Supplementary materials

Urban and Remote cheMistry modELLing with the new chemical mechanism URMELL: Part I gas-phase mechanism development

M. L. Luttkus*[a], E. H. Hoffmann[b], A. Tilgner[b], R. Wolke[a], H. Herrmann[b], I. Tegen[a]

[a] Department Modelling of Atmospheric Processes, Leibniz Institute for Tropospheric Research (TROPOS), Leipzig, Germany

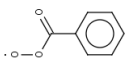
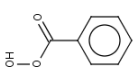
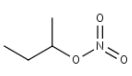
[b] Atmospheric Chemistry Department, Leibniz Institute for Tropospheric Research (TROPOS), Leipzig, Germany

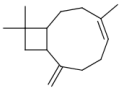
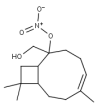
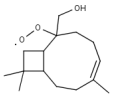
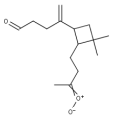
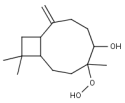
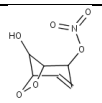
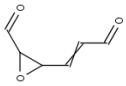
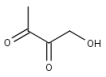
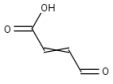
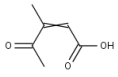
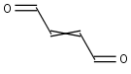
* Correspondence: luttkus@tropos.de

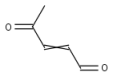
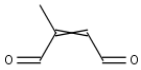
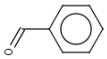
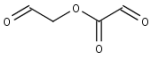
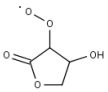
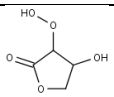
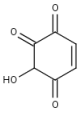
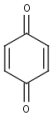
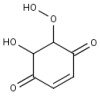
Supplement S1 – Gas-phase chemical mechanism URMELL

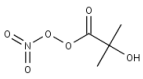
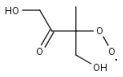
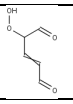
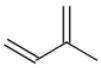
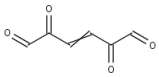
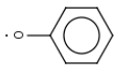
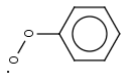
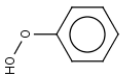
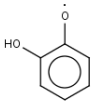
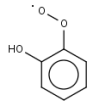
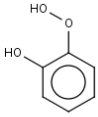
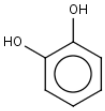
The chemical mechanism URMELL contains of 313 species (listed in Table S1-1), 733 chemical reactions (listed in Table S1-2) and 183 photolysis reactions (listed in Table S1-3). Table S1-1 contains species name, chemical and structural formula, a short description and the Alias set for the deposition scheme. Table S1-2 lists all chemical reactions, the rate coefficient as well as references and comments. Table S1-3 summarizes all photo-dissociation reactions and photolysis parameters are given in Table S1-4. Images for the chemical structures are e.g. taken from the MCM3.3.1 (http://mcm.york.ac.uk/home.htt), Wennberg *et al.*[1], Vereecken *et al.*[2] or are created using GECKO-A (http://geckoa.lisa.u-pec.fr/index.php).

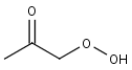
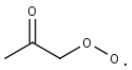
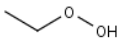
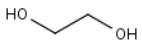
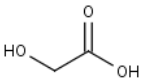
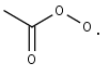
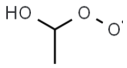
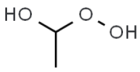
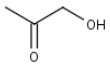
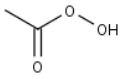
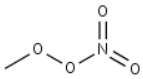
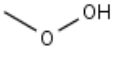
Table S1-1: List of 308 species used in URMELL chemistry mechanism including chemical & structural formula, description and assigned Alias for deposition scheme (new species bold).

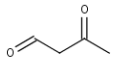
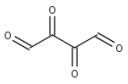
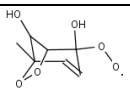
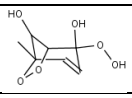
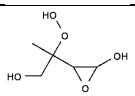
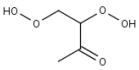
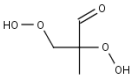
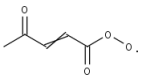
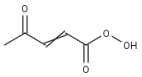
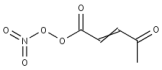
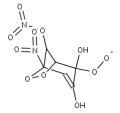
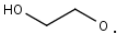
URMELL species	Chemical formula	Structural formula	Description	Alias for depos.
ACBZO2	C7H5O3		Acylperoxy radical from benzaldehyde	RO2
ACBZOOH	C7H6O3		Perbenzoic acid	PAA
ALKNO3	C5H11NO3		Alkyl nitrates from BIGALK oxidation (shown is SC4H9NO3)	ORA
ALKO2	C5H11O2		Peroxy radicals from BIGALK (shown is SC4H9O2)	RO2
ALKOH	C5H12		Lumped alcohol from BIGALK (shown is BUT2OL)	

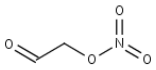
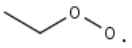
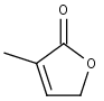
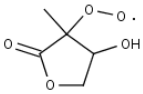
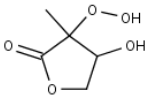
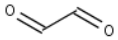
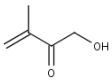
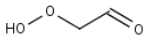
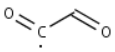
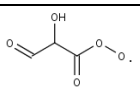
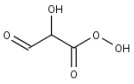
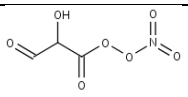
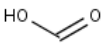
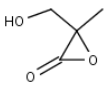
ALKOOH	C5H12O2		Organic hydroperoxides from BIGALK (shown is SC4H9OOH)	OP
APIN	C10H16		α-Pinene	
BCARY	C15H24		β-Caryophyllene and other sesquiterpenes	
BCNO3	C15H25NO4		Organonitrate from β-caryophyllene OH/O_3 + NO chemistry	ORA
BCO2	C15H25O3		Peroxy radical from β-caryophyllene OH/O_3 chemistry	RO2
BCOO	C15H24O3		Peroxy radical from β-caryophyllene O_3 chemistry	RO2
BCOOH	C15H26O3		Hydroperoxide from β-caryophyllene OH/O_3 + HO2 chemistry	OP
BENZ	C6H6		Benzene	
BENZ=O	C6H6O4		Bicyclic carbonyl oxidation product from benzene chemistry	ORA
BENZN	C6H7NO6		Bicyclic hydroxynitrate from benzene chemistry	ORA
BENZO2	C6H7O5		Bicyclic peroxy radical from benzene chemistry	RO2
BENZOOH	C6H8O5		Bicyclic hydroperoxide from benzene chemistry	OP
BEPOMUC	C6H6O3		Unsaturated epoxide-dialdehyde from OH + benzene	MeCHO
BIACETOH	C4H6O3		1-Hydroxy-2,3-butanedione	ORA
BIGACID1	C4H4O3		4-Oxo-2-butenoic acid, a product of aromatic oxidation	ORA
BIGACID2	C5H6O3		4-Oxo-2-pentenoic acid, a product of aromatic oxidation	ORA
BIGACID3	C6H8O3		3-methyl-4-oxo-2-pentenoic acid, a product of xylene oxidation	ORA
BIGALD1	C4H4O2		1,4-Butenedial, a ring-opening product of aromatic chemistry	MeCHO

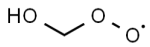
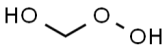
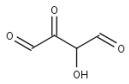
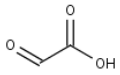
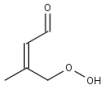
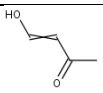
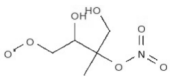
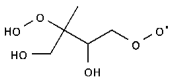
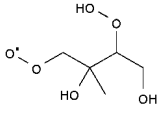
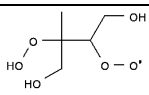
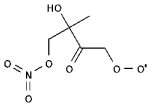
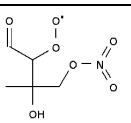
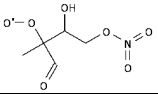
BIGALD2	C5H6O2		Unsaturated dicarbonyl, a product of aromatic oxidation	MeCHO
BIGALD3	C5H6O2		Unsaturated dialdehyde, a product of aromatic oxidation	MeCHO
BIGALD4	C6H8O2		Lumped unsaturated dicarbonyls, products of xylene oxidation	MeCHO
BIGALK	C5H12		Lumped alkanes C>3	
BIGENE	C4H8		Lumped alkenes C>3	
BPIN	C10H16		β-Pinene	
BZALD	C7H6O		Benzaldehyde	MeCHO
BZFUO	C4H4O4		BZFUO ring-opening product from BZFUONE chemistry	MeCHO
BZFUONE	C4H4O2		2(5H)-Furanone, reaction product from aromatic chemistry	MeCHO
BZFUONEO2	C4H6O5		Peroxy radical from 2(5H)-Furanone OH/NO_3 chemistry	RO2
BZFUONEOOH	C4H6O5		Hydroperoxide from 2(5H)-Furanone OH/NO_3 + HO_2 chemistry	PAA
BZQCO	C6H5O4		3-Hydroxycyclohex-5-ene-1,2,4-trione from quinone chemistry	ORA
BZQO2	C6H5O5		Peroxy radical from quinone chemistry	RO2
BZQONE	C6H4O2		Quinone, reaction product from phenol chemistry	MeCHO
BZQOOH	C6H6O5		Hydroperoxide from quinone chemistry	PAA
C	CH4		Methane	
C2H2	C2H2		Ethyne (acetylene)	
C2H4	C2H4		Ethene/ ethylene	
C33CO	C3H2O3		Oxopropanedial, reaction procuct of quinone chemistry	MeCHO
C3H6	C3H6		Propene	

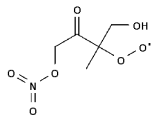
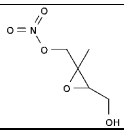
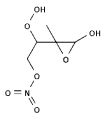
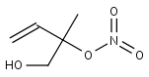
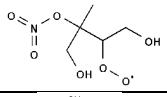
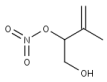
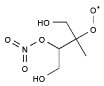
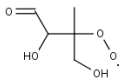
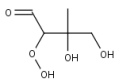
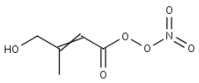
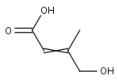
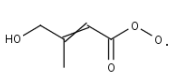
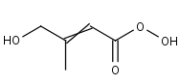
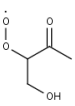
C3MDIALO2	C4H5O4		Peroxy radical from MACR	RO2
C3MDIALOH	C4H6O3		Hydroxy dialdehyde from MACR chemistry	ORA
C3MDIALOOH	C4H6O4		Hydroperxy dialdehyde from MACR chemistry	PAA
C4PAN5	C4H7NO6		Peroxynitrate from MBO chemistry	PAN
C59O2	C5H9O5		peroxy radical from ISOPOOH, IEPOX, HPALD	RO2
C5DIALOOH	C5H6O4		Hydroperxy dialdehyde from BEPOMUC chemistry	PAA
C5DIALO2	C5H5O4		Peroxy radical from BEPOMUC chemistry	RO2
C5H8	C5H8		Isoprene	
C615CO2O2	C6H7O4		Peroxy radical from TEPOMUC chemistry	RO2
C615CO2OOH	C6H8O4		Hydroperxy dialdehyde from TEPOMUC chemistry	PAA
C6CO4DB	C6H4O4		Reaction product of quinone chemistry	MeCHO
C6H5O	C6H5O		Phenoxy radical	
C6H5O2	C6H5O2		Phenylperoxy radical	RO2
C6H5OOH	C6H6O2		Phenyl hydroperoxide	OP
CATEC1O	C6H5O2		(2-Hydroxyphenyl) oxidanyl radical from catechol chemistry	
CATEC1O2	C6H5O3		Peroxy radical from catechol	RO2
CATEC1OOH	C6H6O3		Hydroperoxide from catechol	OP
CATECHOL	C6H6O2		Catechol	
CC	C2H6		Ethane	

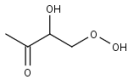
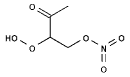
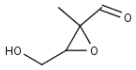
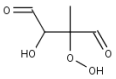
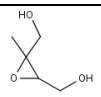
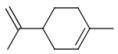
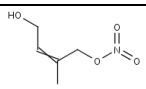
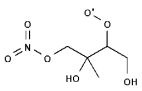
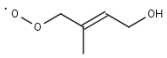
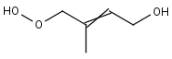
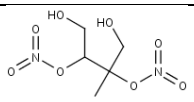
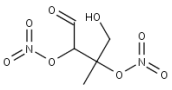
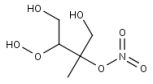
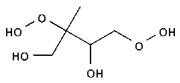
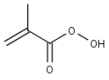
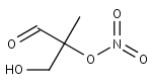
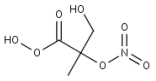
CC(=O)COO	C3H6O3		Acetone hydroperoxide	PAA
CC(=O)CO[O]	C3H5O3		Propyldioxy, peroxy radical from acetone	RO2
CCC	C3H8		Propane	
CCOO	C2H6O2		Ethyl hydroperoxide	OP
CH2OHCH2OH	C2H6O2		Ethylene glycol	
CH2OHCOOH	C2H4O3		Glycolic acid	ORA
CH3C(O)O2	C2H3O3		Acetylperoxy radical	RO2
CH3CH(OH)OO	C2H5O3		(1-Hydroxyethyl) dioxidanyl from ozone C3H6 chemistry	RO2
CH3CH(OH)OOH	C2H6O3		1-Hydroperoxyethanol from ozone C3H6 chemistry	OP
CH3CHO	C2H4O		Acetaldehyde	MeCHO
CH3COCH2OH	C3H6O2		Hydroxyacetone	ORA
CH3COCH3	C3H6O		Acetone	MeCHO
CH3COCOOH	C3H4O3		Pyruvic acid	ORA
CH3COOH	C2H4O2		Acetic acid	ORA
CH3COOOH	C2H4O3		Peracetic acid	PAA
CH3O2	CH3O2		Methylperoxy radical	RO2
CH3O2NO2	CH3NO4		(nitroperoxy)Methane	PAN
CH3OH	CH4O		Methanol	
CH3OOH	CH4O2		Methyl hydroperoxide	OP
CO	CO		Carbon monoxide	

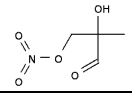
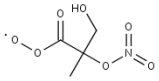
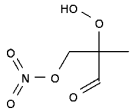
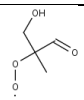
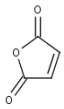
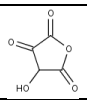
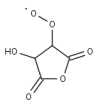
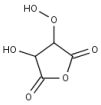
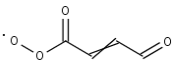
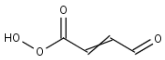
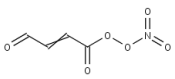
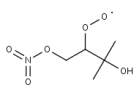
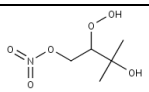
CO2C3CHO	C4H6O2		3-Oxobutanal	MeCHO
CO2C4DIAL	C4H2O4		2,3-Dioxobutanedial, reaction product of quinone chemistry	MeCHO
CO2H3CHO	C4H6O3		2-Hydroxy-3-oxobutanal	ORA
CRESO2	C7H9O6		Bicyclic peroxy radical from cresol chemistry	RO2
CRESOL	C7H8O		Lumped cresols from toluene oxidation	
CRESOOH	C7H10O6		Bicyclic hydroperoxide from cresol chemistry	OP
DHHPEPOX	C5H10O5		Lumped dihydroxy-hydroperoxy-epoxide from isoprene chemistry	PAA
DHPMEK	C4H8O5		Dihydroperoxy methyl ketone from isoprene chemmistry	PAA
DHPMPAL	C4H8O5		Dihydroperoxy methyl aldehyde from isoprene chemistry	PAA
DICARBO2	C5H5O4		Acylperoxy radical formed from aromatic oxidation, via unsaturated dicarbonyl chemistry	RO2
DICARBOOH	C5H6O4		Acylhydroperoxide formed from aromatic oxidation	PAA
DICARBPAN	C5H5NO6		Hydroxy-peroxyacyl nitrate from DICARBO2	PAN
DNCATECO2	C6H5N2O11		Dinitro-peroxyradical from nitrocatechol NO_3 chemistry	RO2
ELVOC			Extremely low volatile organic compound from monoterpene chemistry	PAA
ENEO2	C4H7O3		Lumped hydroxy peroxide alkene C>3 from BIGENE	RO2
EO	C2H5O2		Hydroxyalkoxy radical from OH ethene chemistry	
EO2	C2H5O3		Hydroxyperoxy radical from OH ethene chemistry	RO2
EOOH	C2H6O3		Hydroxyhydroperoxide from OH ethene chemistry	OP
EPOXDIALD	C4H4O3		Epoxydialdehyde from TEPOMUC chemistry	ORA

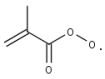
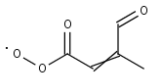
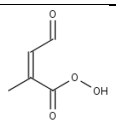
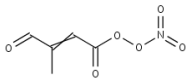
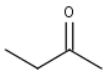
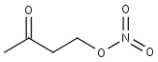
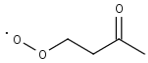
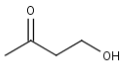
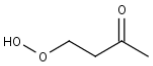
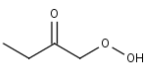
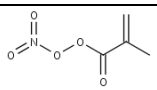
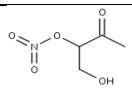
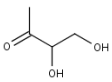
ETHLN	C2H3NO4		2-Oxoethyl nitrate	ORA
ETHPX	C2H5O2		Ethylperoxy radical	RO2
ETOH	C2H6O		Ethanol	
FUONE	C5H6O2		3-Methyl-2(5H)-furanone	MeCHO
FUONEO2	C6H7O5		Peroxy radical from FUONE chemistry	RO2
FUONEOOH	C6H8O5		Hydroperoxide from from FUONE chemistry	PAA
GLY	C2H2O2		Glyoxal	MeCHO
H2	H2		Hydrogen	
H2O2	H2O2		Hydrogen peroxide	H2O2
HCHO	CH2O		Formaldehyde	HCHO
HCOC5	C5H8O2		2-Hydroxy-3-methyl-3-butenal, from isoprene chemistry	ORA
HCOCH2OOH	C2H4O3		Hydroperoxyacetaldehyde	PAA
HCOCO	C2HO2		Formyl(oxo)methylium, product of glyoxal OH chemistry	
HCOCOHCO3	C3H3O5		Hydroxy dicarbonyl peroxide	RO2
HCOCOHCO3H	C3H4O5		Hydroxy dicarbonyl hydroperoxide	PAA
HCOCOHPAN	C3H3NO7		Hydroxy dicarbonyl peroxynitrate	PAN
HCOOH	CH2O2		Formic acid	ORA
HMML	C4H6O3		3-(Hydroxymethyl)-3-methyloxirane-2-one product from isoprene chemistry	ORA
HNO3	HNO3		Nitric acid	HNO3
HNO4	HNO4		Hydroxy nitrate	

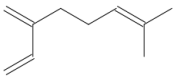
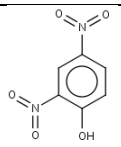
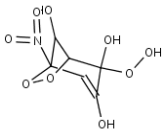
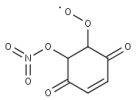
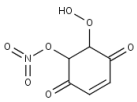
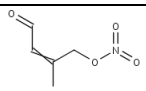
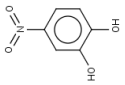
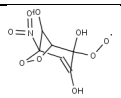
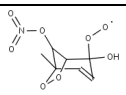
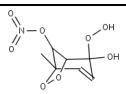
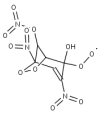
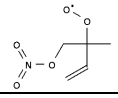
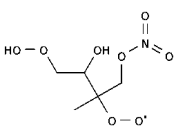
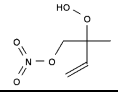
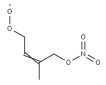
HO2	HO2		Hydroperoxyl radical	
HOCH2OO	CH3O3		Hydroxymethylperoxy radical from formaldehyde chemistry	RO2
HOCH2OOH	CH4O3		Hydroperoxymethanol from formaldehyde chemistry	OP
HOCOC4DIAL	C4H4O4		2-Hydroxy-3-oxobutanedial, product of quinone chemistry	MeCHO
HONO	HONO		Nitrous acid	HONO
HOOCCHO	C2H2O3		Glyoxylic acid	ORA
HPALD	C5H8O3		Unsaturated hydroperoxyaldehyde, from isoprene chemistry	PAA
HVMK	C4H6O2		4-Hydroxy-3-buten-2-one from IHNE chemistry	ORA
IBUTALOH	C4H8O2		Hydroxymethylpropanal, OH+MBO product	ORA
IBUTALOHO2	C4H7O4		Peroxy radical from IBUTALOH oxidation	RO2
IBUTALOHOOH	C4H8O4		hydroperoxide from IBUTALOH oxidation	PAA
IBUTALOOH	C4H8O3		2-Hydroxyisobutyric acid from IBUTALOH oxidation	ORA
IDHNBOO	C5H10NO7		Peroxy radical from isoprene NO3 chemistry	RO2
IDHPOO1	C5H11O6		Peroxy radical from ISOPBOOH/ LISOPACOOH OH chemistry	RO2
IDHPOO2	C5H11O6		Peroxy radical from ISOPDOOH/ LISOPACOOH OH chemistry	RO2
IDHPOO3	C5H11O6		Peroxy radical from ISOPBOOH/ ISOPDOOH OH chemistry	RO2
IHNC1O2	C5H8NO7		Peroxide from IHNE OH chemistry	RO2
IHNC2O2	C5H8NO7		Peroxide from IHNE OH chemistry	RO2
IHNC3O2	C5H8NO7		Peroxide from IHNE OH chemistry	RO2

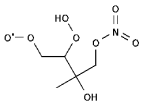
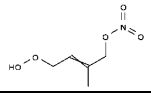
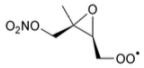
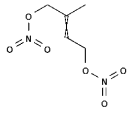
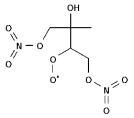
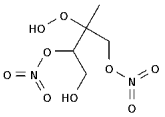
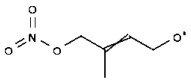
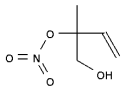
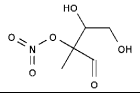
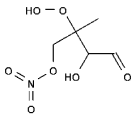
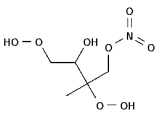
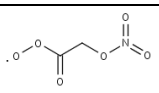
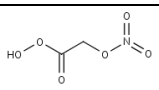
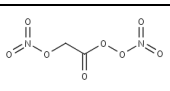
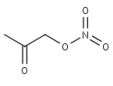
IHNC4O2	C5H8NO7		Peroxide from IHNE OH chemistry	RO2
IHNE	C5H9NO5		Hydroxynitrate epoxide from isoprene chemistry	ORA
IHNEOOH	C5H9NO7		Hydroxy-hydroperoxynitrate epoxide from isoprene chemistry	ORA
ISOPBNO3	C5H9NO4		1,4-hydroxynitrate from OH+isoprene chemistry	ORA
ISOPBNO3O2	C5H10NO7		Peroxy radical from ISOPBNO3	RO2
ISOPBO2	C5H9O3		1,-isomer of isoprene peroxy radical	RO2
ISOPBOOH	C5H10O3		hydroxyhydroperoxide from isoprene chemistry	OP
ISOPDNO3	5H9NO4		Hydroxynitrate from isoprene chemistry	ORA
ISOPDNO3O2	C5H10NO7		Peroxy radical from ISOPDNO3	RO2
ISOPDO2	C5H9O3		2,-Isomer of isoprene peroxy radical	RO2
ISOPDOOH	C5H10O3		Hydroxyhydroperoxide from isoprene chemistry	OP
LC578O2	C5H9O5		Dihydroxy aldehyde peroxy radical from isoprene chemistry	RO2
LC578OOH	C5H10O5		Dihydroxy aldehyde hydroperoxide from isoprene chemistry	PAA
LC5PAN1719	C5H7NO6		Lumped hydroxy-peroxyacyl nitrate for C=5	PAN
LHC4ACCHO	C5H8O2		Lumped hydroxyaldehyde from isoprene chemistry	ORA
LHC4ACCO2H	C5H8O3		Lumped 4-hydroxy acid from isoprene chemistry	ORA
LHC4ACCO3	C5H7O4		Lumped hydroxyl-acylperoxy radical C=5	RO2
LHC4ACCO3H	C5H8O4		Lumped hydroxyl-acylhydroperoxide	PAA
LHMVKABO2	C4H7O4		Lumped acetyl-hydroxy peroxide radical	RO2

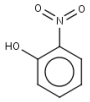
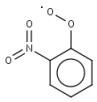
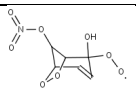
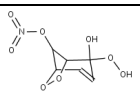
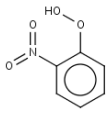
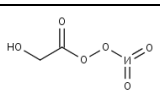
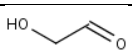
LHMVKABOOH	C4H8O4		Lumped acetyl-hydroxy hydroperoxide	PAA
LHMVKNOOH	C4H7NO6		Acetyl-hydroperoxy-nitrate from isoprene NO3 chemistry	ORA
LIECHO	C5H8O3		Lumped hydroxy-epoxide aldehyde from isoprene chemistry IEOPX quelle	ORA
LIECO3H	C5H8O5		Hydroperoxide from LIECHO	PAA
LIEPOX	C5H10O3		Isoprene derived epoxydiols 97% IOPOXB	PAA
LIMONENE	C10H16		Limonene	
LISOPACNO3	C5H9NO4		Lumped hydroxynitrate from isoprene chemistry	ORA
LISOPACNO3O2	C5H10NO7		Peroxy radical from LISOPACNO3	RO2
LISOPACO2	C5H9O3		Hydroxyl-peroxy radical from isoprene chemistry	RO2
LISOPACOOH	C5H10O3		Hydroxy-hydroperoxide from isoprene chemistry	OP
LISOPNO3NO3	C5H10N2O8		Dihydroxy-dinitrate from isoprene chemistry	ORA
LISOPNO3NO3=O	C5H8N2O8		Dinitrate-hydroxyketone from isoprene chemistry	ORA
LISOPNO3OOH	C5H11NO7		Dihydroxy-hydroperoxy nitrate	ORA
LISOPOOHOOH	C5H12O6		Lumped dihydroperoxide from isiprene OH chemistry	OP
MACO2H	C4H6O2		Methacrylic acid	ORA
MACO3H	C4H6O3		Acylhydroperoxide from MACR	PAA
MACR	C4H6O		Methacrolein	MeCHO
MACR2N3OH	C4H7NO5		Hydroxynitrate from MACR chemistry	ORA
MACR2NOOH	C4H7NO6		Acylhydroperoxide from MACRNO2	ORA
MACRENOL	C4H6O2		Hydroxy methacrolein	ORA

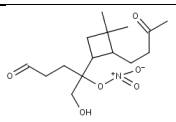
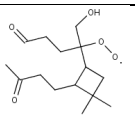
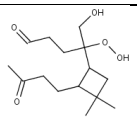
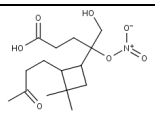
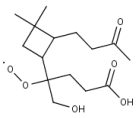
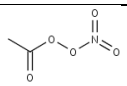
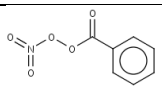
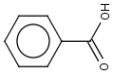
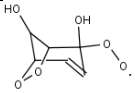
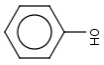
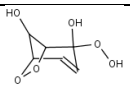
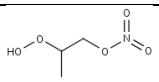
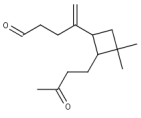
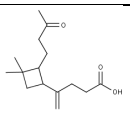
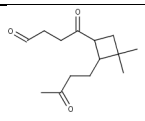
MACRN	C4H7NO5		Hydroxynitrate from isoprene NO_3 chemistry	ORA
MACRNO2	C4H6NO7		Acylperoxy radical from MACR2N3OH chemistry	RO2
MACRNOOH	C4H7NO6		Hydroperoxynitrate from MACRN chemistry	ORA
MACRO2	C4H7O4		Hydroxy peroxy radical from methacrolein chemistry	RO2
MACROH	C4H8O3		Dihydroxy-acetyl from MACR chemistry	ORA
MACROOH	C4H8O4		Hydroxy-hydroperoxide from methacrolein	PAA
MALANHY	C4H2O3		Maleic anhydride	MeCHO
MALANHYCO	C4H2O5		Hydroxy-ketone from MALANHY	
MALANHYO2	C4H3O6		Hydroxy-peroxide from MALANHY	RO2
MALANHYOOH	C4H4O6		Hydroxy-hydroperoxide from MALANHY	PAA
MALO2	C4H3O4		Acylperoxy radical from OH reaction with BIGALD1	RO2
MALOOH	C4H4O4		Acylhydroperoxide from MALO2	PAA
MALPAN	C4H3NO6		Acylperoxynitrate from MALO2	PAN
MBO	C5H10O		2-Methyl-3-buten-2-ol	
MBONO3O2	C5H10NO6		Peroxy radical from NO_3+MBO	RO2
MBONO3OOH	C5H11NO6		Hydroperoxy-nitrate from MBO chemistry	ORA
MBOO2	C5H11O4		Hydroxyl-peroxy radical from MBO chemistry	RO2
MBOOOH	C5H12O4		Hydroxy-hydroperoxide from MBO chemistry	OP

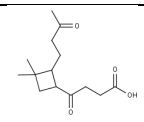
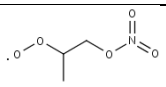
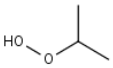
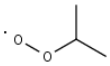
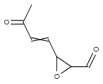
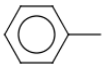
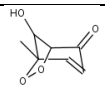
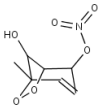
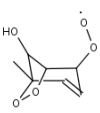
MCO3	C4H5O3		Acylperoxy radical from OH abstraction reaction with MACR	RO2
MDIALO2	C5H5O4		Peroxy radical from OH addition to BIGALD3	RO2
MDIALOOH	C5H6O4		Lumped Acyl-hydroperoxy-aldehyde	PAA
MDIALPAN	C5H5NO6		Acylperoxynitrate from MDIALO2	PAN
MEK	C4H8O		Methyl ethyl ketone	MeCHO
MEKANO3	C4H7NO4		Nitrate from MEK chemistry	ORA
MEKAO2	C4H7O3		Peroxy radical from MEK chemistry	RO2
MEKAOH	C4H8O2		C4 Hydroxy butanone	ORA
MEKAOOH	C4H8O3		Hydroperoxide from MEK chemistry	PAA
MEKBO2	C4H7O3		Peroxy radical from MEK chemistry	RO2
MEKBOH	C4H8O2		C4 Hydroxy butanone	ORA
MEKBOOH	C4H8O3		Hydroperoxide from MEK chemistry	PAA
MEKCO2	C4H7O3		Peroxy radical from MEK chemistry	RO2
MEKCOH	C4H8O2		C4 Hydroxy butanone	ORA
MEKCOOH	C4H8O3		Hydroperoxide from MEK chemistry	PAA
MGLY	C3H4O2		Methyl glyoxal	MeCHO
MPAN	C4H5NO5		Methacryloyl peroxynitrate	PAN
MVK	C4H6O		Methyl vinyl ketone	MeCHO
MVKN	C4H7NO5		Hydroxy nitrate from MVK chemistry	ORA
MVKOH	C4H8O3		Dihydroxy-acetyl from MVK chemistry	ORA

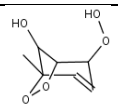
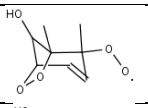
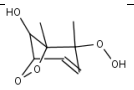
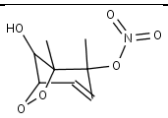
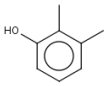
MYRC	C10H16		Myrcene	
N2O5			Dinitrogen pentoxide	
N2PHEN	C6H4N2O5		2,4-Dinitrophenol	ORA
NAROMOLOOH			Lumped peroxyhidrate from phenols with one or two nitro groups, completely conversion to SOA (structure shown for NCATECO2 + HO_2 product)	ORA
NBZQO2	C6H4NO7		Peroxy radical from quinone NO_3 chemistry	RO2
NBZQOOH	C6H5NO7		Hydroperoxide from quinone chemistry	ORA
NC4CHO	C5H7NO4		Nitrooxy-aldehyde from NO_3+isoprene chemistry	ORA
NCATECHOL	C6H5NO4		4-Nitrocatechol	ORA
NCATECO2	C6H6NO9		Bicyclic peroxy radical from 4-nitrocatechol OH chemistry	RO2
NCRESO2	C7H8NO8		Bicyclic peroxy radical from cresol NO_3 chemistry	RO2
NCRESOOH	C7H9NO8		Hydroperoxide from cresol chemistry	ORA
NDNPHENO2	C6H4N3O12		Bicyclic eroxy radical from 2,4-Dinitrophenol NO_3 chemistry	RO2
NH3			Ammonia	NH3
NISOPBO2	C5H8NO5		Peroxy radical from isoprene NO_3 oxidation	RO2
NISOPBOO	C5H11NO8		Peroxy radical from isoprene NO_3 chemistry with nitrate, hydroxyl, hydroperoxy and inner peroxy group	RO2
NISOPBOOH	C5H9NO5		Hydroperoxy-nitrate from isoprene NO_3 chemistry	ORA
NISOPDO2	C5H8NO5		Peroxy radical from isoprene NO_3 oxidation	RO2

NISOPDOO	C5H11NO8		Peroxy radical from isoprene NO_3 chemistry with nitrate, hydroxyl, hydroperxy and terminal peroxy group	RO2
NISOPDOOH	C5H9NO5		Hydroperoxy-nitrate from isoprene NO_3 chemistry	ORA
NISOPEOO1E	C5H8N1O6		Peroxy-nitrate radical from isoprene NO_3 chemistry with cyclic ether ring	RO2
NISOPEOO1Z	C5H8N1O6		Peroxy-nitrate radical from isoprene NO_3 chemistry with cyclic ether ring	RO2
NISOPN	C5H8N2O6		Lumped dinitrate from isoprene NO_3 chemistry	ORA
NISOPNOO	C5H9N2O8		Lumped peroxy radical from NISOPN	RO2
NISOPNOOH	C5H10N2O9		Lumped hydroxy-hydroperoxy dinitrate from isoprene chemistry	ORA
NISOPO	C5H9NO4		Nitrate-oxyradical from isoprene chemistry	
NISOPOH	C5H9NO4		Lumped Hydroxynitrate from isoprene NO_3 chemistry	ORA
NISOPOHOH=O	C5H9NO6		Dihydroxy-nitrate-aldehyde from isoprene NO_3 chemistry	ORA
NISOPOOHOH=O	C5H9NO7		Hydroperoxynitrate-Hydroxy-aldehyde form isoprene NO_3 chemistry	ORA
NISOPOOHOOH	C5H11NO8		Hydroxynitrate dihydrperoxide from isoprene NO_3 chimistry	ORA
NO	NO		Nitric oxide	NO
NO2	NO2		Nitrogen dioxide	NO2
NO3	NO3		Nitrate radical	NO3
NO3CH2CO3	C2H2NO6		Acylperoxyradical of 2-oxoethyl nitrate	RO2
NO3CH2CO3H	C2H2NO6		Acylhydroperoxy of 2-oxoethyl nitrate	ORA
NO3CH2PAN	C2H2N2O8		Peroxyacetyl-dinitrate	PAN
NOA	C3H5NO4		2-Oxopropyl-nitrate from NO_3+propene chemistry	ORA

NPHEN	C6H5NO3		2-Nitrophenol	ORA
NPHENO	C6H4NO3		2-Nitrophenoxyradical	
NPHENO2	C6H4NO4		2-Nitrophenperoxyradical	RO2
NPHENOLO2	C6H6NO8		Bicyclic peroxy radical from phenol NO_3 chemistry	RO2
NPHENOLOOH	C6H7NO8		Hydroperoxide from phenol chemistry	ORA
NPHENOOH	C6H5NO4		1-Hydroperoxy-2-nitrobenzene	ORA
NTERPNO3			Second generation products from monterpene+NO_3 chemistry	ORA
NTERPO2			Peroxy radical from NO_3+monoterpene chemistry	RO2
NTERPOOH			Hydroperoxide from NO_3+monoterpene chemistry	ORA
O1D	O		Excited oxygen atom	
O3	O3		Ozone	
O3PX	O3PX		Ground-state oxygen atom	
O=C(OO)C=O	C2H2O4		2-Oxoethaneperoxoic acid	PAA
O=CC(=O)O[O]	C2HO4		Glyoxyloylperoxyradical	RO2
OCC(=O)OO	C2H4O4		Ethaneperoxoic acid	PAA
OCC(=O)OON(=O)=O	C2H3NO6		2-Hydroxy-1-(nitroperoxy)ethanone	PAN
OCC(=O)O[O]	C2H3O4		2-Hydroxyacetylperoxy-radical	RO2
OH	OH		Hydroxyl radical	
OHCCH2OH	C2H4O2		Gglycolaldehyde	ORA

P1NO3	C15H25NO6		Higher generation Nitrate from β-caryophyllene OH/O_3 chemistry	ORA
P1O2	C15H25O5		Higher generation peroxy radical from β-caryophyllene OH/O_3 chemistry	RO2
PSQTOOH	C15H26O5		Higher generation non-volatile hydroperoxide from β-caryophyllene OH/O_3 chemistry	PAA
P2NO3	C15H25NO7		Higher generation non-volatile Nitrate from β-caryophyllene OH/O_3 chemistry	ORA
P2O2	C15H25O6		Higher generation peroxy radical from β-caryophyllene O_3 chemistry	RO2
PAN	C2H3NO5		Peroxy acetyl nitrate	PAN
PBZNIT	C7H5NO5		Peroxy benzoyl nitrate	PAN
PHCOOH	C7H6O2		Benzoic acid	ORA
PHENO2	C6H7O6		Bicyclic peroxy radical from phenol	RO2
PHENOL	C6H6O		Phenol, product of benzene chemistry	
PHENOOH	C6H8O6		Bicyclic hydroperoxide from phenol	OP
PO2	C3H7O3		Propene-derived peroxy radical	RO2
POOH	C3H8O3		Propene-derived hydroxy hydroperoxide	OP
PR2O2HNO3	C3H7NO5		Hydroperoxy-alkylnitrate from propene NO_3 chemistry	ORA
PROD1	C15H24O2		Lumped second generation products from β-caryophyllene OH/O_3 chemistry	MeCHO
PROD2	C15H24O3		Second generation acid from β-caryophyllene O_3 chemistry	ORA
PROD3	C14H22O3		Lumped hIgher generation products from β-caryophyllene OH/O_3 chemistry	MeCHO

PROD4	C14H22O4		Higher generation acid from β-caryophyllene O_3 chemistry	ORA
PRONO3BO2	C3H6NO5		Alkylnitrate-peroxy radical from propene NO_3 chemistry	RO2
PROPOOH	C3H8O2		Propyl hydroperoxide	OP
PROPPX	C3H7O2		Propylperoxy radical	RO2
SO2	SO2		Sulfure dioxide	SO2
SULF	H2SO4		Sulfuric acid	SULF
TEPOMUC	C7H8O3		Dialdehyde with cyclic ether from toluene and xylene chemistry	MeCHO
TERP2O2			Lumped peroxy radical from second generation monoterpene oxidation	RO2
TERP2OOH			Lumped second generation monoterpene hydroperoxide	PAA
TERPNO3			Lumped hydroxynitrates from monoterpene OH chemistry	ORA
TERPO2			Lumped peroxy radical from monoterpenes OH chemistry	RO2
TERPOOH			Lumped hydroperoxide from monoterpene OH chemistry	OP
TERPROD1			Lumped first generation monoterpene oxidation products	MeCHO
TERPROD2			Lumped second generation monoterpene oxidation product	MeCHO
TOL	C7H8		Toluene	
TOL=O	C7H8NO4		Bicyclic carbonyl oxidation product from toluene chemistry	ORA
TOLN	C7H9NO6		Bicyclic hydroxynitrate from toluene chemistry	ORA
TOLO2	C7H9O5		Bicyclic peroxy radical from toluene	RO2

TOLOOH	C7H10O5		Bicyclic hydroperoxide from toluene	OP
XYL	C8H10		Lumped xylene species	
XYLENO2	C8H11O5		Bicyclic peroxy radical from xylene OH chemistry	RO2
XYLENOOH	C8H12O5		Bicyclic hydroperoxide from xylene OH chemistry	OP
XYLNO3	C8H11NO6		Bicyclic hydroxynitrate from xylene chmeistry	ORA
XYLOL	C8H10O		Dimethyl-phenol from xylene chemistry	

URMELL contains several complex rate coefficients, which are provided hereafter. The corresponding parameter values are given in Table S1-2 as well as the related references.

$$k_{O3PX}(P_1, P_2) = M \times P_1 \times \left(\frac{T}{300}\right)^{P_2}$$

$$k_{HO2O3}(P_1, P_2, P_3) = P_1 \times \left(\frac{T}{300}\right)^{P_2} \times \exp\left(\frac{P_3}{T}\right)$$

$$k_{HO2}(P_1, P_2, P_3, P_4) = P_1 \times \exp\left(\frac{P_2}{T}\right) + M \times P_3 \times \exp\left(\frac{P_4}{T}\right)$$

$$k_{tro}(P_1, P_2, P_3, P_4, P_5, P_6, P_7) = \frac{k_0 \times k_\infty}{k_0 + k_\infty} \times P_7^{\frac{1}{1+k_1}}$$

$$k_1 = \left(\frac{log10\left(\frac{k_0}{k_\infty}\right)}{0.75 - 1.27 \times log10(P_7)}\right)^2$$

$$k_0 = M \times P_1 \times \left(\frac{T}{300}\right)^{P_2} \times \exp\left(\frac{P_3}{T}\right)$$

$$k_\infty = P_4 \times \left(\frac{T}{300}\right)^{P_5} \times \exp\left(\frac{P_6}{T}\right)$$

$$k_{HNO3}(P_1, P_2, P_3, P_4, P_5, P_6) = k_0 + \frac{k_2}{1 + k_2/k_1}$$

$$k_0 = P_1 \times \exp\left(\frac{P_2}{T}\right)$$

$$k_1 = P_3 \times \exp\left(\frac{P_4}{T}\right)$$

$$k_2 = M \times P_5 \times \exp\left(\frac{P_6}{T}\right)$$

$$k_{CO}(P_1, P_2) = P_1 \times \left(1 + \frac{M}{P_2}\right)$$

$$k_{iso}(P_1, P_2, P_3) = P_1 \times \exp\left(-\frac{P_2}{T}\right) \times \exp\left(\frac{P_3}{T^3}\right)$$

Table S1-2: Chemical reactions of URMELL, their reaction rate coefficient as well as references and comments. Complex rate coefficients are summarized beforehand. Next to the MCM3.3.1 and IUPAC data the following references have been used for the mechanism development: Schultz *et al.*[3], Chen *et al.*[4], Cox *et al.*[5], Jenkin *et al.*[6], Wennberg *et al.*[1], Vereecken *et al.*[2], Sheps *et al.*[7], Teng *et al.*[8], Müller *et al.*[9], Jenkin *et al.*[10], Khan *et al.*[11], Jenkin *et al.*[12] and Bates *et al.*[13]. All reaction equations marked with an X or a number from 1 to 5 deviate from original JAMv2b formula.

Reaction			**Rate coefficient**	**Reference & comments**	
O_x chemistry					
O3PX	$\xrightarrow{O_2}$	O3	$k_{O3PX}(6.0\times10^{-34}, -2.6)$	IUPAC	X
O3PX + O3	→		$8.0\times10^{-12}\times \exp(-2060/T)$	[3], IUPAC	
O1D	$\xrightarrow{O_2}$	O3PX	$3.2\times10^{-11}\times \exp(67/T)$	IUPAC	X
O1D	$\xrightarrow{N_2}$	O3PX	$2.15\times10^{-11}\times\exp(110/T)$	[3], IUPAC	
O1D	$\xrightarrow{H_2O}$	OH + OH	2.14×10^{-10}	IUPAC	X

HO_x chemistry					
H2 + OH	→	HO2	$7.7\times10^{-12}\times\exp(-2100/T)$	IUPAC, MCM	X
OH + O3	→	HO2	$1.7\times10^{-12}\times\exp(-940/T)$	[3], IUPAC	
HO2 + O3	→	OH	$k_{HO2O3}(2.03\times10^{-16}, 4.57, 6.93)$	[3], IUPAC	
HO2 + HO2	$\xrightarrow{M}$	H2O2	$k_{HO2}(2.2\times10^{-13}, 600, 1.93\times10^{-13}, 980)$	[3], IUPAC	
HO2 + HO2	$\xrightarrow{H_2O}$	H2O2	$k_{HO2}(3.08\times10^{-34}, 2800, 2.66\times10^{-54}, 3180)$	[3], IUPAC	
H2O2 + OH	→	HO2	$2.9\times10^{-12}\times\exp(-160/T)$	IUPAC	X
OH + HO2	→		$4.8\times10^{-11}\times\exp(250/T)$	[3], IUPAC	

NO_x chemistry					
NO +O3PX	$\xrightarrow{M}$	NO2	$k_{tro}(1\times10^{-31}, -1.6, 0, 5\times10^{-11}, -0.3, 0, 0.85)$	IUPAC	X
NO2 + O3PX	→	NO	$5.1\times10^{-12}\times\exp(198/T)$	IUPAC	X

NO2 + O3PX	$\xrightarrow{M}$	NO3	$k_{tro}(1.3\times10^{-31}, -1.5, 0, 2.3\times10^{-11}, 0.24, 0, 0.6)$	IUPAC	X
NO + NO	$\xrightarrow{O_2}$	NO2 + NO2	$4.25\times10^{-39}\times\exp(663.5/T)$	IUPAC	X
NO2 + NO3	→	NO + NO2	$4.5\times10^{-14}\times\exp(-1260/T)$	MCM	X
NO2 + NO3	$\xrightarrow{M}$	N2O5	$k_{tro}(3.6\times10^{-30}, -4.1, 0, 1.9\times10^{-12}, 0.2, 0, 0.35)$	IUPAC	X
HO2 + NO	→	OH + NO2	$3.45\times10^{-12}\times\exp(270/T)$	IUPAC	X
NO + O3	→	NO2	$2.07\times10^{-12}\times\exp(-1400/T)$	IUPAC	X
NO2 + O3	→	NO3	$1.4\times10^{-13}\times\exp(-2470/T)$	IUPAC	X
NO3 + HO2	→	OH + NO2	4.0×10^{-12}	IUPAC, MCM	X
N2O5	$\xrightarrow{M}$	NO2 + NO3	$k_{tro}(1.3\times10^{-3}, -3.5, -11000, 9.7\times10^{14}, 0.1, -11080, 0.35)$	IUPAC	X
NO + OH	$\xrightarrow{M}$	HONO	$k_{tro}(7.4\times10^{-31}, -2.4, 0, 3.3\times10^{-11}, -0.3, 0, 0.81)$	IUPAC	X
HONO + OH	→	NO2	$2.5\times10^{-12}\times\exp(260/T)$	IUPAC	X
NO2 + OH	$\xrightarrow{M}$	HNO3	$k_{tro}(3.2\times10^{-30}, -4.5, 0, 3\times10^{-11}, 0, 0, 0.41)$	IUPAC	X
HNO3 + OH	→	NO3	$k_{HNO3}(2.4\times10^{-14}, 460, 2.7\times10^{-17}, 2199, 6.5\times10^{-34}, 1335)$	[3], IUPAC	
NO + NO3	→	NO2 + NO2	$1.8\times10^{-11}\times\exp(110/T)$	IUPAC	X
NO2 + HO2	$\xrightarrow{M}$	HNO4	$k_{tro}(1.4\times10^{-31}, -3.1, 0, 4\times10^{-12}, 0, 0, 0.4)$	IUPAC	X
HNO4 + OH	→	NO2	$3.2\times10^{-13}\times\exp(690/T)$	IUPAC	X
HNO4	$\xrightarrow{M}$	HO2 + NO2	$k_{tro}(4.1\times10^{-5}, 0, -10650, 6\times10^{15}, 0, -11170, 0.4)$	IUPAC	X
NO3 + OH	→	HO2 + NO2	2.0×10^{-11}	IUPAC	X
NH3 + OH	→		$3.5\times10^{-12}\times\exp(-925/T)$	[3], IUPAC	X

Sulfur chemistry					
SO2 + OH	$\xrightarrow{M}$	SULF	$k_{tro}(2.8\times10^{-31}, -2.6, 0, 2\times10^{-12}, 0, 0, 0.53)$	IUPAC with F_c for 298K	X

C1 chemistry					
CH4 + OH	→	CH3O2	$1.85\times10^{-12}\times\exp(-1690/T)$	MCM	X
CH3O2 + NO	→	HCHO + HO2 + NO2	$2.3\times10^{-12}\times\exp(360/T)$	IUPAC	X
CH3O2 + CH3O2	→	HCHO + HO2 + HCHO + HO2	$7.4\times10^{-13}\times\exp(-520/T)$	[3], IUPAC	
CH3O2 + CH3O2	→	HCHO + CH3OH	$2.33\times10^{-14}\times\exp(678/T)$	[3], IUPAC	
CH3O2 + OH	→	0.95 HCHO + 1.9 HO2 + 0.0275 HOCH2OOH + 0.02 HCHO + 0.02 H2O2 + 0.0025 HCOOH	$3.7\times10^{-11}\times\exp(350/T)$	IUPAC; for sCI see sec. 2.6	X
CH3O2 + HO2	→	0.9 CH3OOH + 0.1 HCHO	$3.8\times10^{-13}\times\exp(780/T)$	IUPAC	X
CH3O2 + NO2	$\xrightarrow{M}$	CH3O2NO2	$k_{tro}(2.5\times10^{-30}, -5.5, 0, 1.8\times10^{-11}, 0, 0, 0.36)$	IUPAC	X
CH3O2 + NO3	→	HCHO + HO2 + NO2	1.2×10^{-12}	IUPAC	X
CH3O2NO2	$\xrightarrow{M}$	CH3O2 + NO2	$k_{tro}(9\times10^{-5}, 0, -9690, 1.1\times10^{16}, 0, -10560, 0.36)$	IUPAC	X
CH3OOH + OH	→	0.6 CH3O2 + 0.4 HCHO + 0.4 OH	$5.3\times10^{-12}\times\exp(190/T)$	MCM	X
HCHO + OH	→	HO2 + CO	$1.25\times10^{-17}\times T^2\times\exp(615/T)$	IUPAC	X
HCHO + HO2	→	HOCH2OO	$9.7\times10^{-15}\times\exp(625/T)$	[3], IUPAC	
HCHO + NO3	→	HNO3 + CO + HO2	5.5×10^{-16}	IUPAC	X
CO + OH	→	HO2	$k_{CO}(1.44\times10^{-13}, 4.2\times10^{19})$	IUPAC	X
CH3OH + OH	→	HCHO + HO2	$6.38\times10^{-18}\times T^2\times\exp(144/T)$	IUPAC	X
HCOOH + OH	→	HO2	4.5×10^{-13}	MCM	X
HOCH2OO	→	HO2 + HCHO	$2.4\times10^{12}\times\exp(-7000/T)$	[3], IUPAC	
HOCH2OO + NO	→	HO2 + HCOOH + NO2	5.6×10^{-12}	IUPAC	X
HOCH2OO + HO2	→	0.5 HCOOH + 0.2 OH + 0.5 HOCH2OOH + 0.2 HO2	$5.6\times10^{-15}\times\exp(2300/T)$	IUPAC; see text sect. 2.2	X
HOCH2OO + HOCH2OO	→	2 HCOOH + 2 HO2	5.5×10^{-12}	IUPAC; see text sect. 2.2	X
HOCH2OOH + OH	→	HOCH2OO	2.9×10^{-11}	[4]	X

C2 chemistry					
C2H2 + OH	$\xrightarrow{M}$	0.636 GLY + 0.636 OH + 0.364 HCOOH + 0.364 CO + 0.364 HO2	$k_{tro}(5\times10^{-30}, -1.5, 0, 1\times10^{-12}, 0, 0, 0.37)$	MCM, IUPAC	X
C2H4 + OH	$\xrightarrow{M}$	EO2	$k_{tro}(8.6\times10^{-29}, -3.1, 0, 9\times10^{-12}, -0.85, 0, 0.48)$	MCM, IUPAC	X
C2H4 + O3	→	1.168 HCHO + 0.168 H2O2 + 0.27 HO2 + 0.17 OH + 0.35 CO + 0.021 HCOOH + 0.18 H2 + 0.231 HOCH2OOH	$6.82\times10^{-15}\times\exp(-2500/T)$	IUPAC, [5]	4
EO2 + HO2	→	EOOH	1.3×10^{-11}	MCM, IUPAC	X
EOOH + OH	→	0.21 EO2 + 0.79 OHCCH2OH + 0.79 OH	$1.45\times10^{-12}\times\exp(684/T)$	[12], MCM	X
EO2 + NO	→	EO + NO2	8.7×10^{-12}	IUPAC, only dominant path	X
EO2 + CH3O2	→	0.5 EO + 0.75 HCHO + 0.5 HO2 + 0.25 CH3OH + 0.25 OHCCH2OH + 0.25 CH2OHCH2OH	$4.0\times10^{-11}\times\exp(1000/T)$	[3]; but considering $R_{-H}O + R'OH$ and $ROH + R'_{-H}O$	X
EO2 + CH3C(O)O2	→	CH3O2 + EO	1.0×10^{-11}	[3]	
EO	→	HO2 + HCHO + HCHO	$1.6\times10^{11}\times\exp(-4150/T)$	[3]	
EO	$\xrightarrow{O_2}$	HO2 + OHCCH2OH	1.0×10^{-14}	[3]	
CH2OHCH2OH + OH	→	OHCCH2OH + HO2	1.45×10^{-11}	MCM	X
CC + OH	→	ETHPX	$1.49\times10^{-17}\times T^2\times\exp(-499/T)$	IUPAC, MCM	X
ETHPX + NO	→	CH3CHO + NO2 + HO2	$2.55\times10^{-12}\times\exp(380/T)$	[3], IUPAC	X
ETHPX + HO2	→	CCOO	$6.4\times10^{-13}\times\exp(710/T)$	[3], IUPAC	X
ETHPX + CH3O2	→	0.7 HCHO + 0.8 CH3CHO + HO2 + 0.3 CH3OH + 0.2 ETOH	2.0×10^{-13}	[3]	
ETHPX + CH3C(O)O2	→	CH3CHO + HO2 + CH3O2	$1.8\times10^{-12}\times\exp(500/T)$	[3]	
ETHPX + ETHPX	→	1.6 CH3CHO + 1.2 HO2 + 0.4 ETOH	7.6×10^{-14}	[3]	
CCOO + OH	→	0.5 ETHPX + 0.5 CH3CHO + 0.5 OH	$1.94\times10^{-12}\times\exp(339/T)$	[3, 12]	X
CH3CHO + OH	→	CH3C(O)O2	$4.7\times10^{-12}\times\exp(345/T)$	[3], IUPAC	X
CH3CHO + NO3	→	HNO3 + CH3C(O)O2	$1.4\times10^{-12}\times\exp(-1860/T)$	[3], IUPAC	X
CH3C(O)O2 + NO	→	NO2 + CH3O2	$7.5\times10^{-12}\times\exp(290/T)$	[3]	

CH3C(O)O2 + NO2	$\xrightarrow{M}$	PAN	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	IUPAC	1
CH3C(O)O2 + NO3	→	NO2 + CH3O2	4.0×10^{-12}	MCM	X
CH3C(O)O2 + HO2	→	0.13 CH3COOH + 0.13 O3 + 0.37 CH3COOOH + 0.5 CH3O2 + 0.5 OH	$1.73\times10^{-12}\times\exp(730/T)$	IUPAC	2
CH3C(O)O2 + CH3O2	→	0.9 CH3O2 + HCHO + 0.9 HO2 + 0.1 CH3COOH	$2.0\times10^{-12}\times\exp(500/T)$	[3]	
CH3COOOH + OH	→	CH3C(O)O2	3.0×10^{-14}	IUPAC main path	X
PAN + OH	→	HCHO + CO + NO2	3.0×10^{-14}	MCM	X
PAN	$\xrightarrow{M}$	CH3C(O)O2 + NO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	IUPAC	X
CH3C(O)O2 + CH3C(O)O2	→	CH3O2 + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	[3]	
OHCCH2OH + OH	→	0.2 GLY + 0.2 HO2 + 0.8 OCC(=O)O[O]	1.0×10^{-11}	[3]	
OHCCH2OH + NO3	→	OCC(=O)O[O] + HNO3	$1.44\times10^{-12}\times\exp(-1862/T)$	[3]	
OCC(=O)O[O] + HO2	→	0.5 HO2 + 0.5 HCHO + 0.5 OH + 0.13 CH2OHCOOH + 0.13 O3 + 0.37 OCC(=O)OO	$2.11\times10^{-12}\times\exp(730/T)$	[6]	2
OCC(=O)OO + OH	→	OCC(=O)O[O]	$1.13\times10^{-12}\times\exp(497/T)$	[3, 12]	
OCC(=O)O[O] + NO	→	NO2 + HO2 + HCHO	$7.5\times10^{-12}\times\exp(290/T)$	MCM	2
OCC(=O)O[O] + NO3	→	NO2 + HO2 + HCHO	4.0×10^{-12}	[3]	
OCC(=O)O[O] + NO2	$\xrightarrow{M}$	OCC(=O)OON(=O)=O	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
OCC(=O)OON(=O)=O + OH	→	HCHO + CO + NO2	1.12×10^{-12}	MCM	X
OCC(=O)OON(=O)=O	$\xrightarrow{M}$	OCC(=O)O[O] + NO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	MCM, IUPAC	X
OCC(=O)O[O] + CH3O2	→	1.9 HCHO + 1.8 HO2 + 0.1 CH2OHCOOH	$2.0\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
OCC(=O)O[O] + CH3C(O)O2	→	HCHO + HO2 + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
CH2OHCOOH + OH	→	HCHO + HO2	2.73×10^{-12}	MCM	X
GLY + OH	→	HCOCO	$6.6\times10^{-18}\times T^2\times\exp(820/T)$	IUPAC	4

GLY + NO3	→	HCOCO + HNO3	4.0×10^{-16}	IUPAC	4
HCOCO	$\xrightarrow{O_2}$	0.12 O=CC(=O)O[O] + 0.64 OH + 1.12 CO + 0.24 HO2	2.1×10^{-11}	MCM for T=298K	4
HCOCO	→	2 CO + HO2	$7\times10^{11}\times\exp(-3160/T)$	MCM	4
O=CC(=O)O[O] + HO2	→	0.13 HOOCCHO + 0.13 O3 + 0.37 O=C(OO)C=O + 0.5 HO2 + 0.5 CO + 0.5 OH	$2.11\times10^{-12}\times\exp(730/T)$	[6]	2
O=C(OO)C=O + OH	→	O=CC(=O)O[O]	$2.13\times10^{-11}\times\exp(600/T)$	[12], MCM	X
O=CC(=O)O[O] + NO	→	HO2 + CO + NO2	$7.5\times10^{-12}\times\exp(290/T)$	MCM	2
O=CC(=O)O[O] + NO3	→	HO2 + CO + NO2	4.0×10^{-12}	[3]	
O=CC(=O)O[O] + NO2	$\xrightarrow{M}$	HO2 + CO + NO3	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
O=CC(=O)O[O] + CH3O2	→	0.9 CO + 1.8 HO2 + HCHO + 0.1 HOOCCHO	$2.0\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
O=CC(=O)O[O] + CH3C(O)O2	→	CO + HO2 + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
HOOCCHO + OH	→	CO + HO2	$1.81\times10^{-12}\times\exp(588/T)$	[15], MCM	X
HCOCH2OOH + OH	→	0.76 GLY + 0.76 OH + 0.24 CO + 0.24 HO2 + 0.24 HCHO	$7.24\times10^{-12}\times\exp(178/T)$	[12], MCM	X
CH3COOH + OH	→	CH3O2	$8.4\times10^{-20}\times T^2\times\exp(1356/T)$	IUPAC, MCM	X
ETOH + OH	→	0.95 CH3CHO + 0.95 HO2 + 0.05 EO2	$6.7\times10^{-18}\times T^2\times\exp(511/T)$	IUPAC, MCM	X
ETHLN + OH	→	NO3CH2CO3	3.4×10^{-12}	[1]	X
ETHLN + NO3	→	NO3CH2CO3 + HNO3	$1.4\times10^{-12}\times\exp(-1860/T)$	[1]	X
NO3CH2CO3 + NO	→	HCHO + 2 NO2	$7.5\times10^{-12}\times\exp(920/T)$	[1]	X
NO3CH2CO3 + NO3	→	HCHO + 2 NO2	4.0×10^{-12}	[1]	X
NO3CH2CO3 + NO2	$\xrightarrow{M}$	NO3CH2PAN	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
NO3CH2CO3 + HO2	→	0.63 HCHO + 0.63 NO2 + 0.37 OH + 0.13 O3 + 0.37 NO3CH2CO3H	$2.8\times10^{-12}\times\exp(730/T)$	[6]	X
NO3CH2CO3 + CH3O2	→	2 HCHO + NO2 + 0.9 HO2	$2.0\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2 chemistry	X
NO3CH2CO3 + CH3C(O)O2	→	HCHO + 2 NO2 + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2 chemistry	X
NO3CH2CO3H + OH	→	NO3CH2CO3	3.63×10^{-12}	[1]	X

NO3CH2PAN	$\xrightarrow{M}$	NO3CH2CO3 + NO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	MCM	X
NO3CH2PAN + OH	→	HCHO + CO + 2 NO2	1.12×10^{-14}	MCM	X

C3 chemistry					
C3H6 + OH	$\xrightarrow{M}$	PO2	$k_{tro}(8\times10^{-27}, -3.5, 0, 3\times10^{-11}, -1, 0, 0.5)$	[3], IUPAC	
C3H6 + O3	→	1.02384 HCHO + 0.3246 OH + 0.432 CH3CHO + 0.523 CO + 0.4426 HO2 + 0.0684 H2 + 0.08778 HOCH2OOH + 0.11584 H2O2 + 0.00798 HCOOH + 0.1 C + 0.05 CH3OH + 0.0715 CH3CH(OH)OOH + 0.0065 CH3COOH	$5.77\times10^{-15}\times\exp(-1880/T)$	[5]	4
C3H6 + NO3	→	PRONO3BO2	$4.6\times10^{-13}\times\exp(-1156/T)$	[3]	
CH3CH(OH)OOH + OH	→	CH3CH(OH)OO	2.8×10^{-11}	[2] for T=298	X
CH3CH(OH)OO	→	HO2 + CH3CHO	$2.4\times10^{12}\times\exp(-7000/T)$	Analog to HOCH2OO	X
CH3CH(OH)OO + NO	→	CH3O2 + HCOOH + NO2	5.6×10^{-12}	Analog to HOCH2OO	X
CH3CH(OH)OO + HO2	→	0.3 CH3COOH + 0.2 OH + 0.2 HCOOH + 0.2 CH3O2 + 0.5 CH3CH(OH)OOH	$5.6\times10^{-15}\times\exp(2300/T)$	Analog to HOCH2OO	X
CH3CH(OH)OO + CH3CH(OH)OO	→	2 HCOOH + 2 CH3O2	5.5×10^{-12}	Analog to HOCH2OO	X
PO2 + NO	→	CH3CHO + HCHO + HO2 + NO2	8×10^{-12}	[3]	
PO2 + NO3	→	CH3CHO + HCHO + HO2 + NO2	2.3×10^{-12}	MCM	X
PO2 + HO2	→	POOH	$7.5\times10^{-13}\times\exp(700/T)$	[3]	
PO2 + CH3O2	→	0.5 CH3CHO + 1.25 HCHO + HO2 + 0.5 CH3COCH2OH + 0.25 CH3OH	8.3×10^{-13}	[3]	
PO2 + CH3C(O)O2	→	CH3CHO + HCHO + HO2 + CH3O2	1.0×10^{-11}	[3]	
POOH + OH	→	0.14 PO2 + 0.86 OH + 0.86 CH3COCH2OH	$7.24\times10^{-13}\times\exp(1011/T)$	[3, 12]	X
CCC + OH	→	PROPPX	$1.65\times7\times T^2\times\exp(-87/T)$	[3,] IUPAC	X
PROPPX + NO	→	0.727 CH3COCH3 + NO2 + HO2 + 0.4095 CH3CHO	$2.7\times10^{-12}\times\exp(360/T)$	MCM (main path), ratios based on CCC + OH	X

				distribution, C_2H_5CHO approximated with 1.5 CH_3CHO	
PROPPX + HO2	→	PROPOOH	$7.5\times10^{-13}\times\exp(700/T)$	[3]	
PROPPX + CH3O2	→	HCHO + 2 HO2 + 0.727 CH3COCH3 + 0. 4095 CH3CHO	$3.75\times10^{-13}\times\exp(-40/T)$	[3], yields adopted from NO reaction	X
PROPPX + CH3C(O)O2	→	CH3O2 + HO2 + 0.727 CH3COCH3 + 0. 4095 CH3CHO	1.0×10^{-11}	[3], yields adopted from NO reaction	X
PROPOOH + OH	→	0.26 PROPPX + 0.55 CH3COCH3 + 0.74 OH + 0.285 CH3CHO	$2.27\times10^{-12}\times\exp(493/T)$	[12], MCM	X
CH3COCH3 + OH	→	CC(=O)CO[O]	$8.8\times10^{-12}\times\exp(-1320/T)$	MCM	X
CH3COCH3 + OH	→	CC(=O)CO[O]	$1.7\times10^{-14}\times\exp(423/T)$	MCM	X
CC(=O)CO[O] + NO	→	CH3C(O)O2 + HCHO + NO2	$2.9\times10^{-12}\times\exp(300/T)$	[3], IUPAC, MCM	
CC(=O)CO[O] + NO3	→	CH3C(O)O2 + HCHO + NO2	2.3×10^{-12}	MCM	X
CC(=O)CO[O] + HO2	→	0.15 CH3C(O)O2 + 0.15 HCHO + 0.15 OH + 0.85 CC(=O)COO	$1.36\times10^{-13}\times\exp(1250/T)$	MCM	X
CC(=O)CO[O] + CH3O2	→	0.3 CH3C(O)O2 + 0.2 CH3COCH2OH + 0.8 HCHO + 0.5 CH3OH + 0.3 HO2 + 0.5 MGLY	3.8×10^{-12}	IUPAC	X
CC(=O)CO[O] + CH3C(O)O2	→	0.5 CH3COOH + 0.5 MGLY + 0.5 CH3O2 + 0.5 CH3C(O)O2 + 0.5 HCHO	5.0×10^{-12}	IUPAC	X
CC(=O)COO + OH	→	0.52 CC(=O)CO[O] + 0.48 MGLY + 0.48 OH	$1.12\times10^{-12}\times\exp(500/T)$	[12], MCM	X
CH3COCOOH + OH	→	CH3C(O)O2	$4.9\times10^{-14}\times\exp(280/T)$	IUPAC, MCM	X
MGLY + OH	→	CH3C(O)O2 + CO	$1.9\times10^{-12}\times\exp(575/T)$	MCM	X
MGLY + NO3	→	CH3C(O)O2 + CO + HNO3	5.0×10^{-16}	IUPAC, MCM	X
CH3COCH2OH + OH	→	MGLY + HO2	$1.083\times10^{-12}\times\exp(307/T)$	[12], MCM	X
PRONO3BO2 + NO	→	0.83 HO2 + 0.83 NOA + 0.17 HCHO + 0.17 CH3CHO + 1.17 NO2	$2.7\times10^{-12}\times\exp(360/T)$	[3], MCM	X
PRONO3BO2 + NO3	→	0.83 HO2 + 0.83 NOA + 0.17 HCHO + 0.17 CH3CHO + 1.17 NO2	2.3×10^{-12}	[3], MCM	X
PRONO3BO2 + HO2	→	PR2O2HNO3	$1.5132\times10^{-13}\times\exp(1300/T)$	[3], MCM	X
PRONO3BO2 + CH3O2	→	0.915 HO2 + 0.915 NOA + 0.835 HCHO + 0.085 CH3CHO + 0.25 CH3OH + 0.085 NO2	1.0×10^{-12}	[3] added NO2	X
PRONO3BO2 + CH3C(O)O2	→	0.83 HO2 + 0.83 NOA + 0.17 HCHO + 0.17 CH3CHO + 0.17 NO2 + CH3O2	1.0×10^{-11}	[3]	

PR2O2HNO3 + OH	→	0.5 PRONO3BO2 + 0.5 NOA + 0.5 OH	7.0×10^{-12}	[3]	
NOA + OH	→	MGLY + NO2	$8.24\times10^{-13}\times\exp(-351/T)$	[3, 12]	X
HCOCOHCO3 + HO2	→	0.5 HO2 + 0.5 OH + 0.5 GLY + 0.5 HCOCOHCO3H	$2.62\times10^{-12}\times\exp(730/T)$	[6], MCM	X
HCOCOHCO3 + NO	→	HO2 + GLY + NO2	$7.5\times10^{-12}\times\exp(290/T)$	MCM	X
HCOCOHCO3 + NO2	$\xrightarrow{M}$	HCOCOHPAN	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
HCOCOHCO3 + NO3	→	HO2 + GLY + NO2	4.0×10^{-12}	MCM	X
HCOCOHCO3 + CH3O2	→	HCHO + 2 HO2 + GLY	$2.0\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	X
HCOCOHCO3 + CH3C(O)O2	→	HO2 + GLY + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	X
HCOCOHCO3H + OH	→	HCOCOHCO3	$5.44\times10^{-12}\times\exp(406/T)$	[12], MCM	X
HCOCOHPAN + OH	→	GLY + CO + NO2	6.97×10^{-11}	MCM	X
HCOCOHPAN	$\xrightarrow{M}$	HCOCOHCO3 + NO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	MCM	X
C33CO + OH	→	3 CO + HO2	$3.55\times10^{-12}\times\exp(591/T)$	[12], MCM	X

C4 chemistry					
BIGENE + OH	→	ENEO2	5.4×10^{-11}	[3]	
ENEO2 + NO	→	CH3CHO + 0.5 HCHO + 0.5 CH3COCH3 + HO2 + NO2	$4.2\times10^{-12}\times\exp(180/T)$	[3]	
ENEO2 + HO2	→	1.333 POOH	$7.5\times10^{-13}\times\exp(700/T)$	[3]	
ENEO2 + CH3O2	→	0.665 CH3COCH2OH + 0.5 CH3OH + 0.5 CH3CHO + 0.25 CH3COCH3 + 0.75 HCHO + HO2	1.0×10^{-12}	[3]	
ENEO2 + CH3C(O)O2	→	CH3CHO + 0.5 HCHO + 0.5 CH3COCH3 + HO2 + CH3O2	1.0×10^{-11}	[3]	
MEK + OH	→	0.294 MEKAO2 + 0.62 MEKBO2 + 0.086 MEKCO2	$1.5\times10^{-12}\times\exp(-90/T)$	[12], IUPAC, MCM	X
MEKAO2 + NO3	→	NO2 + 0.5 HCHO + 0.5 HO2 + 0.5 CO2C3CHO + 0.5 EO2	2.3×10^{-12}	MCM	X
MEKBO2 + NO3	→	CH3CHO + CH3C(O)O2 + NO2	2.3×10^{-12}	MCM	X
MEKCO2 + NO3	→	NO2 + HCHO + 1.5 CH3C(O)O2	2.3×10^{-12}	MCM, $C_2H_5CO_3$ approximated with 1.5 $CH_3C(O)O_2$	X

MEKAO2 + NO	→	0.967 NO2 + 0.4835 HCHO + 0.4835 HO2 + 0.4835 CO2C3CHO + 0.4835 EO2 + 0.033 MEKANO3	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
MEKBO2 + NO	→	CH3CHO + CH3C(O)O2 + NO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
MEKCO2 + NO	→	NO2 + HCHO + 1.5 CH3C(O)O2	$2.7\times10^{-12}\times\exp(360/T)$	MCM, $C_2H_5CO_3$ approximated with 1.5 $CH_3C(O)O_2$	X
MEKANO3 + OH	→	NO2 + CO2C3CHO	1.5×10^{-12}	[12], MCM	X
MEKAO2 + HO2	→	MEKAOOH	$1.81875\times10^{-13}\times\exp(1300/T)$	MCM	X
MEKBO2 + HO2	→	MEKBOOH	$1.81875\times10^{-13}\times\exp(1300/T)$	MCM	X
MEKCO2 + HO2	→	MEKCOOH	$1.81875\times10^{-13}\times\exp(1300/T)$	MCM	X
MEKAOOH + OH	→	OH + CO2C3CHO	$1.1\times10^{-13}\times\exp(1359/T)$	[12], MCM	X
MEKAOOH + OH	→	MEKAO2	$0.368\times10^{-12}\times\exp(635/T)$	[12], MCM	X
MEKBOOH + OH	→	OH + 2 CH3C(O)O2	$6.08\times10^{-13}\times\exp(678/T)$	[12], MCM	X
MEKBOOH + OH	→	MEKBO2	$0.368\times10^{-12}\times\exp(635/T)$	[12], MCM	X
MEKCOOH + OH	→	CO + 1.33 MGLY	$1.46\times10^{-12}\times\exp(298/T)$	[12], MCM; EGLYOX approximated with 1.33 MGLY	X
MEKCOOH + OH	→	MEKCO2	$0.368\times10^{-12}\times\exp(635/T)$	[12], MCM	X
MEKAO2 + CH3O2	→	0.2 CH3OH + 0.6 HO2 + 0.8 HCHO + 0.2 MEKAOH + 0.5 CO2C3CHO + 0.3 HCHO + 0.3 EO2	1.0×10^{-12}	RO_2 chemistry	X
MEKBO2 + CH3O2	→	0.2 CH3OH + 0.6 HO2 + 0.2 MEKBOH + 0.8 HCHO + CH3C(O)O2 + 0.6 CH3CHO	1.0×10^{-12}	RO_2 chemistry	X
MEKCO2 + CH3O2	→	0.5 CH3OH + 0.3 HO2 + 0.2 MEKCOH + 0.8 HCHO + 0.67 MGLY + 0.45 CH3C(O)O2	3.8×10^{-12}	Analog to CC(=O)CO[O], EGLYOX approximated with 1.33 MGLY and $C_2H_5CO_3$ with 1.5 $CH_3C(O)O_2$	X
MEKAO2 + CH3C(O)O2	→	0.4 EO2 + 0.4 HCHO + 0.6 CO2C3CHO + 0.4 HO2 + 0.8 CH3O2 + 0.2 CH3COOH	1.0×10^{-11}	RO_2 chemistry	X
MEKBO2 + CH3C(O)O2	→	0.8 CH3CHO + 1.2 CH3C(O)O2 + 0.8 CH3O2 + 0.2 CH3COOH	1.0×10^{-11}	RO_2 chemistry	X
MEKCO2 + CH3C(O)O2	→	0.5 HCHO + 0.75 CH3C(O)O2 + 0.67 MGLY + 0.5 CH3O2 + 0.5 CH3COOH	5.0×10^{-12}	Analog to CC(=O)CO[O], EGLYOX approximated	X

				with 1.33 MGLY and $C_2H_5CO_3$ with 1.5 $CH_3C(O)O_2$	
MEKAOH + OH	→	HO2 + CO2C3CHO	$1.334\times10^{-13}\times\exp(1334/T)$	[12], MCM	X
MEKBOH + OH	→	HO2 + 2 CH3C(O)O2	$7.3\times10^{-13}\times\exp(628/T)$	[12], MCM	X
MEKCOH + OH	→	HO2 + 1.33 MGLY	$1.66\times10^{-12}\times\exp(270/T)$	[12], MCM, EGLYOX approximated with 1.33 MGLY	X
CO2C3CHO + NO3	→	CC(=O)CO[O] + HNO3	$5.76\times10^{-12}\times\exp(-1862/T)$	MCM	X
CO2C3CHO + OH	→	CC(=O)CO[O]	$5.57\times10^{-12}\times\exp(-405/T)$	[12], MCM	X
MACR + O3	→	0.88 MGLY + 0.12 CH3C(O)O2 + 0.12 CO + 0.12 OH + 0.044 HCOOH + 0.472 HCHO + 0.352 H2O2 + 0.484 HOCH2OOH	$1.4\times10^{-15}\times\exp(-2100/T)$	[1]	5
MACR + OH	→	0.964 MACRO2 + 0.036 CC(=O)COO + 0.036 CO + 0.036 HO2	$4.4\times10^{-12}\times\exp(380/T)$	[1]	5
MACR + OH	→	MCO3	$2.7\times10^{-12}\times\exp(470/T)$	[1]	5
MACR + NO3	→	0.32 HNO3 + 0.32 MCO3 + 0.68 OH + 0.68 CO + 0.68 NOA	$1.8\times10^{-13}\times\exp(-1190/T)$	[1]	5
MACRO2 + NO	→	0.03 MACR2N3OH + 0.97 NO2 + 0.8342 CO + 0.8342 CH3COCH2OH + 0.1358 HCHO + 0.1358 MGLY + 0.8342 HO2	$2.7\times10^{-12}\times\exp(360/T)$	[1]	5
MACRO2 + NO3	→	NO2 + 0.85 CO + 0.85 CH3COCH2OH + 0.15 HCHO + 0.15 MGLY + HO2	2.3×10^{-12}	MCM	5
MACRN + OH	→	NOA + OH	$2.7\times10^{-12}\times\exp(470/T)$	[1]	5
MACR2N3OH + OH	→	MACRNO2	$1.39\times10^{-11}\times\exp(380/T)$	[1]	X
MACRNO2 + HO2	→	0.63 CH3COCH2OH + 0.37 OH + 0.63 NO2 + 0.13 O3 + 0.37 MACR2NOOH	$3.14\times10^{-12}\times\exp(580/T)$	[1], [6]	X
MACR2NOOH + OH	→	MACRNO2	4.42×10^{-12}	[1]	X
MACRNO2 + NO	→	CH3COCH2OH + 2NO2	$7.5\times10^{-12}\times\exp(290/T)$	[1]	X
MACRNO2 + NO3	→	CH3COCH2OH + 2NO2	4.0×10^{-12}	[1]	X
MACRNO2 + NO2	$\xrightarrow{M}$	MPAN + NO2	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	[1] (mini)	1
MACRNO2 + CH3O2	→	CH3COCH2OH + NO2 + 0.7 HO2 + HCHO	$2.9\times10^{-12}\times\exp(500/T)$	[1], CH3C(O)O2 chemistry	X
MACRO2 + HO2	→	0.41 MACROOH + 0.507 CO + 0.507 CH3COCH2OH + 0.507 HO2 + 0.59 OH + 0.083 HCHO + 0.083 MGLY	$2.12\times10^{-13}\times\exp(1300/T)$	[1], CH3C(O)O2 chemistry	5

MACROOH + OH	→	CH3COCH2OH + OH + CO	3.77×10^{-11}	MCM	5
MACRO2 + CH3O2	→	0.75 CO + 0.75 CH3COCH2OH + HCHO + 1.5 HO2 + 0.25 MACROH	9.2×10^{-14}	[3]	
MACROH + OH	→	0.16 C3MDIALOH + HO2 + 0.21 CH3COCH2OH + 0.84 CO + 0.63 OH + 0.63 CH3C(O)O2	$2.4\times10^{-11}\times\exp(70/T)$	[1]	5
MVKOH + OH	→	0.4 CO2C3CHO + 0.6 BIACETOH + HO2	$8.7\times10^{-12}\times\exp(70/T)$	[1]	5
MACRO2 + CH3C(O)O2	→	0.85 CO + 0.85 CH3COCH2OH + 0.15 HCHO + 0.15 MGLY + HO2 + CH3O2	1.0×10^{-11}	[3]	
MACRO2	→	CO + CH3COCH2OH + OH	$2.9\times10^{7}\times\exp(-5297/T)$	[1]	5
MCO3 + NO	→	NO2 + HCHO + 0.35 CH3C(O)O2 + 0.65 CH3O2 + 0.65 CO	$8.7\times10^{-12}\times\exp(290/T)$	[1]	5
MCO3 + NO3	→	NO2 + HCHO + 0.35 CH3C(O)O2 + 0.65 CH3O2 + 0.65 CO	4.0×10^{-12}	[3]	
MCO3 + HO2	→	0.37 MACO3H + 0.13 O3 + 0.13 MACO2H + 0.5 OH + 0.5 HCHO + 0.325 CH3O2 + 0.325 CO + 0.175 CH3C(O)O2	$2.39\times10^{-12}\times\exp(730/T)$	[1], [6]	2
MCO3 + CH3O2	→	0.1 MACO2H + 1.9 HCHO + 0.9 HO2 + 0.315 CH3C(O)O2 + 0.585 CH3O2 + 0.585 CO	$2.0\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
MCO3 + CH3C(O)O2	→	HCHO + 0.35 CH3C(O)O2 + 1.65 CH3O2 + 0.65 CO	$2.9\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
MCO3 + NO2	$\xrightarrow{M}$	MPAN	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
MPAN	→	MCO3 + NO2	$1.58\times10^{16}\times\exp(-13500/T)$	[1]	5
MPAN + OH	→	0.25 CH3COCH2OH + NO3 + 0.25 CO + 0.75 HMML	2.9×10^{-11}	[1]	5
MPAN + O3	→	HCHO + CH3C(O)O2 + NO3	8.2×10^{-18}	MCM	5
MACO2H + OH	→	HCHO + CH3C(O)O2	1.51×10^{-11}	[3]	
MACO3H + OH	→	0.212 MCO3 + 0.134 HMML + 0.654 CH3COCH2OH + 0.654 CO + 0.788 OH	1.66×10^{-11}	MCM	5
HMML + OH	→	0.3 CH3C(O)O2 + 0.3 HCOOH + 0.7 OH + 0.7 MGLY	4.33×10^{-12}	[1]	5
MVK + O3	→	0.545 MGLY + 0.38 CH3C(O)O2 + 0.1 HO2 + 0.08 OH + 0.18 CO + 0.075 CH3COCOOH + 0.8 HCHO + 0.245 H2O2 + 0.275 HOCH2OOH + 0.025 HCOOH	$8.5\times10^{-16}\times\exp(-1520/T)$	[1], [7]	5
MVK + OH	→	LHMVKABO2	$2.6\times10^{-12}\times\exp(610/T)$	[1]	5
LHMVKABO2 + NO	→	0.04 MVKN + 0.96 NO2 + 0.23232 HCHO + 0.23232 MGLY + 0.23232 HO2 + 0.72768 CH3C(O)O2 + 0.72768 OHCCH2OH	$2.7\times10^{-12}\times\exp(360/T)$	[1] (mini)	5

MVKN + OH	→	0.449 MGLY + 0.449 HCOOH + 0.69 NO3 + 0.241 HCHO + 0.241 CH3COCOOH + 0.29 CO2H3CHO + 0.31 NO2 + 0.04 MCO3 + 0.02 OH	$1.24\times10^{-12}\times\exp(380/T)$	[1] (mini)	5
LHMVKABO2 + NO3	→	NO2 + 0.242 HCHO + 0.242 MGLY + 0.242 HO2 + 0.758 CH3C(O)O2 + 0.758 OHCCH2OH	2.5×10^{-12}	MCM	5
LHMVKABO2 + HO2	→	0.335 LHMVKABOOH + 0.36 CH3C(O)O2 + 0.665 OH + 0.36 OHCCH2OH + 0.305 HO2 + 0.05 MGLY + 0.05 HCHO + 0.255 BIACETOH	$2.12\times10^{-13}\times\exp(1300/T)$	[1] (mini)	5
LHMVKABOOH + OH	→	OH + 0.53 BIACETOH + 0.47 CO2H3CHO	5.77×10^{-11}	[1] (mini)	5
LHMVKABO2 + CH3O2	→	0.9 HCHO + 0.35 OHCCH2OH + 0.65 HO2 + 0.35 CH3C(O)O2 + 0.175 BIACETOH + 0.25 CH3OH + 0.25 MACROH + 0.25 MGLY + 0.075 CO2H3CHO	1.0×10^{-12}	[3]	
LHMVKABO2 + CH3C(O)O2	→	0.3 HCHO + 0.3 MGLY + 0.3 HO2 + 0.7 CH3C(O)O2 + 0.7 OHCCH2OH + CH3O2	1.0×10^{-11}	[3]	
BIACETOH + OH	→	HO2 + CH3C(O)O2 + 2 CO	$2.0\times10^{-12}\times\exp(70/T)$	[1]	5
CO2H3CHO + OH	→	HO2 + MGLY	$5.0\times10^{-12}\times\exp(470/T)$	[1] (for sens. study CO2H3CO3 pathways are added)	5
CO2H3CHO + NO3	→	HO2 + MGLY + HNO3	$5.6\times10^{-12}\times\exp(-1860/T)$	MCM	5
MALO2 + NO	→	0.4 GLY + HO2 + 0.4 CO + 0.6 MALANHY + NO2	$7.5\times10^{-12}\times\exp(290/T)$	MCM	X
MALO2 + HO2	→	0.2 GLY + 0.3 MALANHY + 0.5 HO2 + 0.2 CO + 0.5 OH + 0.13 O3 + 0.13 BIGACID1 + 0.37 MALOOH	$2.62\times10^{-12}\times\exp(730/T)$	[6]	2
MALOOH + OH	→	MALO2	4.0×10^{-11}	MCM	X
MALO2 + NO2	$\xrightarrow{M}$	MALPAN	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
MALPAN + OH	→	GLY + 2 CO + NO2	3.7×10^{-11}	MCM	X
MALPAN	$\xrightarrow{M}$	NO2 + MALO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	MCM	X
MALO2 + NO3	→	0.4 GLY + HO2 + 0.4 CO + 0.6 MALANHY + NO2	4.0×10^{-12}	MCM	X
MALO2 + CH3O2	→	0.36 GLY + 0.9 HO2 + 0.9 HO2 + 0.36 CO + 0.54 MALANHY + HCHO + 0.1 BIGACID1	$2.0\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
MALO2 + CH3C(O)O2	→	0.4 GLY + HO2 + 0.4 CO + 0.6 MALANHY + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2

MALANHY + OH	→	MALANHYO2	1.4×10^{-12}	MCM	X
MALANHYO2 + HO2	→	MALANHYOOH	$1.8125\times10^{-13}\times\exp(1300/T)$	MCM	X
MALANHYO2 + NO	→	NO2 + HCOCOHCO3	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
MALANHYO2 + NO3	→	NO2 + HCOCOHCO3	2.3×10^{-12}	MCM	X
MALANHYO2 + CH3O2	→	0.3 HCOCOHCO3 + 0.3 HO2 + 0.5 HCHO + 0.5 CH3OH + 0.8 MALANHYCO	3.8×10^{-12}	Analog to CC(=O)C=[O]	X
MALANHYO2 + CH3C(O)O2	→	0.5 HCOCOHCO3 + 0.5 CH3O2 + 0.5 CH3COOH + 0.5 MALANHYCO	5.0×10^{-12}	Analog to CC(=O)CO[O]	X
MALANHYCO + OH	→	3 CO + HO2	5.68×10^{-12}	MCM	X
MALANHYOOH + OH	→	MALANHYCO + OH	4.66×10^{-11}	MCM	X
IBUTALOH + OH	→	IBUTALOHO2	1.4×10^{-11}	[3]	
IBUTALOHO2 + NO	→	HO2 + CH3COCH3 + NO2	$7.5\times10^{-12}\times\exp(290/T)$	MCM	X
IBUTALOHO2 + NO3	→	HO2 + CH3COCH3 + NO2	4.0×10^{-12}	MCM	X
IBUTALOHO2 + HO2	→	0.37 IBUTALOHOOH + 0.5 CH3COCH3 + 0.5 OH + 0.13 IBUTALOOH + 0.13 O3	$2.62\times10^{-12}\times\exp(730/T)$	[6]	X
IBUTALOOH + OH	→	CH3COCH3 + HO2	$4.66\times10^{-13}\times\exp(326/T)$	[12], MCM	X
IBUTALOHOOH + OH	→	IBUTALOHO2	$7.513\times10^{-13}\times\exp(494/T)$	[12], MCM	X
IBUTALOHO2 + CH3O2	→	HCHO + 1.8 HO2 + 0.9 CH3COCH3 + 0.1 IBUTALOOH	$2.0\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	X
IBUTALOHO2 + CH3C(O)O2	→	HO2 + CH3COCH3 + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	X
IBUTALOHO2 + NO2	$\xrightarrow{M}$	C4PAN5	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
C4PAN5 + OH	→	CH3COCH3 + CO + NO2	4.75×10^{-13}	MCM	X
C4PAN5	$\xrightarrow{M}$	IBUTALOHO2 + NO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	MCM	X
HVMK + OH	→	0.25 CO2H3CHO + 0.25 HO2 + 0.75 OH + 0.75 MGLY + 0.75 HCOOH	$3.35\times10^{-12}\times\exp(983/T)$	[1]	X
MACRENOL + OH	→	CO + 0.87 CH3COCOOH + 0.87 HO2 + 0.13 OH + 0.13 CH3C(O)O2	$3.83\times10^{-12}\times\exp(983/T)$	[1]	X
C3MDIALOH + OH	→	OH + CO + HO2 + CH3C(O)O2	$5.0\times10^{-12}\times\exp(470/T)$	[1]	X

BIGALD1 + OH	→	0.83 MALO2 + 0.34 GLY + 0.17 HO2	5.2×10^{-11}	MCM	X
BIGALD1 + NO3	→	MALO2 + HNO3	$5.6\times10^{-12}\times\exp(-1862/T)$	MCM	X
BIGALD1 + O3	→	1.0675 GLY + 0.125 HCHO + 0.57 OH + 0.82 HO2 + 1.265 CO + 0.1125 HOOCCHO + 0.0675 H2O2	2.0×10^{-18}	MCM	X
HOCOC4DIAL + OH	→	HO2 + CO2C4DIAL	3.67×10^{-11}	MCM	X
CO2C4DIAL + OH	→	HO2 + 4 CO	$3.55\times10^{-12}\times\exp(591/T)$	[12], MCM	X
BIGACID1 + OH	→	0.4 GLY + HO2 + 0.4 CO + 0.6 MALANHY	3.7×10^{-11}	MCM	X
BZFUONE + NO3	→	HNO3 + BZFUONEO2	3.0×10^{-13}	MCM	X
BZFUONE + OH	→	BZFUONEO2	4.45×10^{-11}	MCM	X
BZFUONEO2 + HO2	→	BZFUONEOOH	$2.05\times10^{-13}\times\exp(1300/T)$	MCM	X
BZFUONEO2 + NO	→	NO2 + BZFUO + HO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
BZFUONEO2 + NO3	→	NO2 + BZFUO + HO2	2.3×10^{-12}	MCM	X
BZFUONEO2 + CH3O2	→	BZFUO + 2 HO2 + HCHO	1.0×10^{-12}	MCM, RO2 chemistry	X
BZFUONEO2 + CH3C(O)O2	→	BZFUO + HO2 + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
BZFUONEOOH + OH	→	BZFUONEO2	3.68×10^{-11}	MCM	X
BZFUO + NO3	→	HNO3 + 2 CO + HO2 + HCHO	$11.52\times10^{-12}\times\exp(-1862/T)$	MCM	X
BZFUO + OH	→	2 CO + HO2 + HCHO	3.44×10^{-11}	MCM	X

C5 chemistry					
MDIALO2 + NO	→	0.825 HO2 + 0.175 MGLY + 0.35 CO + 0.175 CH3O2 + 0.175 GLY + NO2 + 0.65 MALANHY	$7.5\times10^{-12}\times\exp(290/T)$	MCM (ratio 50:50 for C3MCODBCO3: MC3CODBCO3)	X
MDIALO2 + NO3	→	0.825 HO2 + 0.175 MGLY + 0.35 CO + 0.175 CH3O2 + 0.175 GLY + NO2 + 0.65 MALANHY	4.0×10^{-12}	MCM	X
MDIALO2 + HO2	→	0.5 OH + 0.4125 HO2 + 0.37 MDIALOOH + 0.0875 MGLY + 0.175 CO + 0.0875 CH3O2 + 0.0875 GLY + 0.325 MALANHY + 0.13 BIGACID2 + 0.13 O3	$2.8\times10^{-12}\times\exp(730/T)$	[6]	2
MDIALOOH + O3	→	0.365 O=C(OO)C=O + 0.17515 MGLY + 0.37056875 GLY + 0.82485 CH3C(O)O2 + 1.08 OH + 0.12015 HO2 + 0.56515 CO +	2.4×10^{-17}	MCM	X

		0.000556875 H2O2 + 0.135 O=CC(=O)O[O] + 0.00928125 HOOCCHO			
MDIALOOH + OH	→	0.5 GLY + 0.5 MGLY + HO2 + 0.5 O=C(OO)C=O + 0.5 OH + 0.5 CH3C(O)O2	4.72×10^{-11}	MCM	X
MDIALO2 + CH3O2	→	1.6425 HO2 + 0.1575 MGLY + 0.315 CO + 0.1575 CH3O2 + 0.1575 GLY + HCHO + 0.585 MALANHY + 0.1 BIGACID2	$2.0\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
MDIALO2 + CH3C(O)O2	→	0.825 HO2 + 0.175 MGLY + 0.35 CO + 0.175 GLY + 1.175 CH3O2 + 0.65 MALANHY	$2.9\times10^{-12}\times\exp(500/T)$	Analog to CH3C(O)O2	2
MDIALO2 + NO2	$\xrightarrow{M}$	MDIALPAN	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
MDIALPAN + OH		0.5 GLY + 0.5 HCHO + 1.5 CO + NO2 + 0.5 MGLY	4.37×10^{-11}	MCM	X
MDIALPAN	$\xrightarrow{M}$	NO2 + MDIALO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	MCM	X
BIGALK + OH	→	ALKO2	3.5×10^{-12}	[3]	
ALKO2 + NO	→	0.36 CH3CHO + 0.225 HCHO + 0.225 CH3COCH3 + 0.9 HO2 + 0.72 MEK + 0.9 NO2 + 0.1 ALKNO3	$4.2\times10^{-12}\times\exp(180/T)$	[3]	
ALKNO3 + OH	→	0.4 CH3CHO + 0.25 HCHO + 0.25 CH3COCH3 + HO2 + 0.8 MEK + NO2	2.0×10^{-12}	[3]	
ALKO2 + HO2	→	ALKOOH	$7.5\times10^{-13}\times\exp(700/T)$	[3]	
ALKOOH + OH	→	ALKO2	$3.8\times10^{-12}\times\exp(200/T)$	[3]	
ALKO2 + CH3O2	→	0.3 CH3CHO + 1.1875 HCHO + 0.1875 CH3COCH3 + 0.75 HO2 + 0.6 MEK + 0.25ALKOH	1.0×10^{-12}	[3]	
ALKOH + OH	→	1.25 MEK + HO2	5.0×10^{-12}	[3]	
ALKO2 + CH3C(O)O2	→	0.4 CH3CHO + 0.25 HCHO + 0.25 CH3COCH3 + HO2 + 0.8 MEK + CH3O2	1.0×10^{-11}	[3]	
MBO + OH	→	MBOO2	$8.1\times10^{-12}\times\exp(610/T)$	[3]	
MBO + O3	→	0.35 CO + 0.5 HCHO + 0.1 CH3COCH3 + 0.9 IBUTALOH + 0.25 HCOOH + 0.06 HO2 + 0.06 OH	1.0×10^{-17}	[3]	
MBO + NO3	→	MBONO3O2	$4.6\times10^{-14}\times\exp(-400/T)$	[3]	
MBOO2 + NO	→	HO2 + 0.67 CH3COCH3 + 0.67 OHCCH2OH + 0.33 HCHO + 0.33 IBUTALOH + NO2	$2.6\times10^{-12}\times\exp(365/T)$	[3]	
MBOO2 + HO2	→	MBOOOH	$7.5\times10^{-13}\times\exp(700/T)$	[3]	

MBOOOH + OH	→	0.5 MBOO2 + 0.625 MACROH + 0.5 OH	$3.8\times10^{-12}\times\exp(200/T)$	[3]	
MBOO2 + CH3O2	→	0.9165 HCHO + 0.625 MACROH + 0.25 CH3OH + HO2 + 0.3335 CH3COCH3 + 0.3335 OHCCH2OH + 0.1665 IBUTALOH	$3.7\times10^{-13}\times\exp(-40/T)$	[3]	
MBOO2 + CH3C(O)O2	→	HO2 + 0.67 CH3COCH3 + 0.67 OHCCH2OH + 0.33 HCHO + 0.33 IBUTALOH + CH3O2	1.0×10^{-11}	[3]	
MBONO3O2 + NO	→	0.35 HCHO + 0.35 IBUTALOH + 1.35 NO2 + 0.43 NOA + 0.65 CH3COCH3 + 0.65 HO2	$2.6\times10^{-12}\times\exp(365/T)$	[3], MCM	X
MBONO3O2 + NO3	→	0.35 HCHO + 0.35 IBUTALOH + 1.35 NO2 + 0.43 NOA + 0.65 CH3COCH3 + 0.65 HO2	2.3×10^{-12}	MCM	X
MBONO3O2 + HO2	→	MBONO3OOH	$4.3\times10^{-13}\times\exp(1040/T)$	[3], MCM	X
MBONO3O2 + CH3O2	→	0.875 HCHO + 0.125 IBUTALOH + 0.12 5NO2 + 0.25 NOA + 0.375 CH3COCH3 + 0.875 HO2 + 0.25 CH3OH + 0.625 MACROH	1.0×10^{-12}	[3]	
MBONO3O2 + CH3C(O)O2	→	0.35 HCHO + 0.35 IBUTALOH + 0.35 NO2 + 0.43 NOA + 0.65 CH3COCH3 + 0.65 HO2 + CH3O2	1.0×10^{-11}	Analog to NO3	X
MBONO3OOH + OH	→	MBONO3O2	$1.9\times10^{-12}\times\exp(910/T)$	[3]	
DICARBO2 + NO	→	0.17 MGLY + 0.17 HO2 + 0.17 CO + 0.83 MALANHY + 0.83 CH3O2 + NO2	$7.5\times10^{-12}\times\exp(290/T)$	MCM	X
DICARBO2 + NO3	→	0.17 MGLY + 0.17 HO2 + 0.17 CO + 0.83 MALANHY + 0.83 CH3O2 + NO2	4.0×10^{-12}	MCM	X
DICARBO2 + NO2	$\xrightarrow{M}$	DICARBPAN	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM	1
DICARBO2 + HO2	→	0.085 MGLY + 0.085 HO2 + 0.085 CO + 0.415 MALANHY + 0.415 CH3O2 + 0.5 OH + 0.37 DICARBOOH + 0.13 BIGACID2 + 0.13 O3	$2.8\times10^{-12}\times\exp(730/T)$	MCM, [6]	2
DICARBPAN	$\xrightarrow{M}$	DICARBO2 + NO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	MCM	X
DICARBPAN + OH	→	MGLY + 2 CO + NO2	5.43×10^{-11}	MCM	X
DICARBO2 + CH3O2	→	0.153 MGLY + 1.053 HO2 + 0.153 CO + 0.747 CH3O2 + 0.747 MALANHY + HCHO + 0.1 BIGACID2	$2.0\times10^{-12}\times\exp(500/T)$	MCM, CH3C(O)O2 chemistry	2
DICARBO2 + CH3C(O)O2	→	0.17 MGLY + 0.17 HO2 + 0.17 CO + 0.83 CH3O2 + 0.83 MALANHY + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	MCM, CH3C(O)O2 chemistry	2
DICARBOOH + OH	→	DICARBO2	3.59×10^{-12}	MCM	X

BIGACID2 + OH	→	0.17 MGLY + 0.17 HO2 + 0.17 CO + 0.83 CH3O2 + 0.83 MALANHY	5.44×10^{-11}	MCM	X
BIGALD2 + OH	→	0.48 DICARBO2 + 0.52 MGLY + 0.52 GLY + 0.52 HO2	6.2×10^{-11}	MCM	X
BIGALD2 + NO3	→	DICARBO2 + HNO3	$3.85\times10^{-12}\times\exp(-1862/T)$	MCM	X
BIGALD2 + O3	→	0.5675 GLY + 0.3475 CH3C(O)O2 + 0.0625 CH3CHO + 0.9175 CO + 0.57 OH + 0.4725 HO2 + 0.0675 H2O2 + 0.05625 CH3COCOOH + 0.5675 MGLY + 0.0625 HCHO + 0.05625 HOOCCHO	2.0×10^{-18}	MCM	X
BIGALD3 + OH	→	0.77 MDIALO2 + 0.23 GLY + 0.23 MGLY + 0.23 HO2	4.41×10^{-11}	MCM	X
BIGALD3 + NO3	→	MDIALO2 + HNO3	$5.95\times10^{-12}\times\exp(-1862/T)$	MCM	X
BIGALD3 + NO3	→	MDIALO2 + HNO3	$5.95\times10^{-12}\times\exp(-1862/T)$	MCM	X
BIGALD3 + O3	→	0.89 OH + 1.335 CO + 0.445 CH3C(O)O2 + 0.555 MGLY + 0.075625 H2O2 + 0.520625 GLY + 0.445 HO2 + 0.034375 HOOCCHO	5.0×10^{-18}	MCM	X
FUONE + NO3	→	NO2 + FUONEO2	1.0×10^{-12}	MCM	X
FUONE + OH	→	FUONEO2	2.42×10^{-11}	MCM (for PXFUONE)	X
FUONEO2 + HO2	→	FUONEOOH	$2.05\times10^{-13}\times\exp(1300/T)$	MCM	X
FUONEO2 + NO	→	NO2 + HO2 + CH3C(O)O2 + HCHO	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
FUONEO2 + NO3	→	NO2 + HO2 + CH3C(O)O2 + HCHO	5.08×10^{-11}	MCM	X
FUONEO2 + CH3O2	→	HO2 + CH3C(O)O2 + HCHO + HO2 + HCHO	1.0×10^{-12}	MCM, RO2 chemistry	X
FUONEO2 + CH3C(O)O2	→	HO2 + CH3C(O)O2 + HCHO + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
FUONEOOH + OH	→	FUONEO2	2.78×10^{-11}	MCM	X
C5DIALO2 + NO	→	BIGALD1 + CO + HO2 + NO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
C5DIALO2 + NO3	→	BIGALD1 + CO + HO2 + NO2	2.3×10^{-12}	MCM	X
C5DIALO2 + HO2	→	C5DIALOOH	$2.05\times10^{-13}\times\exp(1300/T)$	MCM	X
C5DIALOOH + OH	→	OH + MALO2 + CO + HO2	7.25×10^{-11}	MCM	X
C5DIALO2 + CH3O2	→	0.6 HO2 + 0.8 HCHO + 0.2 CH3OH + 0.7 BIGALD1 + CO + 1.2 HO2 + 0.3 MALO2	1.0×10^{-12}	MCM, RO2 chemistry	X
C5DIALO2 + CH3C(O)O2	→	0.8 CH3O2 + 0.2 CH3COOH + 0.8 BIGALD1 + CO + HO2 + 0.2 MALO2	1.0×10^{-11}	MCM, RO2 chemistry	X

C5 isoprene chemistry					
C5H8 + OH	→	0.05 LISOPACO2 + 0.6 ISOPBO2 + 0.35 ISOPDO2	$2.1\times10^{-11}\times\exp(465/T)$	[1], [8], IUPAC	5
C5H8 + O3	→	0.407 CH3O2 + 0.407 CO + 0.416 MACR + 0.16 HO2 + 1.059 HCHO + 0.28 OH + 0.177 MVK + 0.245 H2O2 + 0.319 HOCH2OOH + 0.029 HCOOH	$1.05\times10^{-14}\times\exp(-2000/T)$	[1], [7], IUPAC	5
C5H8 + NO3	→	0.465 NISOPBO2 + 0.535 NISOPDO2	$2.95\times10^{-12}\times\exp(-450/T)$	[1] (for sens. study NISOPO2 pathways asre added)	5
LISOPACO2 + NO	→	0.4 HO2 + 0.88 NO2 + 0.12 LISOPACNO3 + 0.4 LHC4ACCHO + 0.48 CO + 0.48 OH + 0.29 LHMVKABOOH + 0.19 MACROOH	$2.7\times10^{-12}\times\exp(360/T)$	[1] (60% ISOP1CO4OH, 40% ISOP1OH4CO)	
LISOPACO2 + NO3		0.45 HO2 + NO2 + 0.45 LHC4ACCHO + 0.55 CO + 0.55 OH + 0.33 LHMVKABOOH + 0.22 MACROOH	2.3×10^{-12}	[3], k_{RO2NO3}	X
LISOPACNO3 + OH	→	0.94 LISOPACNO3O2 + 0.06 LIEPOX + 0.06 NO2	$2.74\times10^{-11}\times\exp(390/T)$	[1]	X
LISOPACNO3 + OH	→	0.4 NC4CHO + 0.4 HO2 + 0.24 MACRNOOH + 0.6 CO + 0.6 OH + 0.36 LHMVKNOOH	$7.5\times10^{-12}\times\exp(20/T)$	[1]	X
LISOPACO2 + HO2	→	LISOPACOOH	$2.12\times10^{-13}\times\exp(1300/T)$	[1]	X
LISOPACOOH + OH	→	0.46 LIEPOX + 0.46 OH + 0.42 IDHPOO1 + 0.12 IDHPOO2	$3.0\times10^{-11}\times\exp(390/T)$	[1]	X
LISOPACOOH + OH	→	LISOPACO2	$2.0\times10^{-12}\times\exp(200/T)$	[1]	X
LISOPACOOH + OH	→	0.8 OH + 0.5 LHC4ACCHO + 0.2 HPALD + 0.18 HO2 + 0.3 CO + 0.18 DHPMEK + 0.12 DHPMPAL	$1.5\times10^{-11}\times\exp(20/T)$	[1]	X
LISOPACO2 + CH3O2	→	HCHO + 0.725 LHC4ACCHO + 0.275 CO + 0.275 OH + 0.165 LHMVKABOOH + 0.11 MACROOH + 0.725 HO2	2.0×10^{-12}	[1]	X
LISOPACO2 + CH3C(O)O2	→	HO2 + LHC4ACCHO + CH3O2	1.0×10^{-11}	[3]	
LISOPACO2 + ISOPBO2	→	MVK + HCHO + 0.557 LHC4ACCHO + 0.443 CO + 0.443 OH + 0.266 LHMVKABOOH + 0.177 MACROOH + 1.167 HO2	2.49×10^{-12}	[1]; including subsequent reactions according to MCM3.3.1 and the recommendation for the reduced mechanism see sect. 2.5.2	X
LISOPACO2 + ISOPDO2	→	0.705 MACR + 0.705 HCHO + 0.295 HCOC5 + 0.612 LHC4ACCHO + 0.388 CO + 0.388 OH + 0.233 LHMVKABOOH + 0.155 MACROOH + 1.022 HO2	3.94×10^{-12}	[1]; including subsequent reactions according to MCM3.3.1 and the	X

				recommendation for the reduced mechanism see sect. 2.5.2	
LISOPACO2	→	0.4 HO2 + 0.4 HPALD + 0.6 DHPMEK + 0.6 CO + 0.6 OH	$k_{iso}(1.63\times10^{14}, 12200, 1\times10^{8})$	[1]	5
LISOPACO2	→	0.4 HO2 + 0.4 HPALD + 0.6 DHPMPAL + 0.6 CO + 0.6 OH	$k_{iso}(4.34\times10^{7}, 7160, 1\times10^{8})$	[1]	5
DHPMPAL + OH	→	0.32 C3MDIALOOH + 0.68 CO + OH + 0.68 CC(=O)COO	$2.62\times10^{-12}\times\exp(713/T)$	[12], MCM	X
DHPMEK + OH	→	CH3C(O)O2 + 2 CO	$6.6\times10^{-13}\times\exp(1057/T)$	[12], MCM, only dominant pathways	X
C3MDIALOOH + OH	→	C3MDIALO2	$1.402\times10^{-10}\times\exp(227/T)$	[12], MCM	X
C3MDIALO2 + HO2	→	C3MDIALOOH	$1.82\times10^{-13}\times\exp(1300/T)$	MCM	X
C3MDIALO2 + NO	→	NO2 + MGLY + CO + HO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
C3MDIALO2 + NO3	→	NO2 + MGLY + CO + HO2	2.3×10^{-12}	MCM	X
ISOPBO2	→	OH + HCHO + MVK	$1.04\times10^{11}\times\exp(-9746/T)$	[1]	5
ISOPDO2	→	OH + HCHO + MACR	$1.88\times10^{11}\times\exp(-9752/T)$	[1]	5
LIEPOX + OH	→	0.8 LC578O2 + 0.2 LIECHO + 0.2 HO2	$4.4\times10^{-11}\times\exp(-400/T)$	[1], [9]	X
LIECHO + OH	→	0.28 OH + 1.28 CO + 0.28 CH3COCH2OH + 0.72 LHMVKABO2	1.5×10^{-11}	[9]	X
LIECHO + OH	→	CO + HO2 + 0.28 C3MDIALOOH + 0.72 MDIALOOH	$2.2\times10^{-11}\times\exp(-400/T)$	[9]	X
LIECO3H + OH	→	0.888 CO + 0.444 OH + 0.444 HO2 + 0.318 CO2H3CHO + 0.112 LC578O2 + 0.126 C3MDIALOH + 0.444 LHMVKABOOH	2.25×10^{-11}	[1]	X
ISOPBO2 + NO	→	0.86 HO2 + 0.86 NO2 + 0.86 HCHO + 0.86 MVK + 0.14 ISOPBNO3	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
ISOPBNO3 + OH	→	0.15 LIEPOX + 0.15 NO2 + 0.85 ISOPBNO3O2	$8.4\times10^{-12}\times\exp(390/T)$	[9]	X
ISOPBNO3O2 + NO	→	0.26 HCHO + 0.26 HO2 + 0.26 MACR2N3OH + 0.69 OHCCH2OH + 0.69 CH3COCH2OH + 1.64 NO2 + 0.05 LISOPNO3NO3	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
ISOPBNO3O2 + NO3	→	0.272 HCHO + 0.272 HO2 + 0.272 MACR2N3OH + 0.728 OHCCH2OH + 0.728 CH3COCH2OH + 1.728 NO2	2.3×10^{-12}	Products analog to reaction with NO but no organic nitrate formation, MCM KRO2NO3 rate constant	X
ISOPBNO3O2 + HO2	→	0.482 LISOPNO3OOH + 0.059 MACR2N3OH + 0.059 HCHO + 0.459 OHCCH2OH + 0.459 CH3COCH2OH + 0.059 HO2 + 0.459 NO2 + 0.518 OH	$2.6\times10^{-13}\times\exp(1300/T)$	[1]	X

ISOPBNO3O2	→	NISOPOOHOH=O + HO2	$1.875\times10^{13}\times\exp(-10000/T)$	[1]	X
ISOPBO2 + NO3	→	NO2 + MVK + HO2 + HCHO	2.3×10^{-12}	See ISOPBNO3O2	X
ISOPBO2 + HO2	→	0.973 ISOPBOOH + 0.063 MVK + 0.063 OH + 0.063 HO2 + 0.063 HCHO	$2.12\times10^{-13}\times\exp(1300/T)$	[1]	X
ISOPBOOH + OH	→	0.75 ISOPBO2 + 0.125 MVK + 0.25 HO2 + 0.125 MVKOOH + 0.25 CO	$6.1\times10^{-12}\times\exp(200/T)$	[1]	X
ISOPBOOH + OH	→	0.855 LIEPOX + 0.855 OH + 0.095 IDHPOO3 + 0.05 IDHPOO1	$1.7\times10^{-11}\times\exp(390/T)$	[1]	X
ISOPBO2 + CH3O2	→	2 HCHO + MVK + 2 HO2	2.0×10^{-12}	[1]	X
ISOPBO2 + CH3C(O)O2	→	HO2 + HCHO + MVK + CH3O2	1.0×10^{-11}	Analog to RO2 chemistry with RO2+CH3C(O)O2 rate constant from [1]	X
ISOPBO2 + ISOPBO2	→	2 MVK + 2 HO2 + 2 HCHO	6.92×10^{-14}	[1]	X
ISOPDO2 + ISOPDO2	→	1.6 MACR + 1.6 HO2 + 1.6 HCHO + 0.4 HCOC5	5.74×10^{-12}	[1], MCM	X
ISOPBO2 + ISOPDO2	→	0.9 MACR + 1.0 MVK + 1.9 HO2 + 1.9 HCHO + 0.1 HCOC5	3.08×10^{-12}	[1]	X
IDHPOO1 + NO	→	0.82 NO2 + 0.82 HO2 + 0.15 MACROOH + 0.15 HCHO + 0.18 LISOPNO3OOH + 0.67 CH3COCH2OH + 0.67 HCOCH2OOH	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
IDHPOO1 + HO2	→	0.03 MACROOH + 0.4 OH + 0.03 HCHO + 0.4 HO2 + 0.6 LISOPOOHOOH + 0.37 HCOCH2OOH + 0.37 CH3COCH2OH	$2.47\times10^{-13}\times\exp(1300/T)$	[1]	X
IDHPOO1	→	DHHPEPOX + OH	$k_{iso}(6.8\times10^{12}, 11200, 8.46\times10^{7})$	[1]	X
IDHPOO3 + NO	→	0.9 NO2 + 0.9 OH + 0.9 CH3COCH2OH + 0.9 OHCCH2OH + 0.1 LISOPNO3OOH	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
IDHPOO3 + HO2	→	1.3 OH + 0.65 CH3COCH2OH + 0.65 OHCCH2OH + 0.35 LISOPOOHOOH	$2.47\times10^{-13}\times\exp(1300/T)$	[1]	X
IDHPOO3	→	DHHPEPOX + OH	$k_{iso}(1.87\times10^{12}, 9630, 8.02\times10^{7})$	[1]	X
DHHPEPOX + OH	→	OH + 0.571 MACROOH + 0.429 LHMVKABOOH	3.0×10^{-12}	[1]	X
ISOPDO2 + NO	→	0.87 HO2 + 0.87 NO2 + 0.87 HCHO + 0.87 MACR + 0.13 ISOPDNO3	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
ISOPDNO3 + OH	→	0.874 ISOPDNO3O2 + 0.126 LIEPOX + 0.126 NO2	$1.17\times10^{-11}\times\exp(390/T)$	[1]	X

ISOPDNO3O2 + NO	→	0.96 HCHO + 0.96 HO2 + 0.96 MVKN + 0.96 NO2 + 0.04 LISOPNO3NO3	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
ISOPDNO3O2 + NO3	→	HCHO + HO2 + MVKN + NO2	2.3×10^{-12}	See ISOPBNO3O2	X
ISOPDNO3O2 + HO2	→	0.401 LISOPNO3OOH + 0.599 MVKN + 0.599 HCHO + 0.599 HO2 + 0.599 OH	$2.6\times10^{-13}\times\exp(1300/T)$	[1]	X
ISOPDNO3O2	→	NISOPOOHOH=O + HO2	$1.875\times10^{13}\times\exp(-10000/T)$	[1]	X
ISOPDO2 + NO3	→	HCHO + MACR + HO2 + NO2	2.3×10^{-12}	See ISOPBNO3O2	X
ISOPDO2 + HO2	→	0.937 ISOPDOOH + 0.063 MACR + 0.063 OH + 0.063 HO2 + 0.063 HCHO	$2.12\times10^{-13}\times\exp(1300/T)$	[1]	X
ISOPDOOH + OH	→	0.855 LIEPOX + 0.855 OH + 0.095 IDHPOO3 + 0.05 IDHPOO2	$3.0\times10^{-11}\times\exp(390/T)$	[1]	X
ISOPDOOH + OH	→	0.51 ISOPDO2 + 0.16 HCOC5 + 0.33 CO + 0.33 HO2 + 0.165 MACR + 0.165 MACROOH	$4.1\times10^{-12}\times\exp(200/T)$	[1]	X
IDHPOO2 + NO	→	0.87 NO2 + 0.87 HO2 + 0.13 OHCCH2OH + 0.13 CC(=O)COO + 0.13 LISOPNO3OOH + 0.74 LHMVKABOOH + 0.74 HCHO	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
IDHPOO2 + HO2	→	0.24 OH + 0.07 CC(=O)COO + 0.07 OHCCH2OH + 0.24 HO2 + 0.76 LISOPOOHOOH + 0.17 HCHO + 0.17 LHMVKABOOH	$2.47\times10^{-13}\times\exp(1300/T)$	[1]	X
IDHPOO2	→	0.32 LC578OOH + 0.68 DHHPEPOX + OH	$k_{iso}(3.73\times10^{12}, 10400, 9.95\times10^{7})$	[1]	X
ISOPDO2 + CH3O2	→	1.25 HCHO + 0.5 MACR + HO2 + 0.5 HCOC5 + 0.25 CH3OH	2.0×10^{-12}	[1]	X
ISOPDO2 + CH3C(O)O2	→	HO2 + HCHO + MACR + CH3O2	1.0×10^{-11}	See ISOPBO2	X
NISOPBO2 + NO	→	0.97 NO2 + 0.65 NISOPEOO1E + 0.32 NISOPEOO1Z + 0.03 NISOPN	$2.7\times10^{-12}\times\exp(360/T)$	[2]	X
NISOPDO2 + NO	→	0.1272 HO2 + 0.8 NO2 + 0.1272 NC4CHO + 0.6728 NISOPO + 0.2 NISOPN	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
NISOPBO2 + NO3	→	NO2 + 0.68 NISOPEOO1E + 0.32 NISOPEOO1Z	2.3×10^{-12}	[2]	X
NISOPDO2 + NO3	→	0.159 HO2 + 0.159 NC4CHO + NO2 + 0.841 NISOPO	2.3×10^{-12}	[1]	X
NISOPBO2 + HO2	→	0.473 NISOPBOOH + 0.353 NISOPEOO1E + 0.174 NISOPEOO1Z + 0.527 OH	$2.47\times10^{-13}\times\exp(1300/T)$	[1], [2]	X
NISOPDO2 + HO2	→	NISOPDOOH	$2.47\times10^{-13}\times\exp(1300/T)$	[1]	X
NISOPBO2 + CH3O2	→	0.355 NISOPOH + 0.966 HCHO + 0.034 NC4CHO + 0.19552 NISOPEOO1Z + 0.41548 NISOPEOO1E + 0.611 HO2 + 0.034 CH3OH	2.8×10^{-13}	[1], [2]	X

NISOPDO2 + CH3O2	→	0.645 HCHO + 0.401 NC4CHO + 0.355 LISOPACNO3 + 0.244 NISOPBO + 0.336 HO2 + 0.355 CH3OH	1.18×10^{-12}	[1]	X
NISOPBO2 + CH3C(O)O2	→	CH3O2 + 0.68 NISOPEOO1E + 0.32 NISOPEOO1Z	1.92×10^{-12}	[1], [2]	X
NISOPDO2 + CH3C(O)O2	→	0.159 HO2 + 0.159 NC4CHO + CH3O2 + 0.84 NISOPBO	7.71×10^{-12}	[1]	X
NISOPEOO1E	→	2 CO + 0.35 NOA + 0.65 MGLY + 1.65 HO2 + 0.65 NO2 + OH	4.1×10^{-6}	[2], ISOP1N23O4CO5OOH treated as ICNE + HO2	X
NISOPEOO1E + HO2	→	IHNEOOH	$2.52\times10^{-13}\times\exp(1300/T)$	[2]	X
NISOPEOO1E + CH3O2	→	0.76 HCHO + 0.686 HO2 + 0.4 CH3OH + 0.88 CO + 0.154 NOA + 0.286 MGLY + 0.286 NO2 + 0.4 IHNE + 0.16 MACRN	$1.0\times10^{-13}\times\exp(1139/T)$	[2], see sect. 2.5.1	X
NISOPEOO1E + NO3	→	1.13 HO2 + 0.4 CO + 0.07 NOA + 0.13 MGLY + 1.13 NO2 + 0.8 HCHO + 0.8 MACRN	$1.9\times10^{-11}\times\exp(-390/T)$	[2], see sect. 2.5.1	X
NISOPEOO1E + NO	→	1.13 HO2 + 0.4 CO + 0.07 NOA + 0.13 MGLY + 1.13 NO2 + 0.8 HCHO + 0.8 MACRN	$2.7\times10^{-12}\times\exp(360/T)$	[2], only main path, see sect. 2.5.1	X
NISOPEOO1E + CH3C(O)O2	→	1.13 HO2 + 0.4 CO + 0.07 NOA + 0.13 MGLY + 0.13 NO2 + 0.8 HCHO + 0.8 MACRN + CH3O2	1.0×10^{-11}	Analog to RO2+CH3C(O)O2 chemistry	X
NISOPEOO1Z	→	LIECHO + NO2	3.6×10^{-5}	[2]	X
NISOPEOO1Z + HO2	→	IHNEOOH	$2.52\times10^{-13}\times\exp(1300/T)$	[2]	X
NISOPEOO1Z + CH3O2	→	0.6 HCHO + 0.46 HO2 + 0.2 LIECHO + 0.4 CH3OH + 0.8 CO + 0.14 NOA + 0.26 MGLY + 0.46 NO2 + 0.4 IHNE	$1.0\times10^{-13}\times\exp(1139/T)$	[2], ISOP1N23O4CO-> ICNE in Wennberg	X
NISOPEOO1Z + NO3	→	LIECHO + 2NO2	$1.9\times10^{-11}\times\exp(-390/T)$	[2]	X
NISOPEOO1Z + NO	→	LIECHO + 2NO2	$2.7\times10^{-12}\times\exp(360/T)$	Analog to reaction with NO_3, only main path	X
NISOPEOO1Z + CH3C(O)O2	→	LIECHO + NO2 + CH3O2	1.0×10^{-11}	Analog to RO2+CH3C(O)O2 chemistry	X
NISOPBO2 + NISOPDO2	→	0.3808 NISOPEOO1E + 0.1792 NISOPEOO1Z + 0.089 HO2 + 0.038 LISOPACNO3 + 0.399 NISOPOH + 0.532 NC4CHO + 0.474 NISOPO	2.56×10^{-12}	[1], [2]	X
NISOPDO2 + NISOPDO2	→	0.046 HO2 + 0.798 LISOPACNO3 + 0.861 NC4CHO + 0.34 NISOPO	3.71×10^{-12}	[1]	X

NISOPBO2 + NISOPBO2	→	1.3124 NISOPEOO1E + 0.6176 NISOPEOO1Z + 0.07 NISOPOH + 0.07 NC4CHO	1.61×10^{-12}	[1], [2]	X
NISOPBOOH + OH	→	NISOPBO2	$3.4\times10^{-12}\times\exp(200/T)$	[1]	X
NISOPBOOH + OH	→	0.49 OH + 0.49 IHNE + 0.51 NISOPBOO	$8.72\times10^{-12}\times\exp(390/T)$	[1]	X
NISOPBOO + NO	→	NO2 + 0.233 HCHO + 0.408 OH + 0.055 LHMVKABOOH + 0.644 NOA + 0.36 OHCCH2OH + 0.063 NISOPNOOH + 0.47 HO2 + 0.159 MACRNOOH + 0.013 LHMVKNOOH + 0.048 CH3COCH2OH + 0.06 ETHLN + 0.012 CC(=O)COO + 0.006 MACROOH + 0.284 HCOCH2OOH	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
NISOPBOO + HO2	→	0.234 NISOPOOHOOH + 0.326 HO2 + 0.126 HCHO + 1.147 OH + 0.06 MACRNOOH + 0.589 NOA + 0.34 OHCCH2OH + 0.008 LHMVKNOOH + 0.042 CH3COCH2OH + 0.051 ETHLN + 0.058 NO2 + 0.004 MACROOH + 0.009 CC(=O)COO + 0.054 LHMVKABOOH + 0.249 HCOCH2OOH	$2.64\times10^{-13}\times\exp(1300/T)$	[1]	X
NISOPBOO	→	OH + 0.5 NISOPOOHOH=O + 0.5 IHNEOOH	$8.72\times10^{12}\times\exp(-10000/T)$	[1]	X
NISOPDOOH + OH	→	NISOPDO2	$3.4\times10^{-12}\times\exp(200/T)$	[1]	X
NISOPDOOH + OH	→	0.24 OH + 0.08 NO2 + 0.68 NISOPDOO + 0.24 IHNE + 0.08 LIECHO	$2.37\times10^{-11}\times\exp(390/T)$	[1]	X
NISOPDOOH + OH	→	OH + NC4CHO	$7.5\times10^{-12}\times\exp(20/T)$	[1]	X
NISOPDOO + NO	→	0.083 NISOPNOOH + 0.088 OH + 0.312 HCHO + 0.917 NO2 + 0.064 MACRN + 0.541 NOA + 0.541 HCOCH2OOH + 0.829 HO2 + 0.024 MVKN + 0.064 CC(=O)COO + 0.064 ETHLN + 0.021 LHMVKNOOH + 0.203 MACRNOOH	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
NISOPDOO + HO2	→	0.387 NISOPOOHOOH + 0.088 HCHO + 0.646 OH + 0.023 MACRN + 0.471 NOA + 0.471 HCOCH2OOH + 0.58 HO2 + 0.006 MVKN + 0.005 LHMVKNOOH + 0.05 MACRNOOH + 0.054 CC(=O)COO + 0.054 ETHLN	$2.64\times10^{-13}\times\exp(1300/T)$	[1]	X
NISOPDOO	→	OH + NISOPOOHOH=O	$6.55\times10^{12}\times\exp(-10000/T)$	[1]	X
NISOPOOHOH=O + OH	→	CO + NO2 + 0.75 MVKOOH + 0.25 MACROOH	1.0×10^{-11}	[1]	X
NISOPOOHOOH + OH	→	OH + NISOPOOHOH=O	2.0×10^{-12}	[1]	X
NISOPO	$\xrightarrow{O_2}$	NC4CHO + HO2	$2.5\times10^{-14}\times\exp(-300/T)$	[1]	X
NISOPO	→	IDHNBOO	$1.0\times10^{20}\times\exp(-10000/T)$	[1]	X

IDHNBOO + HO2	→	0.379 HO2 + 0.379 OH + 0.621 LISOPNO3OOH + 0.094 MACRN + 0.242 OHCCH2OH + 0.242 NOA + 0.010 MVKN + 0.033 CH3COCH2OH + 0.033 ETHLN + 0.104 HCHO	$2.6\times10^{-13}\times\exp(1300/T)$	[1]	X
IDHNBOO + NO	→	0.302 MACRN + 0.464 NOA + 0.464 OHCCH2OH + 0.024 MVKN + 0.06 ETHLN + 0.06 CH3COCH2OH + 0.85 HO2 + 0.85 NO2 + 0.326 HCHO + 0.15 LISOPNO3NO3	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
NISOPOH + OH	→	IDHNBOO	$8.72\times10^{-12}\times\exp(390/T)$	[1]	X
NISOPN + OH	→	0.26 IHNE + 0.26 NO2 + 0.74 NISOPNOO	$2.37\times10^{-11}\times\exp(390/T)$	[1]	X
NISOPNOO + NO	→	NOA + 1.11 NO2 + 0.11 OHCCH2OH + 0.89 ETHLN + 0.89 HO2	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
NISOPNOO + HO2	→	0.82 NOA + 0.82 OH + 0.18 NISOPNOOH + 0.09 NO2 + 0.09 OHCCH2OH + 0.73 ETHLN + 0.73 HO2	$2.71\times10^{-13}\times\exp(1300/T)$	[1]	X
MACRNOOH + OH	→	CO + OH + NOA	$2.7\times10^{-12}\times\exp(470/T)$	[1]	X
LHMVKNOOH + OH	→	OH + MVKN	5.77×10^{-11}	[1]	X
IHNE + OH	→	0.19 IHNC1O2 + 0.35 IHNC2O2 + 0.02 IHNC3O2 + 0.14 IHNC4O2 + 0.02 MACRENOL + 0.16 HVMK + 0.26 NO2 + 0.18 HCHO + 0.04 NOA + 0.08 HO2 + 0.08 MGLY + 0.24 CO	$3.22\times10^{-11}\times\exp(-400/T)$	[1]	X
IHNC1O2 + HO2	→	0.8 ICHNP + 0.2 NOA + 0.2 CO + 0.2 HO2 + 0.2 HCHO + 0.2 OH	$2.6\times10^{-13}\times\exp(1300/T)$	[1]	X
IHNC1O2 + NO	→	0.0 2LISOPNO3NO3=O + 0.98 NOA + 0.98 CO + 0.98 HO2 + 0.98 HCHO + 0.98 NO2	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
IHNC2O2	→	MACRN + CO + OH	$1.\times10^{7}\times\exp(5000/T)$	[1]	X
IHNC2O2 + HO2	→	0.250 NISOPOOHOH=O + 0.563 MACRN + 0.563 CO + 0.187 NOA + 0.187 OHCCH2OH + 0.75 OH + 0.75 HO2	$2.6\times10^{-13}\times\exp(1300/T)$	[1]	X
IHNC2O2 + NO	→	0.98 NO2 + 0.98 HO2 + 0.24 NOA + 0.24 GLY + 0.74 MACRN + 0.74 CO + 0.02 LISOPNO3NO3=O	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
IHNC3O2	→	MVKN + CO + OH	$1.0\times10^{7}\times\exp(5000/T)$	[1]	X
IHNC3O2 + HO2	→	0.15 NISOPOOHOH=O + 0.638 MVKN + 0.638 CO + 0.212 MGLY + 0.212 ETHLN + 0.85 OH + 0.85 HO2	$2.6\times10^{-13}\times\exp(1300/T)$	[1]	X
IHNC3O2 + NO	→	0.74 MVKN + 0.98 NO2 + 0.98 HO2 + 0.74 CO + 0.24 MGLY + 0.24 ETHLN + 0.02 LISOPNO3NO3=O	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
IHNC4O2 + HO2	→	0.15 NISOPOOHOH=O + 0.638 CH3COCH2OH + 0.85 OH + 1.062 CH3C(O)O2 + 0.85 NO2 + 0.212 HO2 + 0.212 HCHO	$2.6\times10^{-13}\times\exp(1300/T)$	[1], decomposition of MVK3CO4N-> 2 CH3C(O)O2 + NO_2	X

IHNC4O2 + NO	→	1.715 CH3C(O)O2 + 0.245 CH3COCH2OH + 0.735 HO2 + 0.735 HCHO + 1.96 NO2 + 0.02 LISOPNO3NO3=O	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
IHNEOOH + OH	→	0.5 HO2 + 0.5 MACRNOOH + CO + OH + 0.5 NOA	$3.0\times10^{-12}\times\exp(20/T)$	[1]	X
NISOPNOOH + OH	→	0.125 OH + 0.125 LISOPNO3NO3=O + 0.875 NISOPNOO	1.0×10^{-12}	[1]	X
NC4CHO + OH	→	1.08 CO + 0.85 HO2 + 0.58 NOA + 0.5 OH + 0.12 HCHO + 0.12 MGLY + 0.17 NO2 + 0.11 MVKN + 0.05 LIECHO + 0.14 CH3C(O)O2 + 0.14 ETHLN	4.1×10^{-11}	[9]	X
NC4CHO + O3	→	0.555 NOA + 0.89 CO + 0.89 OH + 0.445 MGLY + 0.445 HO2 + 0.075 H2O2 + 0.445 NO2 + 0.52 GLY + 0.035 HOOCCHO	4.4×10^{-18}	[9]	X
NC4CHO + NO3	→	HNO3 + 0.75 NOA + 0.75 CO + 0.75 HO2 +0.25 CH3C(O)O2 + 0.25 ETHLN	$6.0\times10^{-12}\times\exp(-1860/T)$	[9]	X
LHC4ACCHO + OH	→	1.065 OH + 0.355 MGLY + 0.652 CO + 0.297 HO2 + 0.116 LHMVKABOOH + 0.181 MACROOH + 0.35 LC578O2	$4.64\times10^{-12}\times\exp(650/T)$	[1], 60%A, 40%C	X
LHC4ACCHO + O3	→	0.2225 CH3C(O)O2 + 0.89 CO + 0.017188 CH2OHCOOH + 0.075625 H2O2 + 0.017188 HOOCCHO + 0.2775 CH3COCH2OH + 0.6675 HO2 + 0.260313 GLY + 0.2225 HCHO + 0.89 OH + 0.260313 OHCCH2OH + 0.5 MGLY	2.4×10^{-17}	[3]	
LHC4ACCHO + NO3	→	HNO3 + LHC4ACCO3	$6.12\times10^{-12}\times\exp(-1862/T)$	[3]	
LC578O2 + NO	→	0.02 NISOPOHOH=O + 0.98 HO2 + 0.98 NO2 + 0.196 CO + 0.612 MGLY + 0.612 OHCCH2OH + 0.153 MVKOH + 0.043 MACROH + 0.172 GLY + 0.172 CH3COCH2OH	$2.7\times10^{-12}\times\exp(360/T)$	[1], 78%A, 22%C	X
LC578O2 + NO3	→	HO2 + NO2 + 0.2 CO + 0.624 MGLY + 0.624 OHCCH2OH + 0.156 MVKOH + 0.044 MACROH + 0.176 GLY + 0.176 CH3COCH2OH	2.3×10^{-12}	Analog to NO chemistry	X
LC578O2 + HO2	→	0.35 LC578OOH + 0.13 CO + 0.65 OH + 0.65 HO2 + 0.101 MVKOH + 0.406 OHCCH2OH + 0.406 MGLY + 0.029 MACROH + 0.114 GLY + 0.114 CH3COCH2OH	$2.38\times10^{-13}\times\exp(1300/T)$	[1], 78%A, 22%C	X
LC578O2 + CH3O2	→	2 HO2 + 0.2 CO + 0.624 MGLY + 0.624 OHCCH2OH + 0.156 MVKOH + 0.044 MACROH + 0.176 GLY + 0.176 CH3COCH2OH + HCHO	1.0×10^{-12}	Analog to other RO2 chemistry	X
LC578O2 + CH3C(O)O2	→	HO2 + 0.2 CO + 0.624 MGLY + 0.624 OHCCH2OH + 0.156 MVKOH + 0.044 MACROH + 0.176 GLY + 0.176 CH3COCH2OH + CH3O2	1.0×10^{-11}	Analog to other RO2 chemistry	X
LC578O2	→	OH + CO + 0.78 MVKOH + 0.22 MACROH	$1.0\times10^{7}\times\exp(-5000/T)$	[1]	X

LC578O2	→	HO2 + LIECO3H	$1.875\times10^{13}\times\exp(-1000/T)$	[1]	X
LC578OOH + OH	→	CO + 0.5 HO2 + 0.5 OH + 0.5 MACROOH + 0.35 MVKOH + 0.15 MACROH	1.0×10^{-11}	[1]	X
LHC4ACCO3	→	HO2 + MDIALOOH	$4.1\times10^{8}\times\exp(-7700/T)$	[3]	
LHC4ACCO3 + NO	→	0.5 CH3COCH2OH + 0.5 OHCCH2OH + 0.5 CH3C(O)O2 + 0.5 CO + 0.5 HO2 + NO2	$8.1\times10^{-12}\times\exp(270/T)$	[3]	
LHC4ACCO3 + NO3	→	0.5CH3COCH2OH + 0.5OHCCH2OH + 0.5CH3C(O)O2 + 0.5CO + 0.5HO2 + NO2	4.0×10^{-12}	[3]	
LHC4ACCO3 + HO2	→	0.37 LHC4ACCO3H + 0.13 LHC4ACCO2H + 0.13 O3 + 0.5 OH + 0.25 CH3COCH2OH + 0.25 OHCCH2OH + 0.25 CH3C(O)O2 + 0.25 CO + 0.25 HO2	$2.8\times10^{-12}\times\exp(730/T)$	[6]	2
LHC4ACCO3 + CH3O2	→	HCHO + 0.1 LHC4ACCO2H + 0.45 OHCCH2OH + 0.45 CH3COCH2OH + 0.45 CH3C(O)O2 + 0.45 CO + 1.35 HO2	$2.0\times10^{-12}\times\exp(500/T)$	[3], CH3C(O)O2 chemistry	2
LHC4ACCO3 + CH3C(O)O2	→	0.5 CH3COCH2OH + 0.5 OHCCH2OH + 0.5 CH3C(O)O2 + 0.5 CO + 0.5 HO2 + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	[3], CH3C(O)O2 chemistry	2
LHC4ACCO3 + NO2	$\xrightarrow{M}$	LC5PAN1719	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	[3], CH3C(O)O2 chemistry	1
LHC4ACCO2H + OH	→	0.5 CH3COCH2OH + 0.5 OHCCH2OH + 0.5 CH3C(O)O2 + 0.5 CO + 0.5 HO2	2.52×10^{-11}	[3]	
LHC4ACCO3H + OH	→	LHC4ACCO3	2.88×10^{-11}	[3]	
LC5PAN1719 + OH	→	0.5 MACROH + 0.5 MVKOH + CO + NO3	7.79×10^{-11}	MCM	X
LC5PAN1719	$\xrightarrow{M}$	LHC4ACCO3 + NO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	MCM	X
HCOC5 + OH	→	C59O2	$2.7\times10^{-11}\times\exp(390/T)$	[1]	X
C59O2 + NO	→	0.784 CH3COCH2OH + 0.784 CO + 0.98 NO2 + 0.98 HCHO + 0.98 HO2 + 0.196 BIACETOH + 0.02 NISOPOHOH=O	$2.7\times10^{-12}\times\exp(360/T)$	[1]	X
C59O2 + NO3	→	0.8 CH3COCH2OH + 0.8 CO + NO2 + HCHO + HO2 + 0.2 BIACETOH	2.3×10^{-12}	Analog to RO2 chemistry	X
C59O2 + HO2	→	0.35 LC578OOH + 0.65 OH + 0.13 BIACETOH + 0.65 HCHO + 0.65 HO2 + 0.52 CH3COCH2OH + 0.52 CO	$2.38\times10^{-13}\times\exp(1300/T)$	[1]	X
C59O2 + CH3O2	→	0.8 CH3COCH2OH + 0.8 CO + 2 HCHO + 2 HO2 + 0.2 BIACETOH	1.0×10^{-12}	Analog to RO2 chemistry	X

C59O2 + CH3C(O)O2	→	0.8 CH3COCH2OH + 0.8 CO + HCHO + HO2 + 0.2 BIACETOH + CH3O2	1.0×10^{-11}	Analog to RO2 chemistry	X
C59O2	→	HO2 + CO + CO + CH3COCH2OH + OH	$1.875\times10^{13}\times\exp(-10000/T)$	[1]	X
HPALD + OH	→	0.856 OH + 0.385 MDIALOOH + 0.256 BIGALD3 + 0.215 LIECO3H + 0.144 HO2 + 0.144 GLY + 0.144 CC(=O)COO	5.2×10^{-11}	MCM; 60%HPALD1, 40%HPALD2	X
HPALD + NO3	→	MDIALOOH + OH + HNO3	$5.95\times10^{-12}\times\exp(-1862/T)$	MCM; 60%HPALD1, 40%HPALD2	X
HPALD + O3	→	0.438 HCOCH2OOH + 0.39 CH3C(O)O2 + 0.502 MGLY + 0.096 HO2 + 0.582 CO + 1.394 OH + 0.466 GLY + 0.108 CC(=O)COO	2.4×10^{-17}	MCM; 60%HPALD1, 40%HPALD2	X
LISOPOOHOOH + OH	→	0.333 LC578OOH + 0.667 DHHPEPOX + OH	3.0×10^{-12}	[1]	X
LISOPACNO3O2 + NO	→	0.884 HO2 + 0.884 NO2 + 0.116 LISOPNO3NO3 + 0.304 NOA + 0.304 OHCCH2OH + 0.022 MACRN + 0.1 HCHO + 0.48 CH3COCH2OH + 0.48 ETHLN + 0.079 MVKN	$2.7\times10^{-12}\times\exp(360/T)$	[1], 60%A, 40%C	X
LISOPACNO3O2	→	HO2 + NISOPOOHOH=O	$1.875\times10^{13}\times\exp(-10000/T)$	[1]	X
LISOPACNO3O2 + HO2	→	0.533 HO2 + 0.533 OH + 0.467 LISOPNO3OOH + 0.193 NOA + 0.193 OHCCH2OH + 0.011 MACRN + 0.053 HCHO + 0.287 CH3COCH2OH + 0.287 ETHLN + 0.042 MVKN	$2.6\times10^{-13}\times\exp(1300/T)$	[1]	X
LISOPNO3NO3 + OH	→	LISOPNO3NO3=O	2.0×10^{-12}	[1]	X
LISOPNO3NO3=O + OH	→	CO + NO2 + 0.5 MACRN + 0.5 MVKN	4.0×10^{-12}	[1]	X
LISOPNO3OOH + OH	→	0.33 OH + 0.67 HO2 + 0.33 NISOPOHOH=O + 0.67 NISOPOOHOH=O	3.0×10^{-12}	[1]	X
NISOPOHOH=O + OH	→	CO + NO2 + 0.75 MVKOH + 0.25 MACROH	1.0×10^{-11}	[1]	X

C6 chemistry					
BENZ + OH	→	0.327 BENZO2 + 0.14 BEPOMUC + 0.14 HO2 + 0.533 PHENOL + 0.533 HO2	$2.3\times10^{-12}\times\exp(-190/T)$	[10], MCM, IUPAC	X
PHENOL + OH	→	0.06 C6H5O + 0.8 CATECHOL + 0.8 HO2 + 0.14 PHENO2	$4.7\times10^{-13}\times\exp(1220/T)$	[3], MCM	
PHENOL + NO3	→	0.742 C6H5O + 0.742 HNO3 + 0.258 NPHENOLO2	3.8×10^{-12}	MCM	X
PHENO2 + NO	→	0.71 BIGACID1 + 0.71 GLY + NO2 + HO2 + 0.29 BZQONE	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
PHENO2 + NO3	→	0.71 BIGACID1 + 0.71 GLY + NO2 + HO2 + 0.29 BZQONE	2.3×10^{-12}	MCM	X

PHENO2 + HO2	→	PHENOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
PHENO2 + CH3O2	→	2 HO2 + HCHO + 0.71 BIGACID1 + 0.71 GLY + 0.29 BZQONE	1.0×10^{-12}	MCM, RO2 chemistry	X
PHENO2 + CH3C(O)O2	→	HO2 + 0.71 BIGACID1 + 0.71 GLY + CH3O2 + 0.29 BZQONE	1.0×10^{-11}	MCM, RO2 chemistry	X
PHENOOH + OH	→	PHENO2	1.16×10^{-10}	MCM	X
NPHENOLO2+ NO	→	BIGACID1 + GLY + 2 NO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
NPHENOLO2+ NO3	→	BIGACID1 + GLY + 2 NO2	2.3×10^{-12}	MCM	X
NPHENOLO2+ HO2	→	NPHENOLOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
NPHENOLO2+ CH3O2	→	2 HO2 + HCHO + BIGACID1 + GLY + NO2	1.0×10^{-12}	MCM, RO2 chemistry	X
NPHENOLO2+ CH3C(O)O2	→	HO2 + BIGACID1 + GLY + NO2 + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
NPHENOLOOH+ OH	→	NPHENOLO2	1.07×10^{-10}	MCM	X
BZQONE + NO3	→	NBZQO2	3.0×10^{-13}	MCM	X
BZQONE + OH	→	BZQO2	4.6×10^{-12}	MCM, IUPAC	X
NBZQO2 + HO2	→	NBZQOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
NBZQO2 + NO	→	C6CO4DB+ 2 NO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
NBZQO2 + NO3	→	2 NO2 + C6CO4DB	2.3×10^{-12}	MCM	X
NBZQO2 + CH3O2	→	NO2 + C6CO4DB + HO2 + HCHO	1.0×10^{-12}	MCM, RO2 chemistry	X
NBZQO2 + CH3C(O)O2	→	NO2 + C6CO4DB + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
NBZQOOH + OH	→	NBZQO2	6.68×10^{-11}	MCM	X
BZQO2 + HO2	→	BZQOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
BZQO2 + NO	→	HO2 + CO + NO2 + HOCOC4DIAL	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
BZQO2 + NO3	→	HO2 + CO + NO2 + HOCOC4DIAL	2.3×10^{-12}	MCM	X
BZQO2 + CH3O2	→	HO2 + CO + HOCOC4DIAL + HO2 + HCHO	1.0×10^{-12}	MCM, RO2 chemistry	X
BZQO2 + CH3C(O)O2	→	HO2 + CO + HOCOC4DIAL + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
BZQOOH + OH	→	BZQCO + OH	1.23×10^{-10}	MCM	X
BZQCO + OH	→	HO2 + CO + HOCOC4DIAL	6.07×10^{-11}	MCM	X
C6CO4DB + OH	→	3 CO + HO2 + C33CO	7.7×10^{-11}	MCM	X
C6H5O + NO2	→	NPHEN	1.0×10^{-12}	[10]	X

C6H5O + HO2	→	PHENOL	2.3×10^{-13}	[10]	X
C6H5O + O3	→	C6H5O2	2.9×10^{-13}	[10]	X
NPHEN + OH	→	NPHENO	9.0×10^{-13}	MCM	X
NPHEN + NO3	→	NPHENO + HNO3	9.0×10^{-14}	MCM	X
C6H5O2 + HO2	→	C6H5OOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
C6H5O2 + NO	→	C6H5O + NO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
C6H5O2 + NO3	→	C6H5O + NO2	2.3×10^{-12}	[3], MCM	
C6H5O2 + CH3O2	→	C6H5O + HO2 + HCHO	1.0×10^{-12}	[3], MCM, RO2 chemistry	
C6H5O2 + CH3C(O)O2	→	C6H5O + CH3O2	1.0×10^{-11}	[3], MCM, RO2 chemistry	
C6H5OOH + OH	→	C6H5O2	3.6×10^{-12}	MCM	X
BENZO2 + HO2	→	BENZOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
BENZO2 + NO	→	0.92 GLY + 0.92 NO2 + 0.46 BIGALD1 + 0.92 HO2 + 0.46 BZFUONE + 0.08 BENZN	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
BENZO2 + NO3	→	GLY + NO2 + 0.5 BIGALD1 + HO2 + 0.5 BZFUONE	2.3×10^{-12}	MCM	X
BENZO2 + CH3O2	→	GLY + 0.5 BIGALD1 + 2 HO2 + HCHO + 0.5 BZFUONE	1.0×10^{-12}	MCM, RO2 chemistry	X
BENZO2 + CH3C(O)O2	→	GLY + 0.5 BIGALD1 + HO2 + CH3O2 + 0.5 BZFUONE	1.0×10^{-11}	MCM, RO2 chemistry	X
BENZOOH + OH	→	1.4 GLY + 0.6 MALANHY + HO2 + 0.4 CO	9.77×10^{-11}	MCM	X
BENZN + OH	→	NO2 + BENZ=O	7.3×10^{-11}	MCM	X
BENZ=O + OH	→	GLY + MALO2 + HO2	8.16×10^{-11}	MCM	X
CATECHOL + OH	→	CATEC1O	1.0×10^{-10}	[3], MCM, IUPAC	
CATECHOL + NO3	→	CATEC1O + HNO3	9.9×10^{-11}	[3], MCM	
CATEC1O + NO2	→	NCATECHOL	2.08×10^{-12}	MCM	X
CATEC1O + O3	→	CATEC1O2	2.86×10^{-13}	MCM	X
NCATECHOL + OH	→	NCATECO2	3.47×10^{-12}	MCM	X
NCATECHOL + NO3	→	DNCATECO2	2.6×10^{-12}	MCM	X
NCATECO2 + HO2	→	NAROMOLOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
NCATECO2 + NO	→	2 NO2 + HOOCCHO + HO2 + MALANHY	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
NCATECO2 + NO3	→	2 NO2 + HOOCCHO + HO2 + MALANHY	2.3×10^{-12}	MCM	X

NCATECO2 + CH3O2	→	NO2 + HOOCCHO + 2 HO2 + MALANHY + HCHO	1.0×10^{-12}	MCM, RO2 chemistry	X
NCATECO2 + CH3C(O)O2	→	NO2 + HOOCCHO + HO2 + MALANHY + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
DNCATECO2 + HO2	→	NAROMOLOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
DNCATECO2 + NO	→	3 NO2 + HOOCCHO + MALANHY	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
DNCATECO2 + NO3	→	3 NO2 + HOOCCHO + MALANHY	2.3×10^{-12}	MCM	X
DNCATECO2 + CH3O2	→	2 NO2 + HOOCCHO + MALANHY + HO2 + HCHO	1.0×10^{-12}	MCM, RO2 chemistry	X
DNCATECO2 + CH3C(O)O2	→	2 NO2 + HOOCCHO + MALANHY + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
CATEC1O2 + HO2	→	CATEC1OOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
CATEC1O2 + NO	→	CATEC1O + NO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
CATEC1O2 + NO3	→	CATEC1O + NO2	2.3×10^{-12}	[3], MCM	
CATEC1O2 + CH3O2	→	CATEC1O + HO2 + HCHO	1.0×10^{-12}	[3], MCM, RO2 chemistry	
CATEC1O2 + CH3C(O)O2	→	CATEC1O + CH3O2	1.0×10^{-11}	[3], MCM, RO2 chemistry	
CATEC1OOH + OH	→	CATEC1O2	$1.9\times10^{-12}\times\exp(190/T)$	[3], MCM	
NPHENO2 + HO2	→	NPHENOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
NPHENO + O3	→	NPHENO2	2.86×10^{-13}	MCM	X
NPHENO + NO2	→	N2PHEN	2.08×10^{-12}	MCM	X
NPHENOOH + OH	→	NPHENO2	9.0×10^{-13}	MCM	X
NPHENO2 + NO	→	NPHENO + NO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
NPHENO2 + NO3	→	NPHENO + NO2	2.3×10^{-12}	MCM	X
NPHENO2 + CH3O2	→	NPHENO + HO2 + HCHO	1.0×10^{-12}	MCM, RO2 chemistry	X
NPHENO2 + CH3C(O)O2	→	NPHENO + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
N2PHEN + OH	→	DNCATECO2	3.0×10^{-14}	MCM	X
N2PHEN + NO3	→	NDNPHENO2	2.25×10^{-12}	MCM	X
NDNPHENO2 + HO2	→	NAROMOLOOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM, NAROMOLOOH no further oxidation	X
NDNPHENO2 + NO	→	3 NO2 + HNO3 + 2 CO + MALANHY	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
NDNPHENO2 + NO3	→	3 NO2 + HNO3 + 2 CO + MALANHY	2.3×10^{-12}	MCM	X

NDNPHENO2 + CH3O2	→	2 NO2 + HNO3 + 2 CO + MALANHY + HO2 + HCHO	1.0×10^{-12}	MCM, RO2 chemistry	X
NDNPHENO2 + CH3C(O)O2	→	2 NO2 + HNO3 + 2 CO + MALANHY + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
BIGALD4 + OH	→	0.7 CH3C(O)O2 + 0.7 CO2H3CHO + 0.6 MGLY + 0.3 HO2	4.9×10^{-11}	MCM	X
BIGALD4 + O3	→	1.0675 MGLY + 0.125 CH3CHO + 0.57 OH + 0.57 CO + 0.695 CH3C(O)O2 + 0.0675 H2O2 + 0.1125 CH3COCOOH	5.0×10^{-18}	MCM	X
BIGACID3 + OH	→	0.65 MALANHY + 0.65 CH3O2 + 0.35 CH3C(O)O2 + 0.35 HO2 + 0.35 HCHO + 0.7 CO	5.08×10^{-11}	MCM	X
C615CO2O2+ HO2	→	C615CO2OOH	$2.24\times10^{-13}\times\exp(1300/T)$	MCM	X
C615CO2O2+ NO	→	BIGALD2 + CO + HO2 + NO2	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
C615CO2O2+ NO3	→	BIGALD2 + CO + HO2 + NO2	2.3×10^{-12}	MCM	X
C615CO2O2+ CH3O2	→	0.8 HCHO + 0.2 CH3OH + 0.7 BIGALD2 + CO + 1.8 HO2 + 0.3 DICARBO2	1.0×10^{-12}	MCM, RO2 chemistry	X
C615CO2O2+ CH3C(O)O2	→	0.8 CH3O2 + 0.2 CH3COOH + 0.8 BIGALD2 + CO + HO2 + 0.2 DICARBO2	1.0×10^{-11}	MCM, RO2 chemistry	X
C615CO2OOH+ OH	→	OH + DICARBO2 + CO + HO2	9.42×10^{-11}	MCM	X

C7 chemistry					
TOL + OH	→	0.063 BZALD + 0.063 HO2 + 0.1914 CRESOL + 0.4171 HO2 + 0.2237 TEPOMUC + 0.5219 TOLO2	$1.8\times10^{-12}\times\exp(340/T)$	[10], IUPAC	X
CRESOL + OH	→	0.2 CRESO2 + 0.727 CATECHOL + 0.727 HO2 + 0.073 C6H5O	$1.6\times10^{-12}\times\exp(970/T)$	[10], MCM, IUPAC o-cresol	X
CRESOL + NO3	→	0.103 CRESO2 + 0.391 C6H5O + 0.494 HNO3 + 0.506 NCRESO2	1.4×10^{-11}	MCM	X
CRESO2 + HO2	→	CRESOOH	$2.3862\times10^{-13}\times\exp(1300/T)$	MCM	X
CRESO2 + NO	→	0.68 BIGACID2 + 0.68 GLY + NO2 + HO2 + 0.32 BZQONE	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
CRESO2 + NO3	→	0.68 BIGACID2 + 0.68 GLY + NO2 + HO2 + 0.32 BZQONE	2.3×10^{-12}	MCM	X
CRESO2 + CH3O2	→	2 HO2 + HCHO + 0.68 BIGACID2 + 0.68 GLY + 0.32 BZQONE	1.0×10^{-12}	MCM, RO2 chemistry	X
CRESO2 + CH3C(O)O2	→	HO2 + 0.68 BIGACID2 + 0.68 GLY + CH3O2 + 0.32 BZQONE	1.0×10^{-11}	MCM, RO2 chemistry	X
CRESOOH + OH	→	CRESO2	1.15×10^{-10}	MCM	X
NCRESO2+ HO2	→	NCRESOOH	$2.4\times10^{-13}\times\exp(1300/T)$	MCM	X

NCRESO2+ NO	→	2 NO2 + BIGACID2 + GLY	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
NCRESO2+ NO3	→	2 NO2 + BIGACID2 + GLY	2.3×10^{-12}	MCM	X
NCRESO2+ CH3O2	→	HO2 + HCHO + NO2 + 0.771 MGLY + 0.771 BIGACID2 + 0.229 GLY + 0.229 BIGACID3	1.0×10^{-12}	MCM, RO2 chemistry	X
NCRESO2+ CH3C(O)O2	→	NO2 + 0.771 MGLY + 0.771 BIGACID2 + 0.229 GLY + 0.229 BIGACID3 + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X
NCRESOOH+ OH	→	NCRESO2	1.1×10^{-10}	MCM	X
TOLO2 + HO2	→	TOLOOH	$2.3862\times10^{-13}\times\exp(1300/T)$	MCM	X
TOLO2 + NO	→	0.889 NO2 + 0.53 GLY + 0.36 MGLY + 0.889 HO2 + 0.18 BIGALD1 + 0.18 BIGALD2 + 0.18 BIGALD3 + 0.18 BZFUONE + 0.18 FUONE + 0.111 TOLN	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
TOLO2 + NO3	→	NO2 + 0.6 GLY + 0.4 MGLY + HO2 + 0.2 BIGALD1 + 0.2 BIGALD2 + 0.2 BIGALD3 + 0.2 BZFUONE + 0.2 FUONE	2.3×10^{-12}	MCM	X
TOLO2 + CH3O2	→	0.6 GLY + 0.4 MGLY + 2 HO2 + 0.2 BIGALD1 + 0.2 BIGALD2 + 0.2 BIGALD3 + HCHO + 0.2 BZFUONE + 0.2 FUONE	1.0×10^{-12}	MCM, RO2 chemistry	X
TOLO2 + CH3C(O)O2	→	0.6 GLY + 0.4 MGLY + HO2 + 0.2 BIGALD1 + 0.2 BIGALD2 + 0.2 BIGALD3 + CH3O2 + 0.2 BZFUONE + 0.2 FUONE	1.0×10^{-11}	MCM, RO2 chemistry	X
TOLOOH + OH	→	GLY + DICARBO2	9.64×10^{-11}	MCM	X
TOLN + OH	→	NO2 + TOL=O	7.16×10^{-11}	MCM	X
TOL=O + OH	→	GLY + DICARBO2	7.99×10^{-11}	MCM	X
BZALD + OH	→	ACBZO2	$5.9\times10^{-12}\times\exp(225/T)$	[3], MCM, IUPAC	
BZALD + NO3	→	ACBZO2 + HNO3	2.4×10^{-15}	MCM	X
ACBZO2 + HO2	→	0.5 C6H5O2 + 0.5 OH + 0.37 ACBZOOH + 0.13 O3 + 0.13 PHCOOH	$1.1\times10^{-11}\times\exp(364/T)$	[6], MCM, CH3C(O)O2 chemistry	2
ACBZO2 + NO	→	C6H5O2 + NO2	$7.5\times10^{-12}\times\exp(290/T)$	[3]	
ACBZO2 + NO3	→	C6H5O2 + NO2	4.0×10^{-12}	MCM	
ACBZO2 + NO2	$\xrightarrow{M}$	PBZNIT	$k_{tro}(3.28\times10^{-28}, -6.87, 0, 1.125\times10^{-11}, -1.105, 0, 0.3)$	MCM, CH3C(O)O2 chemistry	1
ACBZO2 + CH3O2	→	0.9 C6H5O2 + 0.9 HO2 + HCHO + 0.1 PHCOOH	$2.0\times10^{-12}\times\exp(500/T)$	MCM, CH3C(O)O2 chemistry	2

ACBZO2 + CH3C(O)O2	→	C6H5O2 + CH3O2	$2.9\times10^{-12}\times\exp(500/T)$	MCM, CH3C(O)O2 chemistry	2
PHCOOH + OH	→	C6H5O2	1.1×10^{-12}	MCM	X
ACBZOOH + OH	→	ACBZO2	4.66×10^{-12}	MCM	X
PBZNIT + OH	→	C6H5OOH + CO + NO2	1.06×10^{-12}	MCM	X
PBZNIT	$\xrightarrow{M}$	ACBZO2 + NO2	$k_{tro}(1.1\times10^{-5}, 0, -10100, 1.9\times10^{17}, 0, -14100, 0.3)$	[3], MCM, CH3C(O)O2 chemistry	

C8 chemistry					
XYL + OH	→	0.15 XYLOL + 0.23 TEPOMUC + 0.06 BZALD + 0.06 HO2 + 0.56 XYLENO2 + 0.38 HO2	$7.3\times10^{-12}\times\exp(355/T)$	[3,13], see sect. 4.1.1, RACM	X
XYLOL + OH	→	0.33 CRESO2 + 0.6 CATECHOL + 0.6 HO2 + 0.07 C6H5O	8.4×10^{-11}	[3], MCM, XYLOLO2 approximated with CRESO2	X
XYLOL + NO3	→	0.1 CRESO2 + 0.39 C6H5O + 0.49 HNO3 + 0.51 NCRESO2	3.91×10^{-11}	MCM, XYLOLO2 approximated with CRESO2 and NXYLOLO2 with NCRESO2	X
XYLENO2 + HO2	→	XYLENOOH	$2.5\times10^{-13}\times\exp(1300/T)$	MCM	X
XYLENO2 + NO	→	0.138 XYLNO3 + 0.293 GLY + 0.491 MGLY + 0.043 BIGALD1 + 0.147 BIGALD2 + 0.138 BIGALD3 + 0.233 BIGALD4 + 0.862 NO2 + 0.862 HO2 + 0.259 FUONE + 0.043 BZFUONE + 0.081 CO + 0.081 CH3C(O)O2 + 0.081 HCHO	$2.7\times10^{-12}\times\exp(360/T)$	MCM	X
XYLENO2 + NO3	→	HO2 + 0.34 GLY + 0.57 MGLY + 0.05 BIGALD1 + 0.17 BIGALD2 + 0.16 BIGALD3 + 0.27 BIGALD4 + 0.09 CO + 0.09 CH3C(O)O2 + 0.09 HCHO + 0.3 FUONE + 0.05 BZFUONE + NO2	2.3×10^{-12}	MCM	X
XYLENO2 + CH3O2	→	2 HO2 + HCHO + 0.34 GLY + 0.57 MGLY + 0.05 BIGALD1 + 0.17 BIGALD2 + 0.16 BIGALD3 + 0.27 BIGALD4 + 0.09 CO + 0.09 CH3C(O)O2 + 0.09 HCHO + 0.3 FUONE + 0.05 BZFUONE	1.0×10^{-12}	MCM, RO2 chemistry	X
XYLENO2 + CH3C(O)O2	→	HO2 + 0.34 GLY + 0.57 MGLY + 0.05 BIGALD1 + 0.17 BIGALD2 + 0.16 BIGALD3 + 0.27 BIGALD4 + 0.09 CO + 0.09 CH3C(O)O2 + 0.09 HCHO + 0.3 FUONE + 0.05 BZFUONE + CH3O2	1.0×10^{-11}	MCM, RO2 chemistry	X

XYLENOOH + OH	→	0.48 XYLENO2 + 0.52 MGLY + 0.26 MDIALO2 + 0.26 DICARBO2	9.3×10^{-11}	MCM	X
XYLNO3 + OH	→	NO2 + TOL=O + 0.59 CH3O2	7.19×10^{-11}	MCM	X

C10/C15 chemistry					
APIN + OH	→	TERPO2	$1.34\times10^{-11}\times\exp(410/T)$	[3], IUPAC	X
BPIN + OH	→	TERPO2	$1.62\times10^{-11}\times\exp(460/T)$	[3], IUPAC	X
LIMONENE + OH	→	TERPO2	$3.41\times10^{-11}\times\exp(470/T)$	[3], IUPAC	X
MYRC + OH	→	TERPO2	2.1×10^{-10}	[3]	
BCARY + OH	→	BCO2	2.0×10^{-10}	[11], IUPAC	X
APIN + O3	→	0.07 ELVOC + 0.39 TERPROD1 + 0.27 TERPROD2 + 0.63 OH + 0.57 HO2 + 0.23 CO + 0.52 CH3COCH3 + 0.34 HCHO + 0.05 HCOOH + 0.05 BIGALK + 0.06 CH3C(O)O2 + 0.06 CC(=O)CO[O]	$8.22\times10^{-16}\times\exp(-640/T)$	[3], IUPAC	X
BPIN + O3	→	0.43 TERPROD1 + 0.3 TERPROD2 + 0.63 OH + 0.57 HO2 + 0.23 CO + 0.52 CH3COCH3 + 0.34 HCHO + 0.05 HCOOH + 0.05 BIGALK + 0.06 CH3C(O)O2 + 0.06 CC(=O)CO[O]	$1.39\times10^{-15}\times\exp(-1280/T)$	[3], IUPAC	X
LIMONENE + O3	→	0.07 ELVOC + 0.39 TERPROD1 + 0.27 TERPROD2 + 0.63 OH + 0.57 HO2 + 0.23 CO + 0.52 CH3COCH3 + 0.34 HCHO + 0.05 HCOOH + 0.05 BIGALK + 0.06 CH3C(O)O2 + 0.06 CC(=O)CO[O]	$2.91\times10^{-15}\times\exp(-770/T)$	[3], IUPAC	X
MYRC + O3	→	0.43 TERPROD1 + 0.3 TERPROD2 + 0.63 OH + 0.57 HO2 + 0.23 CO + 0.52 CH3COCH3 + 0.34 HCHO + 0.05 HCOOH + 0.05 BIGALK + 0.06 CH3C(O)O2 + 0.06 CC(=O)CO[O]	$2.69\times10^{-15}\times\exp(-520/T)$	[3], IUPAC	X
BCARY + O3	→	0.9 BCOO + 0.1 BCO2 + 0.1 OH	1.2×10^{-14}	[11], IUPAC	X
APIN + NO3	→	NTERPO2	$1.2\times10^{-12}\times\exp(490/T)$	[3], IUPAC	
BPIN + NO3	→	NTERPO2	2.5×10^{-12}	[3], IUPAC	
LIMONENE + NO3	→	NTERPO2	1.2×10^{-11}	[3], IUPAC	
MYRC + NO3	→	NTERPO2	1.1×10^{-11}	[3], IUPAC	X
BCARY + NO3	→	NTERPO2 + 0.5 TERPROD1	1.9×10^{-11}	[3], IUPAC	X
TERPO2 + NO	→	0.26 TERPNO3 + 0.36 HCHO + 0.045 CH3COCH3 + 0.695 TERPROD1 + 0.74 HO2 + 0.74 NO2	$4.2\times10^{-12}\times\exp(180/T)$	[3]	

TERPO2 + HO2	→	TERPOOH	$7.5\times10^{-13}\times\exp(700/T)$	[3]	
TERPO2 + CH3O2	→	1.15 HCHO + 0.05 CH3COCH3 + 0.945 TERPROD1 + HO2 + 0.25 CH3OH	$2.0\times10^{-12}\times\exp(500/T)$	[3]	
TERPO2 + CH3C(O)O2	→	0.4 HCHO + 0.05 CH3COCH3 + 0.945 TERPROD1 + HO2 + CH3O2	1.0×10^{-11}	[3]	
TERPOOH + OH	→	TERPO2	3.3×10^{-11}	[3]	
TERPROD1 + OH	→	TERP2O2	5.7×10^{-11}	[3]	
TERPROD1 + NO3	→	0.5 TERP2O2 + 0.5 NTERPO2 + 0.5 NO2	1.0×10^{-12}	[3]	
TERP2O2 + HO2	→	TERP2OOH	$7.5\times10^{-13}\times\exp(700/T)$	[3]	
TERP2O2 + NO	→	0.1 TERPNO3 + 0.34 HCHO + 0.27 CH3COCH3 + 0.225 CO + 0.9 TERPROD2 + 0.9 HO2 + 0.9 NO2 + 0.225 OHCCH2OH	$4.2\times10^{-12}\times\exp(180/T)$	[3]	
TERP2O2 + CH3O2	→	TERPROD2 + 0.93 HCHO + 0.25 CH3OH + HO2 + 0.125 CO + 0.125 OHCCH2OH + 0.15 CH3COCH3	$2.0\times10^{-12}\times\exp(500/T)$	[3]	
TERP2O2 + CH3C(O)O2	→	0.34 HCHO + 0.27 CH3COCH3 + 0.225 CO + TERPROD2 + HO2 + 0.225 OHCCH2OH + CH3O2	1.0×10^{-11}	[3]	
TERPNO3 + OH	→	NO2 + TERPROD1	3.5×10^{-12}	[3]	
TERP2OOH + OH	→	TERP2O2	2.3×10^{-11}	[3]	
TERPROD2 + OH	→	0.15 CC(=O)CO[O] + 0.68 HCHO + 0.5 CH3COCH3 + 0.65 CH3C(O)O2 + 0.2 HO2 + 0.7 CO	3.4×10^{-11}	[3]	
NTERPO2 + NO	→	0.26 NTERPNO3 + 0.74 TERPROD1 + 1.48 NO2	$4.2\times10^{-12}\times\exp(180/T)$	[3]	
NTERPO2 + NO3	→	TERPROD1 + NO2 + NO2	2.4×10^{-12}	[3]	
NTERPO2 + HO2	→	NTERPOOH	$7.5\times10^{-13}\times\exp(700/T)$	Analog to TERPO2 and TERP2O2	X
NTERPO2 + CH3O2	→	0.5 NTERPNO3 + 0.75 HCHO + 0.25 CH3OH + 0.5 HO2 + 0.5 TERPROD1 + 0.5 NO2	$2.0\times10^{-12}\times\exp(500/T)$	[3]	
NTERPO2 + CH3C(O)O2	→	TERPROD1 + NO2 + CH3O2	1.0×10^{-11}	[3]	
NTERPNO3 + OH	→	NO2 + TERPROD1	3.5×10^{-12}	[3]	
NTERPOOH + OH	→	NTERPO2	2.0×10^{-11}	MCM	X
ELVOC + OH	→	HO2 + TERPROD1	1.0×10^{-11}	[3]	
BCOO	→	PROD1	100	[11]	X

BCOO	$\xrightarrow{H_2O}$	0.5 PROD1 + 0.5 H2O2 + 0.5 PROD2	2.0×10^{-16}	[11]	X
BCO2 + NO	→	0.753 PROD1 + 0.753 HO2 + 0.753 NO2 + 0.247 BCNO3	$2.54\times10^{-12}\times\exp(360/T)$	[11]	X
BCO2 + NO3	→	NO2 + HO2 + PROD1	2.3×10^{-12}	[11], MCM	X
BCO2 + HO2	→	BCOOH	$2.84\times10^{-13}\times\exp(1300/T)$	[11]	X
BCO2 + CH3O2	→	PROD1 + 2 HO2 + HCHO	1.0×10^{-12}	[11], RO2 chemistry	X
BCO2 + CH3C(O)O2	→	PROD1 + HO2 + CH3O2	1.0×10^{-11}	[11], RO2 chemistry	X
BCNO3 + OH	→	PROD1 + NO2	7.3×10^{-11}	[11]	X
BCOOH + OH	→	PROD1 + OH	9.1×10^{-11}	[11]	X
PROD1 + O3	→	0.836 PROD3 + 0.836 HCHO + 0.164 P1O2 + 0.164 OH	1.1×10^{-16}	[11]	X
PROD1 + OH	→	P1O2	7.9×10^{-11}	[11]	X
P1O2 + NO	→	0.753 PROD3 + 0.753 HCHO + 0.753 HO2 + 0.753 NO2 + 0.247 P1NO3	$2.54\times10^{-12}\times\exp(360/T)$	[11]	X
P1O2 + NO3	→	PROD3 + HCHO + HO2 + NO2	2.3×10^{-12}	[11], MCM	X
P1O2 + HO2	→	PSQTOOH	$2.84\times10^{-13}\times\exp(1300/T)$	[11]	X
P1O2 + CH3O2	→	PROD3 + 2 HCHO + 2 HO2	1.0×10^{-12}	[11], RO2 chemistry	X
P1O2 + CH3C(O)O2	→	PROD3 + HCHO + HO2 + CH3O2	1.0×10^{-11}	[11], RO2 chemistry	X
P1NO3 + OH	→	PROD3 + HCHO + NO2	2.3×10^{-11}	[11]	X
PROD2 + O3	→	0.836 PROD4 + 0.836 HCHO + 0.164 P2O2 + 0.164 OH	1.1×10^{-16}	[11]	X
PROD2 + OH	→	P2O2	7.0×10^{-11}	[11]	X
P2O2 + NO	→	0.753 PROD4 + 0.753 HCHO + 0.753 HO2 + 0.753 NO2 + 0.247 P2NO3	$2.54\times10^{-12}\times\exp(360/T)$	[11]	X
P2O2 + NO3	→	PROD4 + HCHO + HO2 + NO2	2.3×10^{-12}	[11], MCM	X
P2O2 + HO2	→	PSQTOOH	$2.84\times10^{-13}\times\exp(1300/T)$	[11]	X
P2O2 + CH3O2	→	PROD4 + 2 HCHO + 2 HO2	1.0×10^{-12}	[11]	X
P2O2 + CH3C(O)O2	→	PROD4 + HCHO + HO2 + CH3O2	1.0×10^{-11}	[11]	X
PROD3 + OH	→	0.9 TERP2O2 + 1.25 CO2C3CHO	3.7×10^{-11}	[11]	X
PROD4 + OH	→	0.9 TERP2O2 + 1.25 CO2C3CHO	1.2×10^{-11}	[11]	X

Table S1-3: URMELL Photolysis reactions. Photolysis rates are calculated as in MCM3.3.1, therefore the reader is referred to http://mcm.york.ac.uk/parameters/photolysis_param.htt. A few parameters were calculated from IUPAC data. A list of the photolysis parameters is given in Table S1-4. All reaction equations marked with an X or a number from 1 to 5 deviate from original JAMv2b formula.

Photolysis reaction			Photolysis rate as in MCM3.3.1	
O3	→	O1D	J1	
O3	→	O3PX	J2	
H2O2	→	OH + OH	J3	
HONO	→	OH + NO	J7	
NO2	→	NO + O3PX	J4	
N2O5	→	NO3 + NO2	[3], IUPAC	
HNO3	→	OH + NO2	J8	
NO3	→	NO	J5	
NO3	→	NO2 + O3PX	J6	
HNO4	→	0.65 HO2 + 0.65 NO2 + 0.35 OH + 0.35 NO3	[3], IUPAC	
CH3OOH	→	HCHO + HO2 + OH	J41	
HCHO	→	CO + HO2 + HO2	J11	
HCHO	→	H2 + CO	J12	
HOCH2OOH	→	HCOOH + HO2 + OH	IUPAC	
EOOH	→	EO + OH	J41	
CCOO	→	CH3CHO + OH + HO2	J41	
CH3CHO	→	CH3O2 + HO2 + CO	J13	
CH3COOOH	→	CH3O2 + OH	J41	3
PAN	→	0.6 CH3C(O)O2 + 0.6 NO2 + 0.4 CH3O2 + 0.4 NO3	[3], IUPAC	
OHCCH2OH	→	HO2 + HCHO + HO2 + CO	J15	
OCC(=O)OO	→	HCHO + HO2 + OH	J41	
GLY	→	0.87 CO + 0.87 CO + 0.87 H2 + 0.13 HCHO + 0.13 CO	J31+J32	4
GLY	→	CO + CO + HO2 + HO2	J33	
O=C(OO)C=O	→	HO2 + CO + OH	J15	
HOOCCHO	→	HO2 + HO2 + CO	J34	3
CH3CH(OH)OOH	→	HCOOH + CH3O2 + OH	Analog to HOCH2OOH	
POOH	→	CH3CHO + HCHO + HO2 + OH	J41	
PROPOOH	→	0.736 CH3COCH3 + 0.396 CH3CHO + OH + HO2	J41	
CH3COCH3	→	CH3C(O)O2 + CH3O2	J21	
CC(=O)COO	→	CH3C(O)O2 + HCHO + OH	J22	
CC(=O)COO	→	CH3C(O)O2 + HCHO + OH	J41	
CH3COCOOH	→	CH3C(O)O2 + HO2	J34	
MGLY	→	CH3C(O)O2 + CO + HO2	J34	3
CH3COCH2OH	→	CH3C(O)O2 + HCHO + HO2	J22	
PR2O2HNO3	→	0.83 HO2 + 0.83 NOA + 0.17 HCHO + 0.17 CH3CHO + OH	J41	

NOA	→	CH3C(O)O2 + HCHO + NO2	J56	3
MEK	→	CH3C(O)O2 + ETHPX	J22	3
MEKANO3	→	NO2 + 0.5 CO2C3CHO + 0.5 HCHO + 0.5 EO2 + 0.5 HO2	J22	3
MEKANO3	→	NO2 + 0.5 CO2C3CHO + 0.5 HCHO + 0.5 EO2 + 0.5 HO2	J53	3
MEKAOOH	→	0.5 HCHO + 0.5 HO2 + 0.5 CO2C3CHO + 0.5 EO2 + OH	J41	3
MEKAOOH	→	0.5 HCHO + 0.5 HO2 + 0.5 CO2C3CHO + 0.5 EO2 + OH	J22	3
MEKBOOH	→	CH3C(O)O2 + CH3CHO + OH	J41	3
MEKBOOH	→	CH3C(O)O2 + CH3CHO + OH	J22	3
MEKCOOH	→	HCHO + 1.5 CH3C(O)O2 + OH	J41	3
MEKCOOH	→	HCHO + 1.5 CH3C(O)O2 + OH	J22	3
MEKAOH	→	CH3C(O)O2 + EO	J22	X
MEKBOH	→	CH3C(O)O2 + CH3CHO	J22	X
MEKCOH	→	1.5 CH3C(O)O2 + HCHO + HO2	J22	X
CO2C3CHO	→	CC(=O)CO[O] + HCHO	J15	
MACR	→	HO2 + 0.5 MCO3 + 0.5 HCHO + 0.175 CH3C(O)O2 + 0.825 CO + 0.325 CH3O2	J18+J19	5
MACRN	→	NOA + HO2 + CO + OH	J22	5
MACRN	→	NOA + HO2 + CO + OH	J41	5
MACR2N3OH	→	CH3COCH2OH + HO2 + CO + NO2	J56	
MACR2NOOH	→	CH3COCH2OH + OH + NO2	J22	
MACR2NOOH	→	CH3COCH2OH + OH + NO2	J41	
MACR2NOOH	→	CH3COCH2OH + OH + NO2	J51	
MACROOH	→	CH3COCH2OH + CO + HO2 + OH	J17	3
MACROH	→	CH3COCH2OH + CO + HO2 + HO2	J17	3
MACO3H	→	HCHO +0.35 CH3C(O)O2 + OH + 0.65 CH3O2 + 0.65 CO	J41	5
MVK	→	0.50 C3H6 + CO + 0.50 CH3C(O)O2 + 0.50 HCHO + 0.50 HO2	J23+J24	
MVKOH	→	CH3C(O)O2 + OHCCH2OH + HO2	J22	
MVKN	→	1.01 CH3C(O)O2 + 0.69 OHCCH2OH + 0.7 NO2 + 0.3 ETHLN + 0.29 HO2 + 0.01 OH	1.6×J56	3
LHMVKABOOH	→	OH + 0.47 HCHO + 0.47 MGLY + 0.47 HO2 + 0.53 CH3C(O)O2 + 0.53 OHCCH2OH	J17	5
CO2H3CHO	→	0.5 MGLY + 0.5 CO + 1.5 HO2 + 0.5 CH3C(O)O2 + 0.5 GLY	J35	3
BIACETOH	→	CH3C(O)O2 + CO + HO2 + HCHO	J35	3
MALOOH	→	0.4 GLY + HO2 + 0.4 CO + 0.6 MALANHY + OH	2×J20	
MDIALOOH	→	0.5 CH3C(O)O2 + 0.5 GLY + 0.5 CO + 0.5 HO2 + 0.5 MGLY + OH	2×J20	
MALANHYOOH	→	OH + HCOCOHCO3	J41	
HCOCOHCO3H	→	OH + GLY + HO2	J41	
IBUTALOH	→	CH3COCH3 + HO2 + HO2 + CO	J17	3
IBUTALOHOOH	→	HO2 + CH3COCH3 + OH	J41	3
ALKNO3	→	0.4 CH3CHO + 0.25 HCHO + 0.25 CH3COCH3 + HO2 + 0.8 MEK + NO2	J54	3
ALKOOH	→	0.4 CH3CHO + 0.25 HCHO + 0.25 CH3COCH3 + HO2 + 0.8 MEK + OH	J41	
LISOPACNO3	→	0.45 LHC4ACCHO + 0.45 HO2 + 0.55 CO + 0.55 OH + 0.33 MACROOH + 0.22 LHMVKABOOH + NO2	J53	3

LISOPACOOH	→	0.97 LHC4ACCHO + 0.97 HO2 + 1.03 OH + 0.03 CO + 0.012 MACROOH + 0.018 LHMVKABOOH	J41	
DHPMPAL	→	CO + HO2 + OH + CC(=O)COO	J15	
DHPMPAL	→	0.5 MGLY + 1.5 OH + 0.5 HCHO + 0.5 C3MDIALOOH	J41	
DHPMEK	→	0.5 CH3C(O)O2 + 0.5 HCHO + 0.5 MGLY + 0.5 HCOCH2OOH + 1.5 OH	J41	
DHPMEK	→	CH3C(O)O2 + HCOCH2OOH + OH	J22	
HCOCH2OOH	→	OH + HCHO + CO + HO2	J41	
HCOCH2OOH	→	HO2 + CO + HCHO + OH	J22	
C3MDIALOOH	→	MGLY + OH + HO2 + CO	2×J17	
HPALD	→	0.285 CH3C(O)O2 + 0.285 HVMK + 0.285 OHCCH2OH + 1.215 CO + 1.5 OH + 0.215 MACRENOL + 0.215 CH3COCH2OH + 0.215 HO2	0.5×J20	
LIECHO	→	HO2 + 0.28 OH + 1.28 CO + 0.72 LHMVKABO2 + 0.28 CH3COCH2OH	J17	
LIECO3H	→	0.546 OH + CO + 1.454 HO2 + 0.391 CO2H3CHO + 0.155 C3MDIALOH + 0.454 LHMVKABOOH	J41	
LIECO3H	→	0.546 OH + CO + 1.454 HO2 + 0.391 CO2H3CHO + 0.155 C3MDIALOH + 0.454 LHMVKABOOH	2×J22	
ISOPBNO3	→	HCHO + MVK + HO2 + NO2	J55	3
ISOPBOOH	→	HCHO + MVK + HO2 + OH	J41	
DHHPEPOX	→	OH + HO2 + 0.429 MGLY + 0.429 OHCCH2OH + 0.571 GLY + 0.571 CC(=O)COO	J41	
ISOPDNO3	→	HCHO + MACR + HO2 + NO2	J54	3
ISOPDOOH	→	HCHO + MACR + HO2 + OH	J41	
NISOPBOOH	→	NO2 + 0.33 HO2 + 0.67 OH + 0.097 MACR + 0.903 MVK + HCHO	J41	
NISOPDOOH	→	0.125 NC4CHO + 0.125 HO2 + 0.783 OH + 0.217 NO2 + 0.182 ISOPBO2 +0.034 ISOPDO2 + 0.659 NISOPO	J41	
NISOPOOHOH=O	→	0.5 CO + 0.25 LHMVKABOOH + 0.25 MACROOH + 0.5 HO2 + 0.5 OH + NO2 + 0.5 MGLY + 0.5 OHCCH2OH	J41	
NISOPOOHOH=O	→	OH + NO2 + MGLY + OHCCH2OH	J54	
NISOPOOHOH=O	→	CO + 0.5 LHMVKABOOH + 0.5 MACROOH + HO2 + NO2	J22	
NISOPOOHOOH	→	NO2 + IDHPOO1	J54	
NISOPOOHOOH	→	OH + 0.5 IDHNBOO + 0.5 LISOPACNO3O2	2×J41	
NISOPOH	→	NO2 + 0.5 MVK + 0.5 MACR + HO2 + HCHO	J53	
NISOPN	→	1.11 NO2 + 0.455 NC4CHO + 0.455 HO2 + 0.1 MVK + 0.01 MACR + 0.11 HCHO + 0.455 NISOPO	J55	
MACRNOOH	→	NOA + OH + CO + HO2	J17	
LHMVKNOOH	→	CH3C(O)O2 + OH + ETHLN		
LHMVKNOOH	→	CH3C(O)O2 + OH + ETHLN	J53+J22	
IHNEOOH	→	HO2 + OH + NOA + GLY	J41	
NISOPNOOH	→	OH + 0.32 NO2 + 0.32 OHCCH2OH + 0.5 ETHLN + 0.82 NOA + 0.68 HO2 + 0.18 LISOPNO3NO3=O	J41	
NISOPNOOH	→	0.535 OH + NO2 + 0.16 OHCCH2OH + 0.25 NOA + 0.09 HO2 + 0.25 LISOPACNO3O2 + 0.125 IDHNBOO + 0.375 MVKN + 0.375 HCHO + 0.09 HCOCH2OOH	2×J51	
ETHLN	→	HCHO + CO + HO2 + NO2	J56	
NO3CH2CO3H	→	HCHO + OH + NO2	J41	
HVMK	→	0.5 CO + 0.5 MGLY + OH + 0.5 HO2 + 0.5 CH3C(O)O2 + 0.5 GLY	0.5×J20	

MACRENOL	→	CO + CH3COCOOH + 2 OH	0.5×J20	
C3MDIALOH	→	CO + MGLY + 2 HO2	2×J17	
NC4CHO	→	NO2 + 0.184 HO2 + 0.088 HCHO + 0.104 CH3C(O)O2 + 0.056 MGLY + 1.004 CO + 0.016 GLY + 0.552 OH + 0.08 MDIALOOH + 0.08 C3MDIALOOH + 0.144 HVMK + 0.336 MACRENOL + 0.06 LHMVKABO2 + 0.14 CH3COCH3	8×J56	3
LHC4ACCHO	→	0.5 LHC4ACCO3 + 0.3 CH3COCH2OH + 0.2 OHCCH2OH + 0.2 CH3C(O)O2 + 1.3 HO2 + 0.8 CO	J18+J19	3
LC578OOH	→	CO + 1.5 HO2 + 0.5 OH + 0.5 MACROOH + 0.35 MVKOH + 0.15 MACROH	J22	
LC578OOH	→	OH + HO2 + 0.1 HCHO + 0.1 CO2H3CHO + 0.438 CH3COCH2OH + 0.438 GLY + 0.088 OHCCH2OH + 0.088 MGLY + 0.122 CO + 0.122 MACROH	J41	
LHC4ACCO3H	→	0.5 CH3COCH2OH + 0.5 OHCCH2OH + 0.5 CH3C(O)O2 + 0.5 CO + 0.5 HO2 + OH	J41	3
HCOC5	→	OCC(=O)O[O] + CH3C(O)O2 + HCHO	J24	3
MBOOOH	→	HO2 + 0.67 OHCCH2OH + 0.67 CH3COCH3 + 0.33 IBUTALOH + 0.33 HCHO + OH	J41	
MBONO3OOH	→	0.35 HCHO + 0.35 IBUTALOH + 0.35 NO2 + 0.43 NOA + 0.65 CH3COCH3 + 0.65 HO2 + OH	J41	
BIGACID2	→	CH3C(O)O2 + HOOCCHO + CO + HO2	J23+J24	
DICARBOOH	→	0.17 MGLY + 0.17 HO2 + 0.17 CO + 0.83 MALANHY + 0.83 CH3O2 + OH	2xJ20	
LISOPNO3OOH	→	0.65 OH + 0.7 HO2 + 0.35 HCHO + 0.025 MVKN + 0.075 ETHLN + 0.25 MACRN + 0.325 OHCCH2OH + 0.625 CH3COCH2OH + 0.65 NO2 + 0.075 MACROOH + 0.25 HCOCH2OOH + 0.025 CC(=O)COO	J41	
LISOPNO3OOH	→	0.65 OH + 0.7 HO2 + 0.35 HCHO + 0.025 MVKN + 0.075 ETHLN + 0.25 MACRN + 0.325 OHCCH2OH + 0.625 CH3COCH2OH + 0.65 NO2 + 0.075 MACROOH + 0.25 HCOCH2OOH + 0.025 CC(=O)COO	J51	
LISOPOOHOOH	→	1.25 OH + 0.25 OHCCH2OH + 0.25 CH3COCH2OH + 0.75 LC578OOH + 0.75 HO2	2×J41	
LISOPNO3NO3	→	CC(=O)COO + OHCCH2OH + 2 NO2	J55	
LISOPNO3NO3=O	→	0.6 CC(=O)COO + NO2 + 0.6 NO3CH2CO3 + 0.4 HO2 + 0.4 CO + 0.2 MACRN + 0.2 MVKN	J41	
LISOPNO3NO3=O	→	0.6 CC(=O)COO + NO2 + 0.6 NO3CH2CO3 + 0.4 HO2 + 0.4 CO + 0.2 MACRN + 0.2 MVKN	J22	
LISOPNO3NO3=O	→	1.5 NO2 + 0.65 CO + 0.1 MACROH + 0.1 MVKOH + 0.075 MVKN + 0.075 MACRN + 0.275 HO2 + 0.025 GLY + 0.025 NOA + 0.025 MGLY + 0.025 ETHLN + 0.525 CH3COCH2OH + 0.375 HCHO + 0.075 NO2 + 0.15 CH3C(O)O2 + 0.225 NO3CH2CO3	2×J51	
NISOPOHOH=O	→	0.5 HO2 + NO2 + 0.5 CO + 0.375 MVKOH + 0.125 MACROH + 0.5 OCC(=O)O[O] + 0.5 CC(=O)COO	J41	
NISOPOHOH=O	→	0.5 HO2 + NO2 + 0.5 CO + 0.375 MVKOH + 0.125 MACROH + 0.5 OCC(=O)O[O] + 0.5 CC(=O)COO	J22	
NISOPOHOH=O	→	NO2 + 0.5 HO2 + 0.375 OHCCH2OH + 0.375 MGLY + 0.125 GLY + 0.625 CC(=O)COO + 0.5 OCC(=O)O[O]	J51	
BEPOMUC	→	0.5 BIGALD1 + 1.5 HO2 + 1.5 CO + 0.5 C5DIALO2	0.1×J4	3
C5DIALOOH	→	OH + BIGALD1 +CO + HO2	J41	
C5DIALOOH	→	CO + OH + HO2 + BIGALD1	J18+J19	
BIGALD1	→	0.6 MALO2 + 0.6 HO2 + 0.4 BZFUONE	0.14×J4	3
BIGALD2	→	0.6 DICARBO2 + 0.6 HO2 + 0.4 FUONE	0.2×J4	
BIGALD3	→	0.6 CO + 0.6 HO2 + 0.6 MDIALO2 + 0.4 FUONE	0.2×J4	

BIGALD4	→	CH3C(O)O2 + MGLY +HO2 + CO	0.0057×J4	3
PHENOOH	→	0.71 BIGACID1 + 0.71 GLY + HO2 + OH + 0.29 BZQONE	J41	
NPHENOLOOH	→	BIGACID1 + GLY + NO2 + OH	J41	
NBZQOOH	→	OH + NO2 + 2 HO2 + 6 CO	J41	
C6CO4DB	→	2 HO2 + 2 CO + C33CO	2×J34	
C33CO	→	2 HO2 + 3 CO	2×J15	
BZQOOH	→	OH + 2 HO2 + 5 CO	J41	
HOCOC4DIAL	→	2 HO2 + CO + GLY	J34, J15	
CO2C4DIAL	→	2 HO2 + 4 CO	2×J34	
BIGACID1	→	HOOCCHO + CO + HO2 + CO + HO2	J18+J19	
C6H5OOH	→	C6H5O + OH	J41	
BENZOOH	→	GLY + 0.5 BIGALD1 + HO2 + OH + 0.5 BZFUONE	J41	
BENZN	→	NO2 + HO2 + GLY + 0.5 BIGALD1 + 0.5 BZFUONE	J54	
BENZ=O	→	GLY + MALO2	J22	
BZFUONEOOH	→	2 HO2 + 2 CO + OH + HCHO	J41	
BZFUO	→	2 HO2 + 2 CO + HCHO	J34	
CATEC1OOH	→	CATEC1O + OH	J41	
NPHENOOH	→	NPHENO + OH	J41	
TEPOMUC	→	0.5 CH3C(O)O2 + HO2 + CO + 0.5 EPOXDIALD + 0.5 C615CO2O2	J4	3
C615CO2OOH	→	OH + BIGALD2 + CO + HO2	J41	
C615CO2OOH	→	CO + OH + HO2 + BIGALD2	J19+J19	
EPOXDIALD	→	CO + HO2 + GLY + CO + HO2	J17*2	
CRESOOH	→	0.68 BIGACID2 + 0.68 GLY + HO2 + OH + 0.32 BZQONE	J41	
NCRESOOH	→	NO2 + OH + BIGACID2 + GLY	J41	
NCRESOOH	→	OH + NO2 + HO2 + 0.68 BIGACID2 + 0.32 BZQONE + 0.68 GLY	J54	
TOLOOH	→	0.6 GLY + 0.4 MGLY + HO2 + 0.2 BIGALD1 + 0.2 BIGALD2 + 0.2 BIGALD3 + OH + 0.2 BZFUONE + 0.2 FUONE	J41	
TOLN	→	NO2 + 0.6 GLY + 0.4 MGLY + HO2 + 0.2 BIGALD1 + 0.2 BIGALD2 + 0.2 BIGALD3 + 0.2 BZFUONE + 0.2 FUONE	J54	
TOL=O	→	GLY + DICARBO2	J22	
BZOOH	→	BZALD + HO2 + OH	J41	
BZALD	→	0.50 HO2 + 0.50 ACBZO2 + 0.50 HO2 + 0.50 CO + 0.50 C6H5O2	J18+J19	
ACBZOOH	→	C6H5O2 + OH	J41	
BIGACID3	→	HOOCCHO + 2 CH3C(O)O2	J24	
XYLENOOH	→	0.34 GLY + 0.57 MGLY + 0.05 BIGALD1 + 0.17 BIGALD2 + 0.16 BIGALD3 + 0.27 BIGALD4 + 0.09 CO + 0.09 HCHO + 0.09 CH3C(O)O2 + 0.3 FUONE + 0.05 BZFUONE + HO2 + OH	J41	
XYLNO3	→	NO2 + HO2 + 0.22 GLY + 0.78 MGLY + 0.26 BIGALD2 + 0.26 BIGALD3 + 0.11 BIGALD4 + 0.37 FUONE	J54*0.4075	
XYLNO3	→	NO2 + HO2 + 0.42 GLY + 0.42 MGLY + 0.08 BIGALD1 + 0.113 BIGALD2 + 0.097 BIGALD3 + 0.38 BIGALD4 + 0.32 CH3C(O)O2 + 0.25 FUONE + 0.08 BZFUONE	J55*0.5925	
FUONEOOH	→	HO2 + CH3C(O)O2 + HCHO + OH	J41	

TERPOOH	→	0.4 HCHO + 0.05 CH3COCH3 + 0.945 TERPROD1 + HO2 + OH	J41	
TERPNO3	→	TERPROD1 + NO2 + HO2	J41	
TERP2OOH	→	OH + 0.372 HCHO + 0.3 CH3COCH3 + 0.25 CO + TERPROD2 + HO2 + 0.25 OHCCH2OH	J41	
NTERPOOH	→	TERPROD1 + NO2 + OH	J41	
NTERPNO3	→	TERPROD1 + NO2 + OH	J41	
TERPROD1	→	TERPROD2 + HO2 + CO	J15	3
TERPROD2	→	0.15 CC(=O)CO[O] + 0.68 HCHO + 0.5 CH3COCH3 + 1.2 HO2 + 1.7 CO	J15	3
ELVOC	→	OH + HO2 + TERPROD2	J41	
BCOOH	→	PROD1 + HO2 + OH	J41	

Table S1-4: List of photolysis parameters used mainly taking from the MCM3.3.1 (J1-J56). The formula used to calculate the photolysis rates is as follows: $J = l \times \cos(\chi)^m \times \exp(-n \times sec\chi)$ where the solar zenith angle χ is in radians

J	l	m	n
J1	6.073×10^{-5}	1.743	0.474
J2	4.775×10^{-4}	0.298	0.080
J3	1.041×10^{-5}	0.723	0.279
J4	1.165×10^{-2}	0.244	0.267
J5	2.485×10^{-2}	0.168	0.108
J6	1.747×10^{-1}	0.155	0.125
J7	2.644×10^{-3}	0.261	0.288
J8	9.312×10^{-7}	1.230	0.307
J11	4.642×10^{-5}	0.762	0.353
J12	6.853×10^{-5}	0.477	0.323
J13	7.344×10^{-6}	1.202	0.417
J15	2.792×10^{-5}	0.805	0.338
J17	7.914×10^{-5}	0.764	0.364
J18	1.482×10^{-6}	0.396	0.298
J19	1.482×10^{-6}	0.396	0.298
J20	$7.600D\times10^{-4}$	0.396	0.298
J21	7.992×10^{-7}	1.578	0.271
J22	5.804×10^{-6}	1.092	0.377
J23	2.4246×10^{-6}	0.395	0.296
J24	2.424×10^{-6}	0.395	0.296
J31	6.845×10^{-5}	0.130	0.201
J32	1.032×10^{-5}	0.130	0.201
J33	3.802×10^{-5}	0.644	0.312
J34	1.537×10^{-4}	0.170	0.208
J35	3.326×10^{-4}	0.148	0.215
J41	7.649×10^{-6}	0.682	0.279
J51	1.588×10^{-6}	1.154	0.318
J53	2.485×10^{-6}	1.196	0.328
J54	4.095×10^{-6}	1.111	0.316
J55	1.135×10^{-5}	0.974	0.309
J56	4.365×10^{-5}	1.089	0.323
JN_2O_5	7.083×10^{-5}	0.887	0.237
$JHNO_4$	9.036×10^{-6}	1.262	0.327
$JHOCH_2OOH$	8.122×10^{-6}	0.879	0.248
JPAN	8.518×10^{-7}	1.173	0.250

Supplement S2 – Sensitivity studies

Supplement S2 contains all additional information about the box model sensitivity studies including figures, statistics and more detailed insights into the performed sensitivity studies. A summary of the main results are presented in the main manuscript in sect. 4.1 and in terms of sCI in sect. 2.2.1.

S2.1 stabilized Criegee intermediate CH_2OO

The sensitivity study on the branching ratios of the stabilized Criegee intermediate CH_2OO considers ratios recommended by Nguyen *et al.* (fig. 2 dashed yellow line) and Sheps *et al.* (fig. 2 yellow line).[7,14] OH (fig. 2e), HO_2 (fig. 2i), HCHO (fig. 2c) and H_2O_2 (fig. 2m) show only minor increases with highest impacts on H_2O_2 concentrations when using the ratios provided by Sheps *et al.*[7,]. The ratios from Nguyen *et al.*[12] produce three times higher HCOOH (fig. 2p) ratios and an earlier production onset with minimum concentrations between 9-10 p.m. and maximum concentrations around 1pm. For Sheps *et al.*[7], minimum and maximum concentrations are delayed by about eight (6 a.m.) and three hours (4 p.m.), respectively. A similar shift can be seen for JAMv2b (fig. 2 blue line) and the MCM (fig. 2 black line), but fluctuations in the diurnal cycle are weak. Compared to other chemistry mechanisms, URMELL shows a clear diurnal cycle when using the ratios from Sheps *et al.*[7,] which is in better agreement with field measurements[15,16] (Millet et al., 2015; Yuan et al., 2015).

S2.2 Treatment of $NPHENOLO_2$

Sensitivity study on the treatment of $NPHENOLO_2$ produced from the reaction of PHENOL with NO_3. For $NPHENOLO_2$ various approximations are currently used: i) direct treatment, ii) approximation with $PHENO_2$ and iii) approximation with NPHEN (see sect. 2.4). To test the different approaches, we performed sensitivity studies with URMELL for the urb_05_w scenario (Fig. S2-4). While URMELL itself considers the direct treatment of $NPHENOLO_2$ (solid yellow line), for the $PHENO_2$ run $NPHENOLO_2$ is replaced by $PHENO_2$ + NO_2 (dashed yellow line) and for the NPHEN run by NPHEN (dotted yellow line). The further oxidation of $PHENO_2$ leads to HO_2 formation while $NPHENOLO_2$ produces NO_2. This increase in HO_2 and decrease in NO_2 enhance the O_3 and consequently also the OH, and NO_3 while lowering NO concentrations. As a consequent, oxidation processes are boosted lowering the reactant (e.g. C_5H_8 Fig. S2-4d) and increasing the reaction product concentrations (remaining plots of Fig. S2-4). In contrast, the approximation with NPHEN has no significant impact on most of

the analyzed compounds except GLY (Fig. S2-4k), which decreases. The degradation of NPHENOLO$_2$ would lead to NO$_2$, BIGACID1 and GLY formation, whereas NPHEN e.g. produces MALANHY but due to lower reaction coefficients of intermediate products (e.g. N2PHEN), these products build up.

S2.3 Analysis of higher (remote) oxidant concentrations

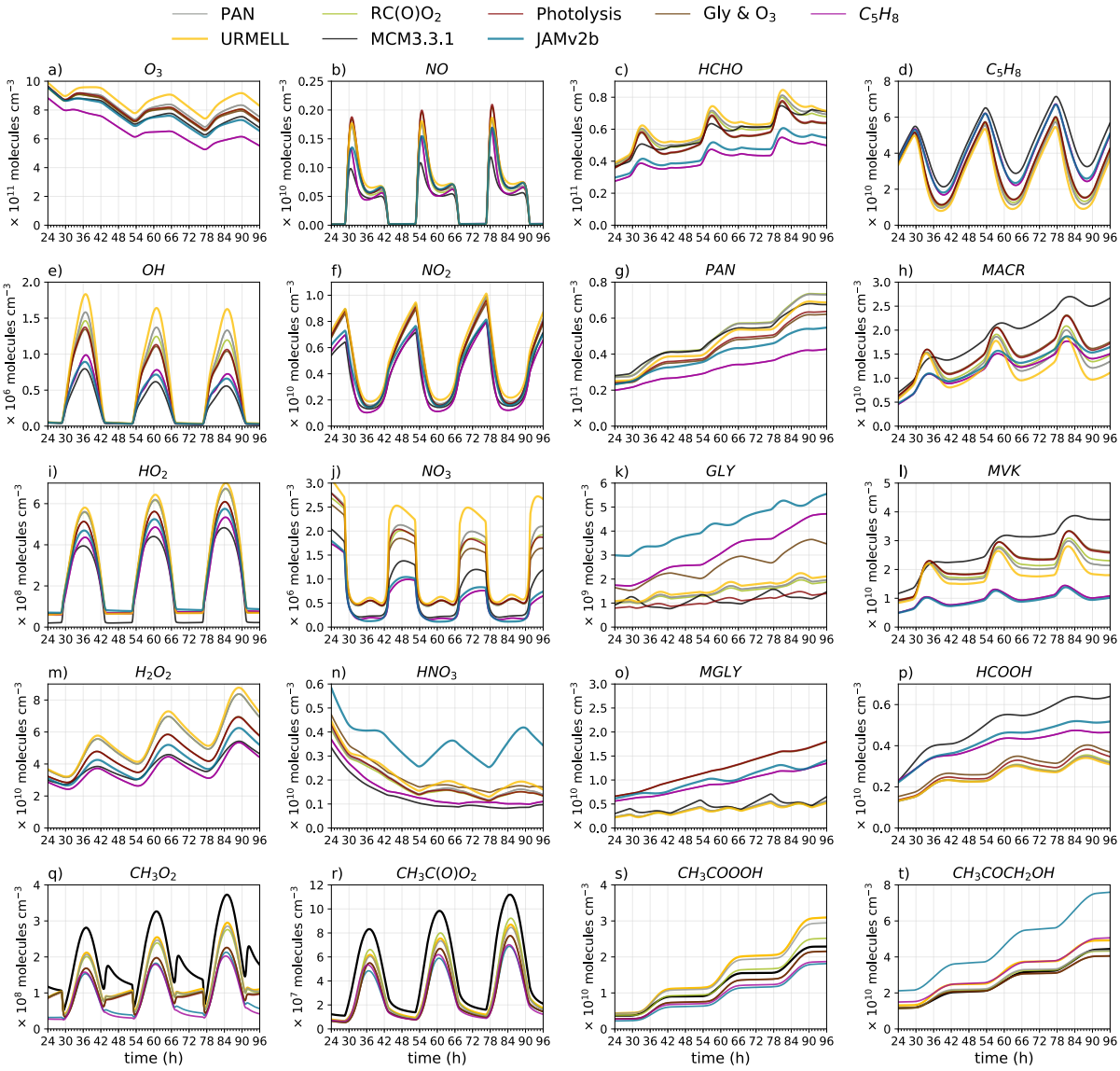


Figure S2-1: Time series of various gas-phase species for the remote summer case with full radiation for several sensitivity runs and additionally showing the MCM3.3.1, JAMv2b and URMELL.

To quantify the contribution of the mechanism adjustments/extensions, multiple sensitivity simulations were performed (overview of performed sensitivity studies is given in Table 5). Starting from the final URMELL mechanism several updates were successively replaced by the

original JAMv2b formulation. Fig. S2-1 illustrates the results of all sensitivity studies, the final URMELL version (yellow line), JAMv2b (blue line) and the MCM3.3.1 (black line).

S2.3.1 $RC(O)O_2$ chemistry with separate PAN simulation

For $RC(O)O_2$ chemistry, the impact of the reaction with NO_2 to produce PAN and PAN-like (Fig. S2-1grey line) species was investigated independent of the other $RC(O)O_2$ chemistry changes (Fig. S2-1green line). For both sensitivity studies, O_3 (Fig. S2-1a), OH (Fig. S2-1e), HO_2 (Fig. S2-1i), NO (Fig. S2-1b), NO_2 (Fig. S2-1f), NO_3 (Fig. S2-1j) and HNO_3 (Fig. S2-1n) peak concentrations are lower with stronger reduction for the PAN simulation. The changed k_{NO2} rate coefficient, resetting it to the faster value (see sect. 2.3) lowers the NO_2 (Fig. S2-1f) day time minimum and increases PAN (Fig. S2-1g) concentrations. As NO_2 photolysis is a major NO and O_3 source and subsequent O_3 photolysis impacts OH, their concentration declines and substance concentrations directly linked (HO_2, H_2O_2, NO_3, HNO_3), too. As a consequence, common reaction partners such as C_5H_8, MACR and MVK increase while their reaction products (HCHO, GLY, CH_3COOOH and CH_3COCH_2OH) decline.

Additional changes to $RC(O)O_2$ chemistry comprise NO, NO_3, CH_3O_2, $CH_3C(O)O_2$ and HO_2 reactions including their reaction rate coefficients and branching ratios (see Table S1-2 for more detail). The slower reaction rate constant of $CH_3C(O)O_2$ with HO_2 (see sect. 2.3) enhances $CH_3C(O)O_2$ concentrations (Fig. S2-1r) and decreases the reaction product CH_3COOOH (Fig. S2-1s). This deceleration also diminishes OH conversion. Furthermore, not all HO_2 + $RC(O)O_2$ pathways in JAMv2b include O_3 and OH formation further reducing OH, O_3 and corresponding subsequent reaction partners. For OH and O_3, the changes to $RC(O)O_2$ chemistry already account for most of the non-isoprene invoked deviations.

S2.3.2 Photolysis

Most changes to photolysis (Fig. S2-1, red line) consider the photolysis rate constant and some (MVKN, CO_2H_3CHO, BIACETOH, BEPOMUC, TEPOMUC, BIGALD1, $MEKNO_3$) also the branching ratios (see Table S1-4). Generally the changed photolysis rates become slower, and thus commonly produced photolysis products (e.g. $CH_3C(O)O_2$, CH_3O_2, HCHO, GLY, OH and HO_2) decline while the sources such as MGLY increase (Fig. S2-1). In the case of the slower photolysis of MGLY a shift towards the OH degradation channel occurs, so instead of releasing HO_2 via photolysis the OH is consumed more frequently lowering HO_x. This reduction in HO_2 concentration also lowers H_2O_2 production (Fig. S2-1m). Lower PAN

(Fig. S2-1g) and CH_3COOOH (Fig. S2-1s) concentration as well a slight day-time NO (Fig. S2-1b) and NO_2 (Fig. S2-1f) increase result from $CH_3C(O)O_2$ (Fig. S2-1r) reduction.

The reductions in OH and O_3 lower the reaction frequency of C_5H_8 (Fig. S2-1d), MVK (Fig. S2-1l) and MACR (Fig. S2-1h) causing a concentration increase. For NO (Fig. S2-1b), also an increase occurs, which is mainly forced by reduced concentrations of oxidation partners including O_3, CH3C(O)O_2, CH_3O_2 and other peroxy radicals. Photolysis differences dominate the non-isoprene induced HO_2, H_2O_2 and HCHO reduction and MGLY increase.

S2.3.3 GLY and ozonolysis implementation updates

GLY (Section 2.1) and ozonolysis changes (Section 2.2) are jointly simulated (brown line in Fig. S2-1). As mentioned in sect 2.1. of the main manuscript, the reaction rate constant of GLY with NO_3 in JAMv2b is four magnitudes higher than in URMELL. On the one hand, an increase of this reaction rate constant reduces NO_3 concentration (Fig. S2-1j) but, on the other hand, leads to a non-expected increase of the GLY concentration (Fig. S2-1k). GLY oxidation is now dominated by NO_3, while beforehand it was mainly oxidized by OH. This also shifts the oxidation pathways of other substances in opposing manner, here the ratio of NO_3 oxidation shrinks, while O_3 and OH become more important. OH and O_3 reaction channels are more efficient GLY sources compared to NO_3 channels leading to a GLY increase. As the reaction of GLY with NO_3 also produces HNO_3 an increase is invoked, too. The increase in HCOOH (Fig. S2-1p) is invoked by ozonolysis changes.

S2.3.4 Isoprene

Additional isoprene related deviations are mainly caused by OH oxidation, as well as MVK and MACR chemistry. When considering all isoprene related changes (purple line in Fig. S2-1), OH (Fig. S2-1e), NO (Fig. S2-1b), NO_2 (Fig. S2-1f), NO_3 (Fig. S2-1j), HCHO (Fig. S2-1c), MGLY (Fig. S2-1o), HCOOH (Fig. S2-1p), Isoprene (Fig. S2-1d), as well as MVK (Fig. S2-1l) and MACR (Fig. S2-1h) become very similar to JAMv2b (blue line in Fig. S2-1).

In JAMv2b the low CH_3O_2 yield of 0.051 (0.407 in URMELL) of C_5H_8 ozonolysis diminishes night-time CH_3O_2 production (Fig S2-1q). The reaction of CH_3O_2 with NO_2 produces nitroperoxy methane ($CH_3O_2NO_2$) and its decomposition is an important nighttime NO_2 source. Therefore, NO_2 nighttime concentrations (Fig. S2-1f) decline reaching similar nighttime peak concentrations as with JAMv2b. As NO chemistry is linked to NO_2, NO concentrations (Fig. S2-1b) also decline.

The integration of H-shift reactions, enabling OH recycling, into isoprene chemistry has the most significant impact on OH (Fig. S2-1e). Therefore, neglecting this OH recycling lowers not just OH but H_2O_2 (Fig. S2-1m) and HO_2 (Fig. S2-1i) concentrations. For compounds with multiple day-time degradation channels (reaction with HO_x, NO_x, O_3, or photolysis) the oxidation is pushed towards the other pathways reducing the oxidant day-time concentrations, too. This has a major impact on O_3 as it is consumed more frequently, while at the same time its formation through $RC(O)O_2 + HO_2$ reaction stagnates. Therefore, O_3 decreases (Fig. S2-1a). The lack of oxidants increases C_5H_8 (Fig. S2-1d) while lowering the reaction product concentrations of MACR (Fig. S2-1h), MVK (Fig. S2-1l) and HCHO (Fig. S2-1c).

Furthermore, the reduction in CH_3O_2 and HO_2 also shifts the oxidation from peroxy radicals towards $CH3C(O)O_2$ and NO_x resulting in lower day time concentrations. As the reactions of $RC(O)O_2$ with HO_2 produce O_3, this further reduces O_3 concentrations. Additionally, a shift of peroxy radical oxidation from CH_3O_2 towards $CH3C(O)O_2$ reduces HO_2 production rates, as CH_3O_2 pathways usually have higher HO_2 yields.

The composition of the ISOPOO pool also plays a role. The chemical degradation of LISOPACO2 seems to have a higher direct impact on O_3 depletion through the reaction of LHC4ACCHO with O_3 (this reaction is not part of Wennberg et al.[1], but kept from Schultz *et al.*[7], the MCM3.3.1 also suggest reactions with O_3) compared to ISOPBO2 and ISOPDO2 leading to MVK/MACR ozonolysis reactions. Note that O_3 is additionally indirectly impacted through NO_x rechanneling, as the degradation pathways of β and δ isoprene nitrates (ISOPBNO3 & ISOPDNO3, LISOPACNO3) differ. Therefore, the contributions of the diverse ISOPOO pool plays an important role for NO_x as well as O_3. As a result, multiple interlinkages changed creating some kind of self-reinforcing effect leading to intensified O_3 reduction. As $NO_2 + O_3$ is the major NO_3 production pathway, NO_3 declines as both precursor decline. But note, that the sources of the higher daytime NO_3 concentrations of URMELL are from the reaction of MPAN (a MACR reaction product) with OH and O_3, both yielding NO_3. In the case of MPAN + OH, JAMv2b postulates NO_2 instead of NO_3 formation while the reaction with O_3 is missing.

The strong increase in HCOOH concentration is due to the high MVK + O_3 production ratio of 0.85 in JAMv2b compared to 0.025 in URMELL. Changes to CH3COCH2OH are also caused by ISOPOO pool composition, with multiple pathways (MACR, HPALD, LIECHO, LHC4ACCHO…). For GLY URMELL shows a stronger day-time production mainly linked to

newly implemented C_5H_8 chemistry (MVK, ISOPOO pool) with a strong photolysis component and only moderate night-time production. Whereas the MCM3.3.1 simulates only minor day-time GLY but stronger night-time ozonolysis production. The main sources are NC4CHO, HPALD, $OHCCH_2OH$ and $HCOCH_2OOH$. Based on the recommendation from Wennberg et al.,[1] URMELL only considers terminal OH addition channels for the C_5H_8 + OH reaction but the MCM3.3.1 also includes internal addition channels which lead to addition GLY ozonolysis formation.

For most species, a reset to the original JAMv2b increases the similarity to JAMv2b. One exception is HNO_3 for which no approximation to JAMv2b is reached, but instead to MCM3.3.1. This is due to the treatment of $HOCH_2CO_3$. In JAMv2b, the reaction of $HOCH_2CO_3$ with NO_2 leads to HCHO + CO_2 + HNO_3 while in MCM and URMELL a PAN-like (PHAN) substance is formed. $HOCH_2CO_3$ is an important day- and nighttime HNO_3 source in JAMv2b while for URMELL OH + NO_2 is the major source. The lower OH and NO_2 concentrations are also in better agreement with the MCM3.3.1 resulting in similar HNO_3 simulations.

Fig. S2-2 till Fig S2-7 show additional plots for the urban and remote scenarios for various summer and winter cases as describe in the main text in sect. 4.1.

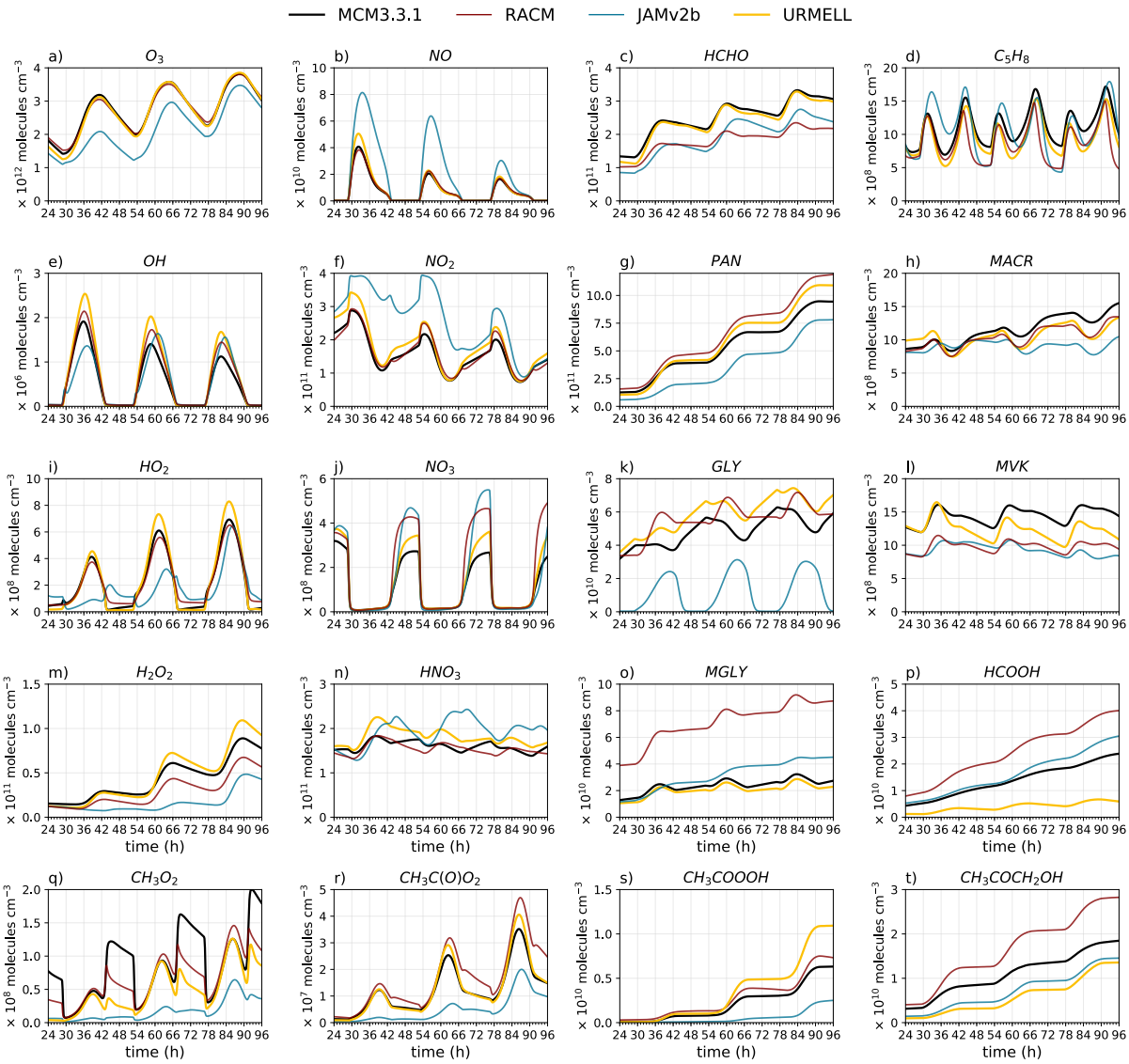


Fig. S2-2: Time series of various gas-phase compounds for the urban summer case with 50% attenuated actinic radiation (urb_s_05) modeled with MCM3.3.1 (black line), RACM (red line), JAMv2b (blue line) and URMELL (yellow line).

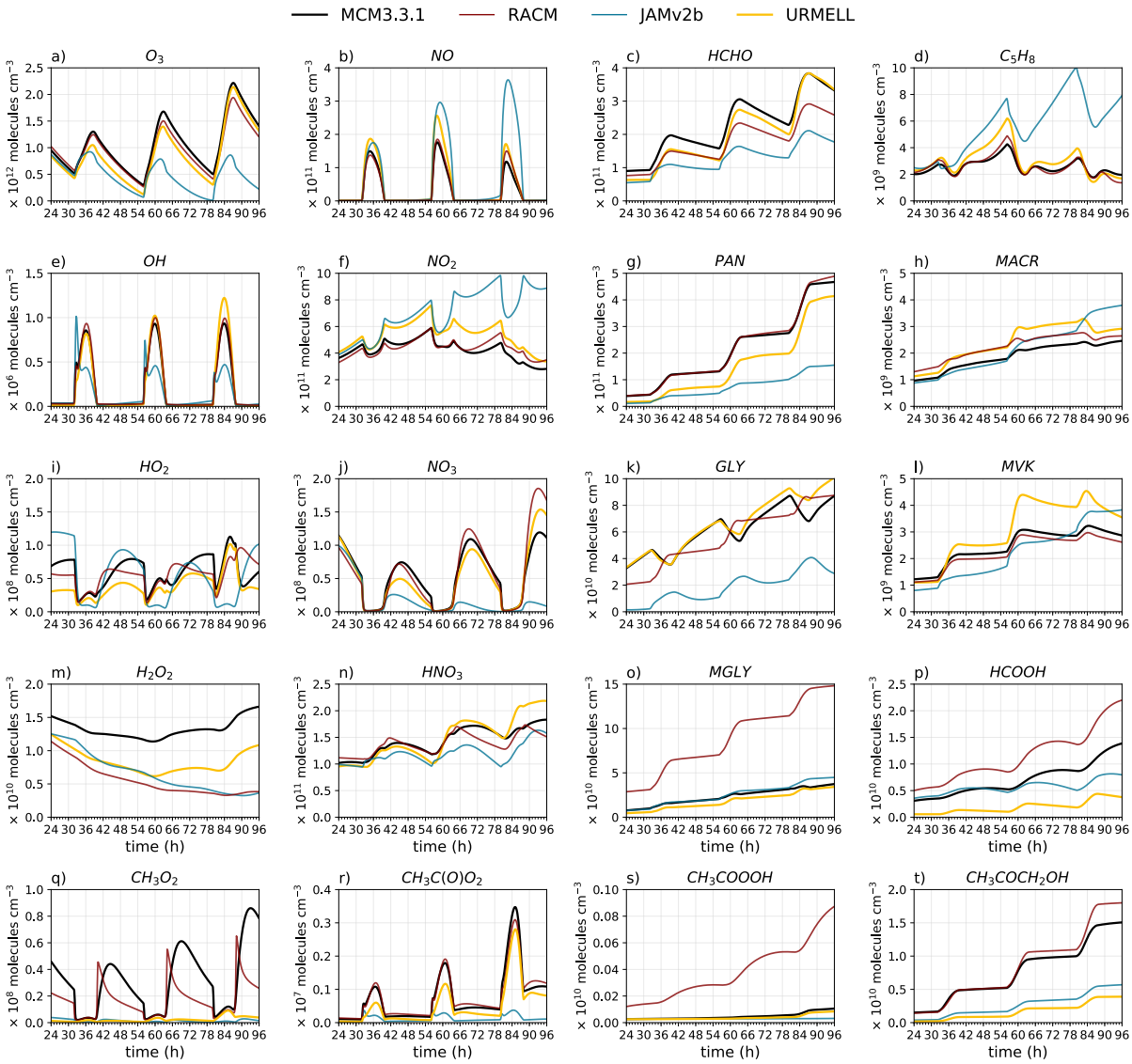


Fig. S2-3: Time series of various gas-phase compounds for the urban winter case with clear sky conditions (urb_w_1) modeled with MCM3.3.1 (black line), RACM (red line), JAMv2b (blue line) and URMELL (yellow line).

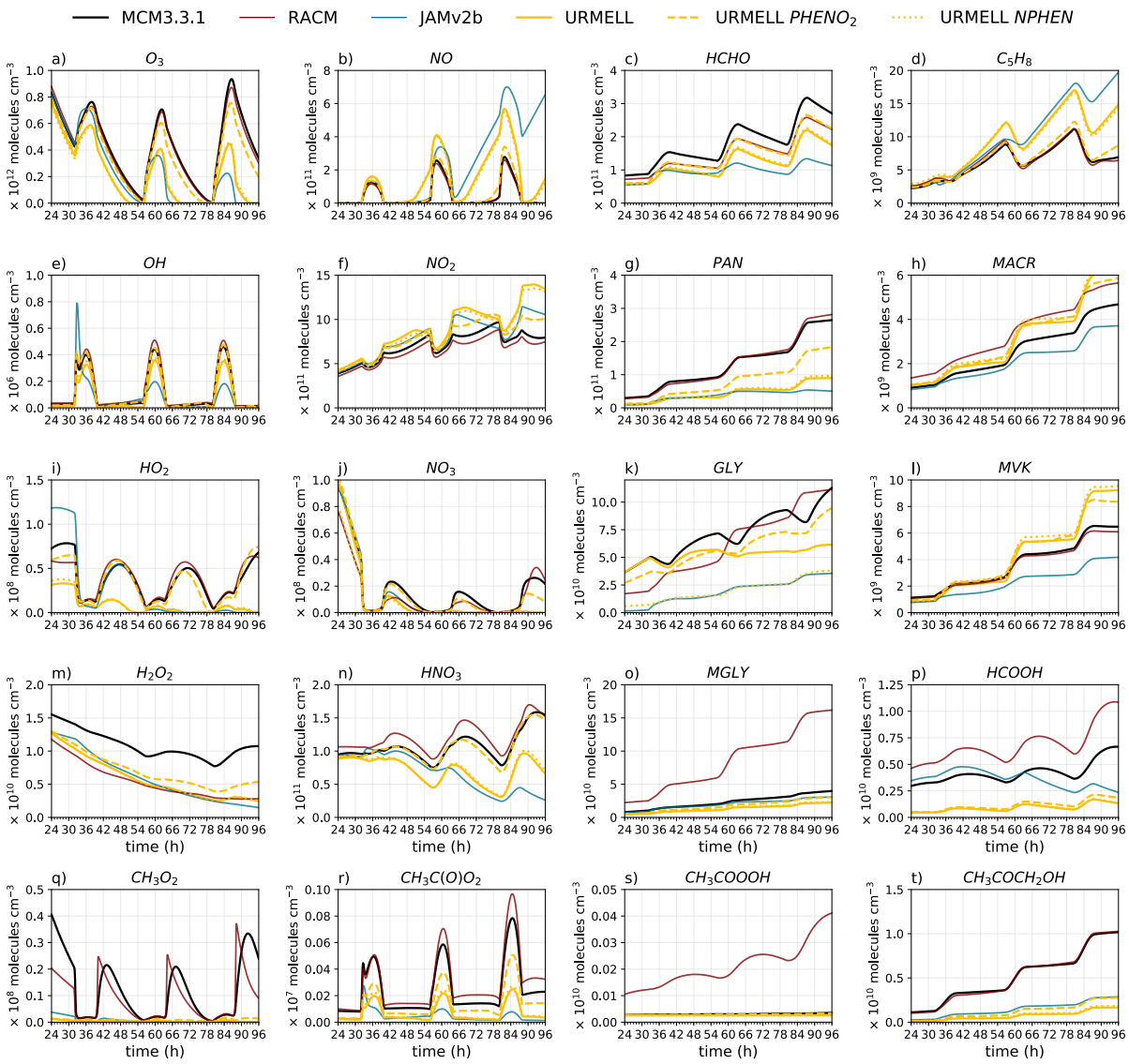


Fig. S2-4: Time series of various gas-phase compounds for the urban winter case with 50% attenuated actinic radiation (urb_w_05) modeled with MCM3.3.1 (black line), RACM (red line), JAMv2b (blue line), URMELL (yellow line) and for XYL+OH reaction rate constant of 2.3×10^{-11} cm^3 $molecule^{-1}$ s^{-1} (yellow dotted line).

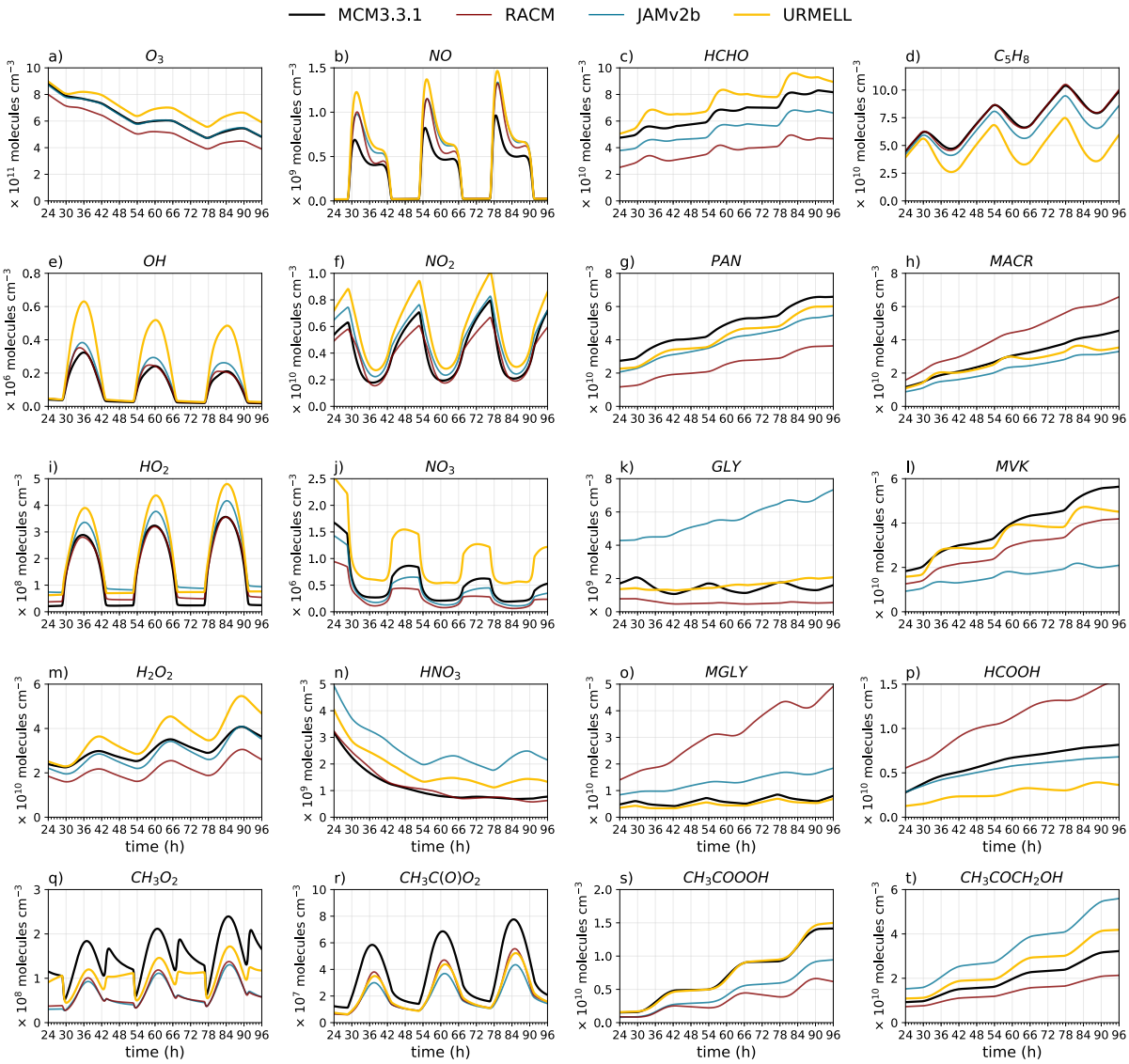


Fig. S2-5: Time series of various gas-phase compounds for the remote summer case with 50% attenuated actinic radiation (rem_s_05) modeled with MCM3.3.1 (black line), RACM (red line), JAMv2b (blue line) and URMELL (yellow line).

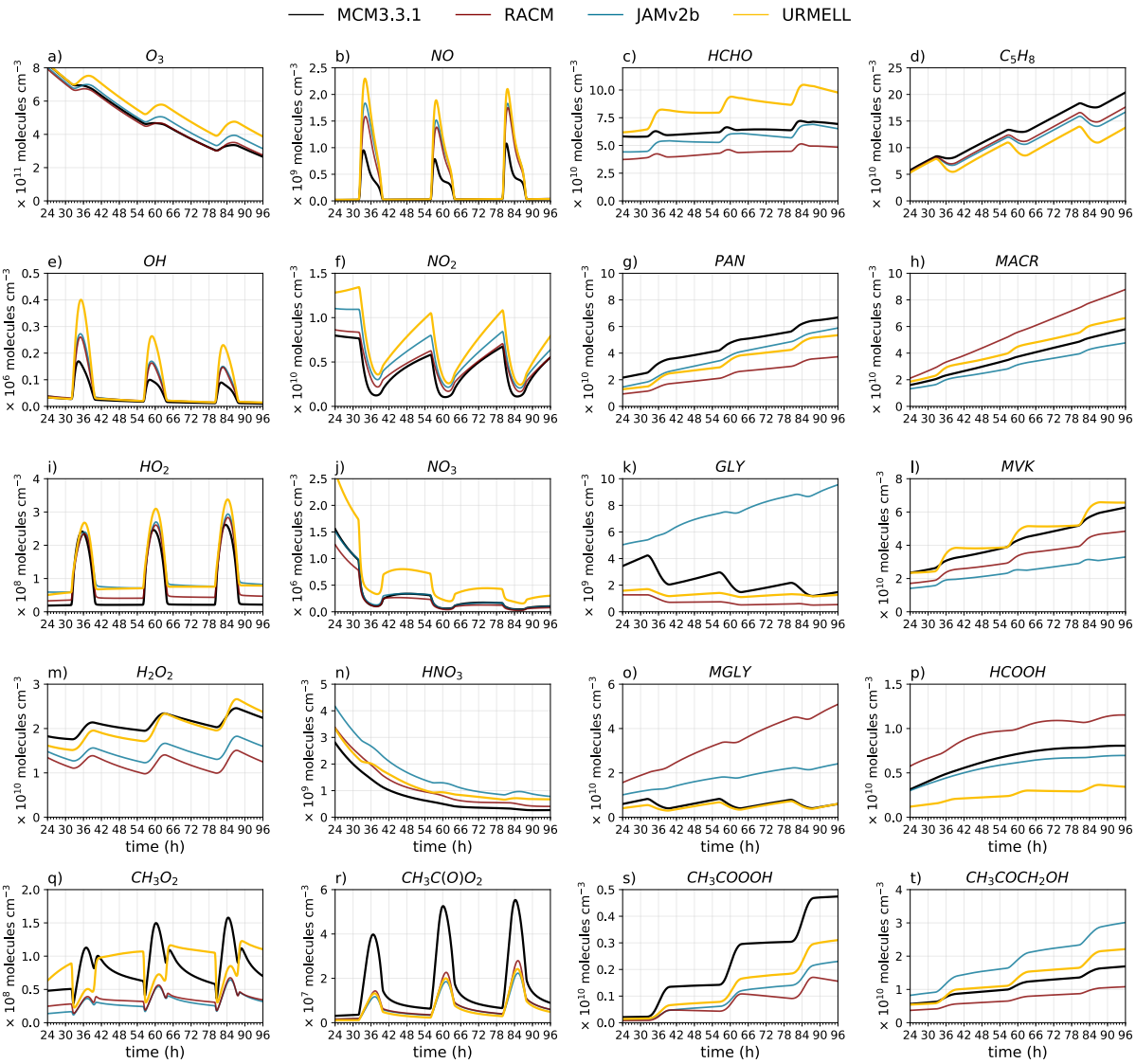


Fig. S2-6: Time series of various gas-phase compounds for the remote winter case with clear sky conditions (rem_w_1) modeled with MCM3.3.1 (black line), RACM (red line), JAMv2b (blue line) and URMELL (yellow line).

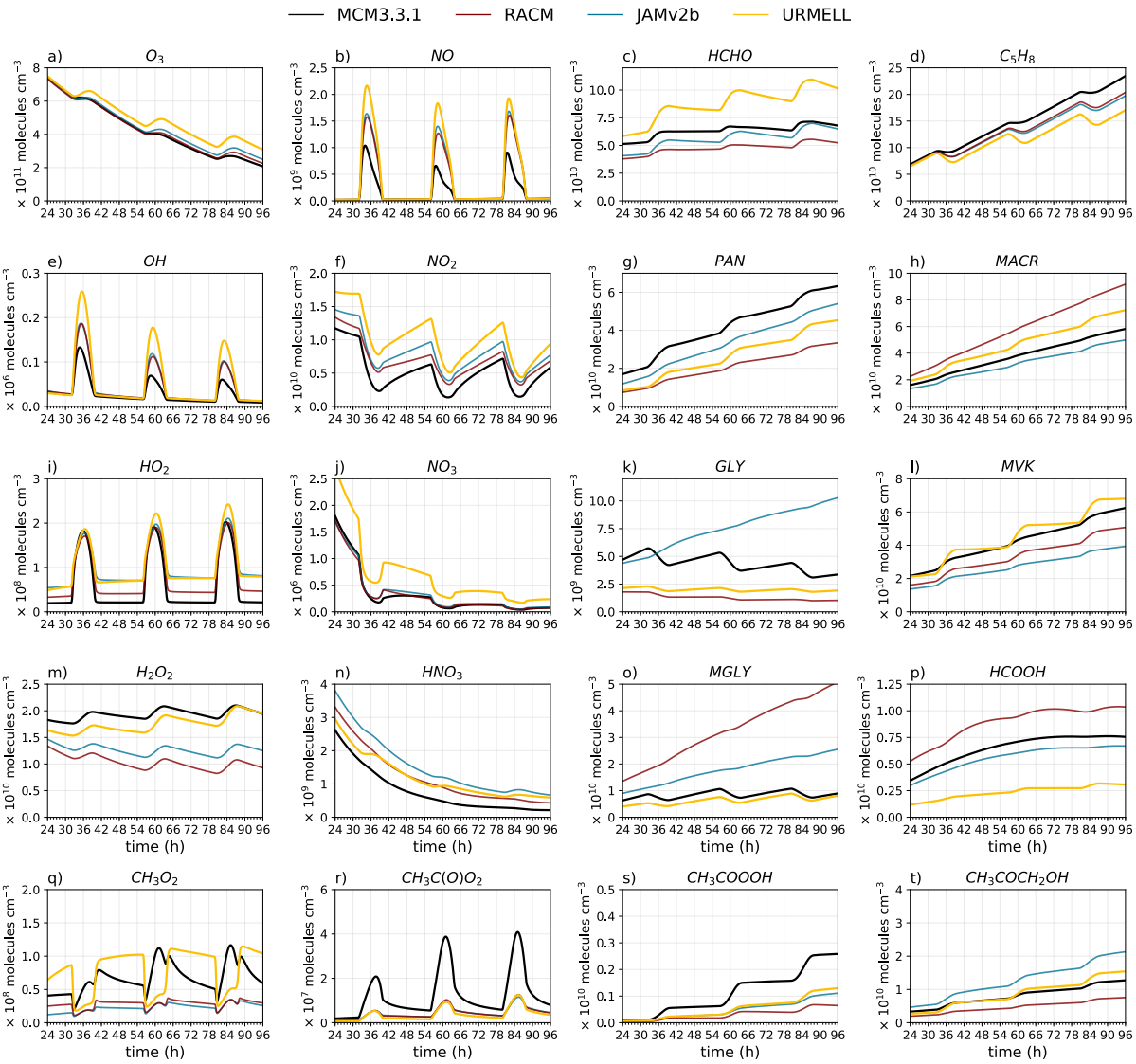


Fig. S2-7: Time series of various gas-phase compounds for the remote winter case with 50% attenuated actinic radiation (rem_w_05) modeled with MCM3.3.1 (black line), RACM (red line), JAMv2b (blue line) and URMELL (yellow line).

Table S2-1: Correlation and COD values between MCM3.3.1 and URMELL, Jamv2b and RACM for box model simulations and the various scenarios indicated by the first three columns: scenario (urban/remote), season (summer s/winter w) and solar radiation (full radiation _1/ 50% attenuated actinic radiation _05). Bold numbers highlight highest R values indicating best representation of MCM3.3.1 concentration trends and lowest COD for closest MCM3.3.1 approximation.

Scenario	Season	Rad.	Species	URMELL		JAMv2b		RACM	
				R	COD	R	COD	R	COD
urban	summer	05	O_3	**0.998**	**0.023**	**0.917**	0.157	0.995	0.015
			NO	**0.997**	**0.080**	**0.920**	0.352	0.996	**0.075**
			NO_2	**0.999**	**0.067**	0.709	0.277	0.975	**0.043**
			OH	**0.995**	0.291	0.889	**0.189**	0.994	**0.144**
			HO_2	**0.998**	**0.237**	0.663	0.511	0.989	0.281
			H_2O_2	**0.999**	**0.083**	0.847	0.474	0.995	0.200
			NO_3	**0.998**	**0.073**	0.956	0.240	0.958	0.180
			HNO_3	**0.857**	**0.066**	0.042	0.122	0.581	**0.040**
			HCHO	**0.998**	**0.030**	0.965	0.158	0.995	0.160
			PAN	**1.000**	**0.061**	0.987	0.268	**1.000**	0.098
			GLY	**0.968**	**0.097**	-0.149	0.725	0.588	0.102
			MGLY	**0.986**	**0.078**	0.848	0.162	0.940	0.498
			C_5H_8	**0.958**	**0.096**	0.734	0.140	0.802	0.165
			MACR	**0.826**	**0.066**	0.278	0.141	**0.963**	**0.055**
			MVK	**0.598**	**0.090**	0.225	0.221	**0.940**	0.190
			HCOOH	0.947	0.556	**0.995**	**0.081**	**0.998**	0.280
			CH_3O_2	**0.622**	**0.395**	0.573	0.692	**0.771**	**0.199**
			$CH_3C(O)O_2$	**0.999**	**0.079**	0.894	0.532	0.978	0.168
			CH_3COOOH	**0.999**	**0.194**	0.940	0.659	**0.999**	0.281
			CH_3COCH_2OH	0.971	0.388	**0.988**	**0.271**	**0.999**	**0.193**
	winter	1	O_3	**0.990**	**0.152**	0.466	0.478	**0.991**	**0.057**
			NO	**0.996**	**0.174**	0.864	0.508	0.989	0.102
			NO_2	**0.925**	**0.121**	-0.202	0.278	0.830	**0.052**
			OH	**0.983**	**0.281**	0.863	0.289	**0.997**	**0.073**
			HO_2	**0.803**	**0.243**	0.411	0.390	0.514	0.165
			H_2O_2	**0.806**	**0.244**	-0.075	0.404	0.105	0.456
			NO_3	**0.947**	**0.180**	0.463	0.633	0.936	**0.136**
			HNO_3	**0.964**	**0.051**	0.798	0.107	0.883	**0.044**
			HCHO	**0.995**	**0.107**	0.991	0.275	**0.999**	0.122
			PAN	0.993	**0.264**	**0.997**	0.491	**1.000**	**0.012**
			GLY	**0.981**	**0.044**	0.720	0.601	0.850	0.138
			MGLY	**0.989**	0.167	0.988	**0.051**	**0.990**	0.577
			C_5H_8	**0.975**	**0.101**	0.298	0.378	0.966	**0.055**
			MACR	**0.981**	0.122	0.934	**0.107**	**0.989**	**0.101**
			MVK	**0.991**	**0.120**	0.904	0.144	**0.999**	**0.042**
			HCOOH	**0.942**	0.603	0.923	**0.141**	**0.999**	0.241
			CH_3O_2	0.116	**0.785**	**0.547**	0.867	**0.638**	**0.327**
			$CH_3C(O)O_2$	**0.987**	**0.309**	0.836	0.681	**0.989**	**0.094**
			CH_3COOOH	**0.992**	**0.105**	0.870	0.257	0.947	0.766

			CH_3COCH_2OH	0.994	0.679	**0.998**	**0.512**	**0.998**	**0.048**
		05	O_3	**0.765**	0.650	0.589	**0.640**	**0.995**	**0.059**
			NO	**0.804**	0.642	0.448	**0.620**	**1.000**	**0.067**
			NO_2	**0.850**	0.123	0.910	**0.073**	**0.999**	**0.044**
			OH	**0.993**	0.435	0.737	**0.386**	**0.998**	**0.136**
			HO_2	0.616	0.703	**0.722**	**0.671**	**0.918**	**0.086**
			H_2O_2	**0.939**	**0.381**	0.905	0.414	0.931	0.391
			NO_3	0.938	0.717	**0.967**	**0.705**	**0.971**	**0.296**
			HNO_3	**0.429**	**0.244**	-0.397	0.346	**0.965**	**0.069**
			HCHO	**0.997**	**0.207**	0.909	0.296	**0.999**	**0.099**
			PAN	**0.997**	**0.489**	0.885	0.525	**0.999**	**0.028**
			GLY	0.888	**0.158**	**0.914**	0.625	**0.912**	0.199
			MGLY	**0.998**	0.280	0.991	**0.075**	0.994	0.545
			C_5H_8	**0.956**	**0.192**	0.812	0.234	**0.987**	**0.040**
			MACR	0.995	**0.089**	**0.997**	0.094	**0.997**	0.154
			MVK	0.993	**0.106**	**0.996**	0.217	**1.000**	**0.019**
			HCOOH	**0.881**	0.653	-0.452	**0.183**	**0.998**	0.235
			CH_3O_2	0.240	**0.865**	**0.583**	0.869	**0.761**	**0.218**
			$CH_3C(O)O_2$	**0.971**	**0.602**	0.596	0.684	**0.985**	**0.135**
			CH_3COOOH	**0.559**	0.087	0.480	**0.060**	**0.951**	0.733
			CH_3COCH_2OH	0.995	0.766	**0.999**	**0.563**	**1.000**	**0.025**

remote	s	05	O_3	0.984	0.067	0.999	0.004	0.999	0.077
			NO	0.982	0.170	0.987	0.154	0.982	0.140
			NO_2	0.970	0.189	0.982	0.104	0.970	0.064
			OH	0.991	0.275	0.998	0.106	0.992	0.061
			HO_2	0.992	0.337	0.991	0.368	0.997	0.216
			H_2O_2	0.997	0.095	0.993	0.045	0.976	0.178
			NO_3	0.981	0.370	0.994	0.168	0.987	0.343
			HNO_3	0.986	0.251	0.958	0.424	0.993	0.050
			HCHO	0.980	0.072	0.997	0.101	0.987	0.269
			PAN	0.999	0.075	0.998	0.110	0.999	0.334
			GLY	-0.051	0.121	-0.121	0.585	0.754	0.452
			MGLY	0.964	0.117	0.777	0.375	0.752	0.663
			C_5H_8	0.727	0.238	0.983	0.063	0.999	0.009
			MACR	0.978	0.061	0.999	0.138	0.999	0.184
			MVK	0.980	0.062	0.967	0.394	1.000	0.156
			HCOOH	0.968	0.393	0.999	0.069	0.989	0.274
			CH_3O_2	0.903	0.182	0.868	0.415	0.865	0.400
			$CH_3C(O)O_2$	0.971	0.249	0.975	0.300	0.972	0.257
			CH_3COOOH	0.999	0.020	0.999	0.252	0.993	0.358
			CH_3COCH_2OH	1.000	0.109	1.000	0.256	1.000	0.170
	w	1	O_3	0.988	0.107	0.997	0.044	0.999	0.014
			NO	0.971	0.241	0.971	0.229	0.970	0.198
			NO_2	0.963	0.316	0.969	0.226	0.979	0.143
			OH	0.981	0.241	0.993	0.167	0.991	0.145
			HO_2	0.982	0.452	0.980	0.466	0.989	0.280

			H_2O_2	0.973	0.046	0.853	0.181	0.612	0.271
			NO_3	0.995	0.446	0.999	0.039	0.999	0.139
			HNO_3	0.995	0.303	0.994	0.412	0.998	0.203
			HCHO	0.929	0.148	0.945	0.069	0.991	0.189
			PAN	0.999	0.173	0.999	0.118	0.999	0.331
			GLY	0.947	0.268	-0.833	0.553	0.948	0.513
			MGLY	0.826	0.110	-0.146	0.501	-0.178	0.686
			C_5H_8	0.953	0.157	0.992	0.080	0.995	0.059
			MACR	0.998	0.080	0.999	0.095	1.000	0.192
			MVK	0.986	0.043	0.993	0.272	0.999	0.134
			HCOOH	0.959	0.445	1.000	0.065	0.993	0.194
			CH_3O_2	-0.053	0.236	0.937	0.460	0.914	0.393
			$CH_3C(O)O_2$	0.972	0.425	0.943	0.367	0.952	0.335
			CH_3COOOH	0.996	0.272	0.995	0.395	0.994	0.496
			CH_3COCH_2OH	0.999	0.089	1.000	0.248	1.000	0.214
		05	O_3	0.992	0.106	0.998	0.044	0.999	0.019
			NO	0.964	0.268	0.957	0.245	0.954	0.228
			NO_2	0.955	0.383	0.985	0.277	0.982	0.218
			OH	0.958	0.229	0.981	0.166	0.979	0.155
			HO_2	0.973	0.450	0.974	0.458	0.988	0.278
			H_2O_2	0.882	0.056	0.270	0.211	-0.103	0.312
			NO_3	0.982	0.480	0.995	0.110	0.995	0.075
			HNO_3	0.992	0.325	0.995	0.409	0.998	0.280
			HCHO	0.985	0.161	0.980	0.069	0.990	0.142
			PAN	0.997	0.248	0.997	0.126	0.998	0.348
			GLY	0.902	0.371	-0.804	0.308	0.845	0.548
			MGLY	0.860	0.161	0.460	0.354	0.438	0.571
			C_5H_8	0.980	0.119	0.996	0.063	0.997	0.052
			MACR	0.999	0.105	0.999	0.085	1.000	0.207
			MVK	0.991	0.044	0.999	0.219	0.999	0.121
			HCOOH	0.964	0.471	0.999	0.075	0.994	0.159
			CH_3O_2	0.092	0.272	0.900	0.488	0.631	0.405
			$CH_3C(O)O_2$	0.969	0.534	0.945	0.427	0.957	0.429
			CH_3COOOH	0.996	0.353	0.996	0.384	0.998	0.546
			CH_3COCH_2OH	0.998	0.066	0.999	0.214	1.000	0.261

Supplement S3 – CTM simulations

Supplement S3 contains the information about the time series analysis including an overview of all selected measurement sites in Table S3-1 and statistics for the entire time series in Table S3-2 und for the mean diurnal cycle of May 2014 in Table S3-3. A map with the dominated land use type distribution and colored ozone correlation values for all considered measurement sites are presented in Fig. S3-1. Time series are shown for selected sites for O_3, NO_2 and NO in fig. S3.2-1 till S3.2-5. For the mechanism comparison in remote areas also plots showing modeled OH, ISO, API+BPI and LIM+MYRC concentration time series for Kellerwald, Simmerath, Schmuecke and Spreewald are shown (Fig. S3.2-6 till S3.2-.

Table S3-1: Overview about the 57 measurement sites considered for the comparisons providing their name, longitude, latitude, station code, classification (24 remote background (BR), 13 urban background (BU), 7 traffic (T) and 12 industrial/traffic and industrial (IR/IU/TI)) and indication of O_3, NO_2 and NO dada availability. Information about the German measurement network used for this study, with links to data and additional information can be found at the station database provided by the German Environment Agency (Umwelt Bundesamt - UBA): https://www.env-it.de/stationen/public/networkList.do

Site	Longitude	Latitude	Station code	Classi-fication	O_3	NO_2	NO
Neuglobsow	13.031662	53.141303	DEUB030	BR	X	X	
Schmuecke	10.769534	50.654066	DEUB029	BR	X	X	X
Waldhof	10.756733	52.800773	DEUB005	BR	X	X	X
Westerland	8.308208	54.924967	DEUB001	BR	X	X	X
Zingst	12.721938	54.436985	DEUB028	BR	X	X	X
Schwedt/Oder	14.285139	53.064262	DEBB029	TI	X		
Eisenhuettenstadt	14.638166	52.146264	DEBB032	TI	X		
Mannheim/Nord	8.465281	49.544078	DEBW005	TI	X	X	X
Salzgitter/Druette	10.455910	52.153690	DENI070	IR	X	X	
Bottrop-Welheim	6.976880	51.525955	DENW021	IU	X	X	
Duisburg-Walsum	6.748363	51.524030	DENW034	IU	X	X	
Trier/Eitzstr.	6.690258	49.784023	DERP047	TI	X	X	
Bitterfeld/Wolfen	12.302866	51.651166	DEST015	TI	X	X	
Niederzier	6.469312	50.883484	DENW074	IR	X		
Leuna	12.032141	51.321364	DEST090	TI	X	X	X
Berlin Marienfelde	13.368103	52.398406	DEBE027	IR	X	X	
Bremen	8.695060	53.117700	DEHB013	IR	X	X	
Neubrandenburg	13.266440	53.559784	DEMV003	T	X	X	
Koblenz	7.596633	50.354403	DERP024	T	X	X	
Erfurt/Kraempferstr.	11.037924	50.979455	DETH020	T	X	X	
Frankfurt/Hoechst	8.542517	50.101750	DEHE005	T	X	X	X
Saarbruecken/Verkehr	7.003174	49.230740	DESL020	T	X	X	X
Karlsruhe/Nordwest	8.355628	49.028594	DEBW081	T	X	X	X
Elsterwerda	13.526796	51.462734	DEBB007	T	X		
Cottbus	14.334470	51.746848	DEBB064	BU	X	X	
Berlin Wedding	13.349326	52.543041	DEBE010	BU	X	X	X

Site	Longitude	Latitude	Station code	Classi-fication	O_3	NO_2	NO
Rostock/Warnemuende	12.080003	54.171330	DEMV021	BU	X	X	
Hamburg/Sternschanze	9.967882	53.564140	DEHH008	BU	X		
Frankfurt/Ost	8.746343	50.125332	DEHE008	BU	X	X	X
Wiesbaden/Sued	8.244949	50.050343	DEHE022	BU	X	X	
Koeln-Chorweiler	6.884571	51.019338	DENW053	T	X	X	X
Osnabrueck	8.052860	52.255340	DENI038	BU	X	X	X
Hannover	9.706120	52.362920	DENI054	BU	X	X	
Halle/Nord	11.979056	51.496185	DEST050	BU	X	X	X
Neuruppin	12.809481	52.931890	DEBB048	BU	X		
Hof/Berliner_Platz	11.897492	50.320611	DEBY020	BU	X	X	
Leipzig-West	12.297411	51.317905	DESN059	BU	X	X	
Potsdam/Zentrum	13.059945	52.401352	DEBB021	BU	X	X	
Radebeul-Wahnsdorf	13.675005	51.119514	DESN051	BR	X		
Schwartenberg	13.465.078	50.659097	DESN074	BR	X		
Riedstadt	8.516798	49.825165	DEHE043	BR	X	X	
Soest/Ost	8.148023	51.570675	DENW068	BR	X	X	
Eggenstein	8.406660	49.076550	DEBW004	BR	X		
Luette	12.561389	52.194225	DEBB065	BR	X		
Spreewald	14.057064	51.897598	DEBB066	BR	X		
Kellerwald	9.031754	51.154843	DEHE060	BR	X		
Neuhaus	11.134593	50.499955	DETH027	BR	X		
Hummelshain	11.661233	50.791616	DETH061	BR	X		
Tiefenbach	12.548869	49.438464	DEBY072	BR	X	X	
Possen	10.867188	51.333333	DETH042	BR	X		
Witzenhausen/Wald	9.774588	51.291757	DEHE024	BR	X		
Carlsfeld	12.611125	50.431322	DESN049	BR	X		
Spessart	9.399441	50.164430	DEHE026	BR	X		
Simmerath(Eifel)	6.281008	50.653234	DENW064	BR		X	
Zinnwald	13.751450	50.731478	DESN052	BR	X	X	
Zartau/Waldstation	11.172327	52.593136	DEST089	BR	X	X	
Collmberg	13.009406	51.303772	DESN076	BR	X	X	

Table S3-2: Summary of min, mean, max, standard deviation (stdv.), correlation (R) and COD values for the measured and modeled O_3, NO_2 and NO concentrations for the 57, 38 and 14 measurement sites considered.

O_3	Measurement sites	Min	Mean	Max	Stdv.	R	COD
	Spessart	**16.040**	**76.301**	**156.718**	**22.647**		
	RACM	38.850	69.382	104.046	14.292	0.546	0.131
	URMELL	25.488	69.783	105.161	15.676	0.611	0.128
	Witzenhausen	**21.671**	**75.954**	**146.570**	**25.560**		
	RACM	28.681	63.438	102.303	15.805	0.523	0.172
	URMELL	22.159	64.051	103.161	16.267	0.611	0.162
	Collmberg	**18.44**	**74.385**	**141.386**	**23.696**		
	RACM	25.581	60.525	118.549	17.520	0.587	0.173
	URMELL	25.755	61.303	121.581	17.872	0.675	0.161
	Possen	**13.782**	**74.043**	**145.719**	**23.844**		
	RACM	27.162	64.026	109.909	16.226	0.617	0.157
	URMELL	23.101	64.675	111.155	16.812	0.707	0.145
	Zingst	**24.500**	**73.455**	**129.900**	**19.076**		
	RACM	38.195	73.317	113.476	15.441	0.624	0.111
	URMELL	36.362	73.471	112.224	15.797	0.563	0.121
	Waldhof	**1.000**	**71.421**	**172.800**	**29.484**		
	RACM	25.571	64.893	121.246	17.060	0.751	0.192
	URMELL	30.865	65.676	119.001	16.788	0.736	0.196
	Cottbus	**7.620**	**70.487**	**146.710**	**26.346**		
	RACM	30.252	66.189	117.381	17.544	0.798	0.143
	URMELL	27.151	66.069	119.188	17.721	0.781	0.148
	Neuglobsow	**3.500**	**70.109**	**139.150**	**26.678**		
	RACM	38.675	71.158	123.702	16.330	0.694	0.195
	URMELL	33.800	71.041	122.656	17.246	0.661	0.199
	Hummelshain	**16.810**	**70.021**	**154.961**	**28.263**		
	RACM	18.398	64.340	113.213	17.115	0.754	0.152
	URMELL	19.298	64.988	110.784	17.629	0.760	0.153
	Radebeul	**18.859**	**69.829**	**143.002**	**23.226**		
	RACM	18.750	59.976	121.460	19.285	0.768	0.137
	URMELL	19.323	60.241	121.923	19.281	0.798	0.129
	Neuhaus	**17.421**	**80.922**	**140.112**	**22.978**		
	RACM	40.788	72.406	98.581	11.986	0.690	0.123
	URMELL	37.793	72.412	102.057	13.474	0.715	0.121
	Tiefenbach	**16.450**	**78.289**	**131.230**	**22.658**		
	RACM	35.307	65.966	103.504	14.132	0.544	0.156
	URMELL	30.348	66.166	105.537	14.681	0.597	0.152
	Carlsfeld	**18.075**	**77.459**	**138.612**	**23.022**		
	RACM	38.631	73.172	105.364	12.939	0.677	0.128
	URMELL	36.939	72.832	107.007	14.538	0.642	0.131

O_3	Measurement sites	Min	Mean	Max	Stdv.	R	COD
	Spreewald	**4.240**	**67.440**	**150.280**	**27.453**		
	RACM	26.479	63.739	117.613	17.831	0.800	0.167
	URMELL	26.040	64.240	117.852	17.364	0.781	0.175
	Hof	**1.350**	**67.056**	**129.430**	**27.375**		
	RACM	23.673	62.562	112.095	16.571	0.760	0.217
	URMELL	26.111	63.088	112.779	16.344	0.733	0.221
	Elsterwerda	**2.000**	**66.979**	**148.500**	**27.124**		
	RACM	24.007	62.082	122.730	18.500	0.816	0.162
	URMELL	23.391	62.191	119.800	18.615	0.783	0.174
	Potsdam	**2.000**	**66.763**	**139.800**	**25.022**		
	RACM	24.177	67.083	122.376	18.677	0.818	0.152
	URMELL	27.816	67.493	123.308	18.648	0.797	0.159
	Bitterfeld	**6.391**	**66.130**	**148.649**	**26.433**		
	RACM	18.880	63.876	122.367	19.013	0.762	0.170
	URMELL	25.691	64.393	125.517	19.309	0.762	0.172
	Leipzig-West	**6.942**	**66.124**	**147.611**	**28.535**		
	RACM	8.262	60.175	120.211	21.024	0.770	0.181
	URMELL	19.915	61.723	120.916	20.505	0.798	0.173
	Kellerwald	**18.054**	**66.081**	**127.947**	**19.595**		
	RACM	24.958	64.913	103.128	15.258	0.603	0.132
	URMELL	29.665	65.910	105.030	15.463	0.692	0.120
	Halle	**5.703**	**65.040**	**160.332**	**26.547**		
	RACM	15.930	57.642	125.261	20.777	0.791	0.168
	URMELL	20.331	59.148	124.936	20.251	0.824	0.156
	Berlin Marienfelde	**0.910**	**64.956**	**142.170**	**27.711**		
	RACM	6.961	61.270	122.450	20.745	0.794	0.187
	URMELL	12.473	61.802	118.289	20.952	0.790	0.196
	Luette	**2.000**	**63.950**	**145.860**	**29.319**		
	RACM	31.034	65.242	112.183	16.964	0.750	0.247
	URMELL	31.386	65.771	114.732	16.941	0.722	0.252
	Mannheim	**1.000**	**63.731**	**165.000**	**31.411**		
	RACM	4.860	56.832	108.557	22.983	0.760	0.242
	URMELL	10.196	57.719	110.845	22.991	0.729	0.253
	Rostock	**1.000**	**62.922**	**139.750**	**24.354**		
	RACM	29.615	68.973	111.766	16.375	0.672	0.206
	URMELL	32.622	69.628	112.403	16.375	0.630	0.212
	Riedstadt	**0.599**	**62.367**	**149.961**	**28.630**		
	RACM	3.867	55.245	111.276	21.925	0.708	0.248
	URMELL	8.366	57.154	113.611	21.711	0.671	0.260
	Hamburg	**1.000**	**61.599**	**146.464**	**26.680**		
	RACM	29.443	70.194	121.969	19.114	0.708	0.224
	URMELL	27.932	69.948	122.466	19.131	0.677	0.227

O_3	Measurement sites	Min	Mean	Max	Stdv.	R	COD
	Berlin Wedding	**1.660**	**61.173**	**139.290**	**26.982**		
	RACM	0.474	59.470	130.237	22.330	0.754	0.232
	URMELL	4.591	60.065	124.438	22.040	0.760	0.228
	Salzgitter	**1.792**	**60.874**	**151.084**	**26.181**		
	RACM	14.480	58.585	112.999	18.339	0.770	0.183
	URMELL	16.565	59.173	113.014	17.953	0.764	0.190
	Hannover	**4.198**	**60.705**	**136.226**	**24.678**		
	RACM	8.037	61.825	123.362	19.813	0.755	0.153
	URMELL	17.128	62.018	125.135	19.650	0.763	0.158
	Eggenstein	**1.000**	**60.702**	**161.000**	**32.636**		
	RACM	6.592	59.533	108.903	22.568	0.804	0.250
	URMELL	18.459	62.599	111.249	20.577	0.755	0.276
	Erfurt	**2.998**	**60.695**	**141.911**	**26.512**		
	RACM	10.980	59.932	108.662	20.003	0.752	0.182
	URMELL	14.611	61.275	111.165	18.860	0.772	0.181
	Niederzier	**0.425**	**58.671**	**119.833**	**25.865**		
	RACM	7.141	58.749	122.138	21.210	0.768	0.219
	URMELL	3.067	59.508	119.701	20.405	0.749	0.230
	Wiesbaden	**1.754**	**58.358**	**156.734**	**29.221**		
	RACM	7.835	57.469	107.436	20.901	0.694	0.246
	URMELL	14.185	58.537	106.404	19.590	0.698	0.248
	Leuna	**1.260**	**58.263**	**148.191**	**25.878**		
	RACM	10.768	57.924	122.123	20.986	0.568	0.229
	URMELL	20.575	59.154	123.164	20.251	0.602	0.221
	Osnabrück	**1.260**	**58.263**	**148.191**	**25.878**		
	RACM	16.629	56.253	125.726	18.481	0.654	0.212
	URMELL	17.133	57.683	118.986	17.892	0.693	0.211
	Frankfurt Ost	**2.284**	**57.614**	**135.732**	**27.155**		
	RACM	3.613	54.569	113.609	22.248	0.754	0.203
	URMELL	10.916	56.121	112.762	21.162	0.744	0.212
	Neubrandenburg	**1.010**	**57.105**	**122.550**	**23.381**		
	RACM	23.861	63.780	114.076	18.738	0.734	0.218
	URMELL	21.652	63.993	111.968	18.714	0.711	0.222
	Soest	**0.873**	**56.551**	**130.004**	**26.367**		
	RACM	13.281	57.788	111.260	19.007	0.798	0.219
	URMELL	16.931	58.253	113.483	19.450	0.797	0.222
	Trier	**1.502**	**56.483**	**157.405**	**29.979**		
	RACM	24.357	65.708	115.468	18.077	0.773	0.273
	URMELL	21.758	66.908	115.664	18.855	0.748	0.278
	Cologne	**0.263**	**55.599**	**141.718**	**29.024**		
	RACM	0.551	47.593	114.010	24.193	0.715	0.277
	URMELL	1.239	48.210	111.934	23.177	0.723	0.275

O_3	Measurement sites	Min	Mean	Max	Stdv.	R	COD
	Karlsruhe	**1.000**	**69.406**	**168.000**	**30.541**		
	RACM	6.592	59.533	108.903	22.568	0.760	0.181
	URMELL	18.459	62.599	111.249	20.577	0.756	0.186
	Zartau	**3.979**	**68.471**	**157.522**	**27.914**		
	RACM	29.925	64.023	117.464	17.216	0.756	0.179
	URMELL	32.354	64.641	118.283	17.317	0.742	0.186
	Schwedt	**8.170**	**68.285**	**152.630**	**25.554**		
	RACM	29.555	65.713	113.991	17.284	0.774	0.154
	URMELL	25.739	66.178	115.249	17.378	0.721	0.164
	Eisenhuettenstadt	**9.960**	**68.163**	**136.060**	**25.193**		
	RACM	28.826	64.291	115.084	17.198	0.768	0.156
	URMELL	26.951	65.668	114.354	17.269	0.699	0.169
	Frankfurt Hoechst	**1.197**	**53.947**	**144.518**	**26.614**		
	RACM	5.135	54.333	106.777	21.795	0.721	0.223
	URMELL	7.519	55.013	104.133	20.899	0.710	0.235
	Koblenz	**0.998**	**49.991**	**133.019**	**27.247**		
	RACM	5.712	57.963	116.734	21.746	0.703	0.268
	URMELL	6.963	59.198	117.651	21.424	0.727	0.267
	Duisburg	**0.494**	**49.372**	**133.737**	**24.802**		
	RACM	3.310	54.189	124.886	22.020	0.677	0.267
	URMELL	2.573	53.718	120.418	21.632	0.671	0.269
	Bottrop	**0.049**	**48.798**	**147.440**	**28.085**		
	RACM	1.779	51.328	122.474	23.246	0.709	0.283
	URMELL	1.480	51.447	113.800	22.526	0.714	0.286
	Neuruppin	**8.510**	**67.739**	**167.010**	**26.175**		
	RACM	29.127	66.324	125.873	18.466	0.791	0.145
	URMELL	26.401	66.691	125.460	18.752	0.769	0.153
	Saarbruecken	**1.240**	**47.185**	**120.830**	**25.213**		
	RACM	26.465	66.936	110.359	17.229	0.725	0.351
	URMELL	25.064	68.935	112.391	17.324	0.662	0.362
	Westerland	**36.450**	**87.524**	**133.600**	**15.685**		
	RACM	35.862	80.094	127.450	15.686	0.542	0.100
	URMELL	40.206	79.132	128.367	16.572	0.525	0.108
	Schmuecke	**18.650**	**85.412**	**154.200**	**25.521**		
	RACM	35.210	72.234	101.708	12.734	0.656	0.139
	URMELL	33.119	72.107	102.843	14.005	0.682	0.139
	Zinnwald	**24.602**	**83.937**	**149.427**	**21.878**		
	RACM	31.618	67.214	110.621	14.017	0.697	0.146
	URMELL	31.718	66.957	109.386	15.022	0.702	0.149
	Schwartenberg	**25.320**	**83.705**	**151.362**	**23.081**		
	RACM	33.327	67.636	108.278	14.113	0.723	0.143
	URMELL	28.729	67.038	111.661	15.878	0.736	0.146

O_3	Measurement sites	Min	Mean	Max	Stdv.	R	COD
	Bremen	**2.260**	**60.533**	**137.050**	**23.827**		
	RACM	27.392	68.426	119.779	17.258	0.668	0.197
	URMELL	25.456	68.047	122.042	17.637	0.672	0.199
NO_2	**Tiefenbach**	**2.820**	**6.282**	**15.920**	**1.842**		
	RACM	0.241	2.322	7.470	1.152	0.399	0.508
	URMELL	0.374	2.469	7.305	1.264	0.336	0.492
	Collmberg	**1.183**	**5.673**	**22.433**	**3.021**		
	RACM	0.642	3.819	11.324	1.860	0.600	0.274
	URMELL	0.634	3.766	11.313	1.844	0.601	0.275
	Zingst	**0.100**	**4.947**	**37.020**	**4.917**		
	RACM	0.384	4.180	27.158	3.319	0.599	0.296
	URMELL	0.371	4.105	24.053	3.073	0.534	0.311
	Waldhof	**0.370**	**4.013**	**17.800**	**3.097**		
	RACM	0.366	2.799	9.379	1.659	0.627	0.249
	URMELL	0.413	2.850	10.592	1.778	0.606	0.253
	Simmerath	**0.066**	**5.685**	**35.267**	**4.664**		
	RACM	0.366	5.583	35.995	5.392	0.566	0.344
	URMELL	0.518	5.900	38.047	5.713	0.548	0.346
	Neuglobsow	**0.100**	**2.113**	**11.300**	**1.592**		
	RACM	0.311	2.382	7.679	1.490	0.671	0.251
	URMELL	0.346	2.453	7.532	1.580	0.679	0.253
	Karlsruhe	**0.000**	**13.750**	**69.000**	**11.760**		
	RACM	2.147	10.880	47.274	6.601	0.774	0.272
	URMELL	2.136	10.013	31.165	5.210	0.650	0.295
	Zartau	**0.331**	**3.906**	**17.900**	**2.515**		
	RACM	0.437	3.073	9.276	1.814	0.665	0.238
	URMELL	0.476	3.054	10.067	1.855	0.643	0.241
	Hof	**1.950**	**11.813**	**53.410**	**7.990**		
	RACM	1.111	4.696	21.396	2.685	0.491	0.451
	URMELL	1.200	4.500	13.362	2.137	0.423	0.458
	Elsterwerda	**1.910**	**9.914**	**40.810**	**5.381**		
	RACM	0.598	3.684	8.794	1.771	0.599	0.479
	URMELL	0.609	3.698	9.205	1.769	0.571	0.476
	Potsdam	**4.560**	**13.962**	**57.800**	**7.951**		
	RACM	1.159	7.807	71.446	7.027	0.556	0.411
	URMELL	1.118	7.234	43.982	5.220	0.527	0.415
	Bitterfeld	**1.397**	**8.918**	**47.312**	**5.993**		
	RACM	1.231	5.031	18.164	2.698	0.422	0.345
	URMELL	1.232	5.107	15.252	2.666	0.415	0.340
	Leipzig-West	**2.985**	**11.622**	**61.448**	**6.911**		
	RACM	1.661	8.608	39.601	5.860	0.521	0.283
	URMELL	1.626	7.880	26.050	4.432	0.611	0.278

NO_2	Measurement sites	Min	Mean	Max	Stdv.	R	COD
	Salzgitter	**3.174**	**11.285**	**40.350**	**5.441**		
	RACM	3.000	8.466	43.679	4.492	0.255	0.261
	URMELL	3.136	8.244	34.341	3.966	0.240	0.265
	Hannover	**4.500**	**16.344**	**58.293**	**8.648**		
	RACM	2.376	11.891	61.038	7.799	0.485	0.300
	URMELL	2.384	11.500	50.883	7.112	0.499	0.300
	Erfurt	**1.913**	**16.080**	**66.659**	**10.184**		
	RACM	1.114	6.030	34.720	4.245	0.496	0.496
	URMELL	1.131	5.707	19.458	3.254	0.515	0.499
	Wiesbaden	**3.442**	**23.711**	**93.624**	**17.319**		
	RACM	1.906	14.102	59.505	9.928	0.645	0.342
	URMELL	1.974	13.718	45.600	8.972	0.657	0.342
	Leuna	**4.002**	**15.586**	**58.761**	**8.689**		
	RACM	1.356	7.085	29.791	4.278	0.407	0.424
	URMELL	1.262	6.676	19.541	3.135	0.470	0.424
	Osnabrück	**4.002**	**15.586**	**58.761**	**8.689**		
	RACM	2.265	9.732	34.418	5.034	0.505	0.304
	URMELL	2.271	9.169	22.911	4.222	0.498	0.312
	Frankfurt Ost	**1.559**	**27.945**	**105.470**	**19.542**		
	RACM	1.639	15.511	71.357	11.314	0.592	0.367
	URMELL	1.764	14.549	51.427	9.603	0.598	0.374
	Neubrandenburg	**4.500**	**18.543**	**59.500**	**10.236**		
	RACM	0.611	3.447	11.178	2.027	0.364	0.682
	URMELL	0.605	3.386	8.876	1.852	0.349	0.683
	Soest	**0.021**	**10.188**	**53.412**	**8.184**		
	RACM	1.301	6.809	23.178	3.837	0.329	0.360
	URMELL	1.460	6.928	23.178	3.837	0.340	0.357
	Trier	**2.429**	**14.949**	**61.404**	**9.600**		
	RACM	1.294	7.285	23.401	4.123	0.491	0.379
	URMELL	1.406	7.285	23.401	4.123	0.505	0.382
	Cologne	**0.546**	**20.289**	**91.004**	**14.404**		
	RACM	5.061	25.451	86.674	13.843	0.388	0.343
	URMELL	5.273	24.256	82.916	12.414	0.391	0.335
	Frankfurt Hoechst	**4.539**	**35.548**	**103.086**	**16.042**		
	RACM	2.409	18.319	82.992	13.809	0.618	0.427
	URMELL	2.495	17.800	65.017	12.479	0.623	0.431
	Koblenz	**3.969**	**33.559**	**80.567**	**15.190**		
	RACM	2.097	14.596	49.360	9.595	0.380	0.465
	URMELL	2.194	13.9923	42.196	8.789	0.431	0.469
	Duisburg	**0.029**	**21.562**	**87.724**	**15.891**		
	RACM	2.094	19.427	54.651	9.962	0.556	0.303
	URMELL	2.071	19.393	56.011	10.167	0.555	0.302

NO_2	Measurement sites	Min	Mean	Max	Stdv.	R	COD
	Berlin Marienfelde	**1.550**	**10.158**	**63.140**	**7.348**		
	RACM	2.320	12.807	92.863	9.810	0.511	0.267
	URMELL	2.490	12.074	48.192	8.272	0.420	0.267
	Mannheim	**1.000**	**20.327**	**94.000**	**15.496**		
	RACM	1.959	13.530	46.508	8.953	0.493	0.319
	URMELL	2.093	13.942	54.479	9.709	0.465	0.322
	Rostock	**0.900**	**12.241**	**65.100**	**11.407**		
	RACM	0.805	4.920	28.057	3.266	0.252	0.469
	URMELL	0.852	4.800	25.992	2.933	0.208	0.474
	Berlin Wedding	**3.850**	**22.217**	**113.780**	**16.423**		
	RACM	2.740	17.629	90.424	14.263	0.603	0.277
	URMELL	2.863	16.528	63.840	11.864	0.577	0.288
	Bottrop	**0.036**	**22.389**	**61.925**	**12.718**		
	RACM	5.689	23.343	60.730	10.886	0.459	0.279
	URMELL	5.889	22.832	67.019	10.507	0.474	0.276
	Cottbus	**1.910**	**9.711**	**48.890**	**5.786**		
	RACM	1.061	4.547	15.628	2.243	0.358	0.409
	URMELL	1.089	4.525	19.013	2.165	0.341	0.407
	Saarbruecken	**4.230**	**37.230**	**107.110**	**18.084**		
	RACM	0.677	4.752	18.697	2.806	0.156	0.757
	URMELL	0.667	4.686	18.508	2.750	0.087	0.759
	Riedstadt	**0.574**	**11.378**	**46.508**	**7.985**		
	RACM	2.767	14.152	70.870	9.148	0.431	0.300
	URMELL	2.775	13.471	50.572	8.064	0.418	0.294
	Westerland	**0.100**	**3.743**	**41.700**	**4.428**		
	RACM	0.149	2.921	13.241	2.030	0.330	0.354
	URMELL	0.149	3.072	14.836	2.213	0.319	0.362
	Schmuecke	**0.310**	**2.548**	**7.700**	**1.492**		
	RACM	0.741	2.861	8.298	1.431	0.271	0.289
	URMELL	0.803	2.923	8.679	1.456	0.323	0.285
	Zinnwald	**1.310**	**5.456**	**30.294**	**3.401**		
	RACM	0.420	2.841	14.668	1.972	0.697	0.146
	URMELL	0.455	3.098	12.595	2.067	0.702	0.149
	Bremen	**1.900**	**14.266**	**71.560**	**9.801**		
	RACM	1.708	5.735	24.791	2.847	0.068	0.448
	URMELL	1.681	5.841	26.687	2.823	0.054	0.445
	Halle	**0.022**	**10.336**	**58.510**	**10.168**		
	RACM	1.303	6.234	19.982	3.625	0.588	0.362
	URMELL	1.339	5.958	17.047	3.157	0.597	0.366

NO	Measurement sites	Min	Mean	Max	Stdv.	R	COD
	Halle	**0.282**	**1.560**	**22.539**	**2.279**		
	RACM	0.061	0.832	6.402	0.899	0.627	0.404
	URMELL	0.057	0.862	6.202	0.957	0.637	0.423
	Mannheim	**0.000**	**3.023**	**54.000**	**6.684**		
	RACM	0.047	2.048	25.085	73.609	0.487	0.745
	URMELL	0.049	2.075	27.501	3.655	0.437	0.750
	Berlin Wedding	**0.100**	**3.572**	**78.470**	**7.220**		
	RACM	0.227	3.013	47.609	4.474	0.546	0.436
	URMELL	0.228	3.114	38.686	4.501	0.416	0.441
	Osnabrück	**0.092**	**1.608**	**58.241**	**4.465**		
	RACM	0.162	1.587	9.809	1.387	0.435	0.426
	URMELL	0.163	1.613	8.668	1.417	0.416	0.430
	Frankfurt Ost	**0.374**	**7.097**	**70.733**	**10.413**		
	RACM	0.137	2.536	42.600	3.740	0.644	0.537
	URMELL	0.139	2.548	26.436	3.514	0.635	0.548
	Cologne	**0.003**	**3.970**	**70.071**	**6.341**		
	RACM	0.249	5.872	85.201	7.874	0.424	0.459
	URMELL	0.243	5.624	51.345	6.731	0.394	0.462
	Frankfurt Hoechst	**0.374**	**13.429**	**100.809**	**11.665**		
	RACM	0.173	3.288	41.325	4.402	0.572	0.672
	URMELL	0.192	3.447	34.463	4.609	0.542	0.678
	Saarbruecken	**0.350**	**26.399**	**184.550**	**25.373**		
	RACM	0.004	0.381	3.649	0.518	0.439	0.967
	URMELL	0.004	0.403	3.393	0.553	0.427	0.966
	Westerland	**0.060**	**0.600**	**37.820**	**2.294**		
	RACM	0.002	0.257	2.045	0.365	0.109	0.619
	URMELL	0.002	0.279	2.279	0.405	0.110	0.621
	Schmuecke	**0.050**	**0.328**	**2.850**	**0.405**		
	RACM	0.012	0.305	1.731	0.320	0.604	0.331
	URMELL	0.011	0.326	1.867	0.355	0.567	0.343
	Zingst	**0.040**	**0.502**	**19.260**	**1.131**		
	RACM	0.003	0.401	3.603	0.555	0.555	0.532
	URMELL	0.003	0.434	3.767	0.591	0.529	0.553
	Waldhof	**0.130**	**0.443**	**4.650**	**0.539**		
	RACM	0.010	0.273	2.137	0.364	0.636	0.492
	URMELL	0.009	0.293	2.297	0.403	0.607	0.510
	Karlsruhe	**0.000**	**1.641**	**62.000**	**5.431**		
	RACM	0.052	1.326	17.899	1.922	0.759	0.776
	URMELL	0.050	1.246	10.179	1.523	0.472	0.784
	Leuna	**0.092**	**1.608**	**58.241**	**4.465**		
	RACM	0.104	0.895	6.046	0.895	0.407	0.360
	URMELL	0.110	0.931	5.222	0.939	0.428	0.367

Table S3-3: R and COD values for the mean diurnal O_3, NO_2 and NO cycles for May 2014 between measured and modeled values using RACM and URMELL.

	O_3		NO_2		NO	
Measurement sites	R	COD	R	COD	R	COD
Neuhaus						
RACM	0.951	0.061				
URMELL	0.950	0.062				
Tiefenbach						
RACM	0.803	0.099	0.764	0.493		
URMELL	0.861	0.094	0.729	0.468		
Carlsfeld						
RACM	0.893	0.038				
URMELL	0.794	0.042				
Spessart						
RACM	0.959	0.052				
URMELL	0.964	0.049				
Witzenhausen						
RACM	0.769	0.109				
URMELL	0.834	0.100				
Possen						
RACM	0.933	0.086				
URMELL	0.970	0.077				
Zingst						
RACM	0.968	0.017	0.597	0.139	0.910	0.477
URMELL	0.926	0.026	0.498	0.152	0.914	0.489
Waldhof						
RACM	0.989	0.053	0.948	0.177	0.937	0.492
URMELL	0.983	0.054	0.939	0.168	0.918	0.507
Collmberg						
RACM	0.804	0.125	0.876	0.221		
URMELL	0.868	0.114	0.900	0.223		
Simmerath						
RACM			0.697	0.127		
URMELL			0.691	0.120		
Cottbus						
RACM	0.992	0.039	0.763	0.357		
URMELL	0.981	0.043	0.716	0.368		
Neuglobsow						
RACM	0.949	0.047	0.944	0.093		
URMELL	0.929	0.049	0.944	0.094		
Hummelshain						
RACM	0.985	0.045				
URMELL	0.977	0.045				

	O_3		NO_2		NO	
Measurement sites	R	COD	R	COD	R	COD
Eisenhuettenstadt						
RACM	0.983	0.037				
URMELL	0.969	0.040				
Neuruppin						
RACM	0.991	0.018				
URMELL	0.982	0.022				
Hof						
RACM	0.919	0.060	0.911	0.453		
URMELL	0.948	0.055	0.948	0.461		
Spreewald						
RACM	0.986	0.044				
URMELL	0.970	0.051				
Elsterwerda						
RACM	0.985	0.045	0.899	0.478		
URMELL	0.987	0.046	0.931	0.462		
Potsdam						
RACM	0.983	0.020	0.772	0.350		
URMELL	0.988	0.019	0.856	0.365		
Bitterfeld						
RACM	0.991	0.024	0.822	0.304		
URMELL	0.978	0.031	0.837	0.297		
Leipzig-West						
RACM	0.963	0.060	0.683	0.217		
URMELL	0.987	0.040	0.817	0.229		
Kellerwald						
RACM	0.962	0.037				
URMELL	0.963	0.027				
Halle						
RACM	0.973	0.073	0.897	0.262	0.964	0.400
URMELL	0.993	0.052	0.954	0.273	0.965	0.427
Berlin Marienfelde						
RACM	0.958	0.048	0.651	0.184		
URMELL	0.959	0.047	0.634	0.175		
Luette						
RACM	0.977	0.054				
URMELL	0.948	0.065				
Mannheim						
RACM	0.985	0.057	0.901	0.205	0.740	0.541
URMELL	0.981	0.055	0.896	0.191	0.730	0.553
Rostock						
RACM	0.970	0.067	0.589	0.427		
URMELL	0.940	0.076	0.380	0.437		

	O_3		NO_2		NO	
Measurement sites	R	COD	R	COD	R	COD
Salzgitter						
RACM	0.977	0.038	0.616	0.176		
URMELL	0.983	0.039	0.556	0.184		
Hannover						
RACM	0.973	0.030	0.920	0.220		
URMELL	0.982	0.027	0.917	0.228		
Eggenstein						
RACM	0.994	0.063				
URMELL	0.970	0.101				
Erfurt						
RACM	0.929	0.051	0.626	0.493		
URMELL	0.966	0.038	0.716	0.498		
Niederzier						
RACM	0.958	0.052				
URMELL	0.972	0.055				
Wiesbaden						
RACM	0.954	0.060	0.944	0.268		
URMELL	0.963	0.061	0.936	0.275		
Leuna						
RACM	0.930	0.054	0.731	0.400	0.786	0.302
URMELL	0.964	0.036	0.830	0.401	0.737	0.335
Osnabrück						
RACM	0.928	0.048	0.821	0.258	0.822	0.287
URMELL	0.952	0.039	0.842	0.274	0.782	0.299
Frankfurt Ost						
RACM	0.950	0.054	0.868	0.325	0.956	0.559
URMELL	0.972	0.037	0.925	0.342	0.940	0.589
Neubrandenburg						
RACM	0.948	0.075	0.158	0.697		
URMELL	0.960	0.076	0.189	0.699		
Soest						
RACM	0.959	0.064	0.852	0.196		
URMELL	0.959	0.070	0.866	0.188		
Trier						
RACM	0.980	0.163	0.796	0.359		
URMELL	0.989	0.170	0.828	0.364		
Cologne						
RACM	0.917	0.100	0.821	0.141	0.971	0.263
URMELL	0.946	0.086	0.847	0.120	0.948	0.281
Frankfurt Hoechst						
RACM	0.953	0.047	0.941	0.362	0.932	0.682
URMELL	0.960	0.048	0.948	0.370	0.917	0.691

	O_3		NO_2		NO	
Measurement sites	R	COD	R	COD	R	COD
Riedstadt						
RACM	0.924	0.092	0.588	0.180		
URMELL	0.937	0.079	0.654	0.154		
Hamburg						
RACM	0.969	0.076				
URMELL	0.965	0.075				
Koblenz						
RACM	0.940	0.102	0.510	0.441		
URMELL	0.962	0.106	0.581	0.454		
Berlin Wedding						
RACM	0.964	0.039	0.811	0.209	0.791	0.352
URMELL	0.973	0.039	0.780	0.220	0.797	0.389
Duisburg						
RACM	0.970	0.070	0.905	0.074		
URMELL	0.968	0.068	0.908	0.075		
Bottrop						
RACM	0.955	0.077	0.903	0.063		
URMELL	0.957	0.084	0.933	0.053		
Saarbruecken						
RACM	0.966	0.223	0.229	0.776	0.737	0.978
URMELL	0.968	0.240	0.213	0.778	0.724	0.976
Karlsruhe						
RACM	0.971	0.078	0.947	0.130	0.899	0.410
URMELL	0.988	0.058	0.906	0.167	0.800	0.441
Zartau						
RACM	0.987	0.042	0.928	0.132		
URMELL	0.983	0.042	0.935	0.129		
Schwedt						
RACM	0.993	0.027				
URMELL	0.983	0.033				
Schwartenberg						
RACM	0.804	0.110				
URMELL	0.857	0.113				
Bremen						
RACM	0.976	0.074	0.516	0.433		
URMELL	0.973	0.072	0.455	0.424		
Westerland						
RACM	0.984	0.046	0.411	0.147	0.831	0.636
URMELL	0.978	0.051	0.354	0.134	0.833	0.623
Schmuecke						
RACM	0.755	0.088	0.571	0.136	0.805	0.258
URMELL	0.844	0.089	0.507	0.137	0.805	0.275

	O_3		NO_2		NO	
Measurement sites	R	COD	R	COD	R	COD
Zinnwald						
RACM	0.912	0.114	0.108	0.342		
URMELL	0.943	0.115	0.097	0.306		
Radebeul						
RACM	0.968	0.085				
URMELL	0.980	0.078				

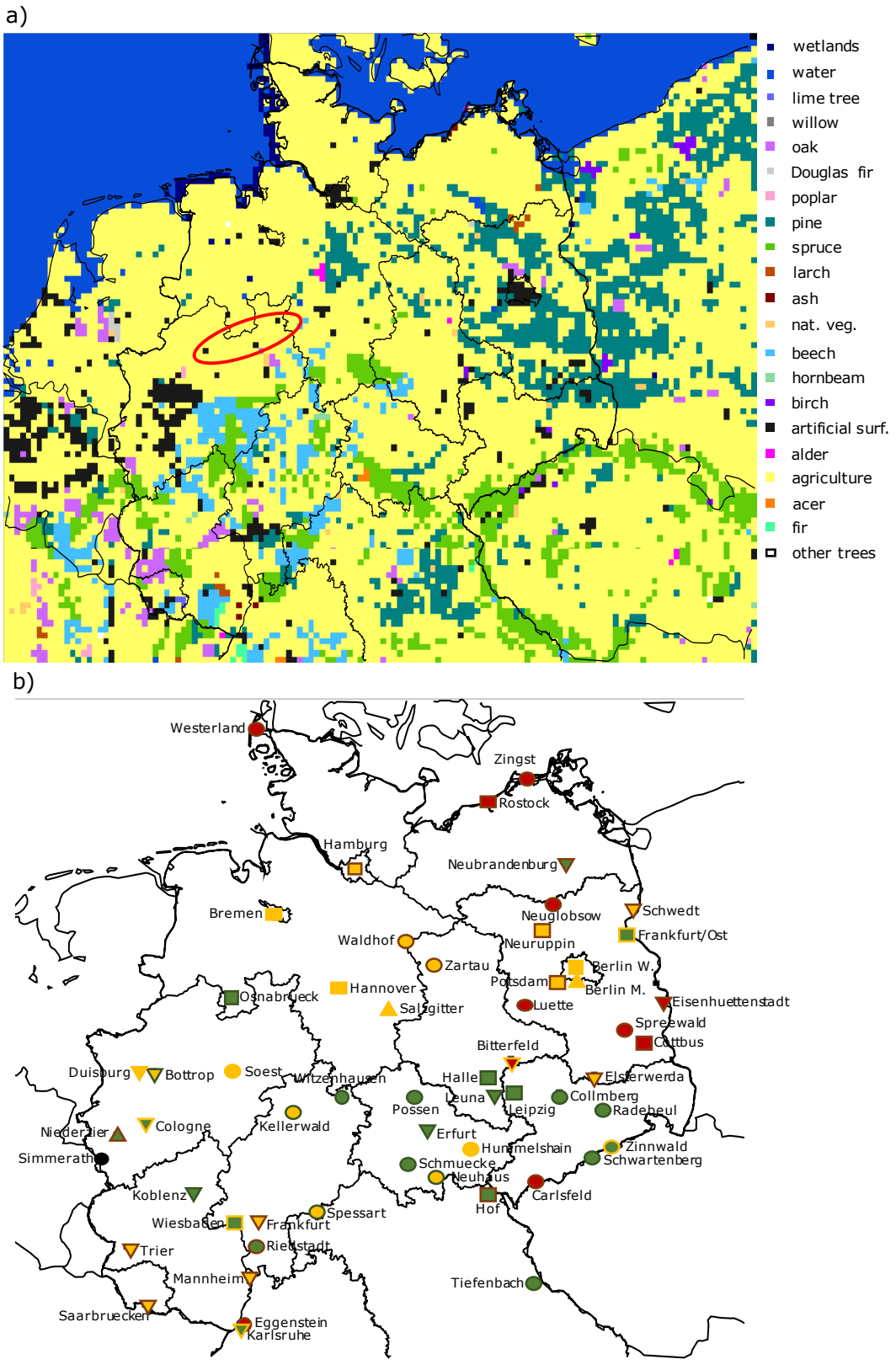


Fig. S3-1: Distribution of the dominant land use type left with red marked area indicating an isoprene-dominated area and b) the selected measurement sites with indication for better ozone correlation values in green for URMELL, red for RACM and yellow if correlation R_{RACM}-R_{URMELL} values are within 0.01 for the entire time series (edge color) and the mean daily concentration cycles (fill color) right. Circles mark the remote background, squares the urban background, triangles traffic/industrial impacted sites.

S3.2 Additional information about remote sites

S3.2.1 BVOC emissions

Table S3.2-1 the BVOC emission parameters of the four common German tree species. Beech (*Fagus sylvatica*) has neither isoprene nor monoterpene pool emissions but releases high amounts of synthesis monoterpenes and OVOCs. Therefore, no isoprene and monoterpene nighttime emission occur for beech. Oak species are the dominant isoprene emitters in Germany (in the case of Simmeranth *Quercus petraea*) with only minor contributions to pool monoterpenes and moderate OVOC emissions. Spruce (*Picea abies*) have moderate isoprene and pool monoterpene but higher synthesis monoterpene and OVOC emissions. Pine trees (*Pinus sylvestris*) do not emit isoprene but higher amounts of pool and synthesis monoterpenes. Therefore, the tree species composition at the measurement site impacts the BVOC mixture which affects the O_3 concentration.

Table S3.2-1 Summary of the standard emission factors for isoprene, monoterpene and OVOCs of the four dominant tree species

Tree species	Isoprene in μg m^{-2} h^{-1} (PAR & T)	Monoterpenes in μg m^{-2} h^{-1}		OVOCs in μg m^{-2} h^{-1} (T)
		MTS (PAR & T)	MTP (T)	
Fagus sylvatica	0.0	7208.74	0.0	3410.0
Quercus petraea	14400.0	0.0	96.0	640.0
Picea abies	1600.0	3360.0	640.0	3680.0
Pinus sylvestris	0.0	1750.0	1750.0	1400.0

Fig. S3.2-1–S3.2-4 show the time series as well as the average daily profiles for the four selected sites. Additional time series of BVOC and OH concentrations are presented in Fig S3.2-2 to S3.2-8. Spreewald is a monoterpene dominated site with only little isoprene contribution (Fig. S3.3-5). Therefore, isoprene chemistry only plays a minor role there. Especially during night, the continuous monoterpene emissions significantly deplete O_3 resulting in a more pronounced daily cycle compared to the diminished cycles at the other three locations. For Spreewald, night time concentrations are nearly matched, while the daytime O_3 peak is under predicted for both simulations. But, the slower O_3 night-time decay causes a slightly lower correlation value for pine. This also transfers to urban environments within low isoprene concentration areas and applies to most of the red marked sites in the east as well as Eggenstein at the south west of the domain in Fig. S3-1b. For Schmuecke (Fig. S3.2-8) and Kellerwald (Fig. S3.2-6), monoterpenes are still dominating, but with much higher portions of synthesis emissions. Furthermore, isoprene and OVOCs become more

important for both sites. Here, O_3 declines after 15 UTC, but this O_3 reduction stagnates or even slightly increases again for a short time between 20 UTC and roughly 2 UTC when NO_3 oxidation becomes sufficient. Afterwards O_3 decreases again to a minimum around 6 UTC. Compared to Kellerwald and Schmuecke, Simmerath does not show so strong night time ozone depletion due to lacking night time BVOC emissions (low monoterpene and isoprene concentration in Fig. S3.2-7), therefore no clear reduction in ozone concentration between 3 and 6 UTC is visible. For Kellerwald and Simmerath, the diurnal O_3 cycle and concentrations are similar compared to the measurements. But, there is a significant offset between the modeled and measured O_3 concentration for Schmuecke of yet unknown cause.

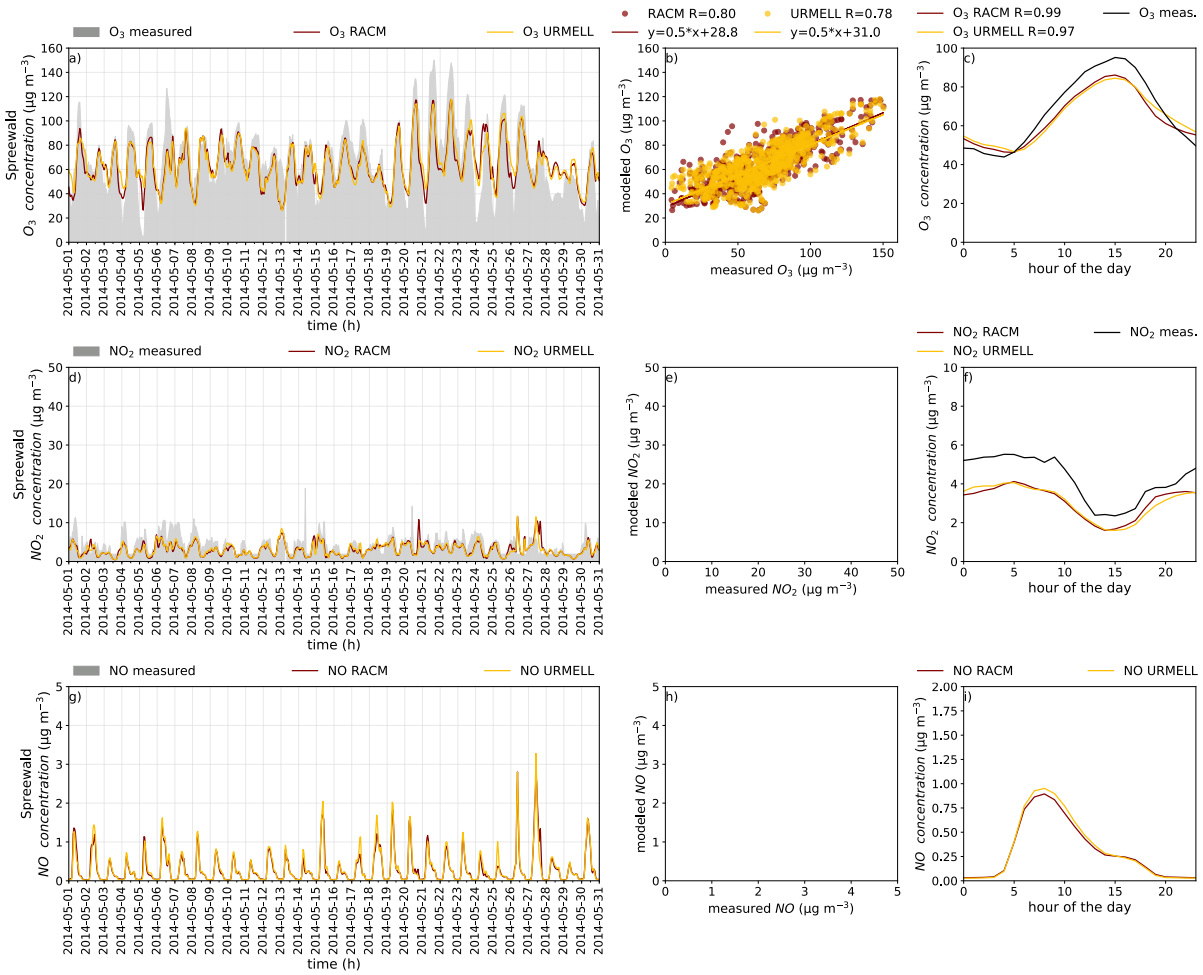


Fig. S3.2-1: Time series of O_3 in a), b) and c); of NO_2 in d), e) and f); of NO in g) h) and i) for Spreewald (pine) measurements in grey for a), d) and g) black line otherwise as well as modeled concentrations using RACM (red line) and URMELL (yellow line).

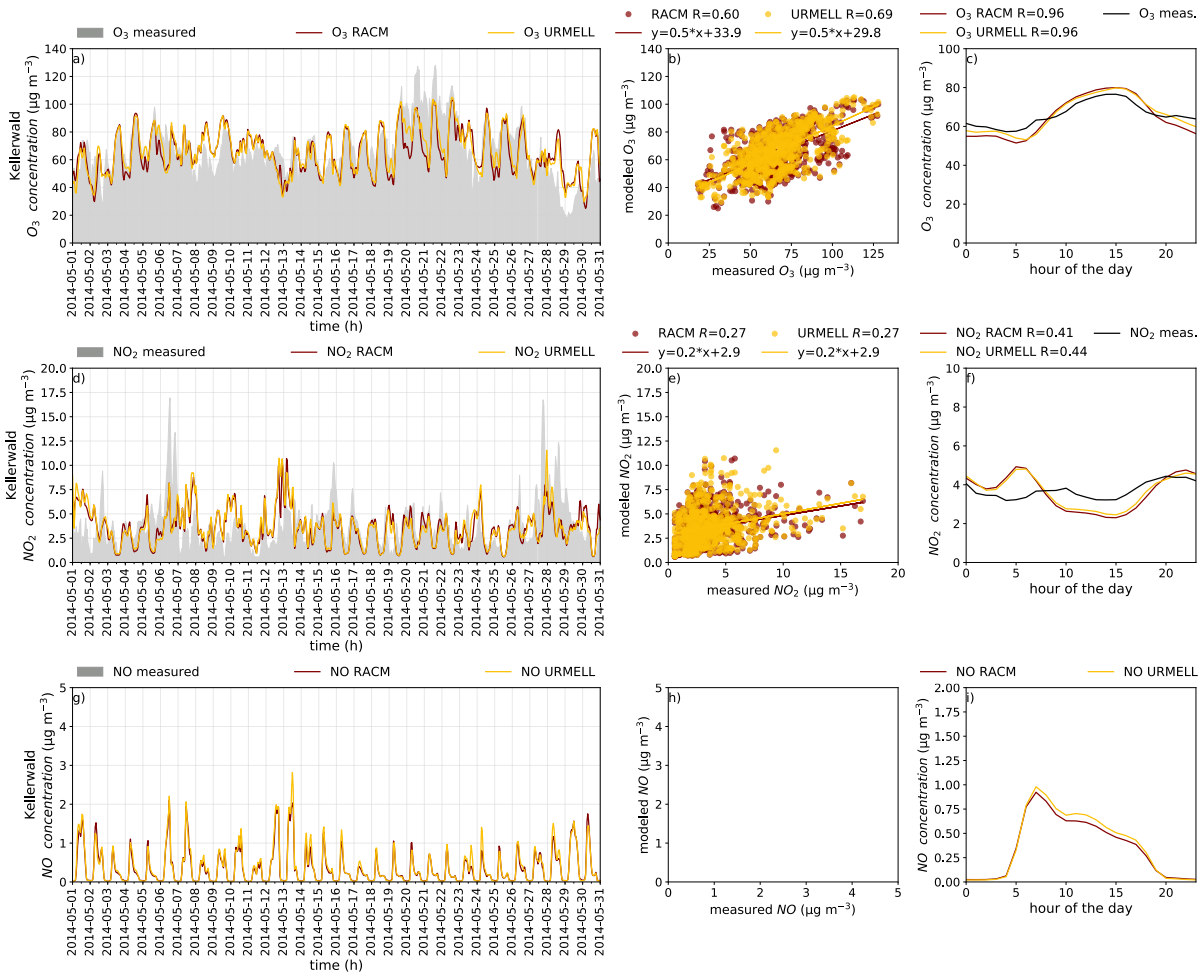


Fig. S3.2-2: Time series of O_3 in a), b) and c); of NO_2 in d), e) and f); of NO in g) h) and i) for Kellerwald (beech) measurements in grey for a), d) and g) black line otherwise as well as modeled concentrations using RACM (red line) and URMELL (yellow line).

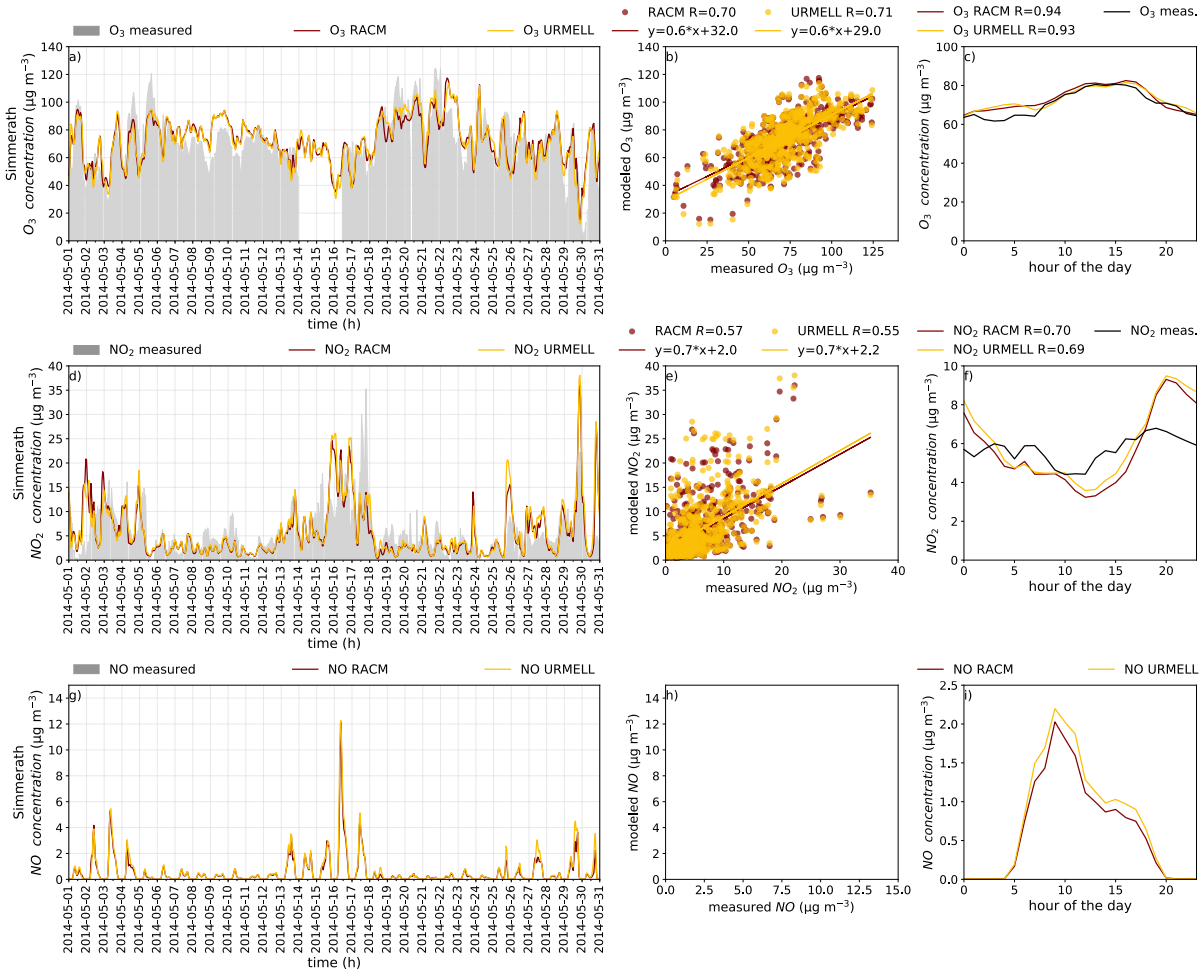


Fig. S3.2-3: Time series of O_3 in a), b) and c); of NO_2 in d), e) and f); of NO in g) h) and i) for Simmerath (oak) measurements in grey for a), d) and g) black line otherwise as well as modeled concentrations using RACM (red line) and URMELL (yellow line).

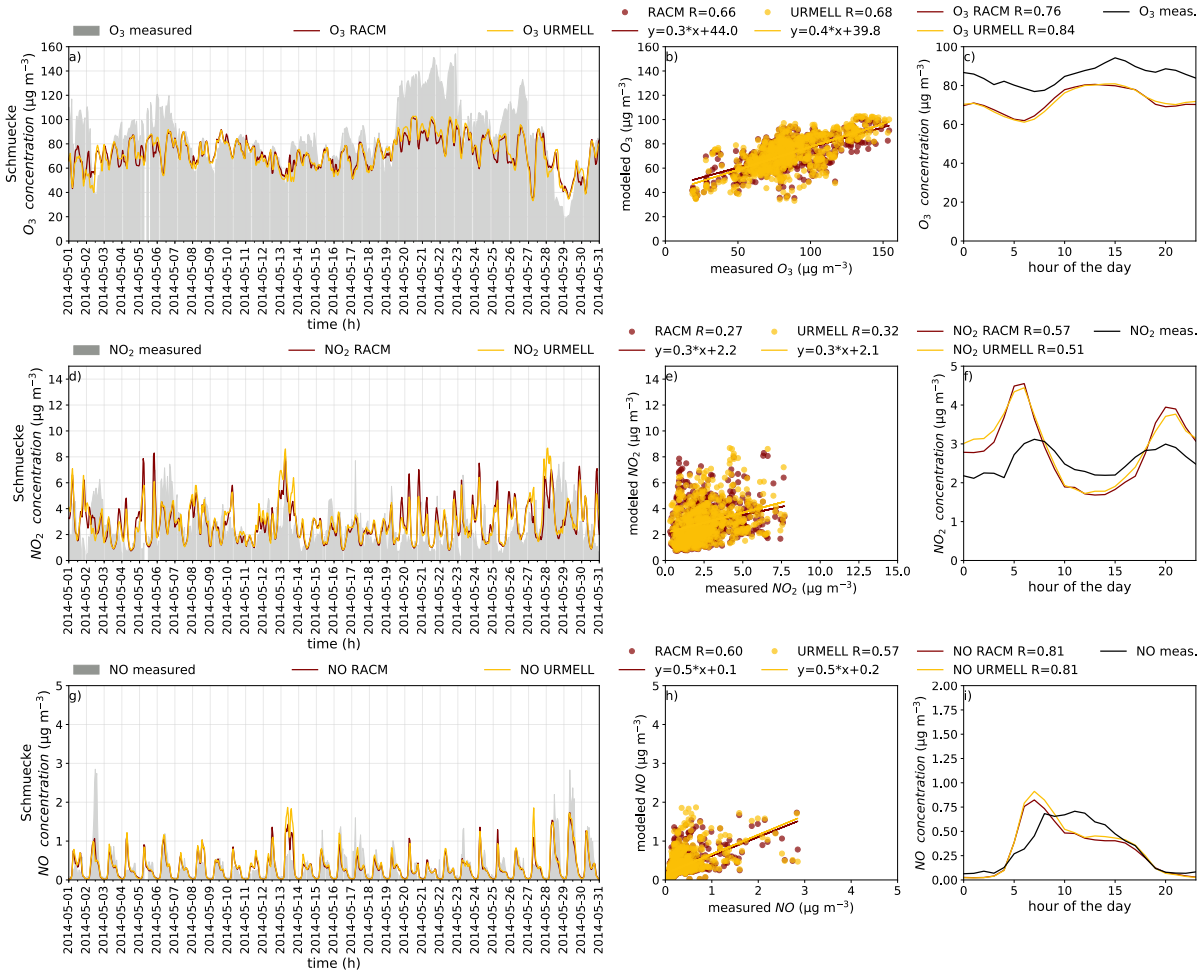


Fig. S3.2-4: Time series of O_3 in a), b) and c); of NO_2 in d), e) and f); of NO in g) h) and i) for Schmuecke (spruce) measurements in grey for a), d) and g) black line otherwise as well as modeled concentrations using RACM (red line) and URMELL (yellow line).

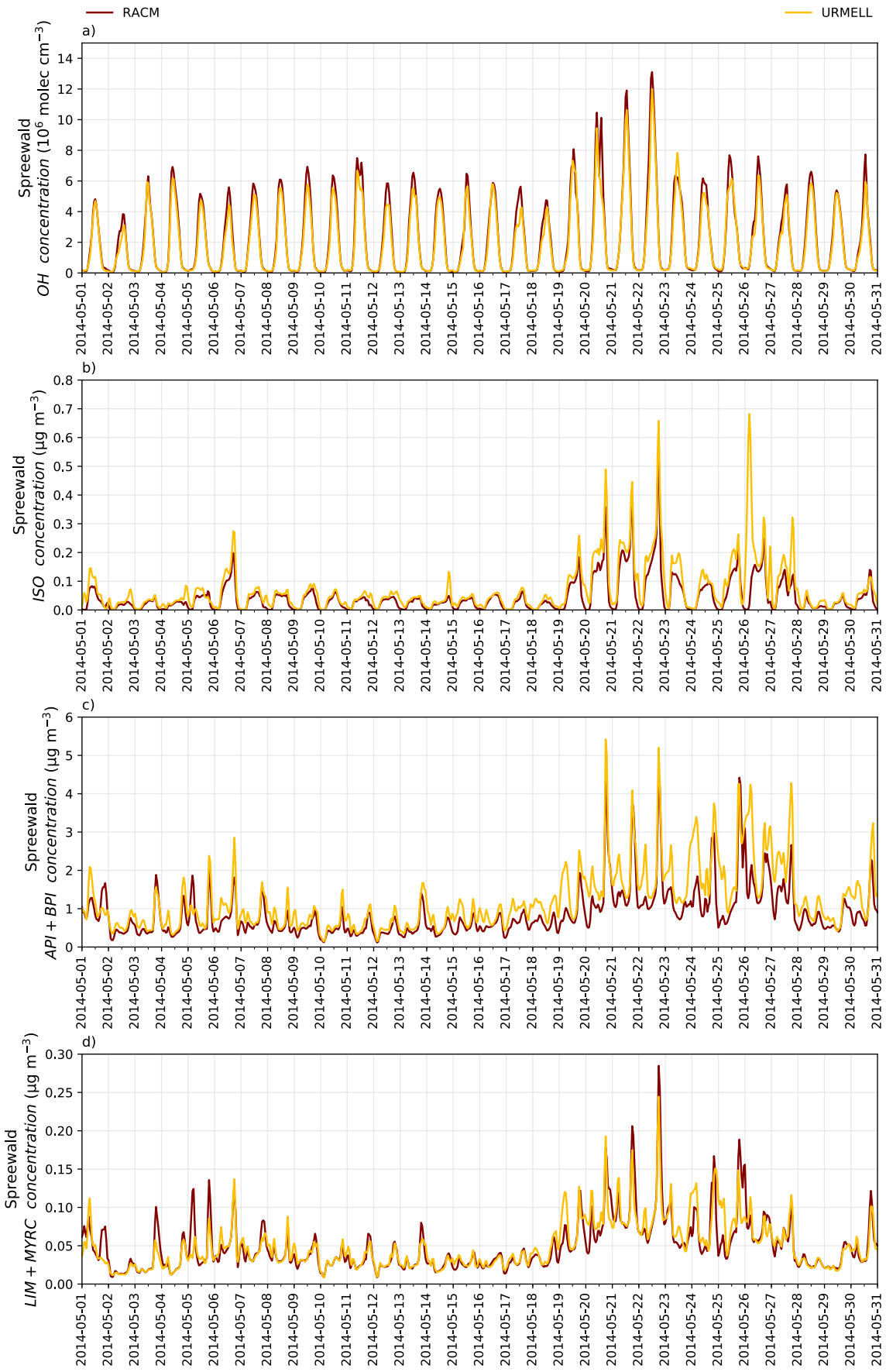


Fig. S3.2-5: Time series of modeled OH in a), isoprene in b), α- and β-pinene in c), limonene and myrcene in d) for Spreewald (pine) using RACM (red line) and URMELL (yellow line).

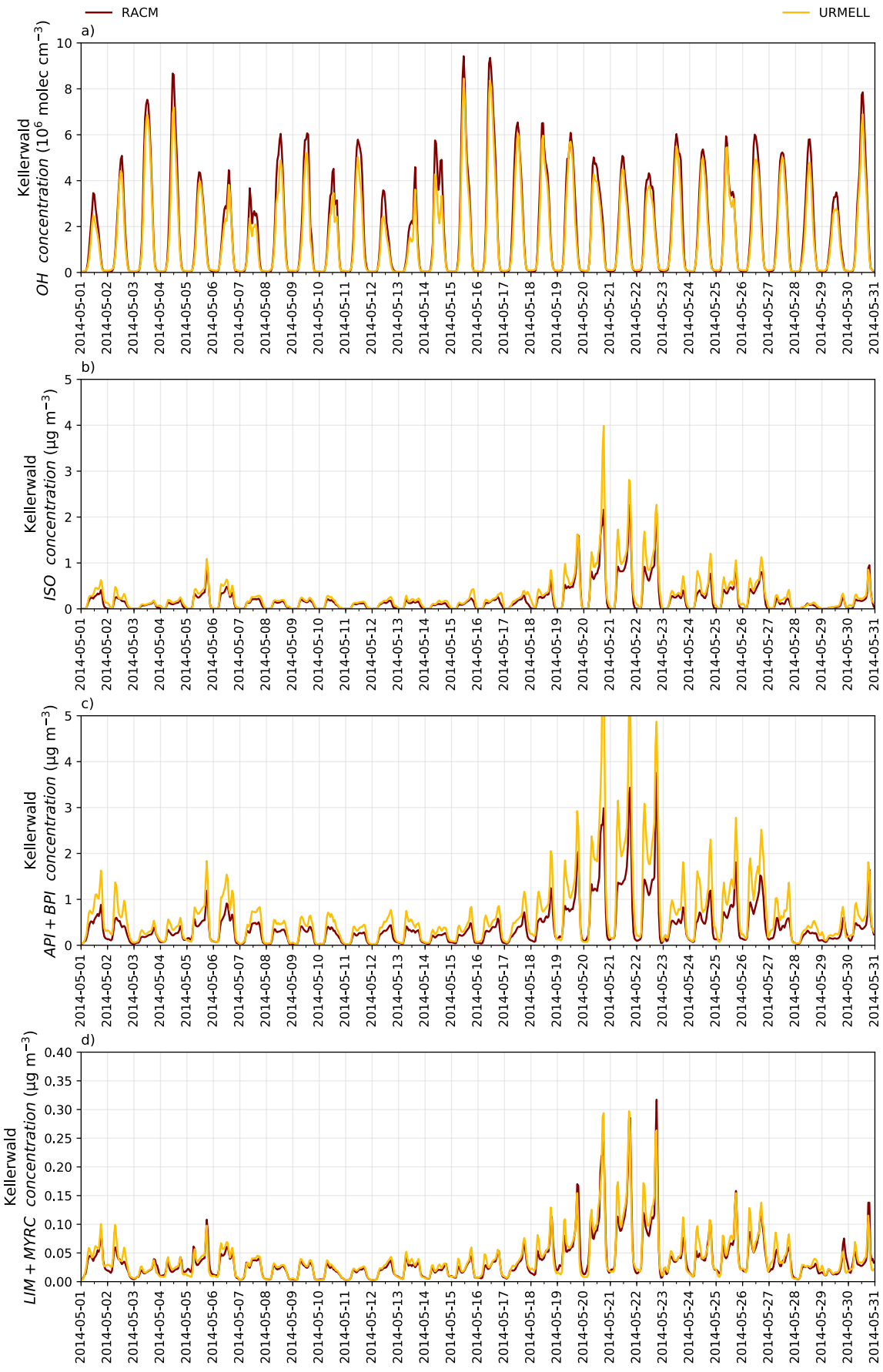


Fig. S3.2-6: Time series of modeled OH in a), isoprene in b), α- and β-pinene in c), limonene and myrcene in d) for Kellerwald (beech) using RACM (red line) and URMELL (yellow line).

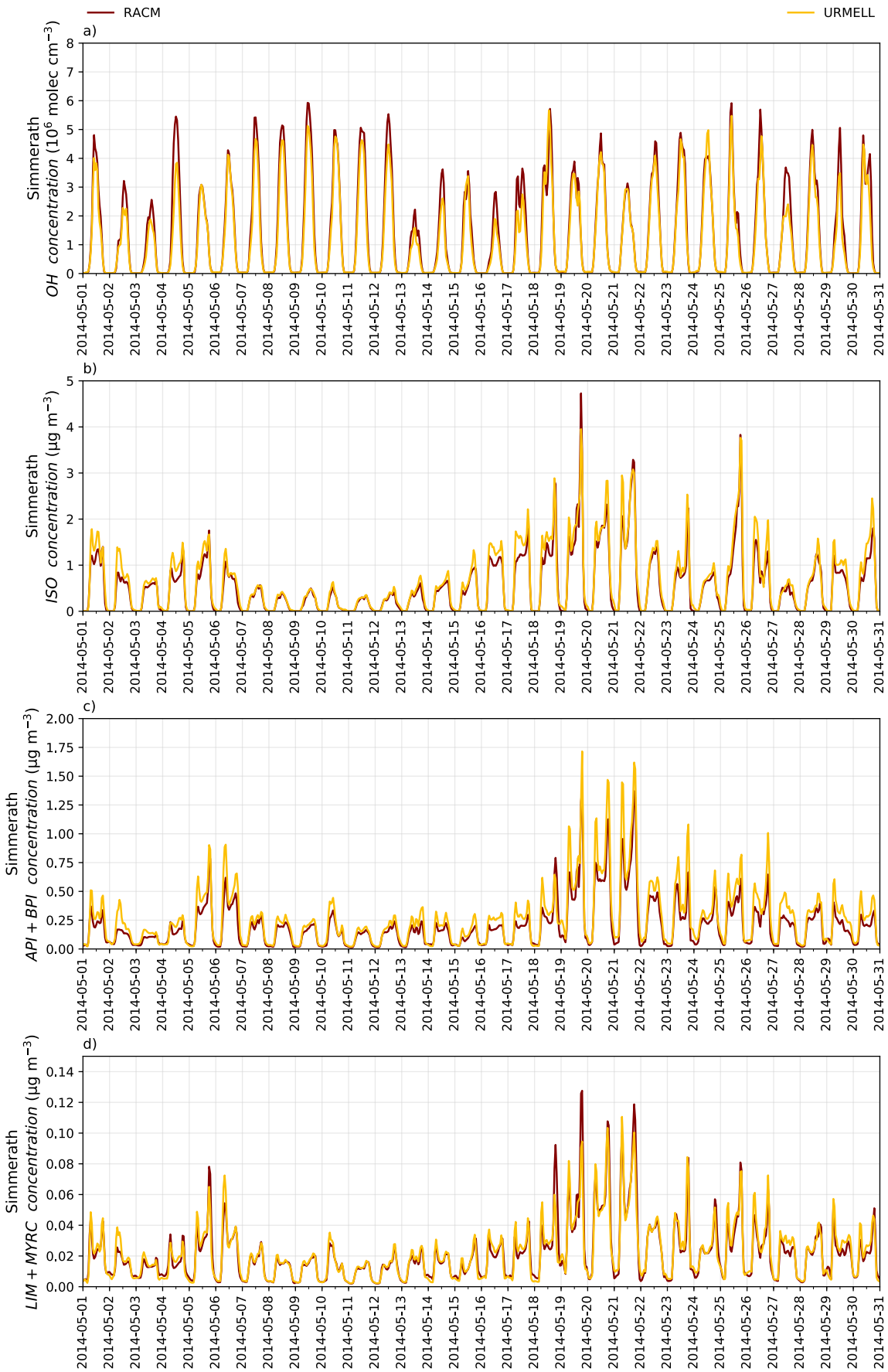


Fig. S3.2-7: Time series of modeled OH in a), isoprene in b), α- and β-pinene in c), limonene and myrcene in d) for Simmerath (oak) using RACM (red line) and URMELL (yellow line).

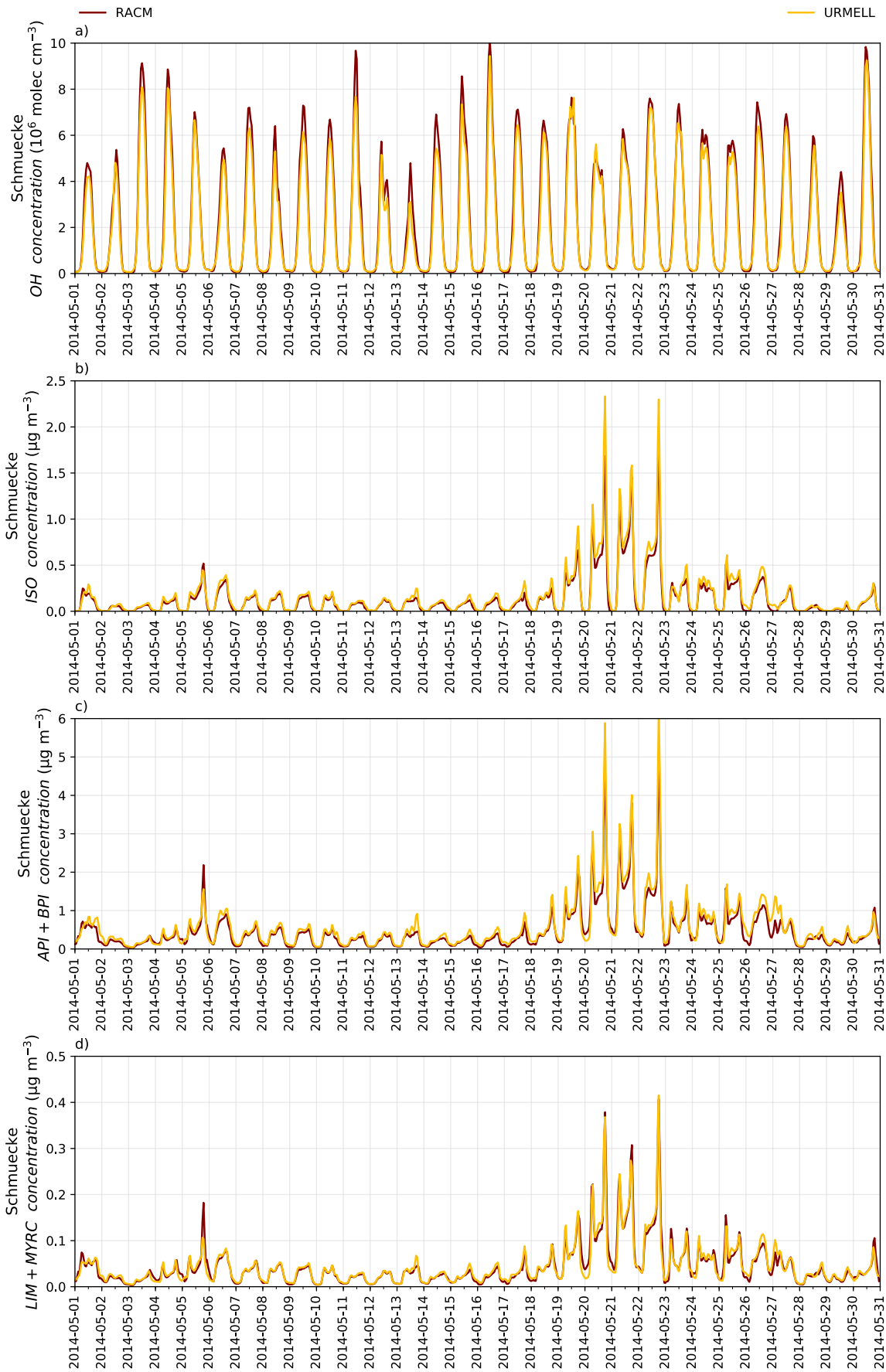


Fig. S3.2-8: Time series of modeled OH in a), isoprene in b), α- and β-pinene in c), limonene and myrcene in d) for Schmuecke (spruce) using RACM (red line) and URMELL (yellow line).

Supplement S4 – CTM simulations

For the model comparison also map plots of NO_2, OH, monoterpene and isoprene concentrations are provided for the 20th of May 2014 for 3, 13 and 19 UTC using RACM and URMELL. Also included is the difference between RACM and URMELL.

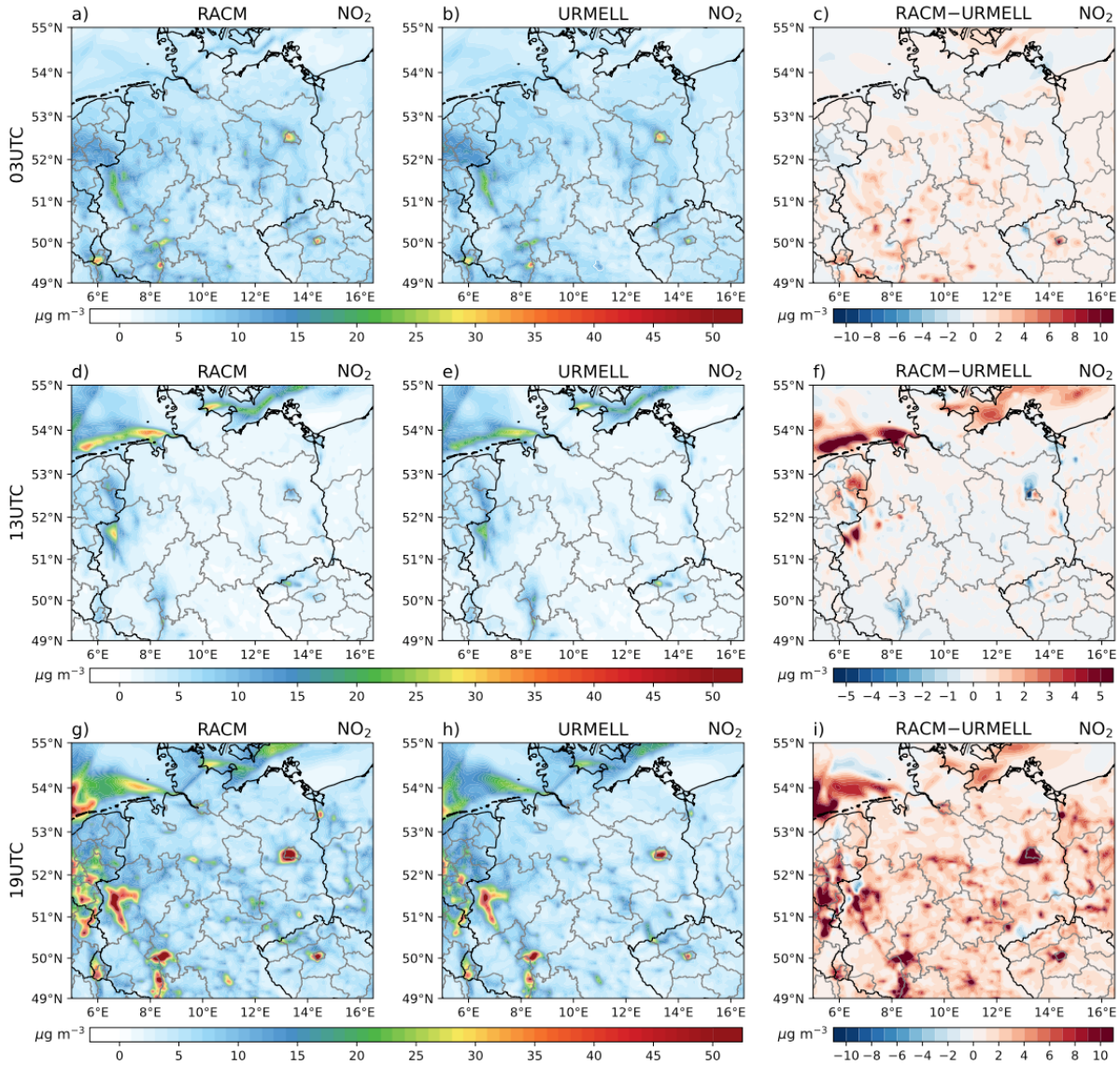


Fig. S4-1: NO_2 concentration for the 20th of May 2014 at 3 UTC, 13 UTC and 19 UTC for RACM (left), URMELL (middle) and the difference between RACM and URMEL (right).

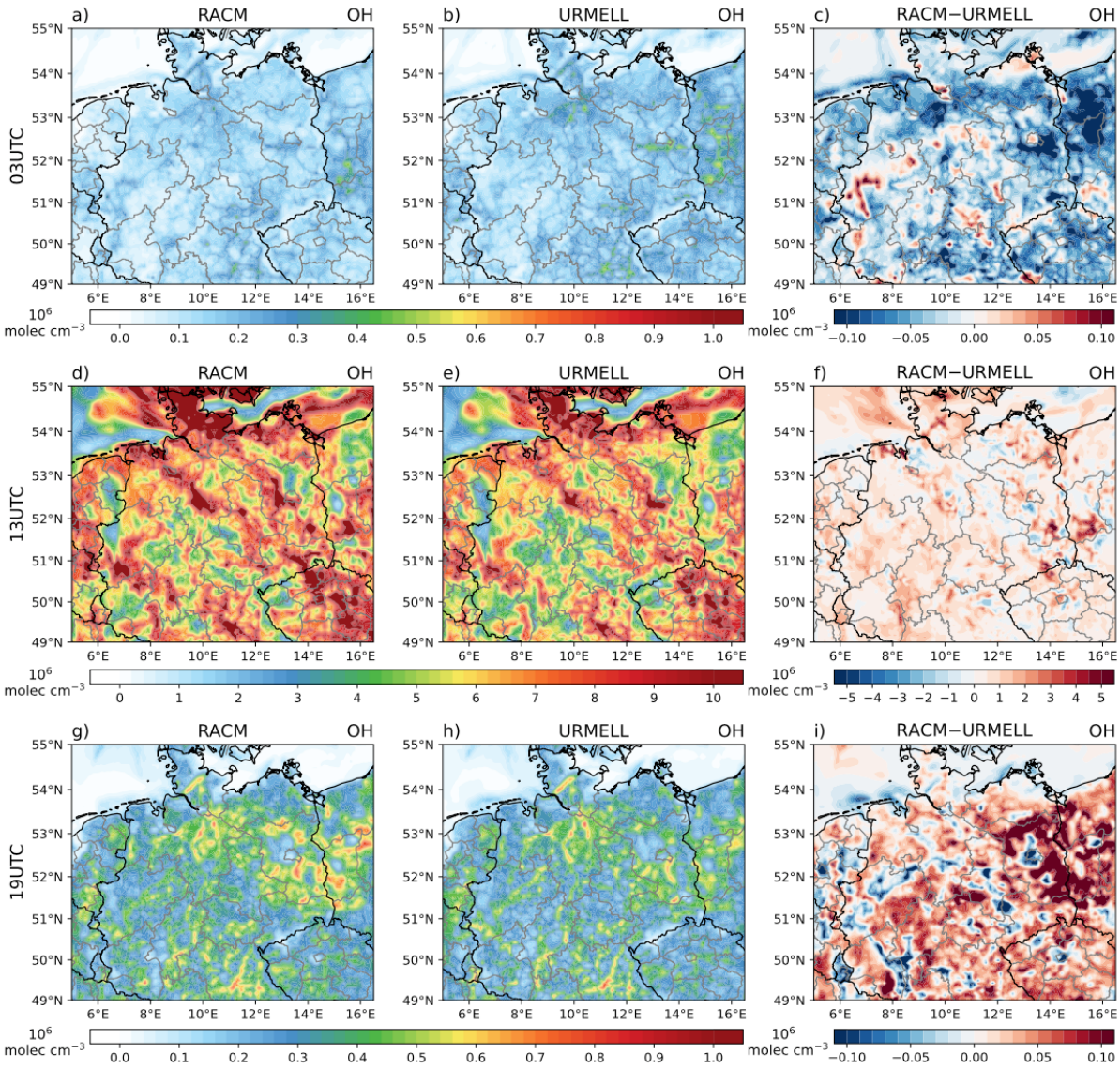


Fig. S4-2: OH concentration for the 20th of May 2014 at 3 UTC, 13 UTC and 19 UTC for RACM (left), URMELL (middle) and the difference between RACM and URMEL (right).

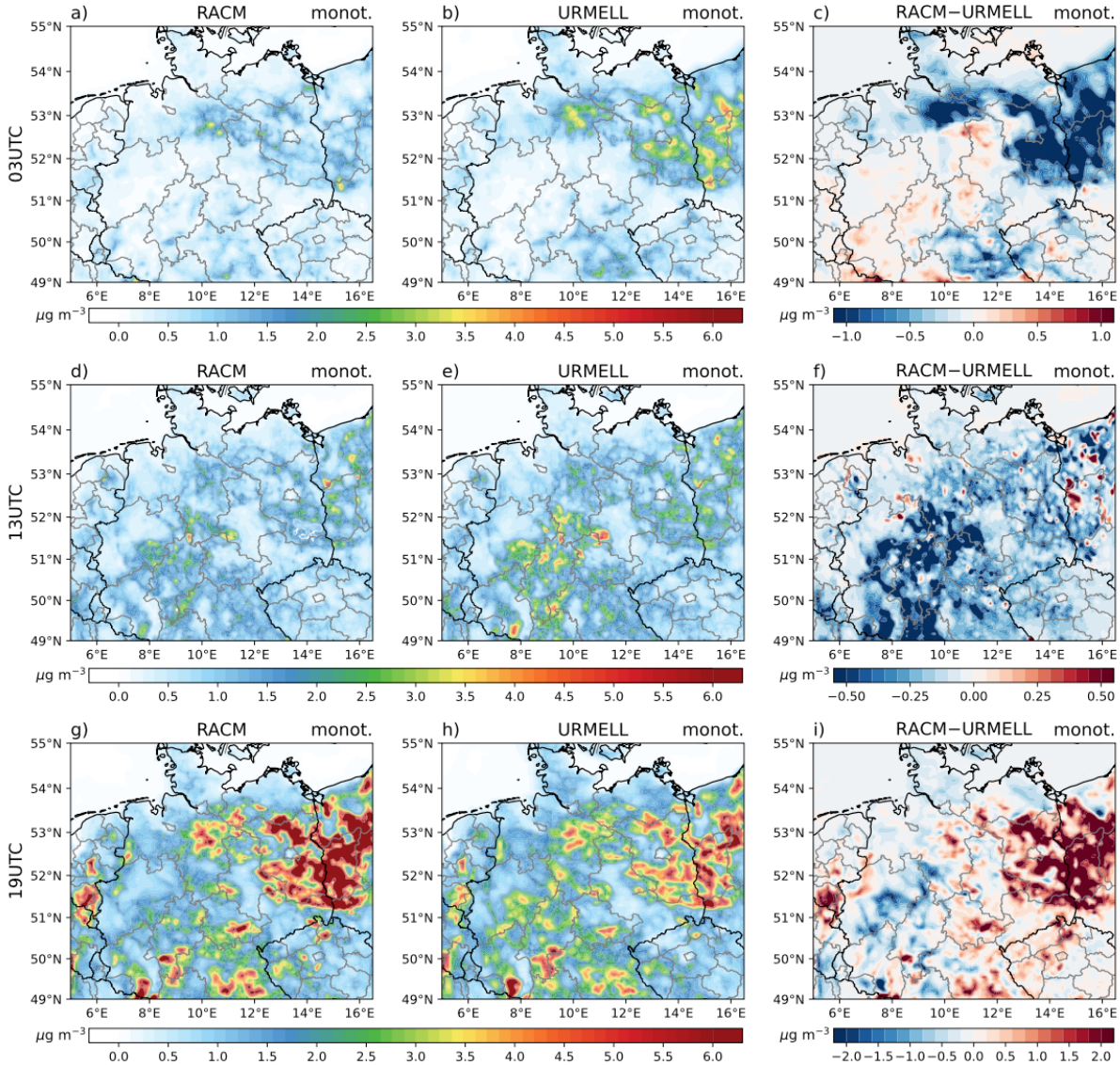


Fig. S4-3: Monoterpene concentration for the 20th of May 2014 at 3 UTC, 13 UTC and 19 UTC for RACM (left), URMELL (middle) and the difference between RACM and URMEL (right).

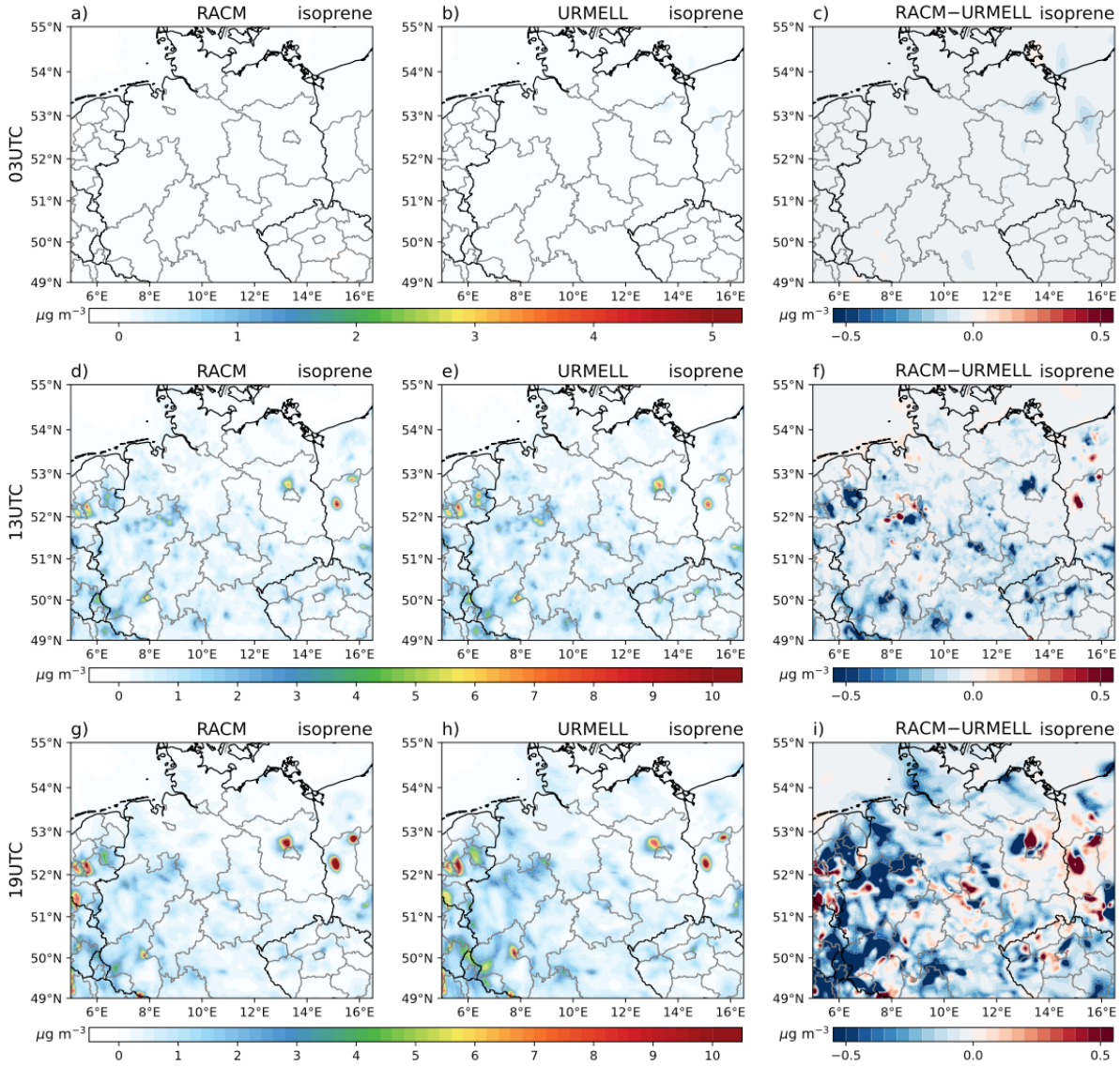


Fig. S4-4: Isoprene concentration for the 20th of May 2014 at 3 UTC, 13 UTC and 19 UTC for RACM (left), URMELL (middle) and the difference between RACM and URMEL (right).

References

1 P. O. Wennberg, K. H. Bates, J. D. Crounse, L. G. Dodson, R. C. McVay, L. A. Mertens, T. B. Nguyen, E. Praske, R. H. Schwantes, M. D. Smarte, J. M. St Clair, A. P. Teng, X. Zhang and J. H. Seinfeld, Gas-Phase Reactions of Isoprene and Its Major Oxidation Products, *Chem. Rev.*, 2018, **118**, 3337–3390.

2 L. Vereecken, P. T. M. Carlsson, A. Novelli, F. Bernard, S. S. Brown, C. Cho, J. N. Crowley, H. Fuchs, W. Mellouki, D. Reimer, J. Shenolikar, R. Tillmann, L. Zhou, A. Kiendler-Scharr and A. Wahner, Theoretical and experimental study of peroxy and alkoxy radicals in the NO_3-initiated oxidation of isoprene, *Phys. Chem. Chem. Phys.*, 2021, **23**, 5496–5515.

3 M. G. Schultz, S. Stadtler, S. Schröder, D. Taraborrelli, B. Franco, J. Krefting, A. Henrot, S. Ferrachat, U. Lohmann, D. Neubauer, C. Siegenthaler-Le Drian, S. Wahl, H. Kokkola, T. Kühn, S. Rast, H. Schmidt, P. Stier, D. Kinnison, G. S. Tyndall, J. J. Orlando and C. Wespes, The chemistry–climate model ECHAM6.3-HAM2.3-MOZ1.0, *Geosci. Model Dev.*, 2018, **11**, 1695–1723.

4 L. Chen, Y. Huang, Y. Xue, Z. Jia and W. Wang, *OH-Initiated Atmospheric Degradation of Hydroxyalkyl Hydroperoxides: Mechanism, Kinetics, and Structure-Activity Relationship*, Aerosols/Atmospheric Modelling/Troposphere/Chemistry (chemical composition and reactions), 2021.

5 R. A. Cox, M. Ammann, J. N. Crowley, H. Herrmann, M. E. Jenkin, V. F. McNeill, A. Mellouki, J. Troe and T. J. Wallington, Evaluated kinetic and photochemical data for atmospheric chemistry: Volume VII – Criegee intermediates, *Atmos. Chem. Phys.*, 2020, **20**, 13497–13519.

6 M. E. Jenkin, R. Valorso, B. Aumont and A. R. Rickard, Estimation of rate coefficients and branching ratios for reactions of organic peroxy radicals for use in automated mechanism construction, *Atmos. Chem. Phys.*, 2019, **19**, 7691–7717.

7 L. Sheps, B. Rotavera, A. J. Eskola, D. L. Osborn, C. A. Taatjes, K. Au, D. E. Shallcross, M. A. H. Khan and C. J. Percival, The reaction of Criegee intermediate CH_2OO with water dimer: primary products and atmospheric impact, *Phys. Chem. Chem. Phys.*, 2017, **19**, 21970–21979.

8 A. P. Teng, J. D. Crounse and P. O. Wennberg, Isoprene Peroxy Radical Dynamics, *J. Am. Chem. Soc.*, 2017, **139**, 5367–5377.

9 J.-F. Müller, T. Stavrakou and J. Peeters, Chemistry and deposition in the Model of Atmospheric composition at Global and Regional scales using Inversion Techniques for Trace gas Emissions (MAGRITTE v1.1) – Part 1: Chemical mechanism, *Geosci. Model Dev.*, 2019, **12**, 2307–2356.

10 M. E. Jenkin, R. Valorso, B. Aumont, A. R. Rickard and T. J. Wallington, Estimation of rate coefficients and branching ratios for gas-phase reactions of OH with aromatic organic compounds for use in automated mechanism construction, *Atmos. Chem. Phys.*, 2018, **18**, 9329–9349.

11 M. A. H. Khan, M. E. Jenkin, A. Foulds, R. G. Derwent, C. J. Percival and D. E. Shallcross, A modeling study of secondary organic aerosol formation from sesquiterpenes using the STOCHEM global chemistry and transport model: SOA FORMATION FROM SESQUITERPENES, *J. Geophys. Res. Atmos.*, 2017, **122**, 4426–4439.

12 M. E. Jenkin, R. Valorso, B. Aumont, A. R. Rickard and T. J. Wallington, Estimation of rate coefficients and branching ratios for gas-phase reactions of OH with aliphatic organic compounds for use in automated mechanism construction, *Atmos. Chem. Phys.*, 2018, **18**, 9297–9328.

13 K. H. Bates, D. J. Jacob, K. Li, P. D. Ivatt, M. J. Evans, Y. Yan and J. Lin, Development and evaluation of a new compact mechanism for aromatic oxidation in atmospheric models, *Atmos. Chem. Phys.*, 2021, **21**, 18351–18374.

14 T. B. Nguyen, G. S. Tyndall, J. D. Crounse, A. P. Teng, K. H. Bates, R. H. Schwantes, M. M. Coggon, L. Zhang, P. Feiner, D. O. Millller, K. M. Skog, J. C. Rivera-Rios, M. Dorris, K. F. Olson, A. Koss, R. J. Wild, S. S. Brown, A. H. Goldstein, J. A. de Gouw, W. H. Brune, F. N. Keutsch, J. H. Seinfeld and P. O. Wennberg, Atmospheric fates of Criegee intermediates in the ozonolysis of isoprene, *Phys. Chem. Chem. Phys.*, 2016, **18**, 10241–10254.

15 B. Yuan, P. R. Veres, C. Warneke, J. M. Roberts, J. B. Gilman, A. Koss, P. M. Edwards, M. Graus, W. C. Kuster, S.-M. Li, R. J. Wild, S. S. Brown, W. P. Dubé, B. M. Lerner, E. J. Williams, J. E. Johnson, P. K. Quinn, T. S. Bates, B. Lefer, P. L. Hayes, J. L. Jimenez, R. J. Weber, R. Zamora, B. Ervens, D. B. Millet, B. Rappenglück and J. A. de Gouw, Investigation of secondary formation of formic acid: urban environment vs. oil and gas producing region, *Atmospheric Chemistry and Physics*, 2015, **15**, 1975–1993.

16 D. B. Millet, M. Baasandorj, D. K. Farmer, J. A. Thornton, K. Baumann, P. Brophy, S. Chaliyakunnel, J. A. de Gouw, M. Graus, L. Hu, A. Koss, B. H. Lee, F. D. Lopez-Hilfiker, J. A. Neuman, F. Paulot, J. Peischl, I. B. Pollack, T. B. Ryerson, C. Warneke, B. J. Williams and J. Xu, A large and ubiquitous source of atmospheric formic acid, *Atmos. Chem. Phys.*, 2015, **15**, 6283–6304.