Reactants	Products	Rate	References	Status
ISOP+HO2	0.628 ISHPA+0.272 ISHPB+0.037 ISHPD+0.063 HO+0.063 HO2+0.063 HCHO+0.025 MACR+0.038 MVK	2.06D-13 exp(1300/T)	(Liu et al., 2013; St. Clair et al., 2015)	Modified
ISHPA+HO	0.75 ISOP+0.25 HC5 +0.125 HO+0.125 H2O	6.13D-12exp(200/T)	(St. Clair et al., 2015)	Added
ISHPB+HO	0.480 ISOP+0.520 HC5+0.26 HO+0.26 H2O	4.14D-12exp(200/T)	(St. Clair et al., 2015)	Modified
ISHPD+HO	0.250 ISOP+0.750 HC5+0.375 HO+0.375 H2O	5.11D-12exp(200/T)	(St. Clair et al., 2015)	Added
ISHPA+HO	0.578 IEPOXA+0.272 IEPOXB+0.850 HO+0.150 HC5P	1.7D-11exp(390/T)	(St. Clair et al., 2015)	Added
ISHPB+HO	0.68 IEPOXA+0.32 IEPOXB+1.00 HO	2.97D-11exp(390/T)	(St. Clair et al., 2015)	Modified
ISHPD+HO	0.50 IEPOXD+0.50 HC5P+0.50 HO	2.92D-11exp(390/T)	(St. Clair et al., 2015)	Added
IEPOXA+HO	IEPOXOO	3.73D-11exp(-400/T)	(Bates et al., 2016)	Added
IEPOXB+HO	IEPOXOO	5.79D-11exp(-400/T)	(Bates et al., 2016)	Modified
IEPOXD+HO	IEPOXOO	3.20D-11exp(-400/T)	(Bates et al., 2016)	Added
ISOP+NO	0.4 MVK+0.26 MACR+0.883 NO2+0.0117 ISOPND+0.1053 ISOPNB+0 .66 HCHO+0.143 UHC+0.08 DIBOO+0.803 HO2	2.7D-12exp(360/T)	(Peeters et al., 2014; Teng et al., 2017)	Modified
ISOPNB+O3	0.541 HCHO+0.506 CO+0.526 HO+0.327 NO2+0.179 HAC+0.102 H2O2+0.349 MACRN+0.112 IMONIT+0.128 CO2+0.327 HO2+0.068 ORA1+0.212 MVKN+0.14 8 MGLY	3.7D-19	(Lee et al., 2014)	Modified
ISOPND+O3	0.266 PROPNN+0.017 ORA2+0.249 GLYC+0.075 H2O2+0.89	2.9D-17	(Lee et al., 2014)	Modified

	HO+0.445 HO2+0.214 CO+0.214 HCHO+0.445 NO2+0.271 ETHLN+0.018 IMONIT+0.445 MGLY+0.289 HAC+0.231 GLY			
ISOPNB+HO	0.88 ISOPNBO2+0.12 IEPOXA+0.12 NO2	2.4D-12exp(745/T)	(Jacobs et al., 2014; Lee et al., 2014)	Modified
ISOPND+HO	ISOPNDO2	1.2D-11exp(652/T)	(Lee et al., 2014)	Modified
ISOPNDO2+NO	0.15 PROPNN+0.44 HAC+0.07 MVKN+0.13 ETHLN+0.31 ORA1+0.31 NO3+0.72 HCHO+0.15 GLYC+1.34 NO2+0.35 HO2+0.34 HKET	2.4D-12exp(360/T)	(Lee et al., 2014)	Modified
ISOPNBO2+NO	0.29 GLYC+0.29 HAC+0.71 HCHO+0.71 HO2+0.461 MACRN+0.249 MVKN+1.29 NO2	2.4D-12exp(360/T)	(Lee et al., 2014)	Modified
MVK+HO	MVKP	2.60D-12exp(610/T)	(Praske et al., 2015)	Modified
MVKP+NO	0.716 GLYC+0.716 ACO3+0.249 MGLY+0.249 HCHO+0.249 HO2+0.035 MVKN+0.965 NO2	2.7D-12exp(350/T)	(Praske et al., 2015)	Modified
MVKP+HO2	0.38 VRP+0.37 GLYC+0.37 ACO3+0.62 HO+0.13 KET+0.25 HO2+0.12 MGLY+0.12 HCHO	1.82D-13exp(1300/T)	(Praske et al., 2015)	Modified
ISO+NO3	INO2	3.15D-12exp(-450/T)	MCM v3.3.1	Modified
INO2+NO3	0.54 ICN+0.42 MVK+0.04 MACR+1.46 NO2+0.54 HO2+0.46 HCHO	2.30D-12	(Schwantes et al., 2015)	Added
INO2+INO2	0.39 INO+0.728 ICN+0.10 MACR+0.616 IHND+0.154 IHNB	5.2D-12	(Schwantes et al., 2015)	Added
INO{+O2}	0.88 ICN+0.88 HO2+0.12 NO2+0.12 HCHO+0.12	2.5D-14exp(-300/T)	(Schwantes et al., 2015)	Added

	MACR			
ICN+NO3	NH4CO3+HNO3	6.3D-12exp(-1860/T)	MCM v3.3.1	Added
NH4CO3+NO	PROPNN+CO+HO2+NO2	7.5D-12exp(-690/T)	MCM v3.3.1	Added
NH4CO3+NH4CO3	0.3 R4N+0.7 PROPNN +0.7 HO2+0.7 CO	1.0D-11	MCM v3.3.1	Added
ICN+HO	0.52 R4NO+ CO+0.52 HO2+0.48 R4N+0.48 HO	4.1D-11	MCM v3.3.1 & Schwantes(2015)	Added
IHND+HO	0.92 IDHNO2D+0.08 IEPOXD+0.08 NO2	1.1D-10	(Schwantes et al., 2015)	Added
IHNB+HO	IDHNO2B	4.2D-11	(Schwantes et al., 2015)	Added
IDHNO2D+NO3	HO2+NO2+0.12 HAC+0.12 ETHLN+0.8 GLYC+0.80 PROPNN+0.08 R4N+0.08 HCHO	2.3D-12	(Schwantes et al., 2015)	Added
IDHNO2B+NO3	HO2+NO2+0.76 HAC+0.76 ETHLN+0.23 R4N+0.23 HCHO	2.3D-12	(Schwantes et al., 2015)	Added
INO2+HO2	0.22 MVK+0.015 MACR+0.235 NO2+0.235 HO+0.235 HCHO+0.54 INPD+0.23 INPB	2.06D-13exp(1300/T)	(Schwantes et al., 2015)	Added
INPD+HO	HO2+INO2	6.9D-12	(Schwantes et al., 2015; St. Clair et al., 2015)	Added
INPB+HO	HO2+INO2	6.9D-12	(Schwantes et al., 2015; St. Clair et al., 2015)	Added
INPD+HO	0.37 INHED+0.37 HO+0.63 INPHO2D	1.1D-10	(Lee et al., 2014; Schwantes et al., 2015)	Added
INPB+HO	0.78 INHEB+0.78 HO+0.22 INPHO2B	4.2D-11	(Lee et al., 2014; Schwantes et al., 2015)	Added

INPHO2B+NO3	NO2+HO2+HCHO+R4NO	2.3D-12	(Schwantes et al., 2015)	Added
INPHO2D+NO3	NO2+HO2+0.92 PROPNN+0.92 GLY+0.08 HAC+0.08 ETHLN	2.3D-12	(Schwantes et al., 2015)	Added
INHED+HO	0.27 HAC+0.73 CO+0.27 NO2+0.27 HCHO+0.27 PROPNN+0.27 GLY+0.46 R4N	8.4D-12	(Bates et al., 2016; Schwantes et al., 2015)	Added
INHEB+HO	0.30 PROPNN+0.30 GLY+0.31 GLYC+0.31 MGLY+0.09 HAC+0.43 NO2+0.39 HCHO+0.01 ETHLN+0.01 HAC+0.12 KET+0.26 R4N	1.25D-11	(Bates et al., 2016; Schwantes et al., 2015)	Added
R4N+HO	PROPNN+HO2+CO	1.7D-11	(Schwantes et al., 2015)	Added
R4NO+HO	PROPNN+HO+CO	1.7D-11	(Schwantes et al., 2015)	Added
INPD+hv	INO+HO	j(Pj_ch3o2h)	MCM v3.3.1 Schwantes et al. (2015)	Added
INPB+hv	INO+HO	j(Pj_ch3o2h)	MCM v3.3.1 Schwantes et al. (2015)	Added
ICN+hv	PROPNN+CO+CO+HO2+HO2	10*j(Pj_noa)	(Müller et al., 2014; Schwantes et al., 2015)	Added
R4N+hv	NO2+ACO3+0.5 ETHP+0.5 MO2	j(Pj_ch3coc2h5)	MCM v3.3.1 Schwantes et al. (2015)	Added
R4NO+hv	HO+MGLY+HCHO+NO2	j(Pj_ch3coc2h5)	MCM v3.3.1 Schwantes et al. (2015)	Added
IHND+hv	HO2+NO2+UHC+DIBOO	j(Pj_onit1)	Same as ISOPND	Added
IHNB+hv	HO2+NO2+UHC+DIBOO	j(Pj_onitOH3)	Same as ISOPNB	Added
PROPNN+hv	NO2+ACO3+HCHO	10*j(Pj_noa)	Müller et al. (2014)	Modified

ETHLN+hv	HO2+CO+HCHO+NO2	10*j(Pj_noa)	(Müller et al., 2014)	Modified
MACRN+hv	NO2+CO+HAC+HO2	10*j(Pj_ibutald)	(Müller et al., 2014)	Modified
MVKN+hv	GLYC+NO2+ACO3	10*j(Pj_noa)	(Müller et al., 2014)	Modified
API+NO3	0.10 TOLNN+0.90 TOLND	8.33D-13exp(490/T)	MCM v3.3.1	Modified
UTONIT+NO3	HONIT	3.15D-13exp(-448/T)	(Fisher et al., 2016)	Added
UTONIN+NO3	HONIT	3.15D-13exp(-448/T)	(Fisher et al., 2016)	Added
TONIN+NO3	HONIT	3.15D-13exp(-448/T)	(Fisher et al., 2016)	Added
TONIT+NO3	HONIT	3.15D-13exp(-448/T)	(Fisher et al., 2016)	Added
TONIH+NO3	HONIT	3.15D-13exp(-448/T)	(Fisher et al., 2016)	Added

Table S1: Isoprene and Monoterpene reactions added to/revised from RACM2_Berkeley.

Species	Description	Species	Description
ISHPA	(1,2) hydroxy hydro peroxides	INO2	Isoprene nitrooxy peroxy radical
ISHPB	(4,3) hydroxy hydro peroxides	ICN	C5 carbonyl nitrate
ISHPD	delta (1,4 and 4,1) hydroxy hydro peroxides	INO	C5 nitrooxyalkoxy radical
IEPOXA	trans-β isoprene-derived dihydroxy epoxide	IHND	C5 hydroxy nitrate – β isomer
IEPOXB	cis-β isoprene-derived dihydroxy epoxide	IHNB	C5 hydroxy nitrate – δ isomer
IEPOXD	delta isoprene-derived dihydroxy epoxide	NH4CO3	Radical from ICN
R4N	C4 carbonyl hydroxynitrate	INPB	C5 nitrooxy hydroperoxide – β isome
R4NO	C4 nitrooxycarbonyl hydroperoxide	INPHO2B	C5 nitrooxy hydroperoxy hydroxy peroxy radical (From β isomers)
IDHNO2D	C5 dihydroxy nitrooxyperoxy radical – δ isomer	INPHO2D	C5 nitrooxy hydroperoxy hydroxy peroxy radical (From δ isomers)
IDHNO2B	C5 dihydroxy nitrooxyperoxy radical– β isomer	INHED	C5 nitrooxy hydroxy epoxide – δ isomer
INPD	C5 nitrooxy hydroperoxide – δ isomer	INHEB	C5 nitrooxy hydroxy epoxide – β isomer

Table S2: New chemical species that are introduced in RACM2_Berkeley2 mechanism.

Species	H* (M atm^{-1})	f0
ISOPND, ISOPNB, IMONIT, MACRN, MVKN, INPD, INPB, ICN, R4N, R4NO, IHND, IHNB, TONIT, UTONIT, TONIN, UTONIN, TONIH	2.00E+06	1
PROPNN	5.0E+5	1
ISHPA, ISHPB, ISHPD	1.0E+14	0
IEPOXA, IEPOXB, IEPOXD, INHEB, INHED	8.0E+7	1
GLYC	2.00E+7	1
HAC	1.4E+6	1
H2O2	5.0E+7	1

Table S3: Changes to dry deposition parameters for isoprene chemistry species and organic nitrate species as recommended by Nguyen et al. (2015). H* is the Henry's law coefficient and f0 is the reactivity factor as defined in Wesely (1989).
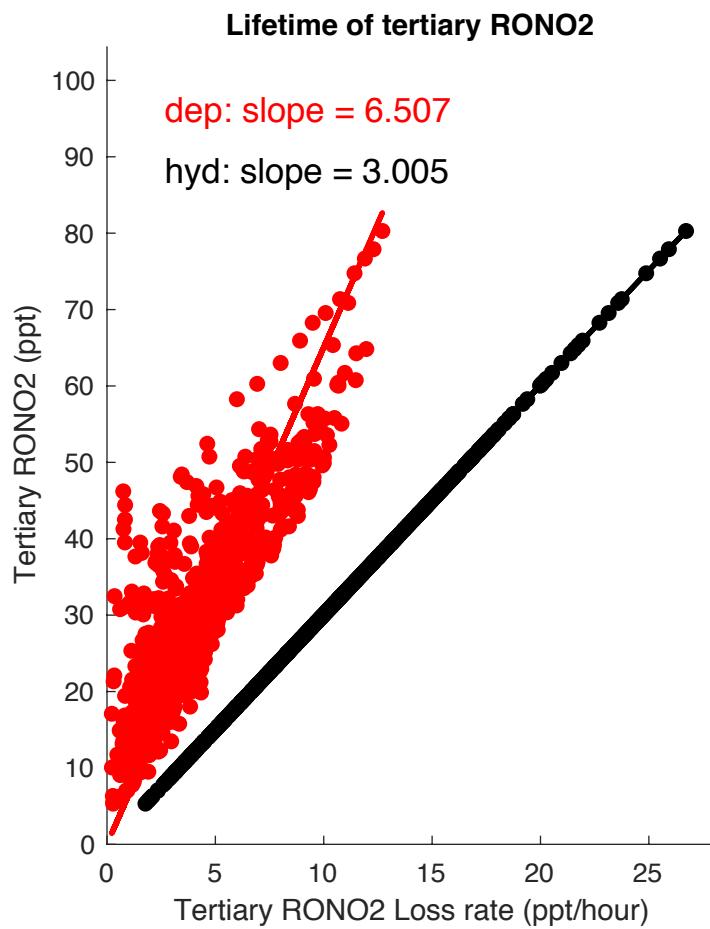
Figure S1: The concentration of tertiary organic nitrates versus their loss rates through deposition and hydrolysis during SOAS. Slopes of the linear fit give the lifetimes against deposition and hydrolysis of tertiary organic nitrates.
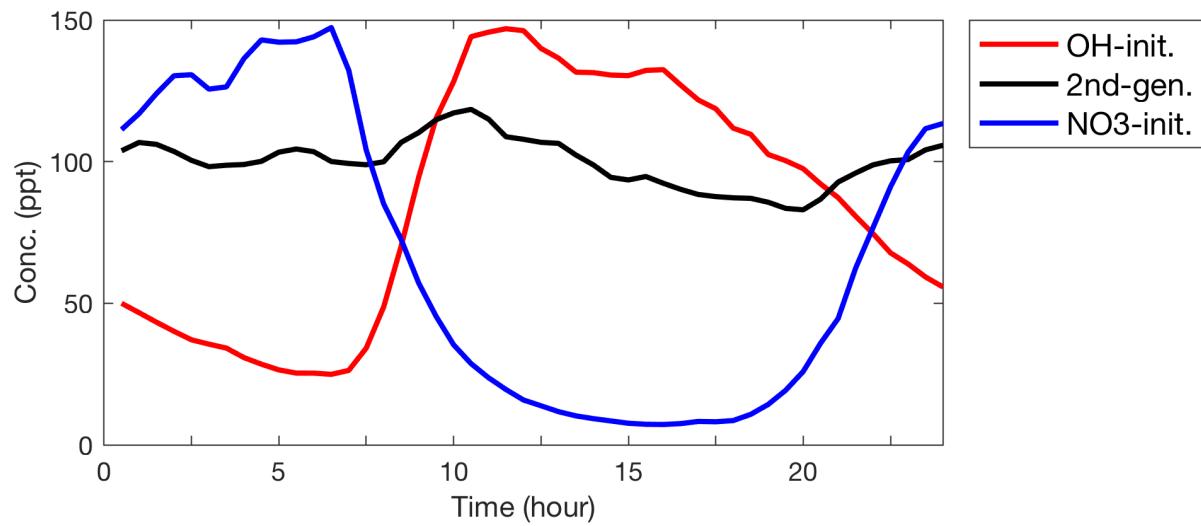
Figure S2: Diurnal cycle of the OH-initiated, NO$_3$-initiated and second-generation organic nitrate concentrations simulated by WRF-Chem using RACM2_Berkeley2 at the CTR site during SOAS.
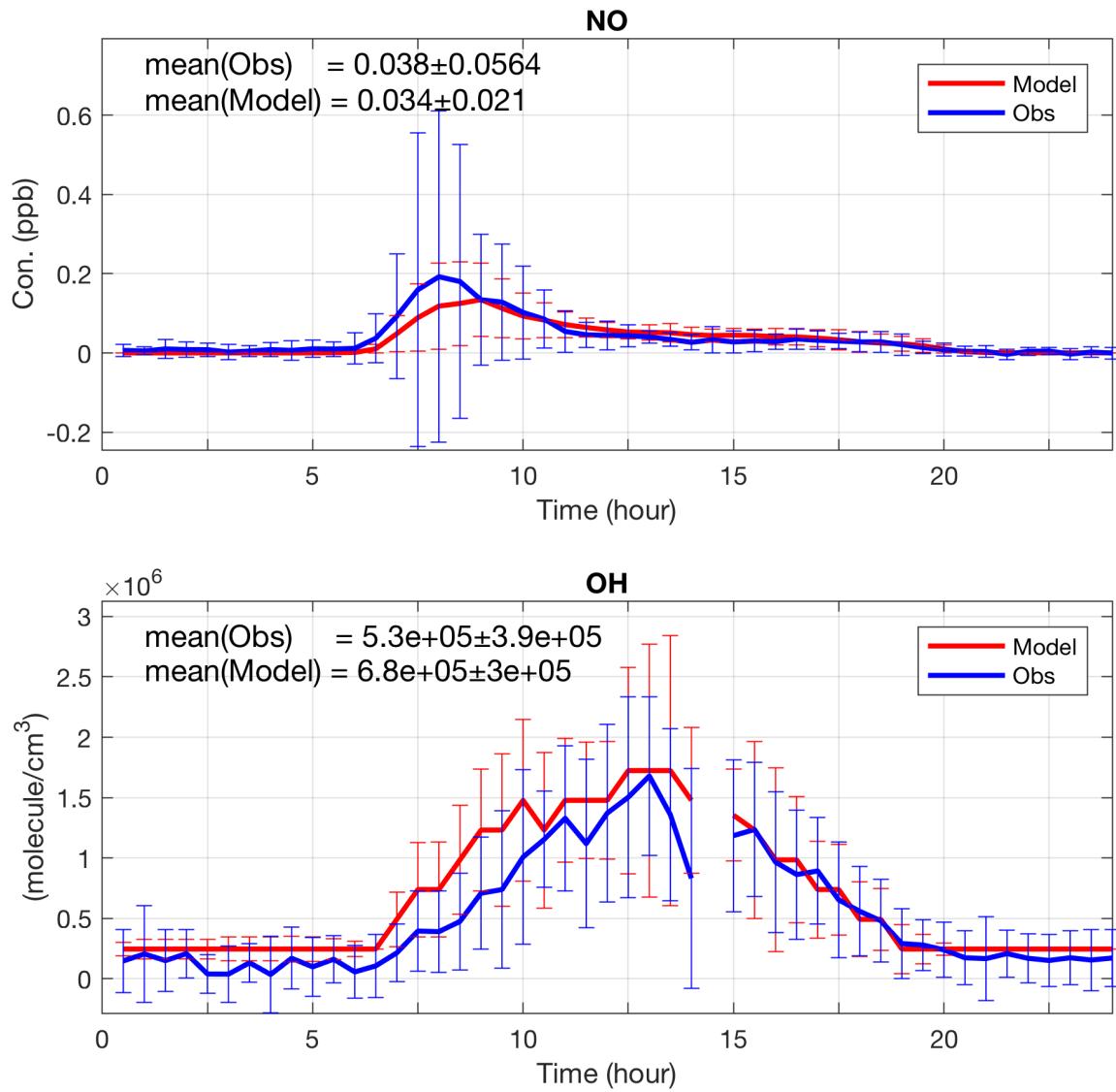
Figure S3: Median diurnal cycles of observed and simulated NO and OH concentrations at Centreville (CTR) during the 2013 SOAS campaign. The vertical bars show the interquartile range of the hourly data. The panel includes mean of the simulated and observed concentrations.
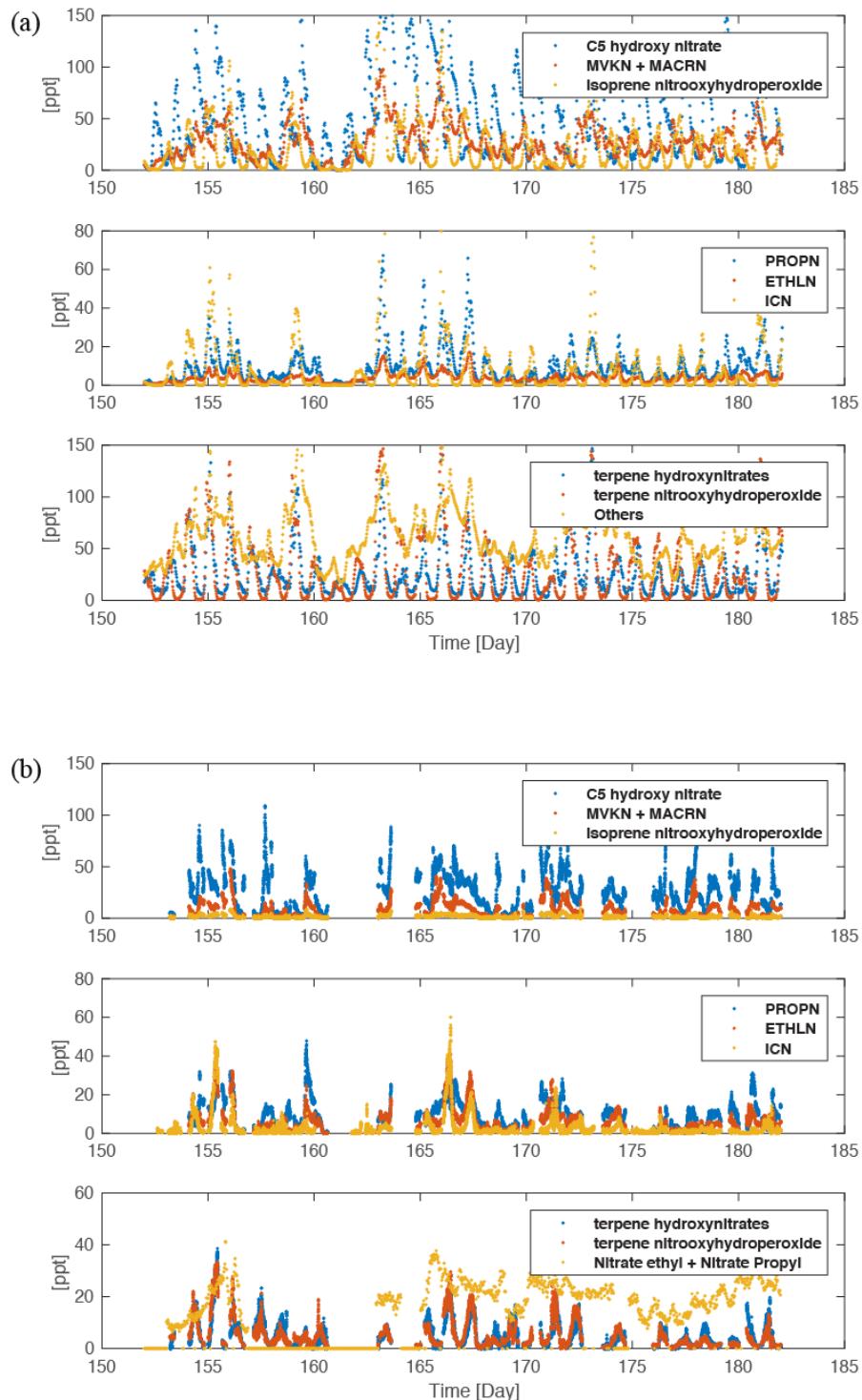
Figure S4: The (a) simulated and (b) observed concentration of C5 hydroxy nitrate, MVKN+MACRN, C5 nitrooxy hydroperoxide [first panel], Propanone nitrate (PROPNN), Ethanal nitrate (ETHLN), C5 carbonyl nitrate (ICN) [second panel], and terpene hydroxynitrates, terpene nitrooxy hydroperoxide, and anthropogenic organic nitrates (Others) [3rd panel] in June 2013 during the SOAS field campaign. At the figure (b) on 3rd panel, observed ethyl Nitrate + propyl Nitrate is shown.
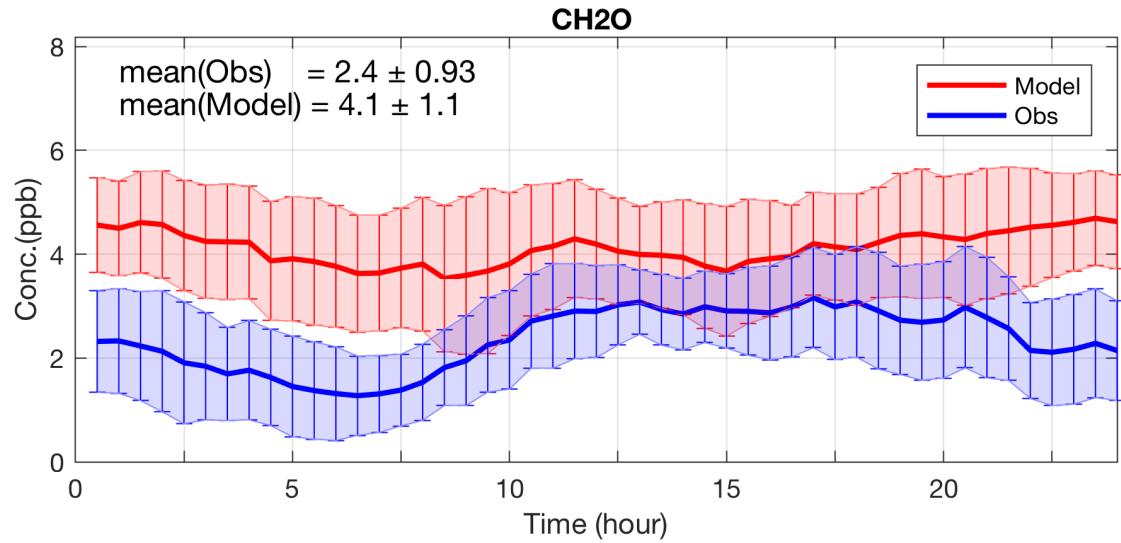
Figure S5: Median diurnal cycles of observed and simulated CH₂O at Centreville during the 2013 SOAS campaign. The vertical bars show the interquartile range of the hourly data. The panel includes mean of the simulated and observed values.
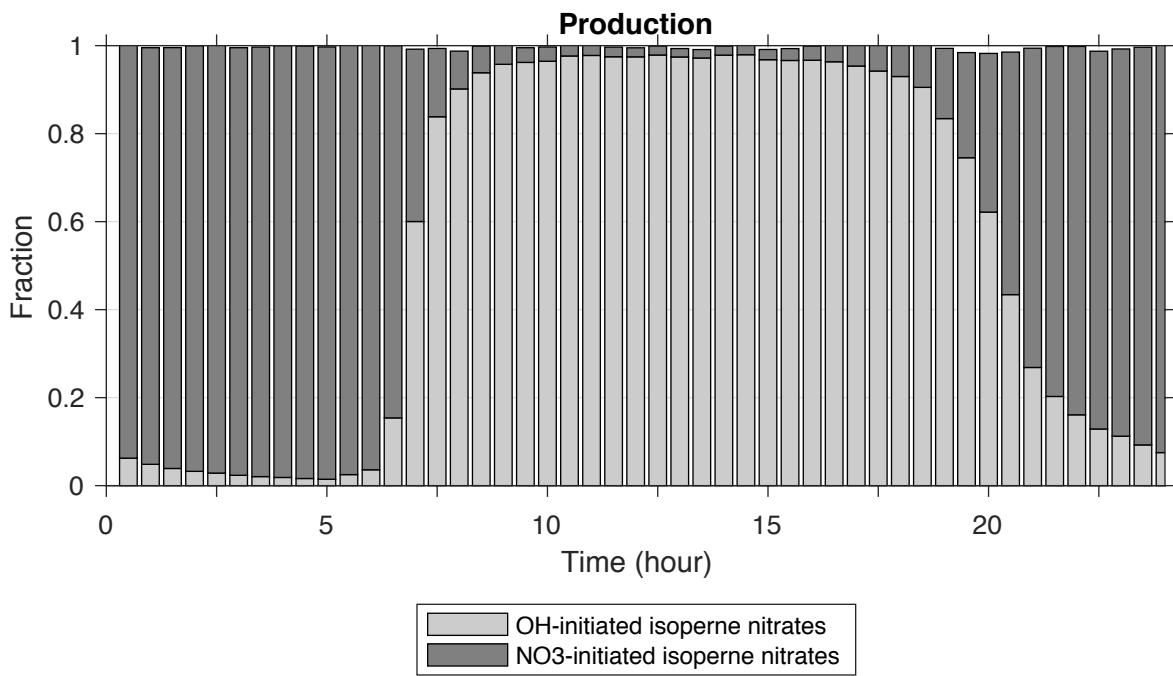
Figure S6: Fraction of isoprene nitrates from OH and NO₃ oxidations to total isoprene nitrate production at boundary layer at the CTR site during SOAS.
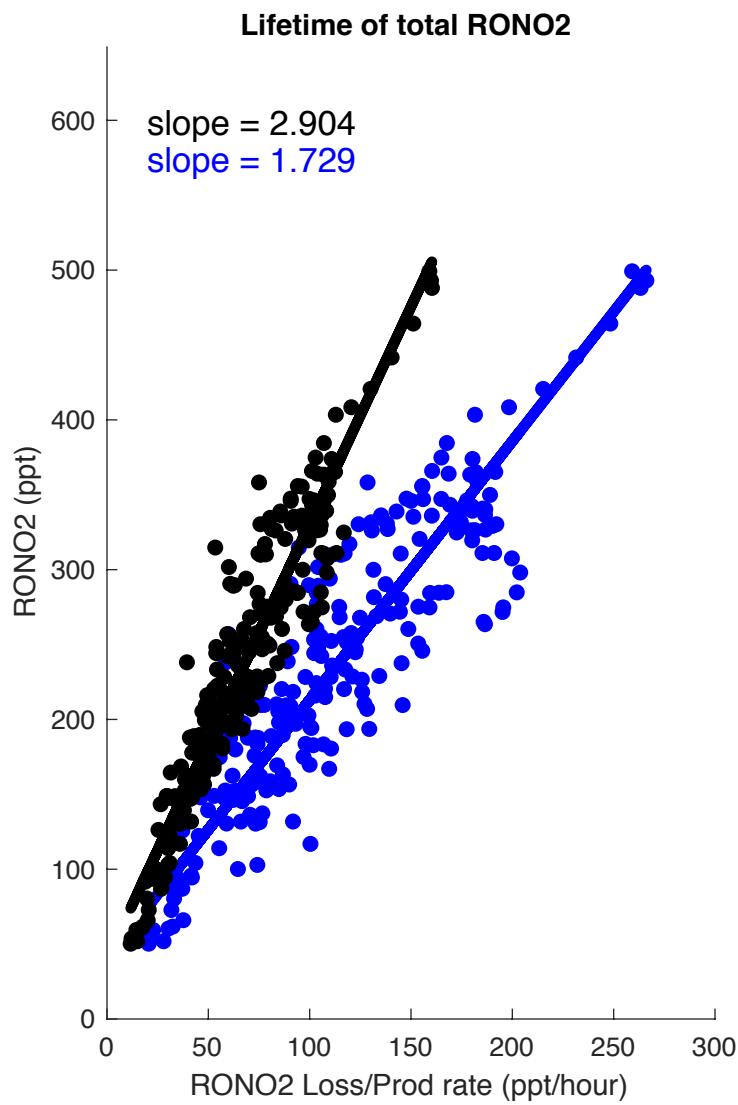
Figure S7: The concentrations of organic nitrates versus their loss rates (black) and production rates (blue) at 12:00-16:00 during SOAS. Slopes of the linear fit give lifetime of organic nitrates.

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