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The global importance of gas-phase peroxy radical accretion reactions for secondary organic aerosol loading

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Supplementary Information: The Global Importance of Gas-phase RO_2 Dimerization Reactions for Secondary Organic Aerosol Loading

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Table S1. Species constrained in the SOAS box models, along with corresponding names in the MCM and GEOS-Chem mechanism. Lumped species, where the sum of species measurements are assigned to one model species, are indicated by merged table entries.

Species Name	MCM Name	GEOS-Chem Name
Formaldehyde	HCHO	CH2O
Isoprene	C5H8	ISOP
α-pinene	APINENE	MTPA
β-pinene	BPINENE	
Limonene	LIMONENE	LIMO
Ethane	C2H6	C2H6
Ethene	C2H4	C2H4
Ethyne	C2H2	C2H2
Benzaldehyde	BENZAL	BALD
Benzene	BENZENE	BENZ
Ethanol	C2H5OH	EOH
Propane	C3H8	C3H8
Propene	C3H6	PRPE
Acetone	CH3COCH3	ACET
Methanol	CH3OH	MOH
Toluene	TOLUENE	TOLU
Ethylbenzene	EBENZ	EBZ
i-butane	IC4H10	ALK4
i-pentane	IC5H12	
n-butane	NC4H10	
n-pentane	NC5H12	
n-hexane	NC6H14	ALK6
n-decane	NC10H22	
o-xylene	OXYL	XYLE
1,3,5-trimethylbenzene	TM135B	
1,2,4-trimethylbenzene	TM124B	

Table S2. SIMLES strings assigned to each GEOS-Chem RO2 for input to the GECKO-A tool.

GEOS-Chem RO_2	Assigned SMILES
A3O2	CCCO[O]
ACRO2	OCC(O[O])C=O
ACO3	[O]OC(=O)C=C
ALK4N1	CC(O[O])CC(ON(=O)=O)C
ALK4O2	CC(CCC)O[O]
ATO2	CC(=O)O[O]
B3O2	OCC(C)O[O]
BENZO2	[O]OCc1ccccc1
BUTO2	OCC(O[O])C=C
BZCO3	[O]OC(=O)c1ccccc1
C4HVP1	CC(O[O])=CCO
C4HVP2	CC(CO)=CO[O]
ETOO	OCCO[O]
ETO2	CCO[O]
HPALD1OO	CC(C=O)(O[O])C(O)COO
HPALD2OO	CC(O)(COO)C(C=O)O[O]
ICHOO	CC(CO)(O[O])C(=O)CO
ICNOO	O=CC(O)C(C)(O[O])CON(=O)=O
IDHNBOO	CC(CO)(O[O])C(CON(=O)=O)OO
IDHNDOO1	CC(CON(=O)=O)(O[O])C(O)COO
IDHNDOO2	CC(CON(=O)=O)(O)C(O[O])COO
IDNOO	CC(CON(=O)=O)(O[O])C(O)CON(=O)=O
IEPOXAOO	CC(C=O)(O[O])C(O)CO
IEPOXBOO	CC(C=O)(O[O])C(O)CO
IHOO1	C/C(=C/CO[O])CO
IHOO4	C/C(=C/CO)CO[O]
IHPNBOO	CC(CO)(O[O])C(CON(=O)=O)OO
IHPNDOO	CC(CON(=O)=O)(O[O])C(O)COO
IHPOO1	CC(CO)(O[O])C(CO)OO
IHPOO2	CC(O)(COO)C(CO)O[O]
IHPOO3	CC(OO)(CO)C(CO)O[O]
INO2B	C=CC(C)(CON(=O)=O)O[O]
INO2D	[O]OCC=C(C)(CON(=O)=O)
ISOPNOO1	CC(CO)(ON(=O)=O)C(CO)O[O]
ISOPNOO2	CC(CO)(O[O])C(CO)ON(=O)=O
KO2	[O]OCCC(=O)C
LIMO2	[O]OC1(C)CCC(CC1O)C(=C)C
APINO2	[O]OC1(C)C(O)CC2CC1C2(C)C
PINO3	[O]OC(=O)CC1CC(C(=O)C)C1(C)C

C96O2	[O]OCC1CC(C(=O)C)C1(C)C
BPINO2	OCC1(O[O])CCC2CC1C2(C)C
BPINOO2	[O]OC1CC(=O)C2CC1C2(C)C
LIMKO2	O=CCC(CCC(=O)C)C(C)(CO)O[O]
LIMO3	[O]OC(=O)CC(CCC(=O)C)C(=C)C
MACR1OO	CC(=C)C(=O)O[O]
MACRNO2	[O]OC(=O)C(C)(CO)ON(=O)=O
MCO3	CC(=O)O[O]
MCROHOO	CC(C=O)(CO)O[O]
MEKCO3	CCC(=O)O[O]
MO2	CO[O]
MVKOHOO	CC(=O)C(O[O])CO
NRO2	[O]OC2C=Cc1ccccc1C2O
OTHRO2	CCO[O]
PIO2	[O]OC1CC2CC(C1(C)O)C2(C)C
PO2	OCC(O[O])C
PRN1	CC(CON(=O)=O)O[O]
R4N1	CCC(ON(=O)=O)C(O[O])
R4O2	CCCC(O[O])
R7O2	CCCC(CC)O[O]
R7N1	CCC(O[O])C(CC)ON(=O)=O
RCO3	CCC(=O)O[O]
TLFUO2	[O]OC1(C)C(=O)OC(C)C1(C)O
ZRO2	[O]OC1C=CC2(C)OOC1C2O
C2BZRO2	[O]OCC(O)c1ccccc1
BPINNRO2	OCC1(CC(O[O])C2CC1C2(C)C)ON(=O)=O
TOLURO2	[O]OC1C=CC2(C)OOC1C2O
PHENRO2	[O]OC1(O)C=CC2OOC1C2O
SQTP3RO2	O=CCCC(CO)(O[O])C1CC(C)(C)C1CCC(=O)C
PLIMALO2	[O]OC1(C)CCC(CC1O)C(=C)C
MCTO2	[O]Oc1ccccc1O
PIPO2	[O]OC1(C)C(O)CC2CC1C2(C)C
LIMRO2	O=CCC(CCC(=O)C)C(C)(CO)O[O]
BENZRO2	[O]OC1C=CC2OOC1C2O
SQTP2RO2	O=CCCC(CO)(O[O])C1CC(C)(C)C1CCC(=O)C
CSLO2	[O]OC1(O)C=CC2(C)OOC1C2O
EBZRO2	[O]OC1C=CC2(CC)OOC1C2O
TMBRO2	[O]OC1C(=CC2(C)OOC1(C)C2O)C
PINRO2	OCC1(CC(O[O])C2CC1C2(C)C)ON(=O)=O
MYRCORO2	O=CCC(CC(=O)C(=O)C)C(C)(C)O[O]
SQTNO2	[O]OC1(C)CCC2C(CC2(C)C)C(=C)CCC1O[N+](=O)[O-]

SQTO2	[O]OC1(C)CCC2C(CC2(C)C)C(=C)CCC1O
PMYRCOO2	O=CCC1CC(O[O])(C(=O)C)C1(C)C
TMB2RO2	[O]OCc1cc(C)cc(C)c1
SQTP4RO2	O=CCCC(CO)(O[O])C1CC(C)(C)C1CCC(=O)C
PMEKRO2	OCC1CC(O[O])(C(=O)C)C1(C)C
APINNRO2	OCC1(CC(O[O])C2CC1C2(C)C)ON(=O)=O
XYLERO2	[O]OC1(C)C=CC2OOC1(C)C2O
OLND	[O]OC1(C)C(ON(=O)=O)CC2CC1C2(C)C
OLNN	[O-][N+](=O)OC1CC(CCC1(C)O[O])C(=C)C
GCO3	OCC(=O)O[O]
AROMCO3	[O]OC(=O)COC(=O)C(=O)C

Table S3. Non-accretion reactions added and removed from the GEOS-Chem mechanism for modified runs

Added Sesquiterpene Chemistry	
Reaction	**Rate**
FARN + OH = SQTO2	2.25d-10
FARN + O3 = 0.89SQTO + 0.16MVK + 0.33ACET + 0.02CH2O + 0.1OH	GCARR_ac(3.5d-12, -2590.0d0)
FARN + NO3 = SQTNO2	2.15d-11
BCAR + OH = SQTO2	2.0d-10
BCAR + O3 = SQTO + 0.08OH	1.2d-14
BCAR + NO3 = SQTNO2	1.9d-11
OSQT + OH = SQTO2	2.1d-10
OSQT + O3 = SQTO + 0.1 OH	6.3d-15
OSQT + NO3 = SQTNO2	2.0d-11
SQTO2 + HO2 = SQTO	GCARR_ac(2.9d-13, 1300.0d0)
SQTO2 + NO = 0.25SQTN + 0.75NO2 + 0.75HO2 + 0.75SQTO	GCARR_ac(2.7d-12, 360.0d0)
SQTO2 + MO2 = SQTO + HO2 + 0.75CH2O + 0.25MOH	GCARR_ac(2.5d-14, -300.0d0)
SQTO2 + NO3 = SQTO + NO2 + HO2	2.3d-12
SQTNO2 + HO2 = SQTN	GCARR_ac(2.9d-13, 1300.0d0)
SQTNO2 + NO = SQTN + NO2 + HO2	GCARR_ac(2.7d-12, 360.0d0)
SQTNO2 + MO2 = SQTN + HO2 + 0.75CH2O + 0.25MOH	GCARR_ac(2.5d-14, -300.0d0)
SQTNO2 + NO3 = SQTN + NO2 + HO2	2.3d-12
SQTN + OH = SQTP2RO2	6.2d-11
SQTN + O3 = 0.1OH + 0.5SQTP4RO2 + 0.15ACET + 0.075MVK + 0.2MYRCO + 0.15CH2O + 0.10CH2OO + 0.3SQTP	GCARR_ac(3.42d-15, -570.0d0)
SQTN + NO3 = SQTP2RO2	3.3d-13

SQTO + OH = SQTP2RO2	6.2d-11
SQTO + O3 = 0.1OH + 0.5SQTP4RO2 + 0.15ACET + 0.075MVK + 0.2MYRCO + 0.15CH2O + 0.10CH2OO + 0.3SQTP	GCARR_ac(3.42d-15, -570.0d0)
SQTO + NO3 = SQTP2RO2	3.3d-13 ;
SQTP + OH = SQTP3RO2	1.0d-11 ;
SQTP + O3 = 0.1OH	1.0d-16 ;
SQTP + NO3 = HNO3 + SQTP3RO2	5.0d-14 ;
SQTP2RO2 + HO2 = SQTP + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0;
SQTP2RO2 + NO = SQTP + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0);
SQTP2RO2 + NO3 = SQTP + NO2 + HO2	2.30d-12;
SQTP3RO2 + HO2 = OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0;
SQTP3RO2 + NO = NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0);
SQTP3RO2 + NO3 = NO2 + HO2	2.30d-12;
SQTP4RO2 + HO2 = OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0;
SQTP4RO2 + NO = NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0);
SQTP4RO2 + NO3 = NO2 + HO2	2.30d-12;
Replaced Aromatic & BVOC Chemistry	
Reaction	**Rate**
STYR + OH = 0.300ZRO2 + 0.700AROMRO2 + 0.700HO2 + CH2O + 0.700BALD	5.8d-11;
STYR + NO3 = AROMRO2 + NO2 + CH2O + BALD	1.5d-12;
EBZ + OH = 0.813AROMRO2 + 0.250CH2O + 0.070ZRO2 + 0.180CSL + 0.400ALD2 + 0.400AROMP5 + 0.800AROMP4 + 0.1800HO2	7.0d-12
EBZ + NO3 = AROMRO2 + HNO3 + CH2O + BALD	1.2d-16
TMB + OH = 0.930AROMRO2 + 0.120CH2O + 0.050ZRO2 + 0.030CSL + 0.600AROMP5 + 0.375AROMP4 + 0.250MGLY + 0.100GLYX + 0.500RCOOH + 0.120CO + 0.030HO2 + 0.150TLFUONE	3.92d-11
TMB + NO3 = AROMRO2 + HNO3 + 0.400AROMP5 + BALD	1.4d-15
BENZ + OH = BRO2 + 0.54PHEN + 0.54HO2 + 0.46AROMRO2 + 0.18GLYX + 0.2CO +0.55AROMP4	GCARR_ac(2.3d-12, -193.0d0)
TOLU + OH = TRO2 + 0.19CSL + 0.19HO2 + 0.81AROMRO2 + 0.06BALD + 0.12GLYX + 0.12MGLY + 0.27CO + 0.04MVK + 0.3AROMP5 + 0.68AROMP4	GCARR_ac(1.8d-12, 340.0d0)

XYLE + OH = XRO2 + 0.15CSL + 0.15HO2 + 0.85AROMRO2 + 0.06BALD + 0.1GLYX + 0.2MGLY + 0.3CO + 0.04MVK + 0.56AROMP5 + 0.28AROMP4 + 0.45RCOOH	1.7d-11
AROMRO2 + HO2 = OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
AROMRO2 + NO = NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
AROMRO2 + NO3 = NO2 + HO2	2.30d-12
AROMRO2 + MO2 = CH2O + HO2 + HO2	GCARR_ac(1.70d-14, 220.0d0)
AROMRO2 + MCO3 = MO2 + HO2 + CO2	GCARR_ac(4.20d-14, 220.0d0)
PHEN + OH = 0.06BENZO + 0.06GLYX + 0.18AROMP4 + 0.14AROMRO2 + 0.8MCT + 0.8HO2	GCARR_ac(4.70d-13, 1220.0d0)
CSL + OH = 0.727MCT + 0.727HO2 + 0.2AROMRO2 + 0.073BENZO + 0.44AROMP5	4.7d-11
CSL + NO3 = 0.5NPHEN + 0.2AROMRO2 + 0.5HNO3 + 0.3BENZO + 0.44AROMP5	1.4d-11
MCT + OH = 0.3BENZO + 0.7AROMRO2 + 1.05AROMP4	2.0d-11
MCT + NO3 = 0.5NPHEN + 0.5HNO3 + 0.3BENZO + 0.2AROMRO2 + 0.3AROMP4	9.9d-11
LIMO + O3 = 0.865OH + 0.15CO + 0.15AROMRO2 + 0.27LIMAL + 0.715LIMO3	GCARR_ac(2.95d-15, -783.0d0)
MTPO + O3 = 0.5ACET + 0.8OH + 0.1CH2O + 0.5MEK + 0.15MVK + 0.4MYRCO + 0.5AROMRO2 + 0.05HO2 + 0.3KO2 + 0.3RCHO	GCARR_ac(2.7d-15, -520.0d0)
APINN + OH = 0.5PINAL + 0.5NO2 + 0.5HO2 + 0.5C96N + 0.5CH2O + 0.5AROMRO2	5.50d-12
C96O2 + NO = 0.16C96N + 0.84NO2 + 0.84AROMRO2 + 0.84ACET + 0.84CH2O + 0.84RCO3 + 0.42MEK	GCARR_ac(2.7d-12, 360.0d0)
C96O2 + NO3 = NO2 + AROMRO2 + ACET + CH2O + RCO3 + 0.5MEK	2.3d-12
C96O2 + MO2 = HO2 + 0.75CH2O + 0.25MOH + 0.25C96O2H + 0.75AROMRO2 + 0.75ACET + 0.75CH2O + 0.75RCO3 + 0.375MEK	GCARR_ac(3.75d-13, 500.0d0)
C96O2H + OH = 0.5C96O2 + 0.5AROMRO2 + 0.5ACET + 0.5CH2O + 0.5RCO3 + 0.25MEK	2.6d-11
C96N + OH = 0.5NO2 + 0.5MONITS + 0.55AROMRO2 + 0.4ACET + 0.4CH2O + 0.4RCO3 + 0.3MEK	2.88d-12
BPINN + OH = 0.5BPINON + 0.5AROMRO2 + CH2O + 0.5NO2 + 0.5HO2 + 0.5BPINO	4.7d-12

LIMAL + NO3 = AROMRO2 + LIMNB	2.6d-13
LIMKET + NO3 = LIMNB + AROMRO2	9.4d-12
LIMN + NO3 = NO2 + LIMNB + AROMRO2	2.6d-13
PIP + OH = 0.3OH + 0.7AROMRO2 + 0.3MVK + 0.3ACET + 0.1CH2O + 0.78MYRCO	GCARR_ac(6.05d-12, 440.0d0)
PIP + O3 = 0.3OH + 0.7AROMRO2 + 0.3MVK + 0.3ACET + 0.1CH2O + 0.78MYRCO	GCARR_ac(1.35d-15, -520.0d0)
PIP + NO3 = 0.5OLNN + 0.5NO2 + 0.15OH + 0.35AROMRO2 + 0.15MVK + 0.15ACET + 0.05CH2O + 0.39MYRCO	GCARR_ac(1.06d-12, 490.0d0)
PIN + OH = 0.7AROMRO2 + 0.7MONITU + 0.3NO2 + 0.3MYRCO	GCARR_ac(6.05d-12, 440.0d0)
PIN + O3 = 0.7AROMRO2 + 0.7MONITU + 0.3NO2 + 0.3MYRCO	GCARR_ac(1.35d-15, -520.0d0)
PIN + NO3 = 0.5OLNN + 1.15NO2 + 0.35AROMRO2 + 0.35MONITU + 0.15MYRCO	GCARR_ac(1.06d-12, 490.0d0)
MYRCO + OH = HO2 + AROMRO2 + 1.5CH2O + MEK + 0.5ACET + 0.5MVK + 0.5GLYC	GCARR_ac(6.05d-12, 440.0d0)
MYRCO + O3 = OH + AROMRO2 + 1.5CH2O + MEK + 0.5ACET + 0.5MVK + 0.5GLYC	GCARR_ac(1.35d-15, -520.0d0)
MYRCO + NO3 = 0.5OLNN + 0.5NO2 + 0.5HO2 + 0.5AROMRO2 + 0.75CH2O + 0.5MEK + 0.25ACET + 0.25MVK + 0.25GLYC	GCARR_ac(1.06d-12, 490.0d0)
C96O2H + hv = OH + AROMRO2 + ACET + CH2O + RCO3 + 0.5MEK	PHOTOL(172)
Replacement Aromatic and BVOC Chemistry	
Reaction	**Rate**
STYR + OH = 0.300ZRO2 + 0.700C2BZRO2 + 0.700HO2 + 0.3CH2O	5.8d-11
STYR + NO3 = C2BZRO2 + NO2	1.5d-12
EBZ + OH = 0.75EBZRO2 + 0.070ZRO2 + 0.180CSL + 0.1800HO2	7.0d-12
EBZ + NO3 = C2BZRO2 + HNO3	1.2d-16
TMB + OH = 0.050ZRO2 + 0.030CSL + 0.030HO2 + 0.92TMBRO2	3.92d-11
TMB + NO3 = TMB2RO2 + HNO3	1.4d-15
BENZ + OH = BRO2 + 0.54PHEN + 0.54HO2 + 0.46BENZRO2	GCARR_ac(2.3d-12, -193.0d0)
TOLU + OH = TRO2 + 0.19CSL + 0.19HO2 + 0.81TOLURO2	GCARR_ac(1.8d-12, 340.0d0)
XYLE + OH = XRO2 + 0.15CSL + 0.15HO2 + 0.85XYLERO2	1.7d-11

PHEN + OH = 0.06BENZO + 0.14PHENRO2 + 0.8MCT + 0.8HO2	GCARR_ac(4.70d-13, 1220.0d0)
CSL + OH = 0.727MCT + 0.727HO2 + 0.2CSLO2 + 0.073BENZO	4.7d-11
CSL + NO3 = 0.5PHEN + 0.5HNO3 + 0.2CSLO2 + 0.3BENZO	1.4d-11
MCT + OH = 0.3BENZO + 0.7MCTO2	2.0d-11
MCT + NO3 = 0.5NPHEN + 0.5HNO3 + 0.3BENZO + 0.2MCTO2	9.9d-11
C2BZRO2 + HO2 = CH2O + BALD + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
C2BZRO2 + NO = CH2O + BALD + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
C2BZRO2 + NO3 = CH2O + BALD + NO2 + HO2	2.30d-12
EBZRO2 + HO2 = 0.333CH2O + 0.533ALD2 + 0.533AROMP5 + 1.067AROMP4 + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
EBZRO2 + NO = 0.333CH2O + 0.533ALD2 + 0.533AROMP5 + 1.067AROMP4 + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
EBZRO2 + NO3 = 0.333CH2O + 0.533ALD2 + 0.533AROMP5 + 1.067AROMP4 + NO2 + HO2	2.30d-12
TMBRO2 + HO2 = 0.13CH2O + 0.13CO + 0.652AROMP5 + 0.408AROMP4 + 0.272MGLY + 0.109GLYX + 0.543RCOOH + 0.163TLFUONE + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
TMBRO2 + NO = 0.13CH2O + 0.13CO + 0.652AROMP5 + 0.408AROMP4 + 0.272MGLY + 0.109GLYX + 0.543RCOOH + 0.163TLFUONE + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
TMBRO2 + NO3 = 0.13CH2O + 0.13CO + 0.652AROMP5 + 0.408AROMP4 + 0.272MGLY + 0.109GLYX + 0.543RCOOH + 0.163TLFUONE + NO2 + HO2	2.30d-12
TMB2RO2 + HO2 = 0.400AROMP5 + BALD + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
TMB2RO2 + NO = 0.400AROMP5 + BALD + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
TMB2RO2 + NO3 = 0.400AROMP5 + BALD + NO2 + HO2	2.30d-12
BENZRO2 + HO2 = 0.391GLYX + 0.434CO + 1.196AROMP4 + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
BENZRO2 + NO = 0.391GLYX + 0.434CO + 1.196AROMP4 + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
BENZRO2 + NO3 = 0.391GLYX + 0.434CO + 1.196AROMP4 + NO2 + HO2	2.30d-12

TOLURO2 + HO2 = 0.074BALD + 0.148GLYX + 0.148MGLY + 0.332CO + 0.05MVK + 0.37AROMP5 + 0.84AROMP4 + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
TOLURO2 + NO = 0.074BALD + 0.148GLYX + 0.148MGLY + 0.332CO + 0.05MVK + 0.37AROMP5 + 0.84AROMP4 + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
TOLURO2 + NO3 = 0.074BALD + 0.148GLYX + 0.148MGLY + 0.332CO + 0.05MVK + 0.37AROMP5 + 0.84AROMP4 + NO2 + HO2	2.30d-12
XYLERO2 + HO2 = 0.07BALD + 0.118GLYX + 0.235MGLY + 0.351CO + 0.047MVK + 0.65AROMP5 + 0.32AROMP4 + 0.5RCOOH + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
XYLERO2 + NO = 0.07BALD + 0.118GLYX + 0.235MGLY + 0.351CO + 0.047MVK + 0.65AROMP5 + 0.32AROMP4 + 0.5RCOOH + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
XYLERO2 + NO3 = 0.07BALD + 0.118GLYX + 0.235MGLY + 0.351CO + 0.047MVK + 0.65AROMP5 + 0.32AROMP4 + 0.5RCOOH + NO2 + HO2	2.30d-12
PHENRO2 + HO2 = 1.288AROMP4 + 0.424GLYX + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
PHENRO2 + NO = 1.288AROMP4 + 0.424GLYX + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
PHENRO2 + NO3 = 1.288AROMP4 + 0.424GLYX + NO2 + HO2	2.30d-12
CSLO2 + HO2 = 1.4AROMP5 + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
CSLO2 + NO = 1.4AROMP5 + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
CSLO2 + NO3 = 1.4AROMP5 + NO2 + HO2	2.30d-12
MCTO2 + HO2 = 1.5AROMP4 + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
MCTO2 + NO = 1.5AROMP4 + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
MCTO2 + NO3 = 1.5AROMP4 + NO2 + HO2	2.30d-12
LIMO + O3 = 0.865OH + 0.15CO + 0.15PLIMALO2 + 0.12LIMAL + 0.715LIMO3	GCARR_ac(2.95d-15, -783.0d0)
MTPO + O3 = 0.5PMYRCOO2 + 0.5ACET + 0.8OH + 0.5MEK + 0.15MVK + 0.05HO2 + 0.3KO2	GCARR_ac(2.7d-15, -520.0d0)
APINN + OH = 0.5PINAL + 0.5NO2 + 0.5HO2 + 0.5APINNRO2	5.50d-12
C96O2 + NO = 0.16C96N + 0.84NO2 + 0.84PMEKRO2	GCARR_ac(2.7d-12, 360.0d0)
C96O2 + NO3 = NO2 + PMEKRO2	2.3d-12

C96O2 + MO2 = HO2 + 0.75CH2O + 0.25MOH + 0.25C96O2H + 0.75PMEKRO2	GCARR_ac(3.75d-13, 500.0d0)
C96O2H + OH = 0.5C96O2 + 0.5PMEKRO2	2.6d-11
C96N + OH = 0.5NO2 + 0.5MONITS + 0.5PMEKRO2	2.88d-12
BPINN + OH = 0.5BPINNRO2 + 0.5CH2O + 0.5NO2 + 0.5HO2 + 0.5BPINO	4.7d-12
LIMAL + NO3 = LIMRO2	2.6d-13
LIMKET + NO3 = LIMRO2	9.4d-12
LIMN + NO3 = NO2 + LIMRO2	2.6d-13
PIP + OH = 0.3OH + 0.7PIPO2 + 0.09MVK + 0.09ACET + 0.03CH2O + 0.234MYRCO	GCARR_ac(6.05d-12, 440.0d0)
PIP + O3 = 0.3OH + 0.7PIPO2 + 0.09MVK + 0.09ACET + 0.03CH2O + 0.234MYRCO	GCARR_ac(1.35d-15, -520.0d0)
PIP + NO3 = 0.5OLNN + 0.5NO2 + 0.15OH + 0.35PIPO2 + 0.045MVK + 0.045ACET + 0.015CH2O + 0.117MYRCO	GCARR_ac(1.06d-12, 490.0d0)
PIN + OH = 0.7PINRO2 + 0.3NO2 + 0.3MYRCO	GCARR_ac(6.05d-12, 440.0d0)
PIN + O3 = 0.7PINRO2 + 0.3NO2 + 0.3MYRCO	GCARR_ac(1.35d-15, -520.0d0)
PIN + NO3 = 0.5OLNN + 1.15NO2 + 0.35PINRO2 + 0.15MYRCO	GCARR_ac(1.06d-12, 490.0d0)
MYRCO + OH = HO2 + MYRCORO2 + 0.5CH2O + 0.5ACET + 0.5MVK + 0.5GLYC	GCARR_ac(6.05d-12, 440.0d0)
MYRCO + O3 = OH + MYRCORO2 + 0.5CH2O + 0.5ACET + 0.5MVK + 0.5GLYC	GCARR_ac(1.35d-15, -520.0d0)
MYRCO + NO3 = 0.5OLNN + 0.5NO2 + 0.5HO2 + 0.5MYRCORO2 + 0.25CH2O + 0.25ACET + 0.25MVK + 0.25GLYC	GCARR_ac(1.06d-12, 490.0d0)
C96O2H + hv = OH + PMEKRO2	PHOTOL(172)
APINNRO2 + HO2 = C96N + CH2O + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
APINNRO2 + NO = C96N + CH2O + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
APINNRO2 + NO3 = C96N + CH2O + NO2 + HO2	2.30d-12
PMEKRO2 + HO2 = ACET + CH2O + RCO3 + 0.5MEK + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
PMEKRO2 + NO = ACET + CH2O + RCO3 + 0.5MEK + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
PMEKRO2 + NO3 = ACET + CH2O + RCO3 + 0.5MEK + NO2 + HO2	2.30d-12
BPINNRO2 + HO2 = BPINON + CH2O + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
BPINNRO2 + NO = BPINON + CH2O + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
BPINNRO2 + NO3 = BPINON + CH2O + NO2 + HO2	2.30d-12
LIMRO2 + HO2 = LIMNB + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
LIMRO2 + NO = LIMNB + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)

LIMRO2 + NO3 = LIMNB + NO2 + HO2	2.30d-12
PINRO2 + HO2 = MONITU + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
PINRO2 + NO = MONITU + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
PINRO2 + NO3 = MONITU + NO2 + HO2	2.30d-12
MYRCORO2 + HO2 = CH2O + MEK + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
MYRCORO2 + NO = CH2O + MEK + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
MYRCORO2 + NO3 = CH2O + MEK + NO2 + HO2	2.30d-12
PLIMALO2 + HO2 = LIMAL + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
PLIMALO2 + NO = LIMAL + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
PLIMALO2 + NO3 = LIMAL + NO2 + HO2	2.30d-12
PMYRCOO2 + HO2 = 0.6RCHO + 0.2CH2O + 0.8MYRCO + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
PMYRCOO2 + NO = 0.6RCHO + 0.2CH2O + 0.8MYRCO + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
PMYRCOO2 + NO3 = 0.6RCHO + 0.2CH2O + 0.8MYRCO + NO2 + HO2	2.30d-12
PIPO2 + HO2 = 0.3ACET + 0.3MVK + 0.1CH2O + 0.78MYRCO + OH + HO2	2.91d-13 * EXP(1300.0d0 / TEMP) * 0.82d0
PIPO2 + NO = 0.3ACET + 0.3MVK + 0.1CH2O + 0.78MYRCO + NO2 + HO2	GCARR_ac(2.60d-12, 365.0d0)
PIPO2 + NO3 = 0.3ACET + 0.3MVK + 0.1CH2O + 0.78MYRCO + NO2 + HO2	2.30d-12

Table S4. Example RO_2+RO_2 accretion reactions (of 180892 and 2477 total present in the MCM-Accr and Reduced-GC-Accr Mechanisms respectively), accretion product gas-phase losses used in the GEOS-Chem simulation (49 present in the Reducecd-GC-Accr Mechainsm), reversible gas-particle partitioning reactions (6131 present in the MCM-Accr Mechanism), and 1st-order particle uptake reactions (32 present in the Reduced-GC-Accr Mechanism). The full mechanisms have been made available as supplementary material (see Code and Data Availability).

Reaction	Rate	Reaction Category
IHOO1 + IHOO1 = DI_202_1Em02	1.056d-12	RO2 + RO2 Accretion
IHOO1 + IHOO1 = DI_202_1Em04	2.832d-14	RO2 + RO2 Accretion
IHOO1 + IHOO1 = DI_202_1Em05	1.525d-14	RO2 + RO2 Accretion
IHOO1 + C4HVP1 = DI_188_1Em02	5.389d-13	RO2 + RO2 Accretion
DI_202_1Em02 + OH = DILVOC	1d-11	Accretion Product Gas-phase Loss
DI_202_1Em02 = DI_202_1Em02aer	condenseRxn(TEMP, 2.020E+02, RP, DG, ALPHA, ASA)	Reversible particle condensation

DI_202_1Em02aer = DI_202_1Em02	evapRxn(TEMP, 2.020E+02, RP, DG, ALPHA, ASA, 1.00E-02, COA)	Reversible particle evaporation
DI_400_1Em09 = DI_400_1Em09aer	VOCuptk1stOrd(TEMP, M, 4.000E+02, RP, ASA, 1.000E+00)	1st-order particle-phase uptake

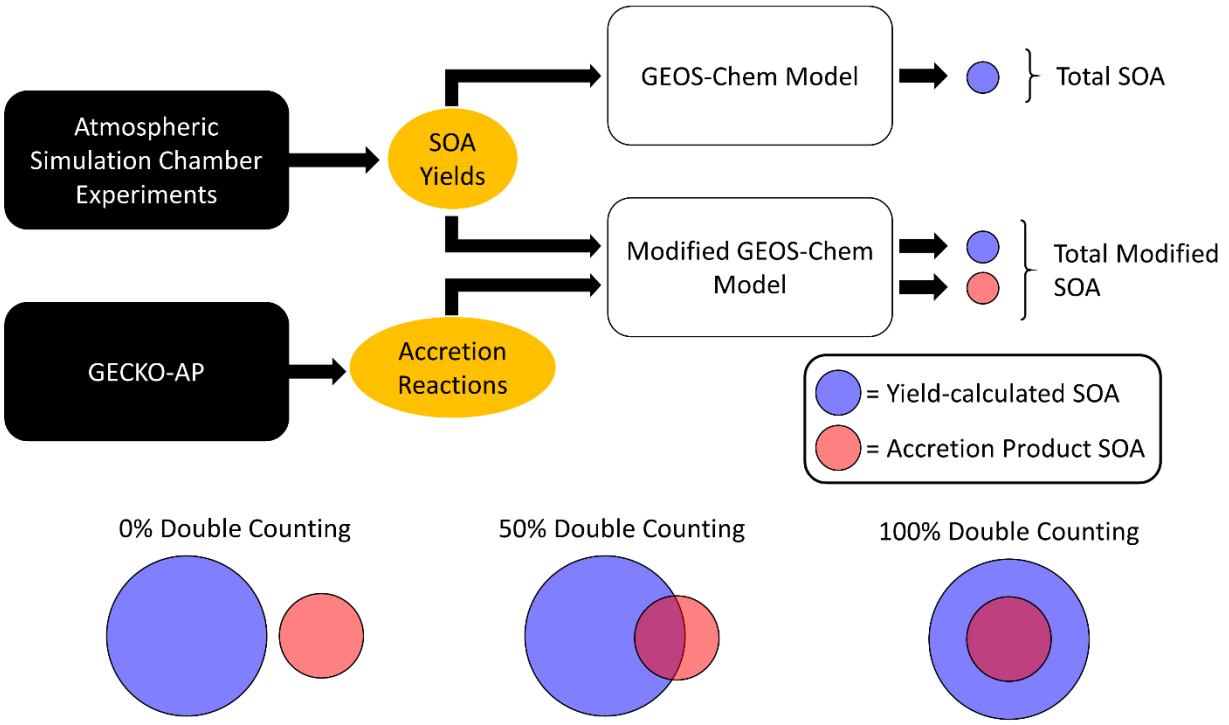

Figure S1. Schematic outlining the addition of accretion product SOA on top of the yield-parameterised SOA already included in the GEOS-Chem base simulation, and the potential double-counting possible if some portion of the accretion product SOA is already accounted for by the yield-parameterised SOA concentrations.

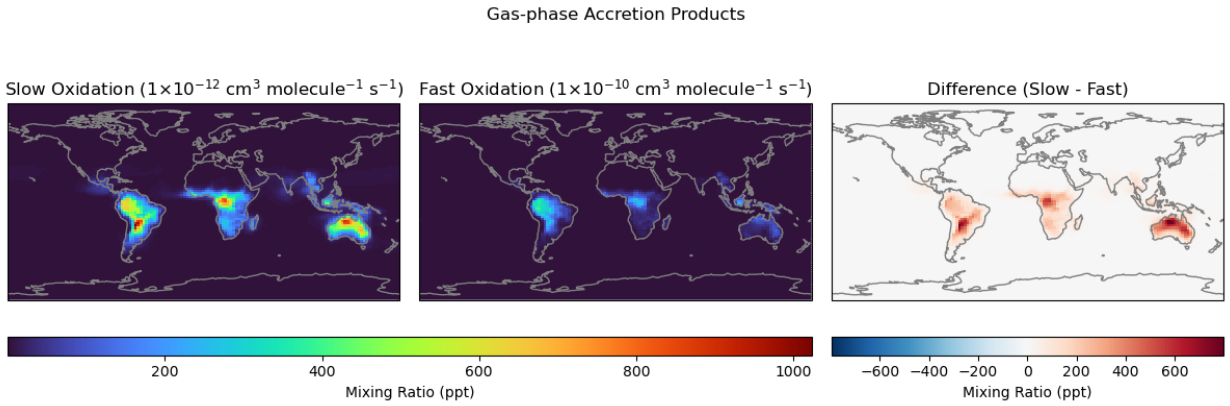

Figure S2. Monthly average gas-phase accretion product mixing ratios in January 2013 from the each of the simulations used to test the sensitivity of the model to choices in the rate constant selected for the reaction of accretion products with OH.

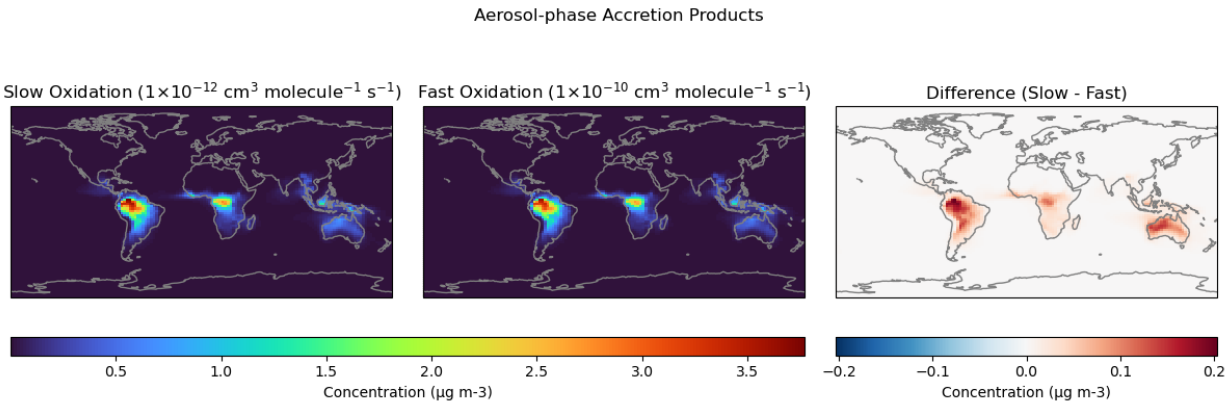

Figure S3. Monthly average aerosol-phase accretion product concentrations in January 2013 from the each of the simulations used to test the sensitivity of the model to choices in the rate constant selected for the reaction of accretion products with OH.

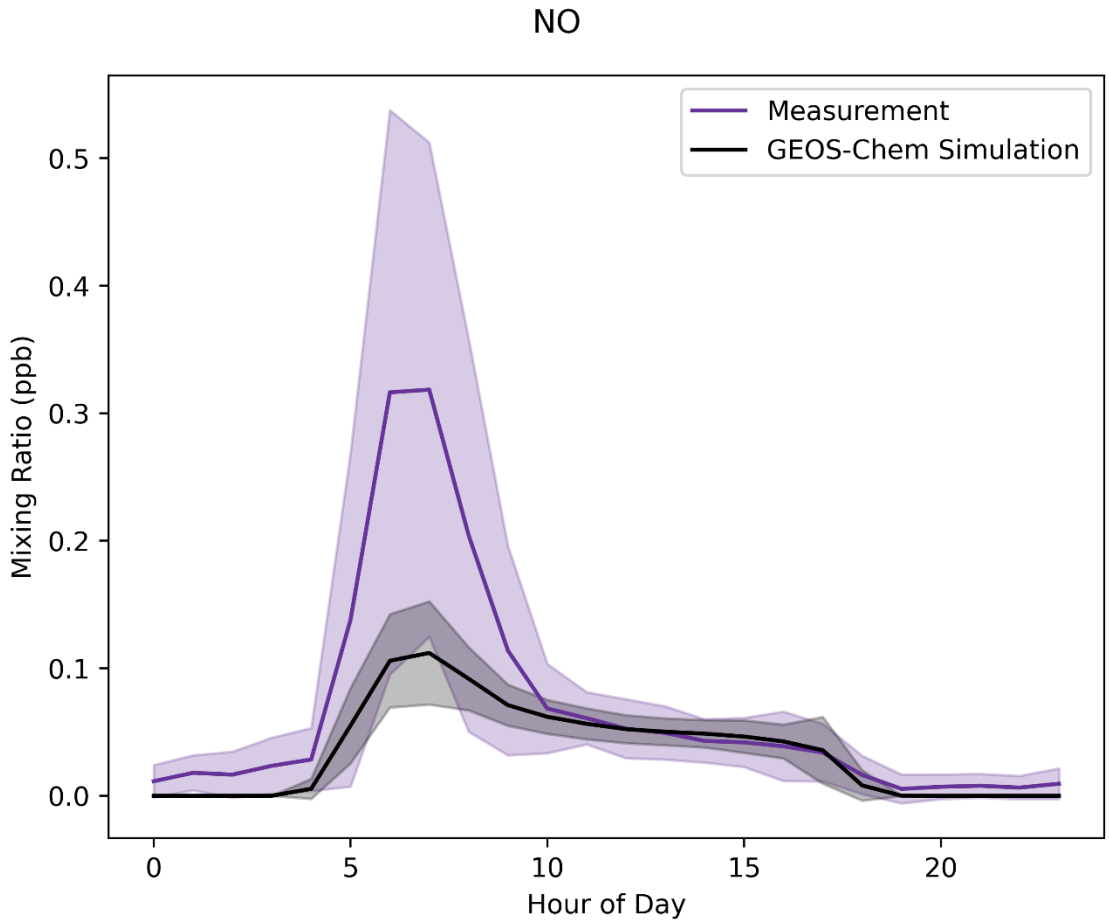

Figure S4. Comparison of simulated NO concentrations in the GEOS-Chem grid-box corresponding to the SOAS measurement location to measured mixing ratios. Each of the box models are constrained to the measured NO mixing ratios. The solid lines show the mean for each hour across the campaign, with the shaded regions showing one standard deviation above and below the mean.

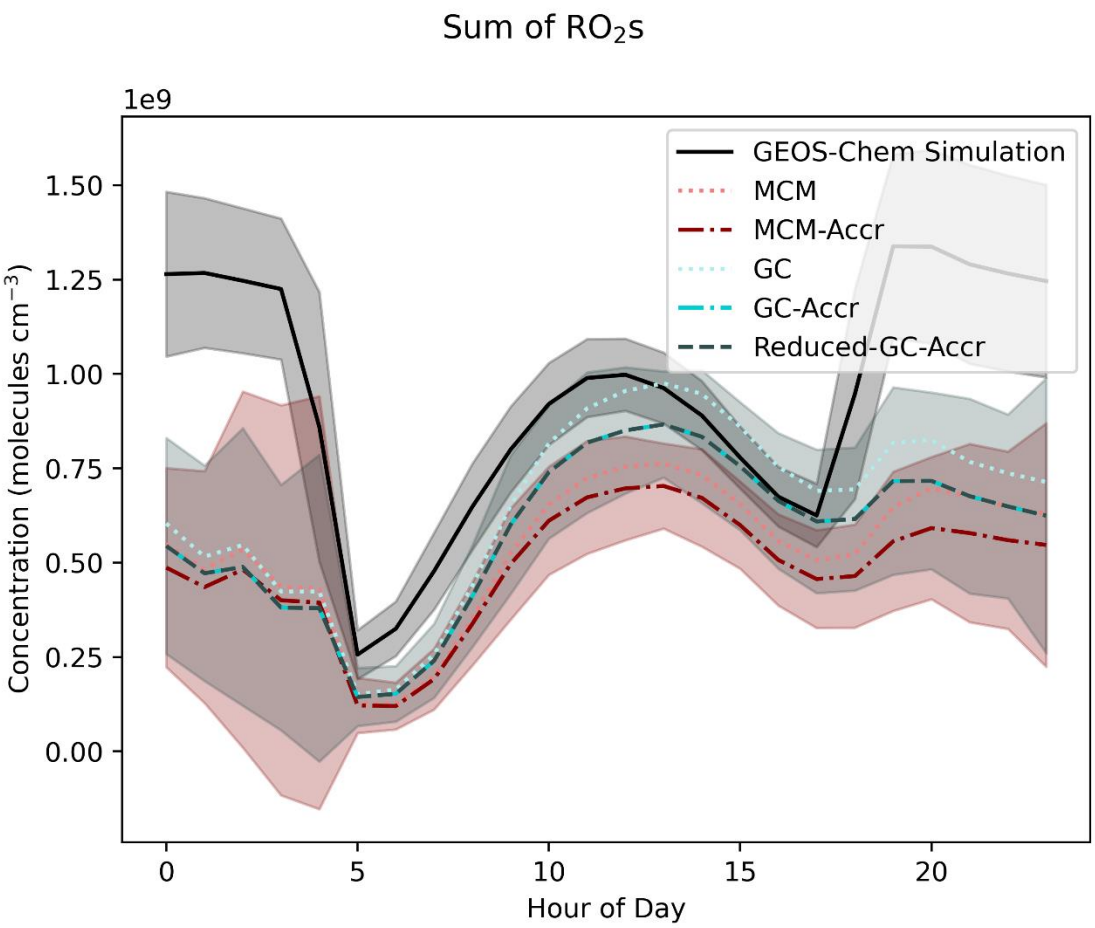

Figure S5. Comparison of simulated RO_2 concentrations in each of the SOAS box models and the GEOS-Chem grid-box corresponding to the SOAS measurement location. The solid lines show the mean for each hour across the campaign, with the shaded regions showing one standard deviation above and below the mean.

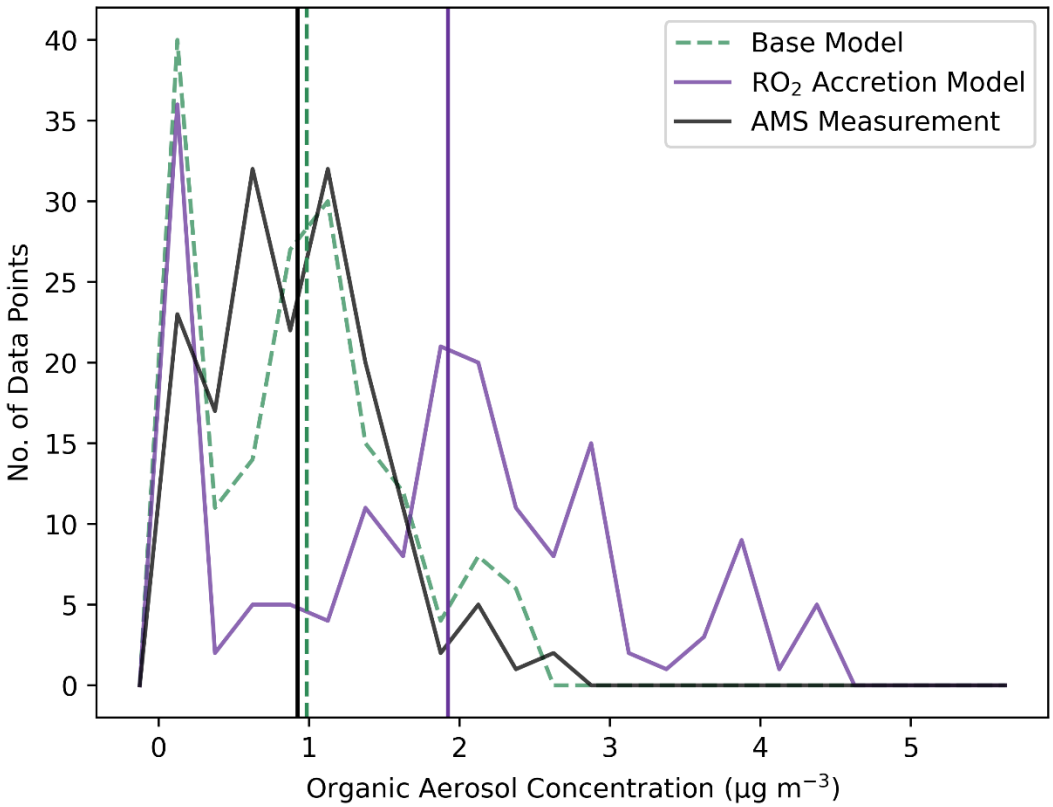

Figure S6. Distribution of measured organic aerosol concentrations (solid black line) compared to organic aerosol concentrations in the GEOS-Chem models over the course of the GOAMAZON flights. Vertical lines show the median of each distribution.

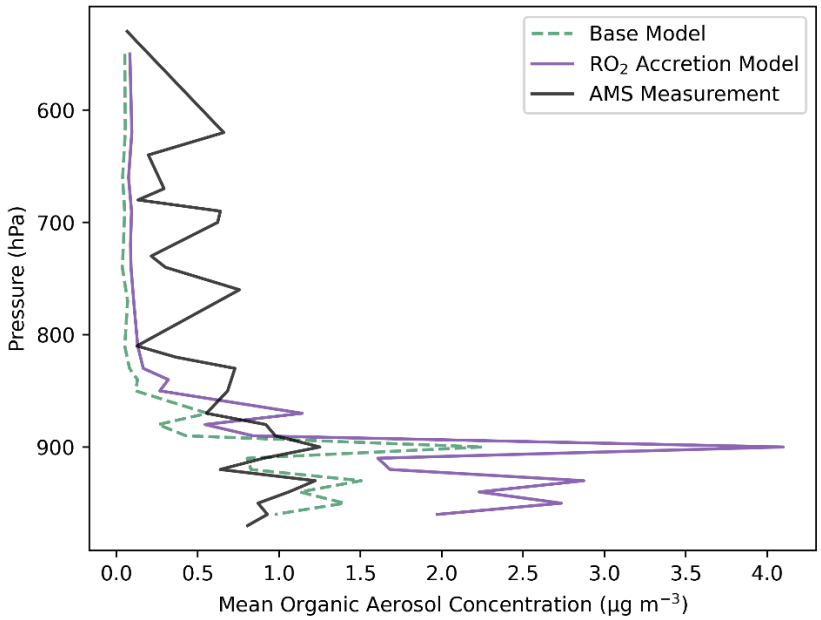

Figure S7. Vertical profile of measured organic aerosol concentrations (solid black line) compared to organic aerosol concentrations in the GEOS-Chem models. Data is binned into 10 hPa groups and the mean value token throughout the GOAMAZON flight trajectory.

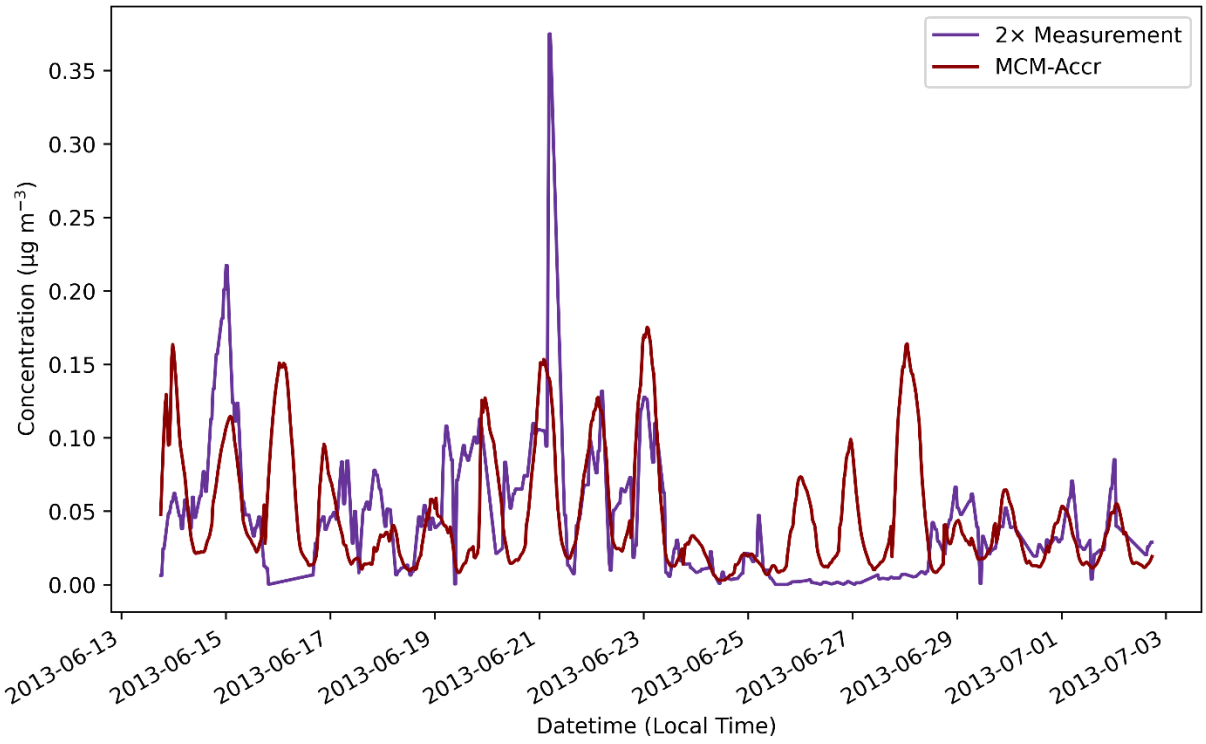

Figure S8. Aerosol-phase concentrations of selected accretion products corresponding to the 41 selected CIMS signals. The red line shows the simulated concentrations from the MCM-Accr model, with the purple line showing measured concentrations multiplied by 2.

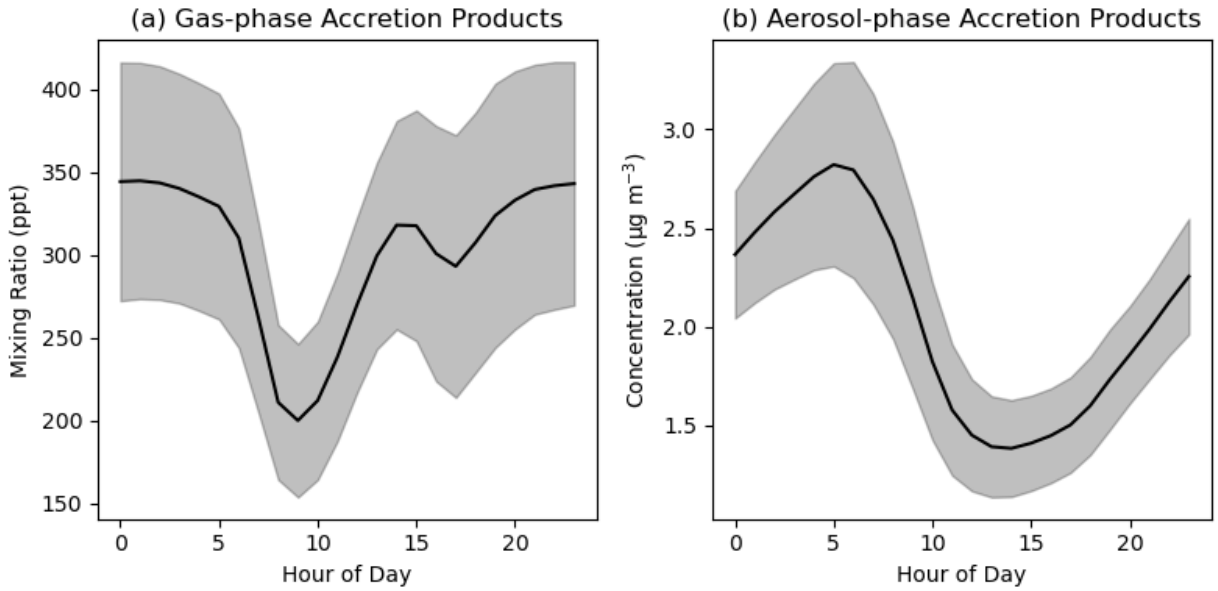

Figure S9. Average modelled ground-level gas-phase (a) and aerosol-phase (b) accretion product concentrations during the GOAMAZON period (2014-02-21 and 2014-03-25) between latitude-longitude coordinates of (-4.0, 62.5) and (0.0, -57.5). The solid lines show the mean for each hour across the campaign, with the shaded regions showing one standard deviation above and below the mean.

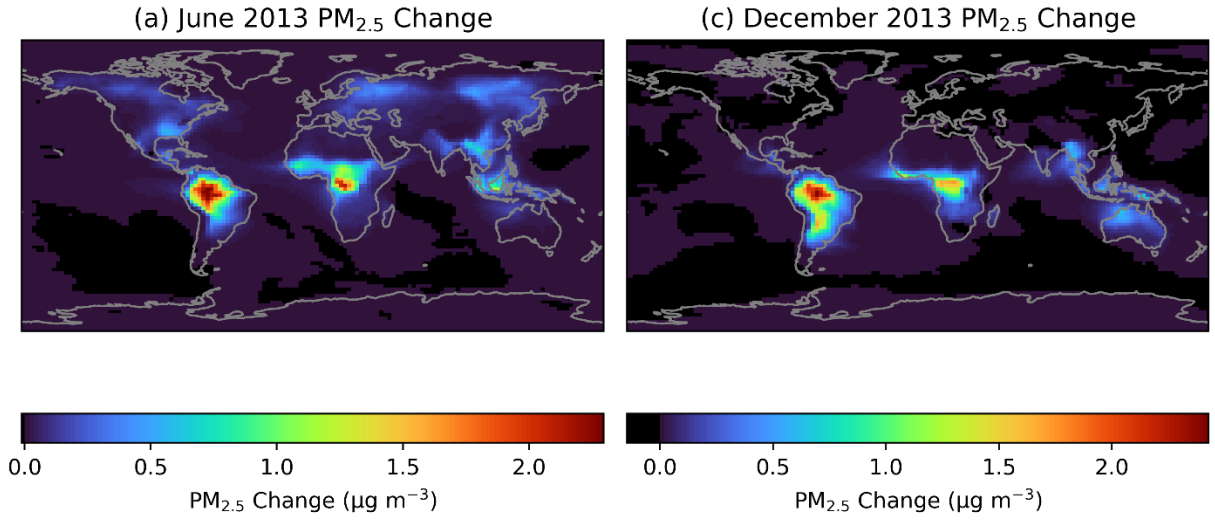

Figure S10. The change in $PM_{2.5}$ concentrations in the first 10 vertical levels when adding RO_2 accretion reactions to GEOS-Chem. (a) and (c) show the absolute change in $PM_{2.5}$ mass concentration in June and January, respectively. (b) and (d) show the change as a percentage of $PM_{2.5}$ in the base model in June and January, respectively.

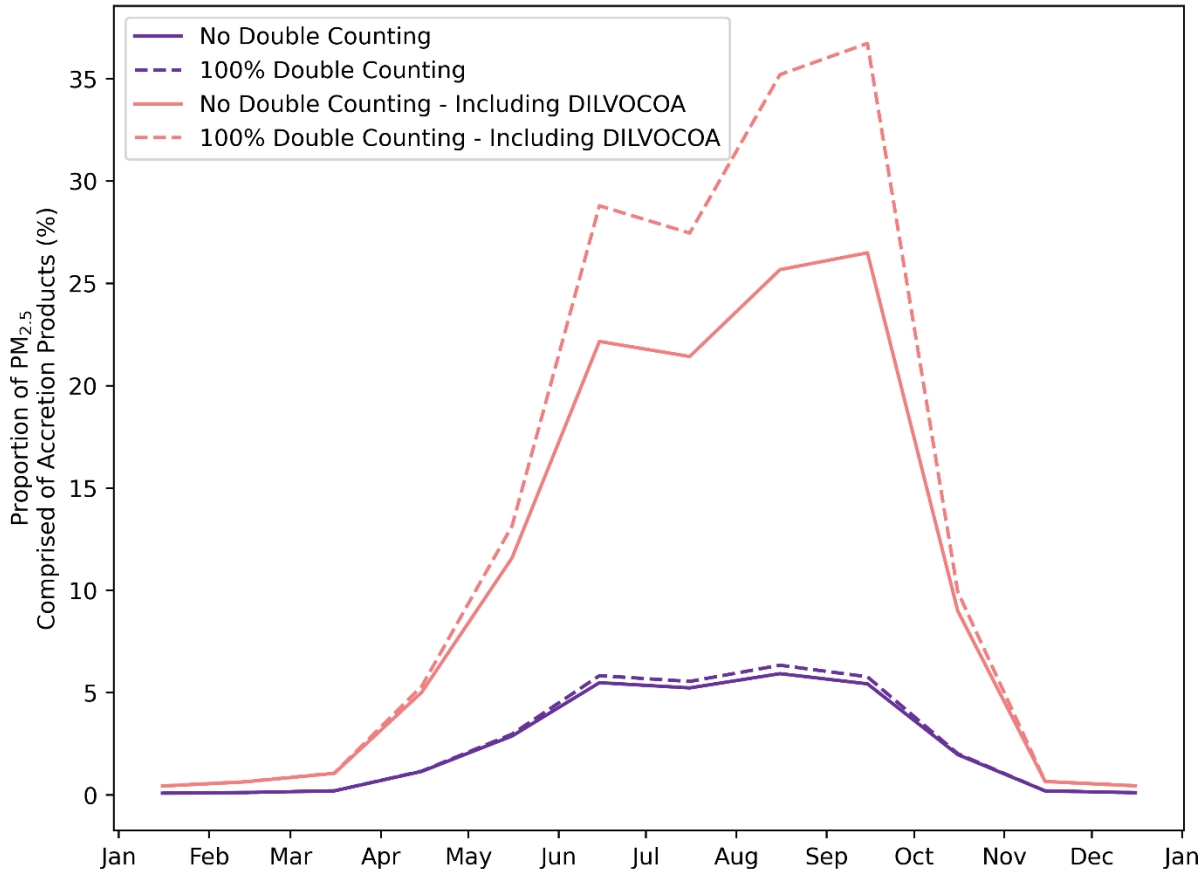

Figure S11. Proportion of $PM_{2.5}$ comprised of RO_2 accretion products, calculated using monthly average surface concentrations throughout 2013 in the south-eastern united states between latitude- longitude coordinates of (31.0, -90.0) and (37.0, -82.0).

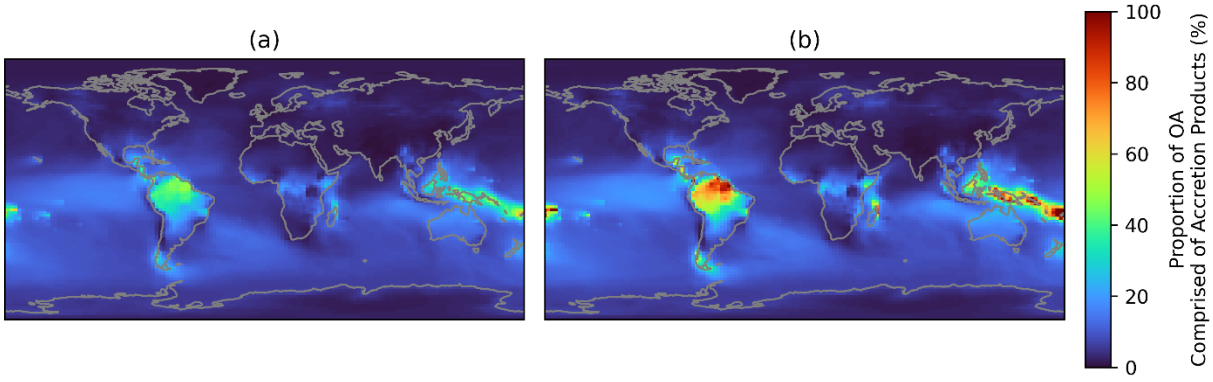

Figure S12. Proportion of organic aerosol (OA) comprised of RO_2 accretion products, calculated using annual average surface concentrations. (a) Simulated accretion product concentrations divided by the simulated OA mass concentration. (b) Assumes 100% double counting of accretion products by subtracting the accretion product concentrations from the OA denominator.

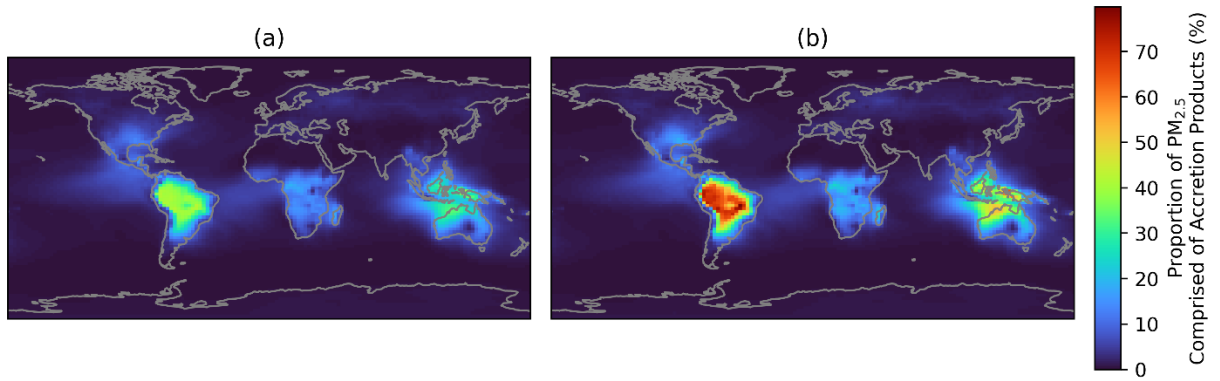

Figure S13. Proportion of $PM_{2.5}$ comprised of RO_2 accretion products, including the products of secondary oxidation of accretion products, DILVOC, calculated using annual average surface concentrations. (a) Simulated accretion product and DILVOC concentrations divided by the simulated $PM_{2.5}$ mass concentration. (b) Assumes 100% double counting by subtracting the accretion product and DILVOC concentrations from the $PM_{2.5}$ denominator.

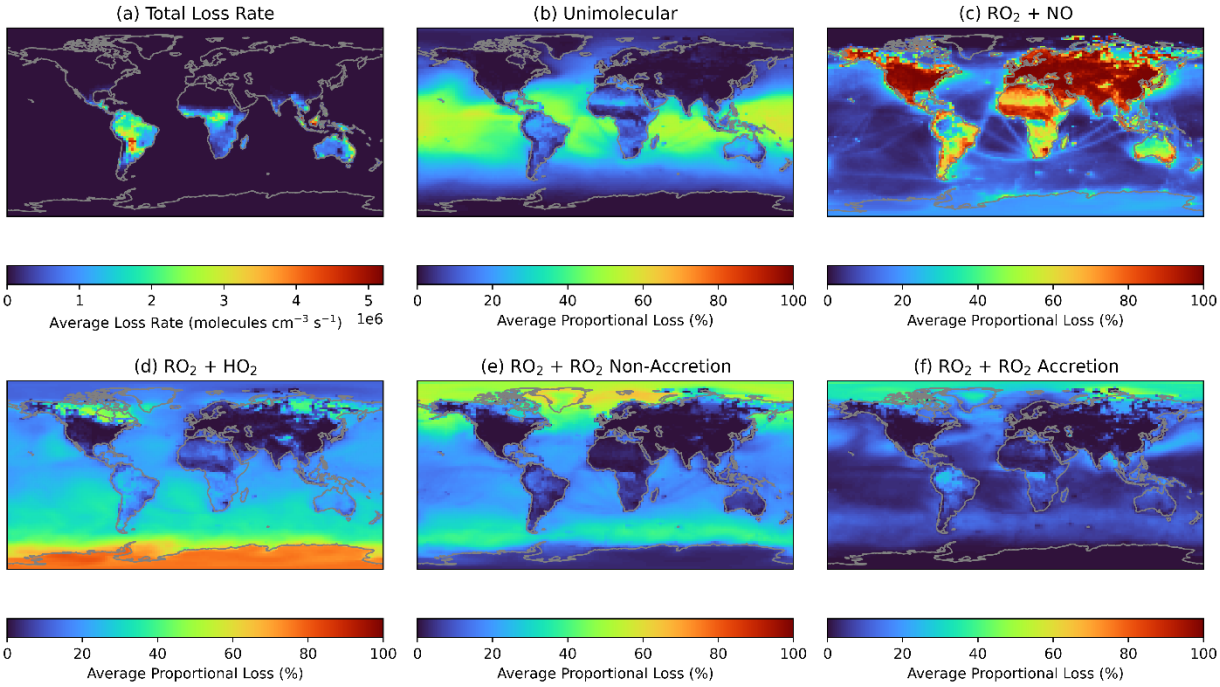

Figure S14. (a) Average total loss rate of the primary isoprene RO_2, IHOO1, during December of the GEOS-Chem simulation. (b-f) Average fractional loss of IHOO1 to each loss pathway, independent of RO_2 concentration.

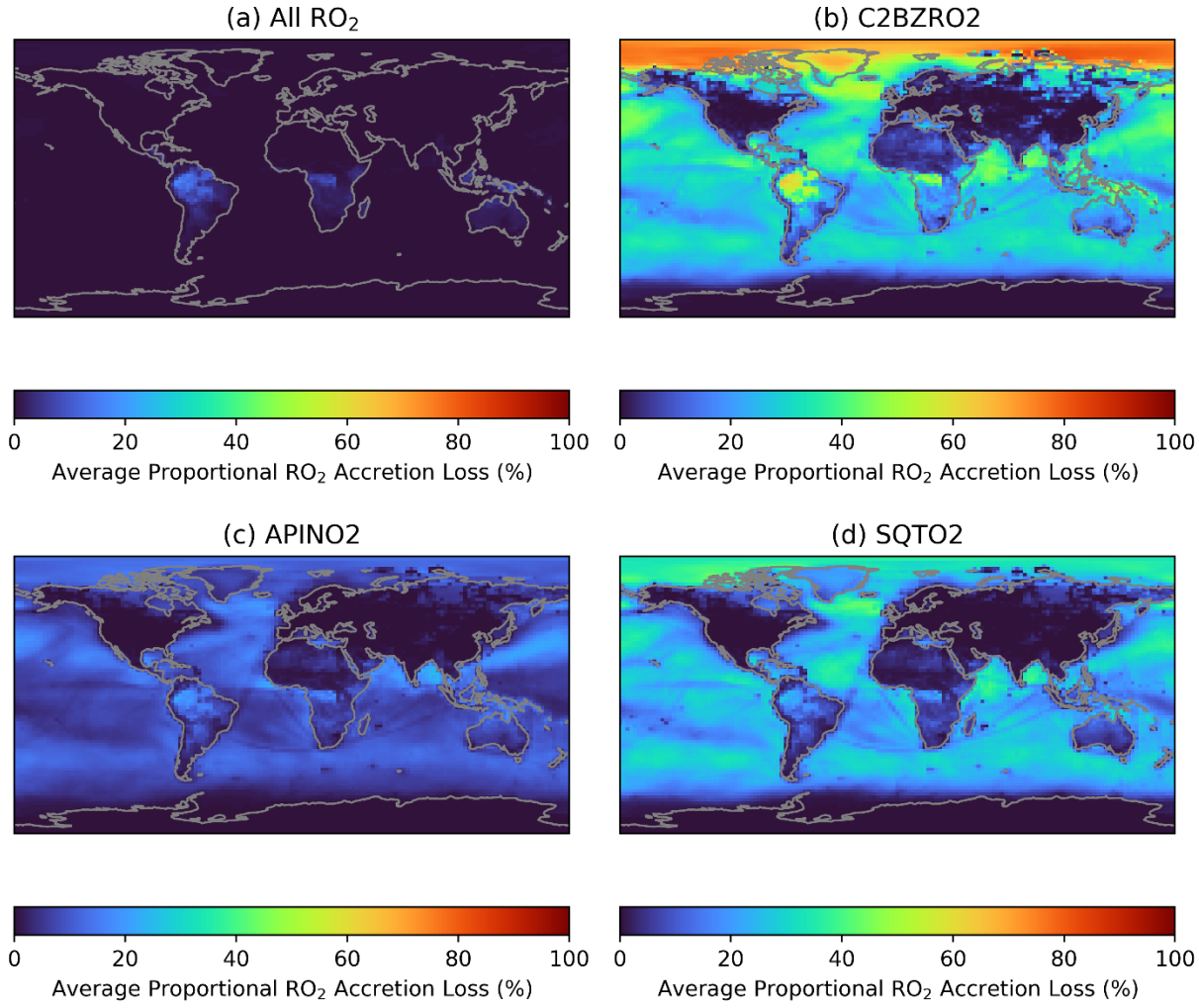

Figure S15. Proportional loss of RO_2 to accretion reactions, independent of RO_2 concentration, during December of the GEOS-Chem simulation. (a) average for all RO_2, (b) primary RO_2 from styrene oxidation (C2BZRO2), (c) primary α-pinene RO_2 (APINO2), (d) primary sesquiterpene RO_2 (SQTO2).

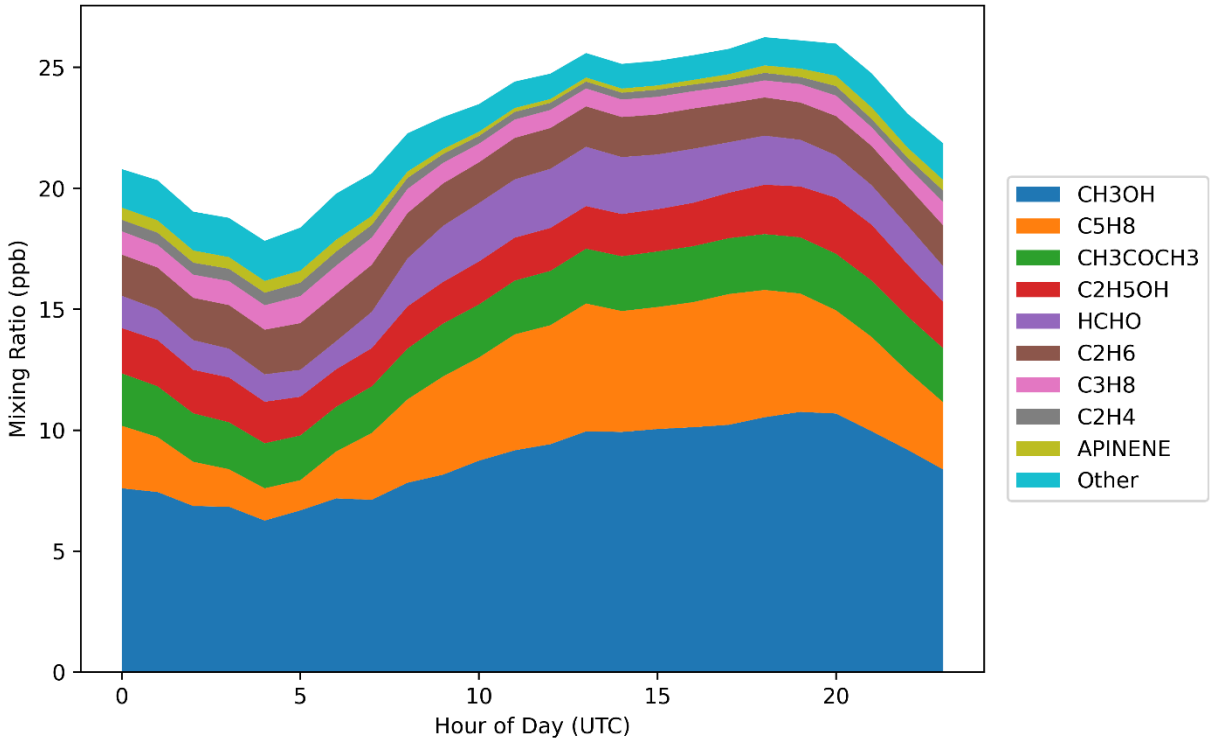

Figure S16. The average diurnal mixing ratios of each constrained VOC (listed in Table S1) in the MCM SOAS box model simulations.