UR8405 + OOH2 + RO23201 + RO2T	k_{51}
569	309	RPR8401 + OH	→	RO28404 + RO2T + H2O	
570	310	RPR8401 + NO3	→	RO28404 + HNO3 + RO2T	
571	311	RPR8401 + UV	→	UR8402 + CO + 2 HO2	
572	312	RO28404 + NO	→	UR8402 + CO2 + NO2 + HO2	
573	313	RO28404 + NO2	→	PAN8401	
574	314[a]	PAN8401	→	RO28404 + NO2	
575	315	RO28404 + HO2	→	UR8401 + O3	
576	316	RO28404 + RO2T	→	UR8402 + CO2 + RO2T + HO2 + O2	k_{126}
577	-[b]	AP6101	→	DUMMY2[e]	
578	-[b]	UR8401	→	AERS12	k_{413}
579	-[b]	UR8402	→	DUMMY[e]	k_{76}
580	-[b]	UR8403	→	DUMMY[e]	k_{76}
581	-[b]	UR8404	→	DUMMY[e]	k_{76}
582	-[b]	UR8405	→	DUMMY[e]	k_{76}
583	88	BIOH + OH	→	RO28501 + RO2T	
584	89	BIOH + NO3	→	RO28502 + RO2T	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
585	90	BIOH + O3	→	0.445 CO + 0.055 H2O2 + 0.89 OH + 0.055 UR8501 + 0.055 UR8502 + 0.445 RO28503 + 0.445 RO28504 + 0.89 RO2T	
586	91	BIOH + O	→	0.75 UR8503 + 0.25 UR8504	
587	197[a]	RO28501 + NO	→	AP8201	
588	197	RO28501 + NO	→	0.3 UR8501 + 0.7 UR8504 + NO2 + HO2	
589	198	RO28501 + RO2T	→	0.3 UR8501 + 0.7 UR8504 + RO2T + HO2 + O2	k_{50}
590	199[a]	RO28501 + HO2	→	0.3 UR8501 + 0.7 UR8504 + OOH1	k_{51}
591	200	RO28502 + NO	→	0.3 UR8501 + 0.7 UR8504 + 2 NO2	
592	201	RO28502 + RO2T	→	0.3 UR8501 + 0.7 UR8504 + NO2 + RO2T + O2	k_{50}
593	202	RO28502 + HO2	→	0.3 UR8501 + 0.7 UR8504 + OOH2 + NO2	k_{51}
594	203	RO28503 + NO	→	AP8502	
595	203	RO28503 + NO	→	RO28505 + NO2 + RO2T	
596	204	RO28503 + RO2T	→	RO28505 + 2 RO2T + O2	k_{50}
597	205[a]	RO28503 + HO2	→	RO28505 + OOH2 + RO2T	k_{51}
598	209	RO28504 + NO	→	UR8505 + RO23201 + NO2 + RO2T	
599	210	RO28504 + RO2T	→	UR8505 + RO23201 + 2 RO2T + O2	k_{50}
600	211[a]	RO28504 + HO2	→	UR8505 + OOH2 + RO23201 + RO2T	k_{51}
601	206	RO28505 + NO	→	RPR8501 + RO23201 + NO2 + RO2T	
602	207	RO28505 + RO2T	→	RPR8501 + RO23201 + 2 RO2T + O2	k_{50}
603	208[a]	RO28505 + HO2	→	OOH2 + RPR8501 + RO23201 + RO2T	k_{51}
604	322	RPR8501 + OH	→	RO28506 + RO2T + H2O	
605	323	RPR8501 + NO3	→	HNO3 + RO28506 + RO2T	
606	324	RPR8501 + UV	→	CO + RO26101 + RO2T + HO2	
607	325	RPR8501 + UV	→	RO28506 + RO2T + HO2	
608	326	RO28506 + NO	→	CO2 + RO26101 + NO2 + RO2T	
609	327	RO28506 + NO2	→	PAN8501	
610	328	PAN8501	→	RO28506 + NO2 + RO2T	
611	329	RO28506 + HO2	→	UR8506 + O3	
612	330	RO28506 + RO2T	→	CO2 + RO26101 + 2 RO2T + O2	k_{126}
613	-[b]	AP6102	→	DUMMY2[e]	
614	-[b]	AP8502	→	DUMMY2[e]	
615	-[b]	UR8501	→	DUMMY[e]	k_{76}
616	-[b]	UR8502	→	AERS12	k_{413}
617	-[b]	UR8503	→	DUMMY[e]	k_{76}
618	-[b]	UR8504	→	DUMMY[e]	k_{76}
619	-[b]	UR8505	→	DUMMY[e]	k_{76}
620	-[b]	UR8506	→	AERS12	k_{413}
621	-[b]	EMS[d]	→	NO2	
622	-[b]	EMS[d]	→	NO	
623	-[b]	EMS[d]	→	CO	
624	-[b]	EMS[d]	→	HCHO	

Table SA2. *Continued*

Number	Previous	Reaction		Rate constants (cm molecule^{-1} s^{-1})
625	-[b]	EMS[d]	→	ALD1
626	-[b]	EMS[d]	→	ALD2
627	-[b]	EMS[d]	→	OLEL
628	-[b]	EMS[d]	→	OLEH
629	-[b]	EMS[d]	→	AROL
630	-[b]	EMS[d]	→	AROH
631	-[b]	EMS[d]	→	PAH
632	-[b]	EMS[d]	→	ISOP
633	-[b]	EMS[d]	→	SO2
634	-[b]	EMS[d]	→	H2SO4
635	-[b]	EMS[d]	→	APIN
636	-[b]	EMS[d]	→	BPIN
637	-[b]	EMS[d]	→	DLMN
638	-[b]	EMS[d]	→	BIOL
639	-[b]	EMS[d]	→	BIOH
640	-[b]	EMS[d]	→	ALKL
641	-[b]	EMS[d]	→	ALKM
642	-[b]	EMS[d]	→	ALKH
643	-[b]	EMS[d]	→	NH3
644	-[b]	NO2	→	DUMMY2[e]
645	-[b]	NO	→	DUMMY2[e]
646	-[b]	O3	→	DUMMY2[e]
647	-[b]	NO3	→	DUMMY2[e]
648	-[b]	N2O5	→	DUMMY2[e]
649	-[b]	HNO3	→	DUMMY2[e]
650	-[b]	HONO	→	DUMMY2[e]
651	-[b]	CO	→	DUMMY2[e]
652	-[b]	H2O2	→	DUMMY2[e]
653	-[b]	SO2	→	DUMMY2[e]
654	-[b]	H2SO4	→	DUMMY2[e]
655	-[b]	HCHO	→	DUMMY2[e]
656	-[b]	ACID	→	DUMMY2[e]
657	-[b]	ALD1	→	DUMMY2[e]
658	-[b]	ALD2	→	DUMMY2[e]
659	-[b]	MCR	→	DUMMY2[e]
660	-[b]	MGLY	→	DUMMY2[e]
661	-[b]	NH3	→	DUMMY2[e]
662	352[a]	AP1401 + OH	→	UR1401 + NO2 + H2O
663	351	AP1402 + OH	→	UR1401 + NO2 + H2O
664	360[b]	AP1501 + OH	→	UR1501 + NO2 + H2O

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
665	361	AP1502 + OH	→	UR1501 + NO2 + H2O	
666	-[b]	RPR2301	→	DUMMY2[e]	
667	-[b]	UR2301	→	DUMMY2[e]	
668	-[b]	PAN2301	→	DUMMY2[e]	
669	-[b]	PAN3201	→	DUMMY2[e]	
670	-[b]	PAN3301	→	DUMMY2[e]	
671	-[b]	PAN6101	→	DUMMY2[e]	
672	-[b]	UR6201	→	DUMMY2[e]	
673	-[b]	PAN6301	→	DUMMY2[e]	
674	-[b]	PAN6302	→	DUMMY2[e]	
675	-[b]	RP6301	→	DUMMY2[e]	
676	-[b]	PAN6303	→	DUMMY2[e]	
677	-[b]	UR6301	→	DUMMY2[e]	
678	-[b]	RP7101	→	DUMMY2[e]	
679	-[b]	RP7102	→	DUMMY2[e]	
680	-[b]	PAN7101	→	DUMMY2[e]	
681	-[b]	UR7102	→	DUMMY2[e]	
682	-[b]	RPR7303	→	DUMMY2[e]	
683	-[b]	RP7304	→	DUMMY2[e]	
684	-[b]	UR7302	→	DUMMY2[e]	
685	-[b]	UR7303	→	DUMMY2[e]	
686	-[b]	RPR7402	→	DUMMY2[e]	
687	-[b]	RP7403	→	DUMMY2[e]	
688	-[b]	RPR7404	→	DUMMY2[e]	
689	-[b]	RP7405	→	DUMMY2[e]	
690	-[b]	RP7406	→	DUMMY2[e]	
691	-[b]	UR7402	→	DUMMY2[e]	
692	-[b]	UR7604	→	DUMMY2[e]	
693	-[b]	UR8401	→	DUMMY2[e]	
694	-[b]	UR8402	→	DUMMY2[e]	
695	-[b]	UR8405	→	DUMMY2[e]	
696	-[b]	RPR8401	→	DUMMY2[e]	
697	-[b]	RPR8501	→	DUMMY2[e]	
698	-[b]	UR8501	→	DUMMY2[e]	
699	-[b]	UR8502	→	DUMMY2[e]	
700	-[b]	UR8505	→	DUMMY2[e]	
701	-[b]	UR8506	→	DUMMY2[e]	
702	-[b]	PAN8401	→	DUMMY2[e]	
703	-[b]	AP6101 + OH	→	ACID + NO2 + H2O	See Griffin et al. 2002 Table 6 (k=0.69x10^{-10} at 300K)
704	-[b]	PAN8501	→	DUMMY2[e]	

Table SA2. *Continued*

Number	Previous	Reaction			Rate constants (cm molecule^{-1} s^{-1})
705	-[b]	AP6102 + OH	→	ACID + NO2 + H2O	k_{703}
706	358[a]	AP8502 + OH	→	UR8503 + NO2 + H2O	
707	-[b]	PINA	→	DUMMY2[e]	
708	-[b]	NRPA	→	DUMMY2[e]	
709	353	AP7101 + OH	→	ARAL + NO2 + H2O	
710	350	AP7301 + OH	→	RPR7302 + NO2 + H2O	
711	354	AP7401 + OH	→	RPR7402 + NO2 + H2O	
712	355	AP7501 + OH	→	RPR7404 + NO2 + H2O	
713	-[b]	RP8101	→	DUMMY2[e]	
714	-[b]	RP8102	→	DUMMY2[e]	
715	-[b]	RP8103	→	DUMMY2[e]	
716	-[b]	PAN8101	→	DUMMY2[e]	
717	-[b]	PAN8102	→	DUMMY2[e]	
718	-[b]	PAN8103	→	DUMMY2[e]	
719	-[b]	UR8101	→	DUMMY2[e]	
720	-[b]	UR8102	→	DUMMY2[e]	
721	-[b]	UR8105	→	DUMMY2[e]	
722	-[b]	UR8106	→	DUMMY2[e]	
723	-[b]	UR8108	→	DUMMY2[e]	
724	359	AP7601 + OH	→	UR7603 + NO2 + H2O	
725	-[b,l]	AP6101 + UV	→	ACID + ALD1 + NO2	5.6×10^{-05}
726	-[b]	UR8203	→	DUMMY2[e]	
727	-[b]	EDLM	→	DUMMY2[e]	
728	-[b]	RP8301	→	DUMMY2[e]	
729	-[b]	RP8302	→	DUMMY2[e]	
730	-[b]	RP8303	→	DUMMY2[e]	
731	-[b]	AP8301	→	DUMMY2[e]	
732	-[b]	AP8302	→	DUMMY2[e]	
733	-[b]	AP8303	→	DUMMY2[e]	
734	-[b]	AP8304	→	DUMMY2[e]	
735	-[b,l]	AP6102 + UV	→	KETL + CO + NO2 + HO2	3.5×10^{-04}
736	-[b]	MVK	→	DUMMY2[e]	
737	-[b]	PAN8301	→	DUMMY2[e]	
738	-[b]	PAN8302	→	DUMMY2[e]	
739	-[b]	UR8301	→	DUMMY2[e]	
740	-[b]	UR8304	→	DUMMY2[e]	
741	-[b]	UR8307	→	DUMMY2[e]	
742	-[b]	UR8308	→	DUMMY2[e]	
743	-[b]	UR8309	→	DUMMY2[e]	
744	-[b]	UR8310	→	DUMMY2[e]	
745	-[b]	UR8311	→	DUMMY2[e]	

Table SA2. *Continued*

Number	Previous	Reaction		Rate constants (cm molecule^{-1} s^{-1})
746	-[b]	UR8312	→ DUMMY2[e]	
747	-[b]	UR8315	→ DUMMY2[e]	
748	-[b]	UR8316	→ DUMMY2[e]	
749	-[b]	UR8317	→ DUMMY2[e]	
750	-[b]	UR8318	→ DUMMY2[e]	
751	-[b]	UR8319	→ DUMMY2[e]	
752	-[b]	UR8322	→ DUMMY2[e]	
753	-[b]	UR8323	→ DUMMY2[e]	
754	-[b]	UR8324	→ DUMMY2[e]	
755	-[b]	AERS12	→ DUMMY2[e]	
756	-[b]	AS3PD	→ DUMMY2[e]	
757	-[b]	AS5PD	→ DUMMY2[e]	
758	-[b]	AS7PD	→ DUMMY2[e]	
759	-[b]	AS10PD	→ DUMMY2[e]	

Table SA2. *Continued*

[a] Reactions with products or yields that differ from the equivalent reaction in Table 2 of Griffin et al. (2002) or Tables S1, S3 and S5 of Chen et al. (2005).

[b] Reactions introduced to the mechanism after the original descriptions given in Table 2 of Griffin et al. (2002) or Tables S1, S3 and S5 of Chen et al. (2005).

[c] Reactions introduced or modified in Chen et al. (2005).

[d] Reactions 621 to 643 describe primary emissions. Emission rates of all species are calculated in the CACHE module sources.f as described above before being passed to the chemistry mechanism for inclusion in calculations of the aggregate rate constant.

[e] DUMMY allows for removal of unreactive species at each timestep to prevent accumulation. DUMMY2 simulates dry deposition. Deposition velocities of all species are calculated in the CACHE module sources.f as described above before being passed to the chemistry mechanism for inclusion in calculations of the aggregate rate constant.

[f] The product yields of these reactions were originally temperature dependent.

[g] The photolysis rates for the peroxide proxy species were increased as part of this work.

[h] The reaction rates for all RO_2^* + RO_2T involving non-acyl peroxy radicals were increased as part of this work.

[i] The reaction rates for all RO_2^* + HO_2 involving non-acyl peroxy radicals were increased as part of this work.

[j] There was a typographical error in the footnotes of Table 6 in Griffin et al. (2002). The coefficient set to 14 should in fact have read 12, which is the value used here.

[k] The reaction rates for all RO_2^* + RO_2T involving acyl peroxy radicals were increased as part of this work.

[l] The reaction rates and products for the photolysis of isoprene-derived nitrates are based on Müller et al., 2014.

MPMPO

Table SA3. Surrogate groups and their species in the MPMPO SOA module.

Surrogate Group[a]	Surrogate Characterisics[b]	Surrogate Species[c]	Species Code	Species	Parent VOC[d]
S1	low C#	oxalic acid	UR6201	keto-propanoic acid	AROL, MVK
			UR6301	oxalic acid	MCR
S2	anthropogenic, aromatic fragments, dissociative	2-methyl-5-formyl-2,4-hexadiendioic acid	RP7405	2-carboxyl-5-methyl-2, 4-hexadiendial	ARAL, ARAC
			RP7304	4-hydroxy-3, 5-dimethyl-2, 4-hexadienalic acid	AROO
			RP7406	2-methyl-5-formyl-2, 4-hexadiendioic acid	ARAL
			UR7303	4-hydroxy-3, 5-dimethyl-2, 4-hexadiendioic acid	AROO
			UR7402	2-methyl-5-carboxy-2, 4-hexadiendioic acid	ARAL
			UR7102	4,5-dimethyl-6-keto-2,4-heptadienoic acid	AROL
			AS3PD[e]	3-hydroxy-2, 4-dimethyl-2, 4-hexadienalic acid	N/A
S3	anthropogenic, aromatic fragments, non-dissociative	3-hydroxy-2,4-dimethyl-2, 4-hexadiendial	RPR7303	4-hydroxy-3, 5-dimethyl-2, 4-hexadiendial	AROO
			RP7403	2-methyl-5-formyl-2, 4-hexadiendial	ARAL
S4	biogenic, dissociative	2-hydroxy-3-isopropyl-5-keto-3-hexenoic acid	UR8401	2-hydroxy-3-isopropyl-6-keto-heptanoic acid	BIOL
			UR8404	2-hydroxy3-isopropyl-6-methyl-cyclohexanone	BIOL
			UR8502	3-isopropyl-6-keto-3-heptenoic acid	BIOH
			UR8506	3-isopropyl-4-hydroxy-2-butenoic acid	BIOH
			RP8101	pinalic-3-acid	APIN
			UR8101	pinonic acid	APIN
			UR8104	pinic acid	APIN
			UR8105	10-hydroxy-pinonic acid	APIN
			UR8106	1-hydroxy-pinonic acid	APIN
			UR8301	limononic acid	DLMN
			UR8304	keto-limononic acid	DLMN
			UR8307	7-hydroxy-limononic acid	DLMN
			UR8308	limonalic acid	DLMN
			UR8309	limonic acid	DLMN
			UR8310	7-hydroxy-keto-limononic acid	DLMN
			UR8311	keto-limonalic acid	DLMN
			UR8312	keto-limonic acid	DLMN
			UR8324	3-acetyl-4-formyl-butanoic acid	DLMN
			UR8102	norpinonic acid	APIN
			AS5PD[e]	2-hydroxyl-3-isopropyl-6-keto-heptanoic acid	N/A

Surrogate Group[a]	Surrogate Characterisics[b]	Surrogate Species[c]	Species Code	Species	Parent VOC[d]
S5	biogenic, non-dissociative	2-hydroxy-3-isopropyl-6-keto-heptanal	UR8405	2-hydroxy-3-isopropyl-hexadial	BIOL
			UR8501	3, 7-dimethyl-6-keto-3-octenal	BIOH
			RP8102	1-hydroxy-pinonaldehyde	APIN
			RP8103	10-hydroxy-pinonaldehyde	APIN
			AP8306	1-hydroxy-2-methyl-2-nitrato-3-formylmethyl-6-keto-heptane	DLMN
			AP8307	2-methyl-2-nitrato-3-formylmethyl-6-keto-heptanal	DLMN
			AP8308	1-methyl-1-nitrato-2-hydroxy-4-acetyl-cyclohexane	DLMN
			AP8309	1-methyl-1-nitrato-2-keto-4-acetyl-cyclohexane	DLMN
			AP8310	2-acetyl-5-keto-hexylnitrate	DLMN
			RP8301	keto-limonaldehyde (3-acetyl-6-keto-heptanal)	DLMN
			RP8302	3,6-dioxo-heptanal	DLMN
			RP8303	3-acetyl-pentadial	DLMN
			UR8315	5-keto-limonaldehyde	DLMN
			UR8316	5-hydroxy-limonaldehyde	DLMN
			UR8317	3-(1-methyl-1,2-dihydroxy-ethyl)-6-keto-heptanal	DLMN
			UR8318	3-acetyl-3-hydroxy-6-keto-heptanal	DLMN
			UR8319	3-acetyl-5-hydroxy-6-keto-heptanal	DLMN
			UR8320	1-methyl-1,2-dihydroxy-4-acetyl-cyclohexane	DLMN
			UR8321	3-hydroxymethyl-2,6-heptanedione	DLMN
			UR8322	3-formyl-2,6-heptanedione	DLMN
			UR8323	3-acetyl-5,6-dioxo-heptanal	DLMN
			AS10PD[e]	1-methyl-1-hydroxy-2-nitrato-3-oxo-4-isopropyl-cyclohexane	N/A
S6	anthropogenic, aromatic, low volatility	3,5-dimethyl-2-nitro- 4-hydroxy-benzoic acid	AP7301	2-nitrooxymethyl-6-methyl-phenol	AROO
			AP7501	4-nitrooxymethyl-benzoic acid	ARAC
			UR7605	2-(dimethyl-propenoic acid)-benzoic acid	PAH
			AS7PD[e]	3, 5-dimethyl-1, 4-dibenzoic acid	N/A
S7	anthropogenic, aromatic, high volatility	3,5-dimethyl-4-formyl-benzoic acid	ADAC	lumped aromatic diacids (terephthalic acid)	ARAL
			RPR7404	4-formyl-benzoic acid	ARAL, ARAC
			RP7601	2-(dimethyl-propenal)-benzaldehyde	PAH
			RP7603	2-(dimethyl-propenal)-benzoic acid	PAH
			UR7302	3-hydroxy-4-methyl-benzoic acid	AROO, ARAC
			UR7401	2-nitro-4-methyl-benzoic acid	ARAL, ARAC
			UR7604	2-carboxy-acetophenone	PAH
S8	anthropogenic, polyaromatic	1-methyl-2-nitrooxymethyl-naphthalene	AP7601	1-methyl-2-nitrooxymethyl-naphthalene	PAH
			UR7601	1, 2-dimethyl-3-hydroxy-naphthalene	PAH
			UR7602	1, 2-dimethyl-3-nitro-naphthalene	PAH
S9	anthropogenic, alkane-derived	8-hydroxy-11-hexadecylnitrate	AP1501	8-hexadecylnitrate	ALKH
			AP1502	8-hydroxy-11-hexadecylnitrate	ALKH
			UR1501	11-hydroxy-8-hexadecanone	ALKH

Table SA3. *Continued*

Surrogate Group[a]	Surrogate Characterisics[b]	Surrogate Species[c]	Species Code	Species	Parent VOC[d]
S10	biogenic, ring-retaining	1-methyl-1- hydroxy-2-nitrato-4-isopropyl-cyclohexane	AP8501	1-methyl-4-nitrato-4-isopropyl-5-hydroxy-cyclohexene	BIOH
			UR8403	1-methyl-3-hydroxy-4-isopropyl-1, 2-cyclohexane epoxide	BIOL
			AP8401	1-methyl-1-nitrato-2, 3-dihydroxy-4-isopropyl-cyclohexane	BIOL
			PINA	pinonaldehyde	APIN
			NRPA	norpinonaldehyde	APIN
			AP8101	2-nitrato-3-hydroxy-pinane	APIN
			AP8102	2-nitrato-3-oxo-pinane	APIN
			PAN8101	peroxy 2,2-dimethyl-3-acetyl-cyclobutyl-acetyl-nitrate	APIN
			PAN8102	peroxy 2,2-dimethyl-3-acetyl-cyclobutyl-formyl-nitrate	APIN
			PAN8103	peroxy 2,2-dimethyl-3-formylmethyl-cyclobutyl-formyl-nitrate	APIN
			UR8107	2,3-dihydroxy-pinane	APIN
			UR8108	2-(2,2-dimethyl-3-formylmethyl-cyclobutyl)-2-keto-acetaldehyde	APIN
			NOPI	nopinone	APIN, BPIN
			AP8201	2-nitrato-10-hydroxy-pinane	BPIN
			AP8202	2-formyl-2-nitrato-6-dimethyl-norpinane	BPIN
			UR8202	2,10-hydroxy-pinane	BPIN
			UR8204	3-hydroxy-nopinone	BPIN
			UR8205	3-oxo-nopinone	BPIN
			EDLM	limonaldehyde (3-isopropenyl-6-keto-heptanal)	DLMN
			AP8301	1-methyl-1-nitrato-2-hydroxy-4-isopropenyl-cyclohexane	DLMN
			AP8302	1-methyl-4-(1-methyl-1-nitrato-2-hydroxy-ethyl)-cyclohexene	DLMN
			AP8303	1-methyl-1-nitrato-2-keto-4-isopropenyl-cyclohexane	DLMN
			AP8304	2-methyl-2-nitrato-2-(4-methyl-4-cyclohexenyl)-acetaldehyde	DLMN
			PAN8301	peroxy 5-formyl-4-isopropenyl-pentionyl nitrate	DLMN
			PAN8302	peroxy 5-formyl-4-acetyl-pentionyl nitrate	DLMN
			UR8313	1-methyl-1,2-dihydroxy-4-isopropenyl-cyclohexane	DLMN
			UR8314	1-methyl-4-(1-methyl-1,2-dihydroxy-ethyl)-cyclohexene	DLMN
S11	biogenic, ring-retaining, low volatility	2,10-dinitrato-pinane	UR8203	2,10-dinitrato-pinane	BPIN
S12	non-volatile dimers of multifunctional acids from monoterpene oxidation	phthalic acid	AERS12	phthalic acid	N/A

Table SA3. *Continued*

[a]Notation of Griffin et al., (2003)
[b]Figure 1 of Griffin et al. (2005)
[c]Griffin et al. (2003), with updates noted in Griffin et al. (2005), Chen et al. (2006), and Chen et al. (2007)
[d]Notation of Griffin et al. (2002) and Chen and Griffin (2005): ALKH = lumped alkanes >C12 (*n*-hexadecane) ; AROL= lumped low SOA yield aromatic species (1,2,3-trimethyl-benzene); AROO = lumped phenolic species (2,6-dimethyl-phenol); ARAL = lumped aromatic monoaldehydes (*p*-tolualdehyde); ARAC = lumped aromatic monoacids (*p*-toluic acid); PAH = lumped gas-phase polycyclic aromatic hydrocarbons (1,2-dimethyl-naphthalene); APIN = α-pinene; BPIN = β-pinene; DLMN = *d*-limonene; BIOL = lumped low SOA yield monoterpene species (α-terpineol); BIOH = lumped high SOA yield monoterpene species (γ-terpinene)
[e]These are aqueous-phase oxidation products (see Chen et al., 2007); they are listed here for completeness but they are not considered in the canopy model.

Appendix B

RACM Chemistry Mechanism

The RACM chemistry scheme is described in full by Stockwell et al. (1997). Other than the additional species and reactions included by Geiger et al. (2003) to incorporate the Mainz Isoprene Mechanism, the scheme is as presented in Tables 1 and 2a-f in Stockwell et al. (1997). Table SB1 lists the species added to those listed in Table 1 (Stockwell et al., 1997); Table SB2 shows the reactions added to those listed in Table 2b or altered from the originals. All of the reaction rate coefficients are calculated as described in Tables 2a-f in Stockwell et al. (1997) and Table 3 in Geiger et al. (2003).

Table SB1. Species names and descriptions for the species added by Geiger et al. (2003) to the original RACM scheme (see Table 1 in Stockwell et al. 1997).

Species No.	Species Code	Species name or description
78	HACE	hydroxyacetone and other C3 ketones
79	ISHP	b-hydroxy hydroperoxides from ISOP+HO_2
80	ISON	b-hydroxyalkylnitrates from ISOP+NO and alkylnitrates from ISO+NO_3
81	MACP	peroxy radicals from MACR+HO
82	MAHP	hydroperoxides from MACP+HO_2
83	MPAN	peroxymethacryloylnitrate and other higher peroxyacylnitrates from isoprene oxidation
84	NALD	nitrooxyacetaldehyde

Table SB2. Reactions added by Geiger et al. (2003) to the original RACM scheme (see Table 2c in Stockwell et al. 1997). See Table 3 in Geiger et al. (2003) for reaction rate coefficients for these reactions.

Reaction No.	Reaction		
(R238)	ISOP + ISOP	→	2MACR + HCHO + HO2
(R239)	ISHP + HO	→	MACR + HO
(R240)	ISON + HO	→	HACE + NALD
(R241)	MACP + NO	→	NO2 + 0.25HACE + 0.25CO + 0.25ACO3 + 0.5MGLY + 0.75HCHO + 0.75HO2
(R242)	MACP + HO2	→	MAHP
(R243)	MACP + MACP	→	HACE + MGLY + 0.5HCHO + 0.5CO + HO2
(R244)	MACP + NO2	→	MPAN
(R245)	MPAN	→	MACP + NO2
(R246)	MPAN + HO	→	HACE + NO2
(R247)	MAHP + HO	→	MACP
(R248)	HACE + HO	→	MGLY + HO2
(R249)	NALD + HO	→	HCHO + CO + NO2
(R70)[a]	ISO + HO	→	ISOP
(R82)[a]	MACR + HO	→	MACP
(R102)[a]	ISO + NO3	→	ISON
(R110)[a]	ISO + O3	→	0.65MACR + 0.58HCHO + 0.1MACP + 0.1ACO3 + 0.08MO2 + 0.28ORA1 + 0.14CO + 0.09H2O2 + 0.25HO2 + 0.25HO
(R113)[a]	MACR + O3	→	0.9MGLY + 0.45ORA1 + 0.32HO2 + 0.22CO + 0.19OH + 0.1ACO3
(R139)[a]	ISOP + NO	→	MACR + NO2 + HCHO + HO2 + 0.046ISON
(R158)[a]	ISOP + HO2	→	ISHP

[a] These reactions, taken from Geiger et al. (2003) replace the reactions shown in Stockwell et al. (1997)

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