Evolution of NO_3 reactivity during the oxidation of isoprene

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Supplementary Information

Box-Model

Table S1: Reactions, rate coefficients and definitions in the model used for analysis. The isoprene oxidation scheme until the 3^{rd} / 4^{th} generation from the Master Chemical Mechansism (MCM) version 3.3.1 is used (Jenkin et al., 2015). Any change from MCMv3.3.1 is annotated.

Reaction	**Reaction constant**	**Annotations**
NOx chemistry		
N2O5 → NO3 + NO2	((1.3e-3*(T/300)@-3.5*exp(-11000/T))*M*(9.7e14*(T/300)@0.1*exp(-11080/T)))/((1.3e-3*(T/300)@-3.5*exp(-11000/T))*M+(9.7e14*(T/300)@0.1*exp(-11080/T)))*10@(log10(0.35)/(1+(log10((1.3e-3*(T/300)@-3.5*exp(-11000/T))*M/(9.7e14*(T/300)@0.1*exp(-11080/T)))/(0.75-1.27*log10(0.35)))@2))	
NO2 + NO3 → N2O5	((3.6e-30*(T/300)@-4.1)*M*(1.9e-12*(T/300)@0.2))/((3.6e-30*(T/300)@-4.1)*M+(1.9e-12*(T/300)@0.2))*10@(log10(0.35)/(1+(log10((3.6e-30*(T/300)@-4.1)*M/(1.9e-12*(T/300)@0.2))/(0.75-1.27*log10(0.35)))@2))	
NO + O3 → NO2 + O2	1.8E-11*exp(110/T)	
NO2 + O3 → NO3 + O2	1.4E-13 * exp (-2470/T)	
NO + O3 → NO2 + O2	2.07E-12 * exp (-1400/T)	
NO3 + CO →	4E-19	Hjorth et al., 1986
OH + NO2 →HNO3	((3.2e-30*(T/300)@-4.5)*M*(3.0e-11))/((3.2e-30*(T/300)@-4.5)*M+(3.0e-11))*10@(log10(0.41)/(1+(log10((3.2e-30*(T/300)@-4.5)*M/(3.0e-11))/(0.75-1.27*log10(0.41)))@2))	
OH + NO3 →HO2 + NO2	2E-11	
HO2 + NO3 → OH + NO2	4E-12	
OH + NO → HONO	((7.4e-31*(T/300)@-2.4)*M*(3.3e-11*(T/300)@-0.3))/((7.4e-31*(T/300)@-2.4)*M+(3.3e-11*(T/300)@-0.3))*10@(log10(0.81)/(1+(log10((7.4e-31*(T/300)@-2.4)*M/(3.3e-11*(T/300)@-0.3))/(0.75-1.27*log10(0.81)))@2))	
HO2 + NO → OH + NO2	3.45E-12*exp(270/T)	
HO2 + NO2 → HO2NO2	((1.4e-31*(T/300)@-3.1)*M*(4.0e-12))/((1.4e-31*(T/300)@-3.1)*M+(4.0e-12))*10@(log10(0.4)/(1+(log10((1.4e-31*(T/300)@-3.1)*M/(4.0e-12))/(0.75-1.27*log10(0.4)))@2))	
HO2NO2 + OH → NO2	3.2e-13*EXP(690/T)	
HO2NO2 → HO2 + NO2	((4.1e-5*exp(-10650/T))*M*(6.0e15*exp(-11170/T)))/((4.1e-5*exp(-10650/T))*M+(6.0e15*exp(-11170/T)))*10@(log10(0.4)/(1+(log10((4.1e-5*exp(-10650/T))*M/(6.0e15*exp(-11170/T)))/(0.75-1.27*log10(0.4)))@2))	

OH + HONO ➝ NO2	2.5e-12*EXP(260/T)	
OH + HNO3 ➝ NO3	2.40E-14*EXP(460/T) + ((6.50E-34*EXP(1335/T)*M)/ (1+(6.50E-34*EXP(1335/T)*M/2.70E-17*EXP(2199/T))))	
HOx chemistry		
OH + O3 ➝ HO2	1.70E-12*EXP(-940/T)	
HO2 + O3 ➝ OH	2.03E-16*(T/300)@4.57*EXP(693/T)	
OH + HO2 ➝	4.8E-11*EXP(250/T)	
HO2 + HO2 ➝ H2O2	2.20E-13*(1+(1.40E-21*EXP(2200/T)*H2O))*EXP(600/T)	
OH + H2O2 ➝ HO2	2.9E-12*exp(-160/T)	
OH + CO ➝ HO2	1.44E-13*(1+(M/4.2E19))	
Primary oxidation of isoprene		
NO3 + C5H8 ➝ NISOPO2	2.95E-12 * exp (-450/T)	IUPAC, 2019
O3 + C5H8 ➝ CH2OOE + MACR	0.3 * 1.03E-14 * exp (-1995/T)	
O3 + C5H8 ➝ CH2OOE + MVK	0.2 * 1.03E-14 * exp (-1995/T)	
O3 + C5H8 ➝ HCHO + MACROOA	0.3 * 1.03E-14 * exp (-1995/T)	
O3 + C5H8 ➝ HCHO + MVKOOA	0.2 * 1.03E-14 * exp (-1995/T)	
OH + C5H8 ➝ CISOPA	0.288*2.7E-11 * exp (390/T)	
OH + C5H8 ➝ CISOPC	0.238*2.7E-11 * exp (390/T)	
OH + C5H8 ➝ ISOP34O2	0.022*2.7E-11 * exp (390/T)	
OH + C5H8 ➝ ME3BU3ECHO + HO2	0.02*2.7E-11 * exp (390/T)	
OH + C5H8 ➝ PE4E2CO + HO2	0.042*2.7E-11 * exp (390/T)	
OH + C5H8 ➝ TISOPA	0.288*2.7E-11 * exp (390/T)	
OH + C5H8 ➝ TISOPC	0.102*2.7E-11 * exp (390/T)	
Secondary oxidation (1st generation)		
NISOPO2 + HO2 ➝ NISOPOOH	0.706*2.91E-13 * EXP(1300/T)	
NISOPO2 + NO3 ➝ NISOPO + NO2	2.3E-12	
NISOPO2 + RO2 ➝ ISOPCNO3	0.2*1.3E-12	
NISOPO2 + RO2 ➝ NC4CHO	0.2*1.3E-12	
NISOPO2 + RO2 ➝ NISOPO	0.6*1.3E-12	
CH2OOE ➝ CH2OO	0.22*1E6	
CH2OOE ➝ CO	0.51*1E6	
CH2OOE ➝ HO2 + CO + OH	0.27*1E6	
MACR + NO3 ➝ MACO3 + HNO3	3.4E-15	

MACR + O3 ➝ HCHO + MGLYOOB	0.12*1.4E-15*EXP(-2100/T)	
MACR + O3 ➝ MGLYOX + CH2OOG	0.88*1.4E-15*EXP(-2100/T)	
MACR + OH ➝ MACO3	0.45*8.0E-12*EXP(380/T)	
MACR + OH ➝ MACRO2	0.47*8.0E-12*EXP(380/T)	
MACR + OH ➝ MACROHO2	0.08*8.0E-12*EXP(380/T)	
MVK + O3 ➝ MGLOOA + HCHO	0.5*8.5E-16*EXP(-1520/T)	
MVK + O3 ➝ MGLYOX + CH2OOB	0.5*8.5E-16*EXP(-1520/T)	
MVK + OH ➝ HVMKAO2	0.3*2.6E-12*EXP(610/T)	
MVK + OH ➝ HMVKBO2	0.7*2.6E-12*EXP(610/T)	
HCHO + NO3 ➝ HNO3 + CO + HO2	5.5E-16	
HCHO + OH ➝ HO2 + CO	5.4E-12 * exp (135/T)	
MACROOA ➝ C3H6	0.255*1E6	
MACROOA ➝ CH3CO3 + HCHO + HO2	0.255*1E6	
MACROOA ➝ MACROO	0.22*1E6	
MACROOA ➝ OH + CO +CH3CO3 + HCHO	0.27*1E6	
MVKOOA ➝ C3H6	0.255*1E6	
MVKOOA ➝ CH3O2 + HCHO + CO + HO2	0.255*1E6	
MVKOOA ➝ MVKOO	0.22*1E6	
MVKOOA ➝ OH + MVKO2	0.27*1E6	
CISOPA + O2 ➝ CISOPAO2	3.5E-12	
CISOPA + O2 ➝ ISOPBO2	3E-12	
CISOPC + O2 ➝ CISOPCO2	2E-12	
CISOPC + O2 ➝ ISOPDO2	3.5E-12	
ISOP34O2 + HO2 ➝ ISOP34OOH	2.91E-13 * EXP(1300/T)	
ISOP34O2 + NO3 ➝ ISOP34O + NO2	2.3E-12	
ISOP34O2 + RO2 ➝ HC4CHO	0.1*2.65E-12	
ISOP34O2 + RO2 ➝ ISOP34O	0.8*2.65E-12	
ISOP34O2 + RO2 ➝ ISOPDOH	0.1*2.65E-12	
ME3BU3ECHO + NO3 ➝ NC526O2	3.3E-13	

ME3BU3ECHO + O3 ➝ CH2OOC + CO2C3CHO	0.33*1.6E-17	
ME3BU3ECHO + O3 ➝ HCHO + CO2C3OOB	0.67*1.6E-17	
ME3BU3ECHO + OH ➝ C530O2	0.712*7.3E-11	
ME3BU3ECHO + OH ➝ ME3BU3ECO3	0.288*7.3E-11	
PE4E2CO + NO3 ➝ NC51O2	1.2E-14	
PE4E2CO + O3 ➝ CH2OOB + CO2C3CHO	0.43*1E-17	
PE4E2CO + O3 ➝ HCHO + CO2C3OOA	0.57*1E-17	
PE4E2CO + OH ➝ C51O2	2.71E-11	
TISOPA + O2 ➝ ISOPAO2	2.5E-12*exp(-480/T)	
TISOPA + O2 ➝ ISOPBO2	3E-12	
TISOPC + O2 ➝ ISOPCO2	2.5E-12*exp(-480/T)	
TISOPC + O2 ➝ ISOPDO2	3.5E-12	
Secondary oxidation (2^{nd} generation)		
NISOPOOH + OH ➝ NC4CHO + OH	1.03E-10	
NISOPO + O2 ➝ NC4CHO + HO2	2.50E-14*EXP(-300/T)	
ISOPCNO3 + OH ➝ INCO2	1.12E-10	
NC4CHO + NO3 ➝ NC4CO3 + HNO3	4.25*1.4E-12*EXP(-1860/T)	
NC4CHO + OH ➝ C510O2	0.52*4.16E-11	
NC4CHO + OH ➝ NC4CO3	0.48*4.16E-11	
NC4CHO + O3 ➝ NOA + GLYOOC	0.5*2.4E-17	
NC4CHO + O3 ➝ GLYOX + NOAOOA	0.5*2.4E-17	
CH2OO + CO ➝ HCHO	1.2E-15	
CH2OO + NO2 ➝ HCHO + NO3	1E-15	
MACO3 + NO3 ➝ CH3C2H2O2 + NO2	1.74 * 2.3E-12	
MACO3 + HO2 ➝ CH3C2H2O2	0.44 * 5.2E-13*EXP(980/T)	
MACO3 + HO2 ➝	0.66 5.2E-13*EXP(980/T)	
MACO3 + RO2 ➝ CH3C2H2O2	0.7*1E-11	
MACO3 + RO2 ➝	0.3*1E-11	

MGLYOOB ➞ MGLYOO	0.18*1E6	
MGLYOOB ➞ OH + CO + CH3CO3	0.82*1E6	
MGLYOX + NO3 ➞ CH3CO3 + CO + HNO3	2.4*1.4E-12*EXP(-1860/T)	
MGLYOX + OH ➞ CH3CO3 + CO	1.9E-12*exp(575/T)	
CH2OOG ➞ CH2OO	0.37*1E6	
CH2OOG ➞ CO	0.47*1E6	
CH2OOG ➞ HO2 + CO + OH	0.16*1E6	
MACRO2 + HO2 ➞ MACROOH	0.625*2.91E-13 * EXP(1300/T)	
MACRO2 + NO3 ➞ MACRO + NO2	2.3E-12	
MACRO2 + RO2 ➞ ACETOL	9.2E-14	
MACROHO2 + HO2 ➞ (MACROHOOH)	0.625*2.91E-13 * EXP(1300/T)	
MACROHO2 + NO3 ➞ MACROHO + NO2	2.3E-12	
MACROHO2 + RO2 ➞ (div)	1.4E-12	
MGLOOA ➞ CH3CHO	0.2*1E6	
MGLOOA ➞ OH + CO + CH3CO3	0.36*1E6	
MGLOOA ➞ CH3CO3 + HCHO + HO2	0.2*1E6	
MGLOOA ➞ MGLOO	0.24*1E6	
CH2OOB ➞ CH2OO	0.24*1E6	
CH2OOB ➞ CO	0.4*1E6	
CH2OOB ➞ HO2 + CO + OH	0.36*1E6	
HMVKAO2 + HO2 ➞ (HMVKAOOH)	0.625*2.91E-13 * EXP(1300/T)	
HMVKAO2 + NO3 ➞ NO2 + HMVKAO	2.3E-12	
HMVKAO2 + RO2 ➞ (div)	2E-12	
HMVKBO2 + HO2 ➞ (HMVKBOOH)	0.625*2.91E-13 * EXP(1300/T)	
HMVKBO2 + NO3 ➞ NO2 + HMVKBO	2.3E-12	
HMVKBO2 + RO2 ➞ (div)	8.8E-13	
C3H6 + O3 ➞ CH2OOB + CH3CHO	0.5*5.5E-15*EXP(-1880/T)	

C3H6 + O3 ➝ CH3CHOOA + HCHO	0.5*5.5E-15*EXP(-1880/T)	
C3H6 + NO3 ➝ PRONO3AO2	0.35*4.6E-13*EXP(-1155/T)	
C3H6 + NO3 ➝ PRONO3BO2	0.65*4.6E-13*EXP(-1155/T)	
C3H6 + OH ➝ HYPROPO2	0.87* ((8e-27*(T/300)@-3.5)*M*(3.0e-11*(T/300)@-1))/ ((8e-27*(T/300)@-3.5)*M+(3.0e-11*(T/300)@-1))* 10@(log10(0.5)/(1+(log10((8e-27*(T/300)@-3.5)*M/ (3.0e-11*(T/300)@-1))/(0.75-1.27*log10(0.5)))@2))	
C3H6 + OH ➝ IPROPOLO2	0.13* ((8e-27*(T/300)@-3.5)*M*(3.0e-11*(T/300)@-1))/ ((8e-27*(T/300)@-3.5)*M+(3.0e-11*(T/300)@-1))* 10@(log10(0.5)/(1+(log10((8e-27*(T/300)@-3.5)*M/ (3.0e-11*(T/300)@-1))/(0.75-1.27*log10(0.5)))@2))	
CH3CO3 + HO2 ➝ CH3CO2H + O3	5.2E-13*EXP(980/T)	
CH3CO3 + NO3 ➝ NO2 + CH3O2	4E-12	
CH3CO3 + RO2 ➝ CH3CO2H	0.3*1E-11	
CH3CO3 + RO2 ➝ CH3O2	0.7*1E-11	
MACROO + CO ➝ MACR	1.2e-15	
MACROO + NO2 ➝ MACR + NO3	1E-15	
CH3O2 + HO2 ➝	3.8E-13*EXP(780/T)*(1-1/(1+498*EXP(-1160/T)))	
CH3O2 + HO2 ➝ HCHO	3.8E-13*EXP(780/T)*(1/(1+498*EXP(-1160/T)))	
CH3O2 + NO3 ➝ CH3O + NO2	1.2E-12	
CH3O2 + RO2 ➝ CH3OH	0.5* 2*1.03E-13*EXP(365/T)*0.5*(1-7.18*EXP(-885/T))	
CH3O2 + RO2 ➝ HCHO	0.5* 2*1.03E-13*EXP(365/T)*0.5*(1-7.18*EXP(-885/T))	
MVKOO + CO ➝ MVK	1.2E-15	
MVKOO + NO2 ➝ MVK + NO3	1E-15	
MVKO2 + HO2 ➝ (MVKOOH)	0.625*2.91E-13 * EXP(1300/T)	
MVKO2 + NO3 ➝ NO2	2.3E-12	
MVKO2 + RO2 ➝ (div)	2E-12	
CISOPAO2 + HO2 ➝ ISOPAOOH	0.706*2.91E-13 * EXP(1300/T)	
CISOPAO2 + NO3 ➝ CISOPAO + NO2	2.3E-12	
CISOPAO2 ➝ C536O2	0.5*2.20E10*EXP(-8174/T)*EXP(1.00E8/T@3)	
CISOPAO2 ➝ C5HPALD1 + HO2	0.5*2.20E10*EXP(-8174/T)*EXP(1.00E8/T@3)	
CISOPAO2 ➝ CISOPA	5.22E15*EXP(-9838/T)	
CISOPAO2 + RO2➝ CISOPAO	0.8*2.4E-12	

CISOPAO2 + RO2 ➝ HC4ACHO	0.1*2.4E-12	
CISOPAO2 + RO2 ➝ ISOPAOH	0.1*2.4E-12	
ISOPBO2 + HO2 ➝ ISOPBOOH	0.706*2.91E-13 * EXP(1300/T)	
ISOPBO2 + NO3 ➝ ISOPBO + NO2	2.3E-12	
ISOPBO2 + RO2 ➝ ISOPBO	0.8*8E-13	
ISOPBO2 + RO2 ➝ ISOPBOH	0.2*8E-13	
CISOPCO2 + HO2 ➝ ISOPCOOH	0.706*2.91E-13 * EXP(1300/T)	
CISOPCO2 + NO3 ➝ CISOPCO + NO2	2.3E-12	
CISOPCO2 ➝ C537O2	0.5*2.20E10*EXP(-8174/T)*EXP(1.00E8/T@3)	
CISOPCO2 ➝ C5HPALD2 + HO2	0.5*2.20E10*EXP(-8174/T)*EXP(1.00E8/T@3)	
CISOPCO2 ➝ CISOPC	3.06E15*EXP(-10254/T)	
CISOPCO2 + RO2 ➝ CISOPCO	0.8*2E-12	
CISOPCO2 + RO2 ➝ HC4CCHO	0.2*2E-12	
CISOPCO2 + RO2 ➝ ISOPAOH	0.2*2E-12	
ISOPDO2 + HO2 ➝ ISOPDOOH	0.706*2.91E-13 * EXP(1300/T)	
ISOPDO2 + NO3 ➝ ISOPDO + NO2	2.3E-12	
ISOPDO2 + RO2 ➝ ISOPDO	0.8*2.9E-12	
ISOPDO2 + RO2 ➝ HCOC5	0.1*2.9E-12	
ISOPDO2 + RO2 ➝ ISOPDOH	0.1*2.9E-12	
ISOP34OOH + OH ➝ HC4CHO + OH	9.73E-11	
ISOP34O ➝ MACR + HCHO + HO2	1E6	
HC4CHO + OH ➝ C58O2	0.829*1.04E-10	
HC4CHO + OH ➝ HC4CO3	0.171*1.04E-10	
ISOPDOH + OH ➝ HCOC5 + HO2	7.38E-11	
NC526O2 + NO3 ➝ NO2 +	2.3E-12	
NC526O2 + RO2 ➝	9.20E-14	
CH2OOC ➝ CH2OO	0.18*1E6	
CH2OOC ➝ HO2 + CO+ OH	0.82*1E6	
CO2C3CHO + NO3 ➝ HNO3 + CO2C3CO3	4* 1.4E-12*EXP(-1860/T)	

CO2C3CHO + OH ➝ CO2C3CO3	7.15E-11	
CO2C3OOB ➝ C4CO2O2 + OH	0.82*1E6	
CO2C3OOB ➝ CO2C3OO	0.18*1E6	
C530O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C530O2 + NO3 ➝ NO2 +	2.3E-12	
C530O2 + RO2 ➝	9.2E-14	
ME3BU3ECO3 + HO2 ➝ C45O2 + OH + NO2	0.44*1.4E-12*EXP(-1860/T)	
ME3BU3ECO3 + HO2 ➝	0.56*2.91E-13 * EXP(1300/T)	
ME3BU3ECO + NO3 ➝ C45O2 + NO2	1.6*2.3E-12	
ME3BU3ECO3 + RO2 ➝ C45O2	1E-11	
NC510O2 + HO2 ➝	0.625*2.91E-13 * EXP(1300/T)	
NC510O2 + NO3 ➝ NO2 +	2.3E-12	
NC510O2 + RO2 ➝	8.8E-12	
CO2C3OOA ➝ C4CO2O2 + OH	0.36*1E6	
CO2C3OOA ➝ CH2COCH2O2 + HO2	0.2*1E6	
CO2C3OOA ➝ CH2COCH3	0.2*1E6	
CO2C3OOA ➝ CO2C3OO	0.24*1E6	
C51O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C51O2 + NO3 ➝ NO2 +	2.3E-12	
ISOPAO2 + HO2 ➝ ISOPAOOH	0.706*2.91E-13 * EXP(1300/T)	
ISOPAO2 + NO3 ➝ NO2 + ISOPAO	2.3E-12	
ISOPAO2 + RO2 ➝ HC4ACHO	0.1*2.4E-12	
ISOPAO2 + RO2 ➝ ISOPAO	0.8*2.4E-12	
ISOPAO2 + RO2 ➝ ISOPAOH	0.1*2.4E-12	
ISOPCO2 + HO2 ➝ ISOPCOOH	0.706*2.91E-13 * EXP(1300/T)	
ISOPCO2 + NO3 ➝ NO2 + ISOPCO	2.3E-12	
ISOPCO2 + RO2 ➝ HC4CCHO	0.1*2E-12	
ISOPCO2 + RO2 ➝ ISOPAOH	0.1*2E-12	
ISOPCO2 + RO2 ➝ ISOPCO	0.8*2E12	
Secondary oxidation (3^{rd} + generation)		
INCO2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
INCO2 + NO3 ➝ NO2 +	2.3E-12	
INCO2 + RO2 ➝	2.9E-12	

NC4CO3 + HO2 ➞ NOA + CO+ HO2 + OH	0.44*5.2E-13*EXP(980/T)	
NC4CO3 + HO2 ➞	0.66*5.2E-13*EXP(980/T)	
NC4CO3 + NO3 ➞ NOA + CO + HO2 + NO2	1.74*2.3E-12	
NC4CO3 + RO2 ➞	0.3*1E-11	
NC4CO3 + RO2 ➞ NOA + HO2 + CO	0.7*1E-11	
NOA + OH ➞ MGLYOX + NO2	1.3E-13	
C510O2 + HO2 ➞	0.706*2.91E-13 * EXP(1300/T)	
C510O2 + NO3 ➞ NO2	2.3E-12	
C510O2 + RO2 ➞	9.2E-14	
GLYOOC ➞ GLYOO	0.11*1E6	
GLYOOC ➞ OH + HO2 + CO + CO	0.89*1E6	
GLYOO + NO2 ➞ GLYOX + NO3	1E-15	
NOAOOA ➞ NOAOO	0.11*1E6	
NOAOOA ➞ OH + NO2 + MGLYOX	0.89*1E6	
NOAOO + NO2 ➞ NOA + NO3	1E-15	
CH3C2H2O2 ➞ CH3CO3 + HCHO	0.35*1E6	
CH3C2H2O2 ➞ HCHO + CH3O2 + CO	0.65*1E6	
MGLYOO + NO2 ➞ MGLYOX + NO3	1E-15	
MACROOH + OH ➞ ACETOL + CO + OH	3.77E-11	
MACRO ➞ ACETOL + CO+ HO2	1E6	
MACROHO ➞ MGLYOX + HCHO + HO2	1E6	
MGLOO + NO2 ➞ MGLYOX + NO3	1E-15	
HMVKAO ➞ MGLYOX + HCHO + HO2	1E6	
HMVKBO ➞ CH3CO3 + HOCH2CHO	1E6	
CH3CHOOA ➞ CH3CHOO	0.24*1E6	

CH3CHOOA ➝ CH3O2 + CO + OH	0.36*1E6	
CH3CHOOA ➝ CH3O2 + HO2	0.2*1E6	
CH3CHOOA ➝	0.2*1E6	
CH3CHOO+ CO ➝ CH3CHO	1.2E-15	
CH3CHOO + NO2 ➝ CH3CHO + NO3	1E-15	
PRONO3AO2 + HO2 ➝	0.520*2.91E-13 * EXP(1300/T)	
PRONO3AO2 + NO3 ➝ NO2 +	2.3E-12	
PRONO3AO2 + RO2 ➝	0.2*6E-13	
PRONO3BO2 + HO2 ➝	0.520*2.91E-13 * EXP(1300/T)	
PRONO3BO2 + NO3 ➝ NO2 +	2.3E-12	
PRONO3BO2 + RO2 ➝	0.2*4E-14	
HYPROPO2 + HO2 ➝	0.520*2.91E-13 * EXP(1300/T)	
HYPROPO2 + NO3 ➝ NO2 +	2.3E-12	
HYPROPO2 + RO2 ➝	8.8E-13	
IPROPOLO2 + HO2 ➝	0.520*2.91E-13 * EXP(1300/T)	
IPROPOLO2 + NO3 ➝ NO2 +	2.3E-12	
IPROPOLO2 + RO2 ➝	2E-12	
MVKOOH + OH ➝ VGLYOX	2.55E-11	
MVKOOH + OH ➝ MVKO2	1.90E-12*EXP(190/T)	
VGLYOX + NO3 ➝	2.0*1.4E-12*EXP(-1860/T)	
CH3CO2H + OH ➝ CH3O2	8E-13	
ISOPAOOH + OH ➝ HC4ACHO	0.05*1.54E-10	
ISOPAOOH + OH ➝ IEPOXA + OH	0.93*1.54E-10	
ISOPAOOH + OH ➝ ISOPAO2	0.02*1.54E-10	
HC4ACHO + NO3 ➝ HC4ACO3 + HNO3	4.25*1.4E-12*EXP(-1860/T)	
HC4ACHO + O3 ➝ ACETOL + GLYOX	0.5*2.4E-17	
HC4ACHO + O3 ➝ CO +	0.5*2.4E-17	
HC4ACHO + OH ➝ C58O2	0.52*4.52E-11	
HC4ACHO + OH ➝ HC4ACO3	0.49*4.52E-11	
C58O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C58O2 + NO3 ➝ NO2 +	2.3E-12	
C58O2 + RO2 ➝	9.2E-14	
HC4ACO3 + HO2 ➝	5.2E-13*EXP(980/T)	
HC4ACO3 + NO3 ➝ NO2 +	1.74*2.3E-12	
HC4ACO3 + RO2 ➝	1E-11	

HC4ACO3 ➝ HO2 +	2.20E10*EXP(-8174/T)*EXP(1.00E8/T@3)	
CISOPAO ➝ C526O2	0.19*1E6	
CISOPAO ➝ HC4CCHO + HO2	0.63*1E6	
CISOPAO ➝ HO2 + M3F	0.18*1E6	
C526O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C526O2 + NO3 ➝ NO2 +	2.3E-12	
C526O2 + RO2 ➝	9.20E-14	
C526O2 ➝ CO + OH	3.00E7*EXP(-5300/T)	
M3F + NO3 ➝ NO2 +	1.9E-11	
M3F + O3 ➝	2E-17	
M3F + OH ➝ HO2 +	9E-11	
C536O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C536O2 + NO3 ➝ NO2 +	2.3E-12	
C536O2 + RO2 ➝	9.20E-14	
C536O2 ➝ CO + OH	3.00E7*EXP(-5300/T)	
C5HPALD1 + NO3 ➝ OH + HNO3 +	4.25*1.4E-12*EXP(-1860/T)	
C5HPALD1 + O3 ➝ MGLYOOA	0.73*2.4E-17	
C5HPALD1 + O3 ➝ MGLYOX	0.27*2.4E-17	
MGLYOOA ➝ MGLYOO	0.11*1E6	
MGLYOOA ➝ CH3CO3 + OH +CO	0.89*1E6	
C5HPALD1 + OH ➝ OH +	5.2E-11	
ISOPAOH + OH ➝ HC4ACHO+ HO2	0.5*9.3E-11	
ISOPAOH + OH ➝ HC4CCHO + HO2	0.5*9.3E-11	
HC4CCHO + NO3 ➝ HC4CCO3 + HNO3	4.25*1.4E-12*EXP(-1860/T)	
HC4CCHO + O3 ➝	2.4E-17	
HC4CCHO + OH ➝ C57O2	0.52*4.52E-11	
HC4CCHO + OH ➝ HC4CCO3	0.48*4.52E-11	
HC4CCO3 + HO2 ➝	5.2E-13*EXP(980/T)	
HC4CCO3 + NO3 ➝ NO2 +	1.74*2.3E-12	
HC4CCO3 + RO2 ➝	1E-11	
C57O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C57O2 + NO3 ➝ NO2 +	2.3E-12	
C57O2 + RO2 ➝	9.20E-14	
ISOPBOOH + OH ➝ IEPOXB + OH	0.92*5E-11	

ISOPBOOH + OH ➝ ISOPBO2	0.08*5E-11	
IEPOXB + OH ➝ IEB1O2	0.5*9.05E-12	
IEPOXB + OH ➝ IEB2O2	0.5*9.05E-12	
IEB1O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
IEB1O2 + NO3 ➝ NO2 +	2.3E-12	
IEB1O2 + RO2 ➝	9.20E-14	
IEB1O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
IEB1O2 + NO3 ➝ NO2 +	2.3E-12	
IEB1O2 + RO2 ➝	8.8E-13	
ISOPBO ➝ MVK + HCHO + HO2	1E6	
ISOPBOH + OH ➝ ISOPBO	3.85E-11	
ISOPCOOH + OH ➝ HC4CCHO + OH	0.05*1.54E-10	
ISOPCOOH + OH ➝ IEPOXC + OH	0.93*1.54E-10	
ISOPCOOH + OH ➝ ISOPCO2	0.02*1.54E-10	
IEPOXC + OH ➝ IEC1O2	0.719*1.5E-11	
IEPOXC + OH ➝	0.281*1.5E-11	
IEC1O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
IEC1O2 + NO3 ➝ NO2 +	2.3E-12	
IEC1O2 + RO2 ➝	9.2E-14	
CISOPCO ➝ C527O2	0.3*1E6	
CISOPCO ➝ HC4ACHO	0.52*1E6	
CISOPCO ➝ HO2 + M3F	0.18*1E6	
C527O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C527O2 + NO3 ➝ NO2 +	2.3E-12	
C527O2 + RO2 ➝	8.8E-13	
C527O2 ➝ CO + OH	3.00E7*EXP(-5300/T)	
C537O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C537O2 + NO3 ➝ NO2 +	2.3E-12	
C537O2 + RO2 ➝	9.2E-14	
C537O2 ➝ CO + OH	3.00E7*EXP(-5300/T)	
C5HPALD2 + NO3 ➝ OH + HNO3 +	4.25*1.4E-12*EXP(-1860/T)	
C5HPALD2 + O3 ➝ MGLYOOC	0.73*2.4E-17	
C5HPALD2 + O3 ➝ MGLYOX	0.27*2.4E-17	
C5HPALD2 + OH ➝ OH	5.2E-11	
ISOPAOH + OH ➝ HC4ACHO + HO2	0.5*9.3E-11	

ISOPAOH + OH ➝ HC4CCHO + HO2	0.5*9.3E-11	
ISOPDOOH + OH ➝ HCOC5 + OH	0.22*1.15E-10	
ISOPDOOH + OH ➝ IEPOXB + OH	0.75*1.15E-10	
ISOPDOOH + ISOPDO2	0.03*1.15E-10	
OH + HCOC5 ➝ C59O2	3.81E-11	
C59O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C59O2 + NO3 ➝ NO2 +	2.3E-12	
C59O2 + RO2 ➝	9.2E-14	
ISOPDO ➝ MACR + HCHO + HO2	1E6	
ISOPDOH + OH ➝ HCOC5	7.38E-11	
HC4CO3 + HO2 ➝	0.56*2.91E-13 * EXP(1300/T)	
HC4CO3 + HO2 ➝ MACR + HO2 + OH	0.44*2.91E-13 * EXP(1300/T)	
HC4CO3 + NO3 ➝ MACR + HO2 + NO2	1.5*2.3E-12	
HC4CO3 ➝ MACR + HO2	1E-11	
CO2C3CO3 + HO2 ➝ CH3COCH2O2	0.44*2.91E-13 * EXP(1300/T)	
CO2C3CO3 + HO2 ➝	0.56*2.91E-13 * EXP(1300/T)	
CO2C3CO3 + NO3 ➝ CH3COCH2O2 + NO2	1.74*2.3E-12	
CO2C3CO3 ➝ CH3COCH2O2	1E-11	
CH3COCH2O2 + HO2 ➝ OH +	0.15*1.36E-13*EXP(1250/T)	
CH3COCH2O2 + HO2 ➝	0.85*1.36E-13*EXP(1250/T)	
CH3COCH2O2 + NO3 ➝ NO2 +	2.3E-12	
CH3COCH2O2 + RO2 ➝ ACETOL	0.2* 2*(3.5E-13*8E-12)@0.5	
CH3COCH2O2 + RO2 ➝	0.6* 2*(3.5E-13*8E-12)@0.5	
CH3COCH2O2 + RO2 ➝ MGLYOX	0.2* 2*(3.5E-13*8E-12)@0.5	
CO2C3OO + CO ➝	1.2E-15	
CO2C3OO + NO2 ➝ NO3 +	1E-15	
C4CO2O2 + HO2 ➝	0.625*2.91E-13 * EXP(1300/T)	
C4CO2O2 + NO3 ➝ NO2 +	2.3E-12	
C4CO2O2 + RO2 ➝	8.8E-12	
C45O2 + HO2 ➝	0.625*2.91E-13 * EXP(1300/T)	
C45O2 + NO3 ➝ NO2 +	2.3E-12	

C45O2 + RO2 ➝	1.3E-12	
ISOPAO ➝ C524O2	0.25*1E6	
ISOPAO ➝ HC4CHO + HO2	0.75*1E6	
C524O2 + HO2 ➝	0.706*2.91E-13 * EXP(1300/T)	
C5242 + NO3 ➝ NO2 +	2.3E-12	
C5242 + RO2 ➝	2.9E-12	
ISOPCOOH + OH ➝ HC4CCHO + OH	0.05*1.54E-10	
ISOPCOOH + OH ➝ IEPOXC + OH	0.93*1.54E-10	
ISOPCOOH + ISOPCO2	0.02*1.54E-10	
ISOPCO ➝ HC4ACHO + HO2	0.75*1E6	
ISOPCO ➝ HC4CCHO + HO2	0.25*1E6	
β-caryophyllene		Jenkin et al., 2012
BCARY + NO3 ➝ NBCO2	1.9E-11	
NBCO2 + NO3 ➝	2.3E-12	
BCARY + O3 ➝ BCAOO	0.435*1.2E-14	
BCARY + O3 ➝ BCBOO	0.435*1.2E-14	
BCARY + O3 ➝	0.13*1.2E-14	
BCAOO ➝ BCSOZ	8E1	
BCBOO ➝ BCSOZ	1.2E2	
SAPHIR chamber		
Y + OH ➝ HO2	1.44E-13*(1+(M/4.2E19))	OH background reactivity; behaving like CO (Fuchs et al., 2013)
Z + wall ➝	3.86E-6	Wall loss for O_3, H_2O_2, HO, HONO and HNO_3
NO3 + wall ➝	1.6E-3	Wall loss NO_3
N2O5 + wall ➝	3.3E-4	Wall loss N_2O_5
Definitions		
RO2	NISOPO2 + ISOP34O2 + CH3C2H2O2 + MACO3 + MACRO2 + MACROHO2 + CH3CO3 + HMVKAO2 + HMVKBO2 + CH3O2 + MVKO2 + CISOPAO2 + ISOPBO2 + CISOPCO2 + ISOPDO2 + NC526O2 + C530O2 + M3BU3ECO3 + C45O2 + NC51O2 + C51O2 + ISOPAO2 + ISOPCO2 + INCO2 + NC4CO3 + C510O2 + PRONO3AO2 + PRONO3BO2 + HYPROPO2 + IPROPOLO2 + C536O2 + C537O2 + INAO2 + C58O2 + HC4CO3 + CO2C3CO3 + CH3COCH2O2 + C4CO2O2 + C527O2 + C526O2 + HC4ACO3 HC4CCO3 + C57O2 + C59O2 + C524O2	organic peroxides
kNO3_all	C5H8*2.95E-12*exp(450/T) + BCARY*1.9E-11 + C3H6*4.6E-13*exp(-1155/T) + (2.3E-12*(NISOPO2 + ISOPAO2 +	overall NO_3 reactivity

	ISOPBO2 + ISOPCO2 + ISOPDO2 + CH3C2H2O2 + MACO3 + MACRO2 + MACROHO2 + HMVKAO2 + HMVKBO2 + MVKO2 + INCO2 + CISOPAO + CISOPAO2 + (NC4CO3*1.74) + C510O2 + NBCO2 + PRONO3AO2 + PRONO3BO2 + HYPROPO2 + IPROPOLO2 + INAO2 + C524O2 + (HC4ACO3*1.74) + (1.6*HC4CO3) + C58O2 + INB1O2 + (HC4CCO3*2.74) + INDO2 + C57O2 + C59O2 + C51O2 + IEB1O2 + IEB2O2 + IEC1O2 + ISOP34O2 + CISOPCO2 + NC526O2 + C527O2 + C526O2 + C536O2 + C537O2 + C530O2 + C45O2 + 1.6*M3BU3ECO3 + INB2O2 + NC51O2 + 1.74*CO2C3CO3 + CH3COCH2O2 + C4CO2O2)) + (4E-12*CH3CO3) + (1.2E-12*CH3O2) + (HO2*4E-12) + (5.5E-16*HCHO) + (4E-19*CO) + 1.4E-12*EXP(-1860/T)*(NC4CHO*4.25 + HC4ACHO*4.25 + HC4CCHO*4.25 + 2.4*MGLYOX + 4*CO2C3CHO + 4.25*C5HPALD1 + 4.25*C5HPALD2 +2*VGLYOX) + 3.3E-13*ME3BU3ECHO + (M3F*1.9E-11) + (1.2E-14*PE4E2CO)	
kNO3_stable	C5H8*2.95E-12*exp(450/T) + BCARY*1.9E-11 + C3H6*4.6E-13*exp(-1155/T) + (5.5E-16*HCHO) + (4E-19*CO) + 1.4E-12*EXP(-1860/T)*(NC4CHO*4.25 + HC4ACHO*4.25 + HC4CCHO*4.25 + 2.4*MGLYOX + 4*CO2C3CHO + 4.25*C5HPALD1 + 4.25*C5HPALD2 +2*VGLYOX) + 3.3E-13*ME3BU3ECHO + (M3F*1.9E-11) + (1.2E-14*PE4E2CO)	NO_3 reactivity measurable by FT-CRDS
M	P*(3.24E16)*(298/T)	Total molecular concentration using measured pressure P in Torr and temperature T in K

Comparison of k^{OH} and k^{NO_3}

During NO3ISOP, k^{OH} was measured with an instrument based on laser photolysis – laser induced fluorescence (LP-LIF) (Hofzumahaus et al., 2009; Lou et al., 2010; Fuchs et al., 2017a; Fuchs et al., 2017b). Ambient air was passed at a flow rate of 19 L min^{-1} through a flow tube and part of the air was drawn into an OH fluorescence detection cell. OH radicals were produced within a few nanoseconds in the flow tube by pulsed laser-photolysis of O_3 (at 266 nm) with subsequent reaction of O(^{1}D) atoms with water vapour. OH concentration profiles were recorded by LIF, with k^{OH} determined from the exponential decay constant after correction for diffusion / wall loss (1.8 ± 0.15 s^{-1}). The time resolution of the k^{OH} measurements was 90 s with a limit of detection of 0.5 s^{-1}. The resulting accuracy of k^{OH} is (5-10) % ± 0.2 s^{-1} at NO mixing ratios below 20 ppbv.

Each isoprene injection results in an increase in reactivity of both OH and NO_3. Within the first few minutes after an isoprene injection, the contribution of secondary oxidation products to both k^{NO_3} and k^{OH} is negligible. Hence, the increase in the OH- and NO_3 reactivity (Δk^{OH} and Δk^{NO_3}) directly after an isoprene injection scales with the amount of isoprene injected and the corresponding rate coefficient ($k_{NO_3+C_5H_8}$ = 6.5 × 10^{-13} cm^3 molecule^{-1} s^{-1}, $k_{OH+C_5H_8}$= 1 × 10^{-10} cm^3 molecule^{-1} s^{-1} at 298 K (IUPAC, 2019)). For any particular injection, both approaches should lead to similar isoprene concentrations as shown in Eq. S1.

$$[\text{Isoprene}] = \frac{\Delta k^{OH}}{k_{\mathrm{OH+C_5H_8}}} = \frac{\Delta k^{NO_3}}{k_{NO_3+C_5H_8}} \qquad \text{(S1)}$$

Figure S1 plots the isoprene mixing ratios derived from measurements of Δk^{OH} versus those derived from Δk^{NO_3}. For experiments with isoprene mixing ratios below ~5 ppbv a slope of 0.88 ± 0.11 was obtained. During two injections, when high concentrations of isoprene (~11 and ~22 ppbv) were injected in the chamber, the Δk^{OH} measurement returns isoprene mixing ratios that are significantly lower than those derived from Δk^{NO_3} and the mixing ratio expected from the amount of isoprene injected. On these days, a combination of the low laser power and a small number of points to fit the (rapid) exponential decay mean that the OH reactivity must be considered a lower-limit.

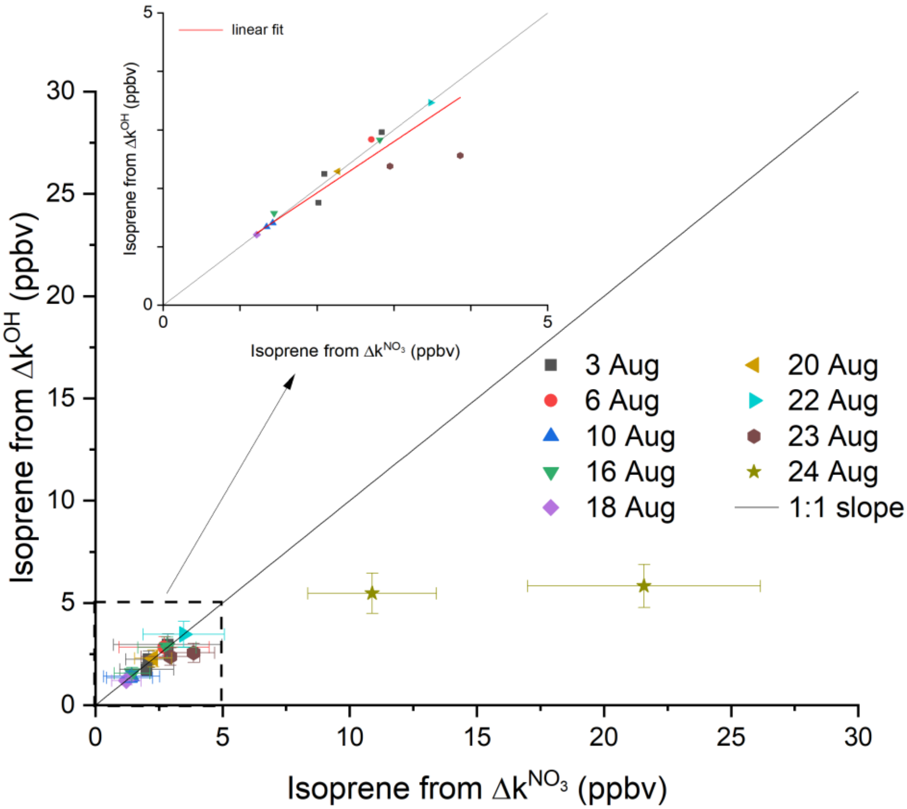


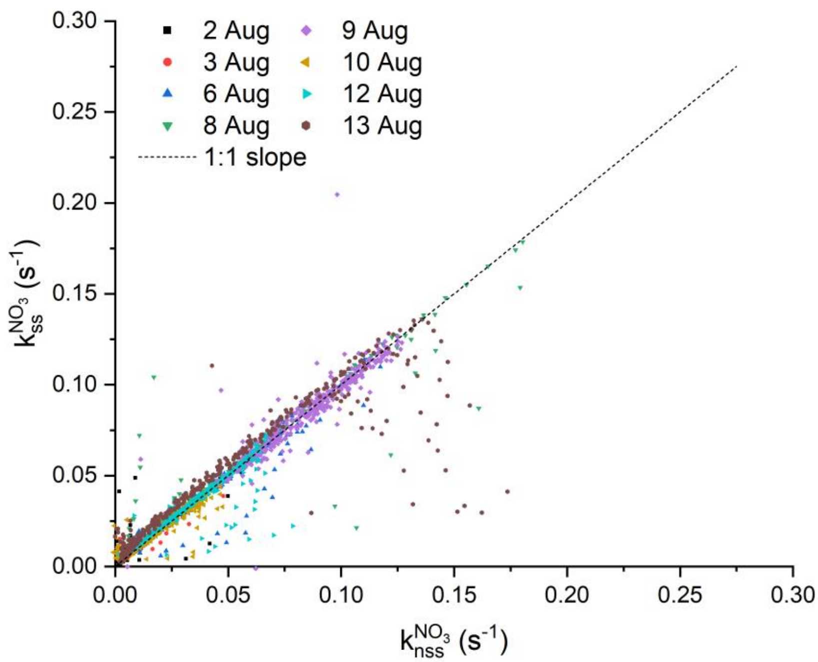
Figure S1: Isoprene mixing ratios deduced from Δk^{OH} against those from Δk^{NO_3} under the usage of Eq. (S1) for isoprene injections of different experiments (days). The error bars denote the associated uncertainties in Δk^{NO_3} (4-70%, Liebmann et al., 2017) and $k_{NO_3+C_5H_8}$ (41% (IUPAC, 2019)) and Δk^{OH} (10%, for [isoprene] < 5 ppbv) and $k_{OH+C_5H_8}$(15% (IUPAC, 2019)). The black line indicates the case of ideal 1:1 correlation, the red line shows an orthogonal linear regression (slope: 0.88 ± 0.11, intercept: 0.17 ± 0.23) for data points < 5 ppbv.

Validity of the steady-state assumption

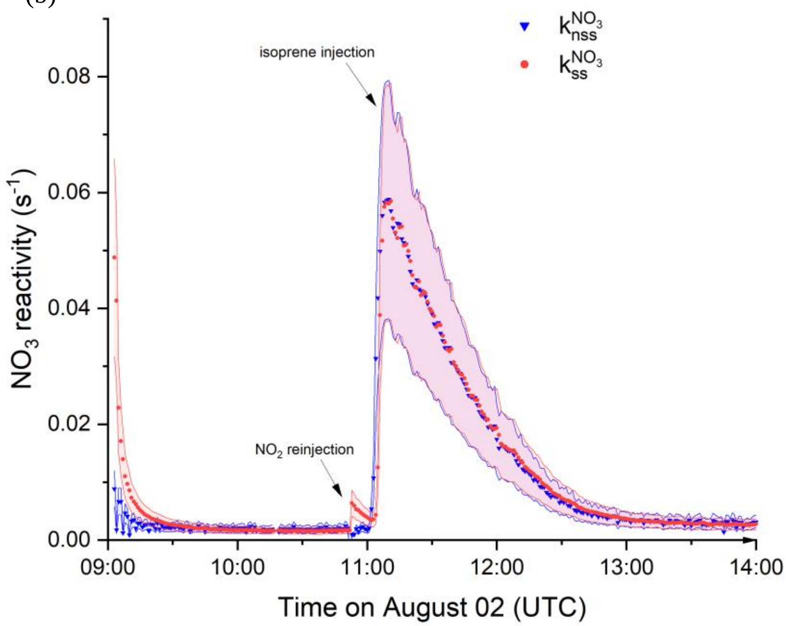
The validity of the steady-state assumption was checked with the help of a correlation plot between the steady-state ($k_{SS}^{NO_3}$) and non-steady-state ($k_{nss}^{NO_3}$) reactivity as depicted in Fig. S2a. A slope close to 1 is found for most of the experiments. At injection points of NO_2 or at low reactivities larger differences are observed which are related to short-term perturbation of the equilibrium between NO_3 and N_2O_5 and deviation from steady-state.

Figure S2b compares $k_{\mathrm{ss}}^{\mathrm{NO3}}$ with $k_{\mathrm{nss}}^{\mathrm{NO3}}$ on the 2nd August. Between 9:00 and 11:00 UTC only NO_2 and O_3 were injected into chamber so that the influence of the chamber alone (reaction with the walls and the dilution flow) determines the NO_3 losses. As the NO_3 loss rate is low under these circumstances, nearly half an hour is necessary to achieve steady-state. This is confirmed by the difference between $k_{\mathrm{nss}}^{\mathrm{NO3}}$ and $k_{\mathrm{ss}}^{\mathrm{NO3}}$. Under the experimental conditions, the equilibrium between NO_3 and N_2O_5 is reached more rapidly than the steady state (Brown et al., 2003). Consequently, $k_{\mathrm{nss}}^{\mathrm{NO3}}$ acquires a constant value earlier than $k_{\mathrm{ss}}^{\mathrm{NO3}}$. A reinjection of NO_2 at ~10:50 perturbs the stationary-state and therefore strongly affects $k_{\mathrm{ss}}^{\mathrm{NO3}}$ whereas $k_{\mathrm{nss}}^{\mathrm{NO3}}$ remains mostly unchanged. After the injection of isoprene the high NO_3-reactivity means that the steady-state assumption becomes valid, which leads to an agreement between the two methods.

(a)



(b)



85 **Figure S2: (a) Steady-state $k_{SS}^{NO_3}$ and non-steady-state $k_{nss}^{NO_3}$ reactivities sorted by experiment. The dotted line through the origin with a slope of 1 represents perfect agreement. (b) Comparison between steady- (red) and non-steady-state (blue) reactivities on the experiment of the 2nd August. The respective uncertainties obtained from error propagation of the uncertainties in k_2 (15%; IUPAC, 2019) and the NO_3 , NO_2 and O_3 mixing ratios (25%, 9% and 5%, respectively) are indicated by areas in the same colour of the data points.**

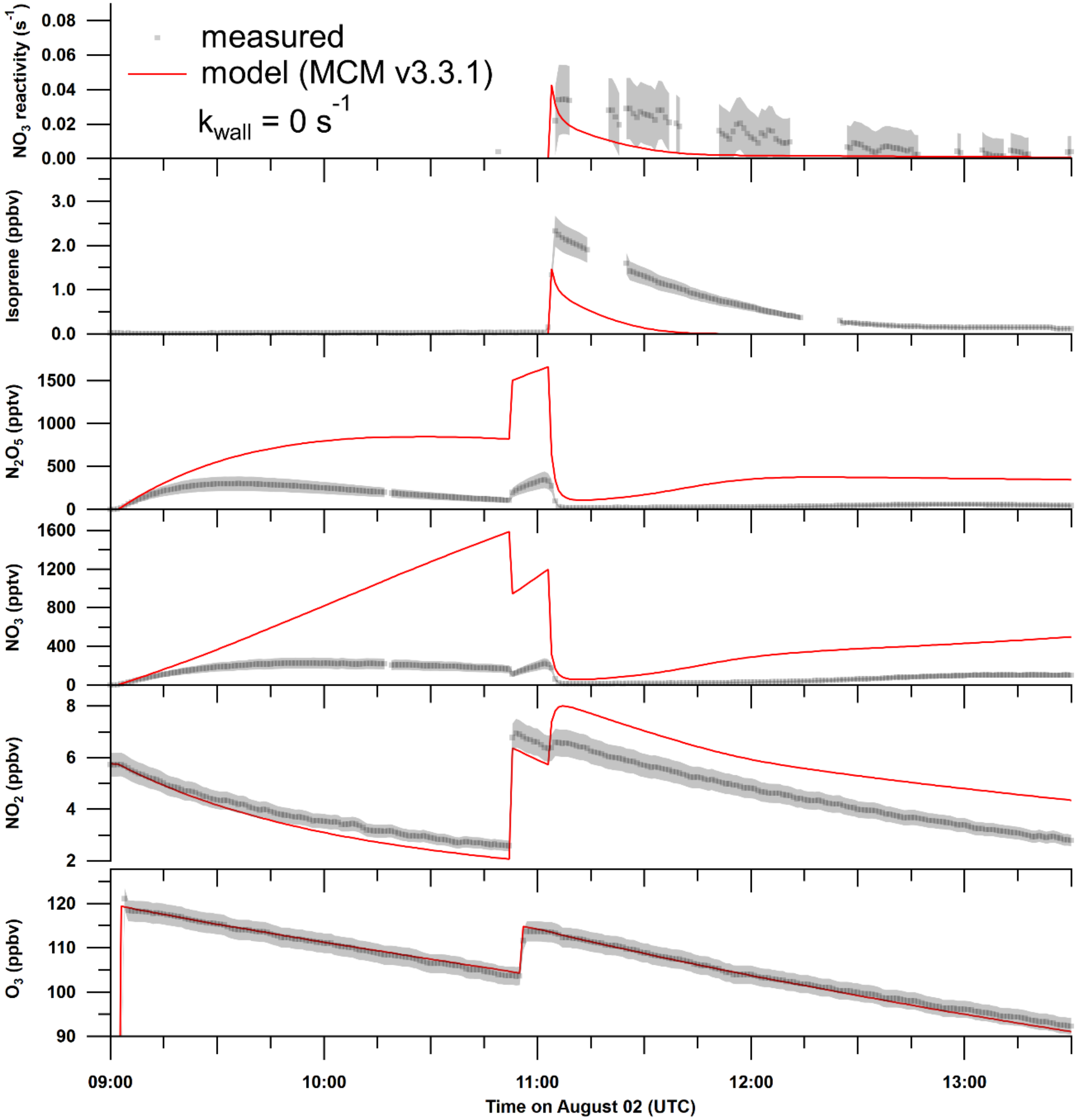


Figure S3: Time-series of the measured O_3, NO_2, NO_3, N_2O_5 and isoprene mixing ratios as well as the NO_3 reactivity on the experiment of the 2nd August (black). The grey shaded area symbolizes the overall uncertainty associated with each measurement. The results of the numerical simulation using MCM v.3.3.1 (with wall loss rates for NO_3 and N_2O_5 set to 0 s^{-1}) for each of the reactants is shown by a red line.

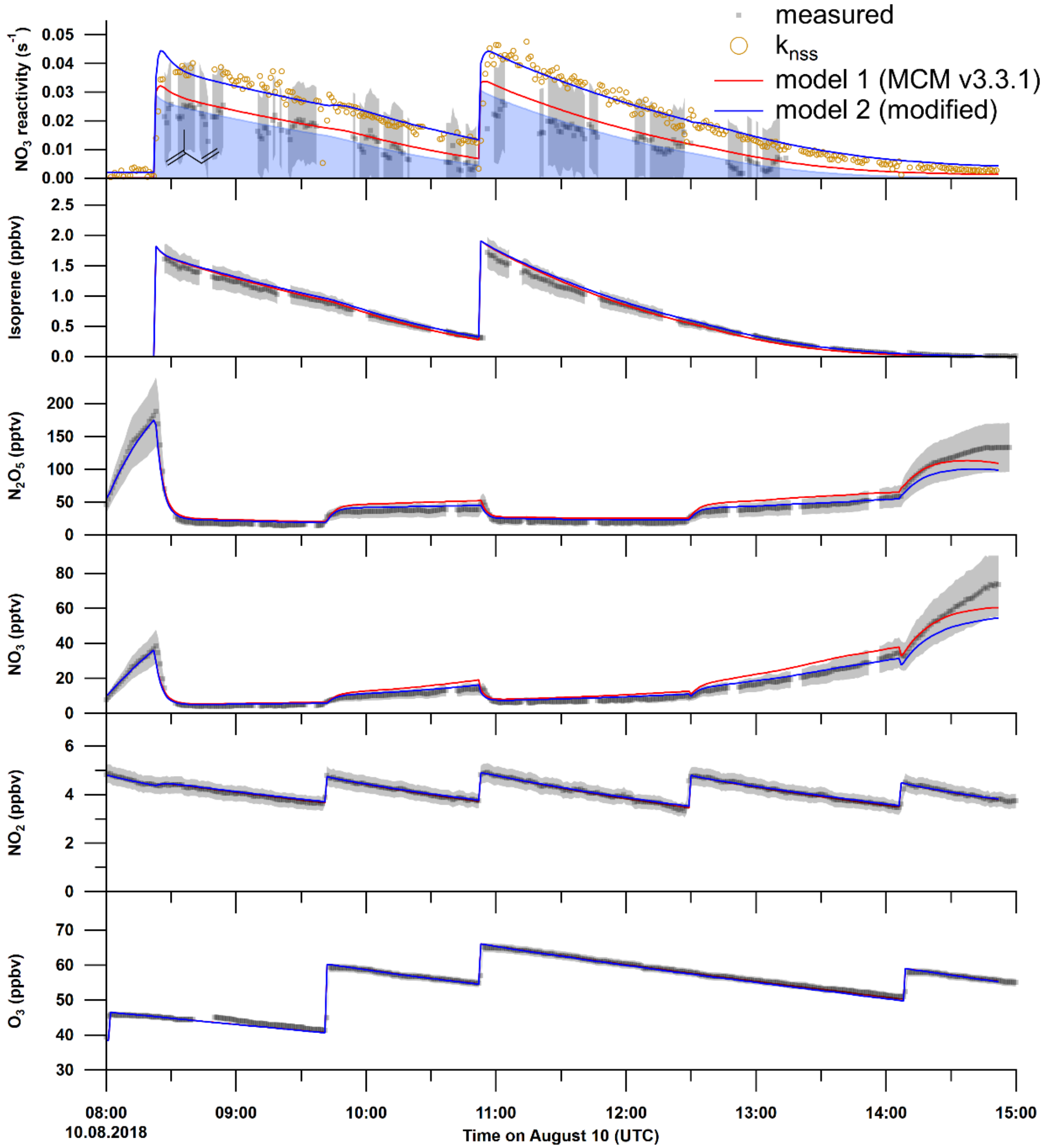


Figure S4: O_3, NO_2, NO_3, N_2O_5 and isoprene mixing ratios as well as the NO_3 reactivity on the experiment of the 10th August (black). The grey shaded area symbolizes the overall uncertainty associated with each measurement. Orange circles denote the non-steady-state reactivity obtained from Eq.(3). The results of the numerical simulation using MCM v.3.3.1 (with NO_3 and N_2O_5 wall loss rate of 0.016 s^{-1} and 3.3 x 10^{-4} s^{-1} respectively) for each of the reactants is shown by a red line, whereas the blue line shows the result of the same model with a doubled reaction constant for NO_3 + RO_2 reactions ($k_{NO_3+RO_2}$= 4.6 x 10^{-12} $cm^3 molecule^{-1} s^{-1}$).

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