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Supplement of

Evolution of NO_3 reactivity during the oxidation of isoprene

Patrick Dewald et al.

Correspondence to: John N. Crowley (john.crowley@mpic.de)

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 (2nd 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 (3rd + 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_2, HONO and HNO_3 (Richter, 2007)
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

Exemplary comparison of isoprene measurements

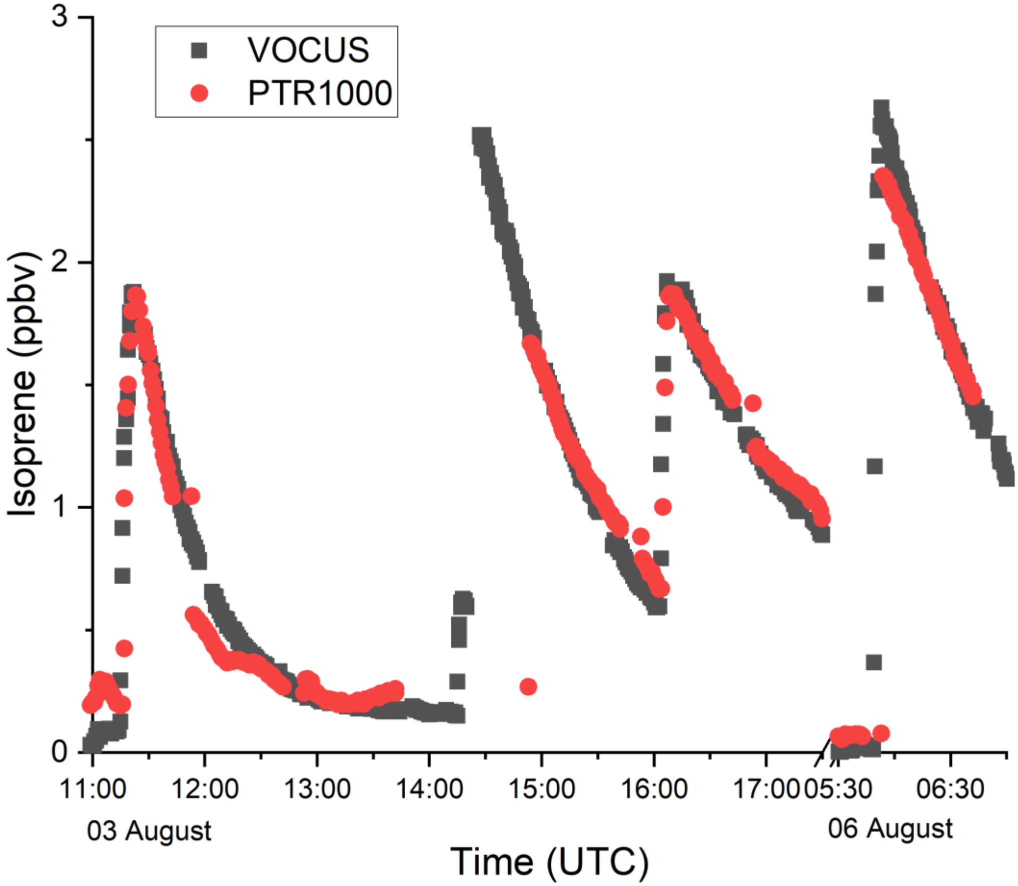

Figure S1: Amounts of isoprene during parts of the experiments on the 3rd and 6th August as measured by the two available PTR-ToF-MS instruments Vocus (black) and PTR1000 (red).

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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 $O(^1D)$ 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.

$$[\text{Isoprene}] = \frac{\Delta k^{OH}}{k_{\text{OH+C}_5\text{H}_8}} = \frac{\Delta k^{NO_3}}{k_{NO_3+C_5H_8}} \quad \text{(S1)}$$

Figure S2 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.

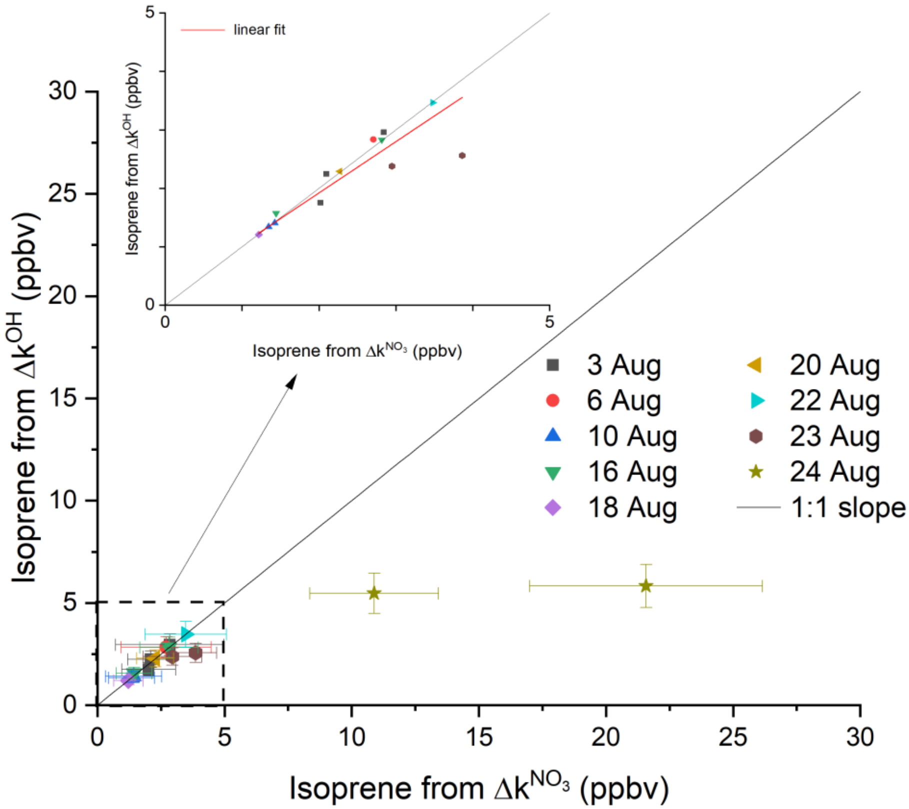


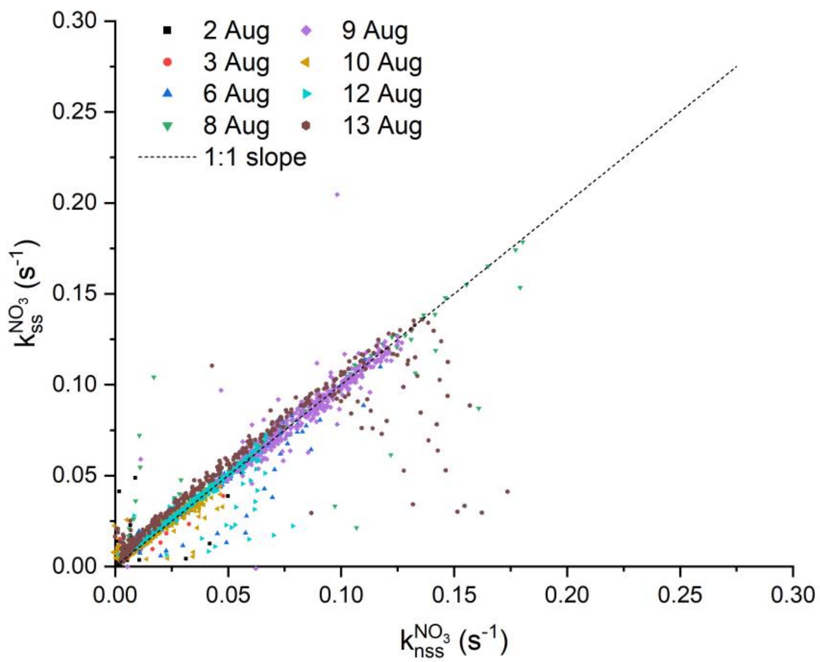
Figure S2: Isoprene mixing ratios deduced from Δk^{OH} against those from Δk^{NO_3} under the usage of Eq. (S1) for isoprene injections of different experiments (days). The error bars denote the associated uncertainties in Δk^{NO_3} (4-70%, Liebmann et al., 2017) and $k_{NO_3+C_5H_8}$ (41% (IUPAC, 2019)) 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. S3a. 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 S3b 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)

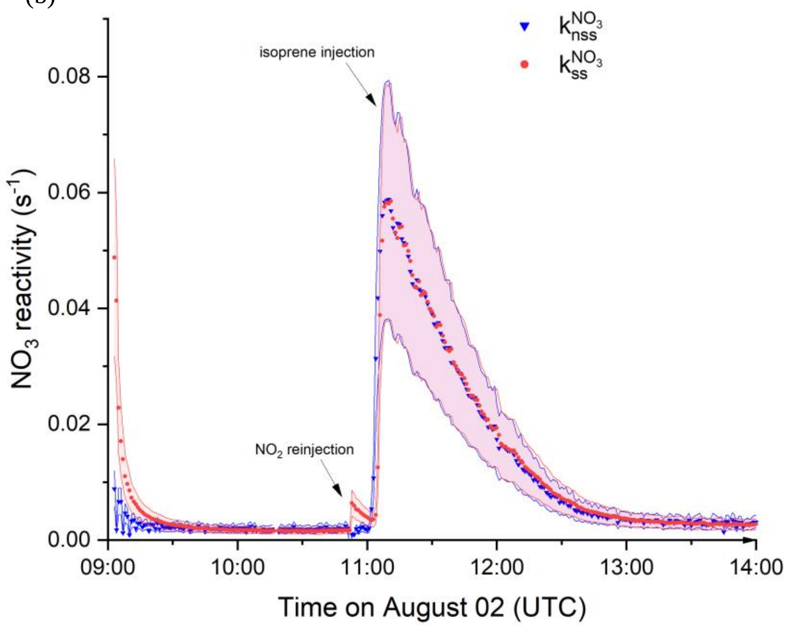


Figure S3: (a) Steady-state $k_{SS}^{NO_3}$ and non-steady-state $k_{nss}^{NO_3}$ reactivities sorted by experiment. The dotted line through the origin with a slope of 1 represents perfect agreement. (b) Comparison between steady- (red) and non-steady-state (blue) reactivities on the experiment of the 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.

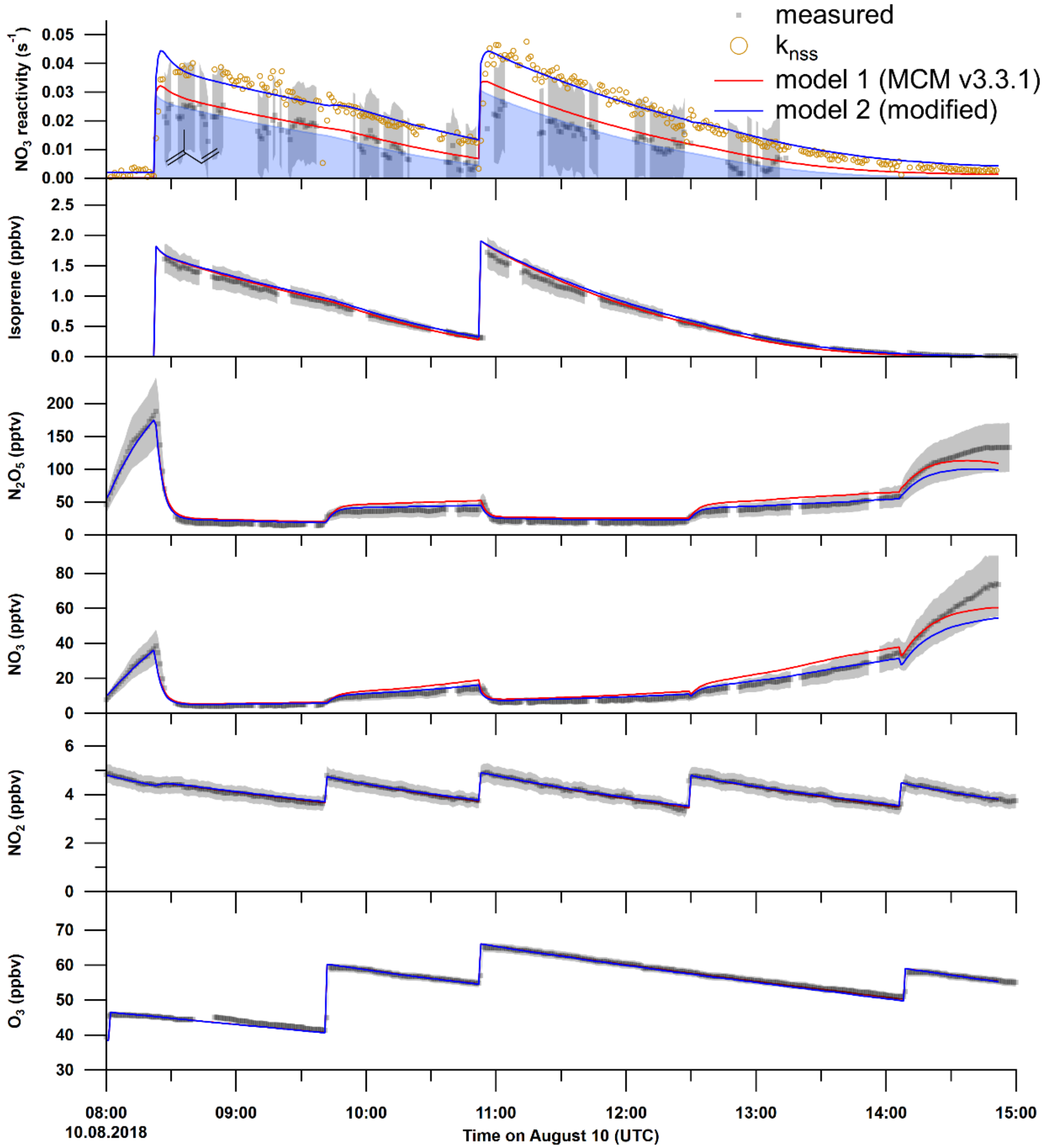


Figure S4: O_3, NO_2, NO_3, N_2O_5 and isoprene mixing ratios as well as the NO_3 reactivity on the experiment of the 10th August (black). The grey shaded area symbolizes the overall uncertainty associated with each measurement. Orange circles denote the non-steady-state reactivity obtained from Eq.(3). 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 (~~$k_{NO_3+RO_2}$= 9.2 x 10^{-12} $cm^3 molecule^{-1} s^{-1}$~~).~~

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