

1 Table S1. New species in the IS scheme (in addition to isoprene nitrates listed in Table1).

Species	Description
DHMOB	dihydroxycarbonyl from HC5
DIBOO	peroxy radical from isoprene+OH
HACET	hydroxyacetone
HC5	C5 hydroxycarbonyl
HC5OO	peroxy radical from HC5
HPALD	hydroperoxymethyl-butenal
IEPOX	dihydroxyepoxide
IEPOXOO	peroxy radical from IEPOX
ISOPNOOB	peroxy radical from ISOPNB
ISOPNOOD	peroxy radical from ISOPND
ISOPO2	peroxy radical from isoprene+OH
ISOPOOH	hydroxyhydroperoxide from ISOPO <sub>2</sub> +HO <sub>2</sub>
MACROO	peroxy radical from MACR
MVKOO	peroxy radical from MVK
NISOPO2	peroxy radical from isoprene+NO <sub>3</sub>
NIT1NO3OOA	acyl peroxy radical from NIT1+NO <sub>3</sub> /OH
NIT1NO3OOB	peroxy radical from NIT1+NO <sub>3</sub>
NIT1OHOO	peroxy radical from NIT1+OH
PYRUACD	pyruvic acid

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1 Table S2. Summary of updates in isoprene oxidation chemistry in the IS scheme to the standard  
 2 SAPRC-07 mechanism (Carter 2010).

Mechanism	Rate Constants	Rate	Products
<b>isoprene with OH</b>			
ISOPRENE + OH = ISOPO2 + ISOPRXN	2.54E-11*exp(410/T)	[1]	[2],[19]
ISOPO2 + NO = 0.40*MVK + 0.26*MACR + 0.883*NO2 + 0.07*ISOPND + 0.047*ISOPNB + 0.66*HCHO + 0.10*HC5 + 0.043*ARO2 + 0.08*DIBOO + 0.803*HO2	2.60E-12*exp(380/T)	[1]	[2]
ISOPO2 + HO2 = 0.880*ISOPOOH + 0.120*OH + 0.047*MACR + 0.073*MVK + 0.120*HO2 + 0.120*HCHO	2.06E-13*exp(1300/T)	[3]	[4]
ISOPO2 + MEO2 = 0.45*HO2 + 0.37*HCHO + 0.23*MVK + 0.15*MACR + 0.05*DIBOO + 0.06*HC5 + 0.02*ARO2 + 0.5*PRD2 + 0.5*HCHO + 0.5*HO2 + 0.25*HCHO + 0.25*MEOH - 0.62*XC	1.80E-12	[3],[5]	[1],[2]
ISOPO2 + RO2C = 0.45*HO2 + 0.37*HCHO + 0.23*MVK + 0.15*MACR + 0.05*DIBOO + 0.06*HC5 + 0.02*ARO2 + 0.5*PRD2 - 0.62*XC	6.80E-13	[3],[5]	[1],[2]
ISOPO2 + ISOPO2 = 0.91*HO2 + 0.75*HCHO + 0.45*MVK + 0.29*MACR + 0.09*DIBOO + 0.11*HC5 + 0.05*ARO2 + PRD2 - 1.24*XC	2.30E-12	[3],[5]	[1],[2]
ISOPO2 + MECO3 = MEO2 + CO2 + 0.91*HO2 + 0.75*HCHO + 0.45*MVK + 0.29*MACR + 0.09*DIBOO + 0.11*HC5 + 0.05*ARO2 - 0.16*XC	4.40E-13*exp(1070/T)	[1]	[1],[2]
ISOPO2 = HO2 + HPALD	4.07E+08*exp(-7694/T)	[6]	[7]
HPALD = OH + HO2 + 0.5*HACET + 0.5*MGLY + 0.25*HOCCHO + 0.25*GLY + HCHO	$J_{HPALD}$	[7]	[7]
HPALD + OH = OH + PRD2 - XC	4.60E-11	[7]	[7],[5]
<b>isoprene with NO<sub>3</sub></b>			
ISOPRENE + NO3 = NISOPO2	3.03E-12*exp(-448/T)	[1]	[8]
NISOPO2 + NO3 = 0.70*NIT1 + 0.035*MVK + 0.035*MACR + 1.3*NO2 + 0.80*HO2 + 0.070*HCHO + 0.23*HC5	2.30E-12	[1]	[8],[5]
NISOPO2 + NO = 0.70*NIT1 + 0.035*MVK + 0.035*MACR + 1.3*NO2 + 0.80*HO2 + 0.070*HCHO + 0.23*HC5	2.60E-12*exp(380/T)	[1]	[8],[5]
NISOPO2 + HO2 = NISOPOOH	2.06E-13*exp(1300/T)	[3]	[12]
NISOPO2 + MEO2 = 0.35*NIT1 + 0.0175*MVK + 0.0175*MACR + 0.15*NO2 + 0.40*HO2 + 0.035*HCHO + 0.115*HC5 + 0.25*NIT1 + 0.25*ISOPND + 0.5*HCHO + 0.5*HO2 + 0.25*HCHO + 0.25*MEOH	1.30E-12	[18]	[1],[8],[5]
NISOPO2 + RO2C = 0.35*NIT1 + 0.0175*MVK + 0.0175*MACR + 0.15*NO2 + 0.40*HO2 + 0.035*HCHO + 0.115*HC5 + 0.25*NIT1 + 0.25*ISOPND	6.04E-13	[18],[5]	[1],[8],[5]
NISOPO2 + NISOPO2 = 0.70*NIT1 + 0.035*MVK + 0.035*MACR + 0.3*NO2 + 0.80*HO2 + 0.070*HCHO + 0.23*HC5 + 0.5*NIT1 + 0.5*ISOPND	1.20E-12	[18]	[1],[8],[5]
NISOPO2 + MECO3 = MEO2 + CO2 + 0.70*NIT1 + 0.035*MVK + 0.035*MACR + 0.3*NO2 + 0.80*HO2 + 0.070*HCHO + 0.23*HC5	4.40E-13*exp(1070/T)	[1]	[1],[8],[5]
<b>isoprene nitrates with OH, O<sub>3</sub>, and NO<sub>3</sub></b>			
ISOPND + OH = ISOPNOOD	2.40E-11*exp(410/T)	[2],[5]	[2]
ISOPNOOD + NO = 0.34*PRD2 + 0.15*PROPNN + 0.44*HACET + 0.07*MVKN + 0.13*ETHLN + 0.31*HCOOH + 0.31*NO3 + 0.72*HCHO + 0.15*HOCCHO + 1.34*NO2 + 0.35*HO2 - 0.68*XC	2.60E-12*exp(380/T)	[1]	[2]
ISOPNOOD + HO2 = RNO3I - XC	2.06E-13*exp(1300/T)	[3]	[5]
ISOPNOOD + MEO2 = 0.17*PRD2 + 0.075*PROPNN + 0.22*HACET + 0.035*MVKN + 0.065*ETHLN + 0.155*HCOOH + 0.155*NO3 + 0.36*HCHO + 0.075*HOCCHO + 0.17*NO2 + 0.175*HO2 +	2.00E-13	[1]	[1],[2]

0.5*RNO3I + 0.25*HCHO + 0.25*MEOH + 0.5*HO2 + 0.5*HCHO - 0.84*XC			
ISOPNOOD + RO2C = 0.17*PRD2 + 0.075*PROPNN + 0.22*HACET + 0.035*MVKN + 0.065*ETHLN + 0.155*HCOOH + 0.155*NO3 + 0.36*HCHO + 0.075*HOCCHO + 0.17*NO2 + 0.175*HO2 + 0.5*RNO3I - 0.84*XC	3.50E-14	[1]	[1],[2]
ISOPNOOD + MECO3 = MEO2 + CO2 + 0.34*PRD2 + 0.15*PROPNN + 0.44*HACET + 0.07*MVKN + 0.13*ETHLN + 0.31*HCOOH + 0.31*NO3 + 0.72*HCHO + 0.15*HOCCHO + 0.34*NO2 + 0.35*HO2 - 0.68*XC	4.40E-13*exp(1070/T)	[1]	[1],[2]
ISOPND + O3 = 0.36*ETHLN + 0.29*PROPNN + 0.70*MGLY + 0.12*RCOOH + 0.39*HO2 + 0.038*HCHO + 0.029*CO + 0.73*OH + 0.017*CO2 + 0.36*NO2 + 0.16*HACET + 0.34*HOCCHO - 0.26*XC	8.70E-15*exp(-1520/T)	[10],[5]	[1],[5],[11]
ISOPNB + OH = ISOPNOOB	3.28E-12*exp(410/T)	[2],[5]	[2]
ISOPNOOB + NO = 0.6*HOCCHO + 0.6*HACET + 0.4*HCHO + 0.4*HO2 + 0.26*MACRN + 0.14*MVKN + 1.6*NO2	2.60E-12*exp(380/T)	[1]	[2]
ISOPNOOB + HO2 = RNO3I - XC	2.06E-13*exp(1300/T)	[3]	[5]
ISOPNOOB + MEO2 = 0.3*HOCCHO + 0.3*HACET + 0.2*HCHO + 0.2*HO2 + 0.13*MACRN + 0.07*MVKN + 0.3*NO2 + 0.5*RNO3I + 0.25*HCHO + 0.25*MEOH + 0.5*HO2 + 0.5*HCHO - 0.5*XC	2.00E-13	[1]	[1],[2]
ISOPNOOB + RO2C = 0.3*HOCCHO + 0.3*HACET + 0.2*HCHO + 0.2*HO2 + 0.13*MACRN + 0.07*MVKN + 0.3*NO2 + 0.5*RNO3I - 0.5*XC	3.50E-14	[1]	[1],[2]
ISOPNOOB + MECO3 = MEO2 + CO2 + 0.6*HOCCHO + 0.6*HACET + 0.4*HCHO + 0.4*HO2 + 0.26*MACRN + 0.14*MVKN + 0.6*NO2	4.40E-13*exp(1070/T)	[1]	[1],[2]
ISOPNB + O3 = 0.12*MVKN + 0.32*MACRN + 0.34*OH + 0.08*HO2 + 0.26*CO + 0.07*CO2 + 0.16*HCOOH + 0.56*HCHO + 0.28*RNO3I + 0.04*HACET + 0.28*NO2 + 0.24*BACL - 0.57*XC	2.13E-14*exp(-1520/T)	[10],[5]	[1],[5],[11]
NIT1 + NO3 = 0.6*NIT1NO3OOA + 0.6*HNO3 + 0.4*NIT1NO3OOB	3.15E-13*exp(-448/T)	[8],[5]	[8],[5]
NIT1NO3OOA + NO3 = NO2 + PROPNNB + CO + CO2 + HO2	4.00E-12	[9]	[9]
NIT1NO3OOA + NO = NO2 + PROPNNB + CO + CO2 + HO2	6.70E-12*exp(340/T)	[1]	[9]
NIT1NO3OOA + NO2 = MAPAN + XN + XC	1.21e-11*(T/300) <sup>-1.07</sup>	[1]	[1]
NIT1NO3OOA + HO2 = 0.75*RCOOH + 0.25*RCOOH + 0.25*O3 + XN + 2*XC	5.20E-13*exp(980/T)	[1]	[1]
NIT1NO3OOA + RO2C = PROPNNB + CO + CO2 + HO2	4.40E-13*exp(1070/T)	[1]	[1],[9]
NIT1NO3OOA + MEO2 = PROPNNB + CO + CO2 + HO2 + HCHO + HO2	2.00E-12*exp(500/T)	[1]	[1],[9]
NIT1NO3OOA + MECO3 = MEO2 + CO2 + PROPNNB + CO + CO2 + HO2	2.90E-12*exp(500/T)	[1]	[1],[9]
NIT1NO3OOB + NO3 = PROPNNB + GLY + NO2 + NO2	2.30E-12	[1]	[1],[11]
NIT1NO3OOB + NO = 0.94*PROPNNB + 0.94*GLY + 0.94*NO2 + 0.06*RNO3I + 0.94*NO2 - 0.06*XC + 0.13*XN	2.60E-12*exp(380/T)	[1]	[1],[11]
NIT1NO3OOB + HO2 = RNO3I - XC + XN	2.06E-13*exp(1300/T)	[3]	[5]
NIT1NO3OOB + RO2C = 0.7*PROPNNB + 0.7*GLY + 0.7*NO2 + 0.3*RNO3I - 0.3*XC + 0.3*XN	3.50E-14	[1]	[1],[5],[11]
NIT1NO3OOB + MEO2 = 0.7*PROPNNB + 0.7*GLY + 0.7*NO2 + 0.3*RNO3I + 0.25*HCHO + 0.25*MEOH + 0.5*HO2 + 0.5*HCHO - 0.3*XC + 0.3*XN	2.00E-13	[1]	[1],[5],[11]
NIT1NO3OOB + MECO3 = MEO2 + CO2 + PROPNNB + GLY + NO2	4.40E-13*exp(1070/T)	[1]	[1],[5],[11]
NIT1 + O3 = 0.3*PROPNNB + 0.45*CO + 0.15*OH + 0.45*HO2 + 0.15*CO2 + 0.7*GLY + 0.7*OH + 0.7*NO2 + 0.7*MGLY	4.15E-15*exp(-1520/T)	[5]	[1],[5],[11]
NIT1 + OH = 0.345*NIT1NO3OOA + 0.655*NIT1OHOO	7.48E-12*exp(410/T)	[1],[11]	[1],[5],[11]

NIT1OHOO + NO = 0.919*PROPNNB + 0.919*GLY + 0.015*CO + 0.015*RNO3I + 0.934*NO2 + 0.934*HO2 + 0.066*RNO3I - 0.096*XC + 0.066*XN	2.60E-12*exp(380/T)	[1]	[1],[5],[11]
NIT1OHOO + HO2 = R6OOH + XN - XC	2.06E-13*exp(1300/T)	[3]	[1]
NIT1OHOO + RO2C = 0.689*PROPNNB + 0.689*GLY + 0.011*CO + 0.011*RNO3I + 0.7*HO2 + 0.3*RNO3I - 0.323*XC	3.50E-14	[1]	[1],[5],[11]
NIT1OHOO + MEO2 = 0.689*PROPNNB + 0.689*GLY + 0.011*CO + 0.011*RNO3I + 0.7*HO2 + 0.3*RNO3I + 0.25*HCHO + 0.25*MEOH + 0.50*HCHO + 0.50*HO2 - 0.323*XC	2.00E-13	[1]	[1],[5],[11]
NIT1OHOO + MECO3 = MEO2 + CO2 + 0.984*PROPNNB + 0.984*GLY + 0.016*CO + 0.016*RNO3I + HO2 - 0.033*XC	4.40E-13*exp(1070/T)	[1]	[1],[5],[11]
NISOPOOH + OH = RNO3I + OH	5.00E-11	[12]	[12],[5]
NISOPOOH + OH = 0.3*NISOPO2 + 0.7*OH + 0.7*NIT1	3.80E-12*exp(200/T)	[12]	[12],[5]
MVKN + OH = 0.65*HCOOH + 0.65*MGLY + 0.35*HCHO + 0.35*PYRUACD + NO3	3.50E-12*exp(140/T)	[2],[5]	[2]
MVKN = MECO3 + NO2 + HOCCHO	J <sub>NOA</sub>	[9]	[9]
MACRN + OH = 0.08*CCOOH + 0.08*HCHO + 0.08*NO3 + 0.07*HCOOH + 0.07*NO3 + 0.07*MGLY + 0.85*HACET + 0.85*NO2 + 0.93*CO2	1.28E-11*exp(405/T)	[2],[5]	[2]
MACRN = HACET + NO2 + CO + HO2	J <sub>C2CHO</sub>	[5]	[9]
ETHLN + OH = HCHO + CO2 + NO2	2.94E-12*exp(365/T)	[2],[5]	[2]
ETHLN = NO2 + HCHO + HO2 + CO	J <sub>NOA</sub>	[9]	[9]
RNO3I + OH = NO2 + HO2 + PRD2	8.00E-12	[12]	[12],[5]
PROPNN + OH = MGLY + NO2	4.00E-13	[13],[12]	[9]
PROPNNB + OH = MGLY + NO2	4.00E-13	[13],[12]	[9]
PROPNN = MECO3 + HCHO + NO2	J <sub>NOA</sub>	[14],[15],[3]	[15]
PROPNNB = MECO3 + HCHO + NO2	J <sub>NOA</sub>	[14],[15],[3]	[15]
<b>MVK with OH</b>			
MVK + OH = MVKOO	2.60E-12*exp(610/T)	[1]	[2]
MVKOO + NO = 0.625*HOCCHO + 0.625*MECO3 + 0.265*MGLY + 0.265*HCHO + 0.265*HO2 + 0.11*MVKN + 0.89*NO2	2.60E-12*exp(380/T)	[1]	[2]
MVKOO + HO2 = ROOH + XC	1.82E-13*exp(1300/T)	[3]	[1]
MVKOO + MEO2 = 0.35*HOCCHO + 0.35*MECO3 + 0.15*MGLY + 0.15*HCHO + 0.15*HO2 + 0.5*MEK + 0.25*HCHO + 0.25*MEOH + 0.5*HCHO + 0.50*HO2	2.00E-13	[1]	[1],[2]
MVKOO + RO2C = 0.35*HOCCHO + 0.35*MECO3 + 0.15*MGLY + 0.15*HCHO + 0.15*HO2 + 0.5*MEK	3.50E-14	[1]	[1],[2]
MVKOO + MECO3 = MEO2 + CO2 + 0.7*HOCCHO + 0.7*MECO3 + 0.3*MGLY + 0.3*HCHO + 0.3*HO2	4.40E-13*exp(1070/T)	[1]	[1],[2]
<b>MACR with OH</b>			
MACR + OH = 0.47*MACROO + 0.53*MACO3	8.00E-12*exp(380/T)	[1]	[2]
MACROO + NO = 0.85*NO2 + 0.85*HO2 + 0.72*HACET + 0.72*CO + 0.13*HCHO + 0.13*MGLY + 0.15*MACRN	2.60E-12*exp(380/T)	[1]	[2],[5]
MACROO + HO2 = ROOH + XC	1.82E-13*exp(1300/T)	[3]	[1]
MACROO + MEO2 = 0.50*HO2 + 0.424*HACET + 0.424*CO + 0.076*HCHO + 0.076*MGLY + 0.5*PRD2 + 0.25*HCHO +	2.00E-13	[1]	[1],[2]

0.25*MEOH + 0.5*HCHO + 0.5*HO2 - XC			
MACROO + RO2C = 0.50*HO2 + 0.424*HACET + 0.424*CO + 0.076*HCHO + 0.076*MGLY + 0.5*PRD2 - XC	3.50E-14	[1]	[1],[2]
MACROO + MECO3 = MEO2 + CO2 + HO2 + 0.15*MGLY + 0.85*HACET + 0.85*CO + 0.15*HCHO	4.40E-13*exp(1070/T)	[1]	[1],[2]
MACO3 + NO = NO2 + CO + CO2 + HCHO + MEO2	6.70E-12*exp(340/T)	[1]	[2]
MACO3 + NO2 = MAPAN	1.21e-11*(T/300) <sup>-1.07</sup>	[1]	[1]
MACO3 + HO2 = 0.75*RCOOOH + 0.25*RCOOH + 0.25*O3 + XC	5.20E-13*exp(980/T)	[1]	[1]
MACO3 + NO3 = NO2 + CO + CO2 + HCHO + MEO2	4.00E-12	[9]	[1],[2]
MACO3 + MEO2 = HCHO + HO2 + CO + CO2 + HCHO + MEO2	2.00E-12*exp(500/T)	[1]	[1],[2]
MACO3 + RO2C = CO + CO2 + HCHO + MEO2	4.40E-13*exp(1070/T)	[1]	[1],[2]
MACO3 + RO2XC = CO + CO2 + HCHO + MEO2	4.40E-13*exp(1070/T)	[1]	[1],[2]
MACO3 + MECO3 = CO2 + MEO2 + CO + CO2 + HCHO + MEO2	2.90E-12*exp(500/T)	[1]	[1],[2]
MACO3 + RCO3 = CO + CO2 + HCHO + MEO2 + RO2C + xHO2 + yROOH + xCCHO + CO2	2.90E-12*exp(500/T)	[1]	[1],[2]
MACO3 + BZCO3 = CO + CO2 + HCHO + MEO2 + BZO + RO2C + CO2	2.90E-12*exp(500/T)	[1]	[1],[2]
MACO3 + MACO3 = 2*CO + 2*CO2 + 2*HCHO + 2*MEO2	2.90E-12*exp(500/T)	[1]	[1],[2]

#### ISOPOOH and IEPOX with OH

ISOPOOH + OH = IEPOX + OH	1.90E-11*exp(390/T)	[4],[12]	[4],[12]
ISOPOOH + OH = 0.387*ISOPO2 + 0.613*HC5 + 0.613*OH	4.75E-12*exp(200/T)	[12]	[12]
ISOPOOH = OH + 0.91*HO2 + 0.75*HCHO + 0.45*MVK + 0.29*MACR + 0.09*DIBOO + 0.11*HC5 + 0.05*ARO2 - 0.16*XC	J <sub>COOH</sub>	[5]	[2],[5]
IEPOX + OH = IEPOXOO	5.78E-11*exp(-400/T)	[4]	[4]
IEPOXOO + HO2 = 0.725*HACET + 0.275*HOCCHO + 0.275*GLY + 0.275*MGLY + 1.125*OH + 0.825*HO2 + 0.200*CO2 + 0.375*HCHO + 0.074*HCOOH + 0.251*CO	2.06E-13*exp(1300/T)	[3]	[4]
IEPOXOO + NO = 0.725*HACET + 0.275*HOCCHO + 0.275*GLY + 0.275*MGLY + 0.125*OH + 0.825*HO2 + 0.200*CO2 + 0.375*HCHO + 0.074*HCOOH + 0.251*CO + NO2	2.60E-12*exp(380/T)	[1]	[4],[5]
IEPOXOO + MEO2 = 0.363*HACET + 0.138*HOCCHO + 0.138*GLY + 0.138*MGLY + 0.063*OH + 0.413*HO2 + 0.100*CO2 + 0.188*HCHO + 0.037*HCOOH + 0.126*CO + 0.5*PRD2 + 0.5*HCHO + 0.5*HO2 + 0.25*HCHO + 0.25*MEOH - 0.5*XC	2.00E-13	[1]	[1],[4]
IEPOXOO + RO2C = 0.363*HACET + 0.138*HOCCHO + 0.138*GLY + 0.138*MGLY + 0.063*OH + 0.413*HO2 + 0.100*CO2 + 0.188*HCHO + 0.037*HCOOH + 0.126*CO + 0.5*PRD2 - 0.5*XC	3.50E-14	[1]	[1],[4]
IEPOXOO + MECO3 = 0.725*HACET + 0.275*HOCCHO + 0.275*GLY + 0.275*MGLY + 0.125*OH + 0.825*HO2 + 0.200*CO2 + 0.375*HCHO + 0.074*HCOOH + 0.251*CO + MEO2 + CO2	4.40E-13*exp(1070/T)	[1]	[1],[4]

#### other main isoprene oxidation products

HC5 + OH = HC5OO	1.42E-11*exp(610/T)	[2],[5]	[2]
HC5OO + NO = NO2 + 0.234*HOCCHO + 0.234*MGLY + 0.216*GLY + 0.216*HACET + 0.29*DHMOB + 0.17*RCOOH + 0.09*PRD2 + 0.09*CO + HO2 + 0.16*XC	2.60E-12*exp(380/T)	[1]	[2]
HC5OO + HO2 = R6OOH - XC	2.06E-13*exp(1300/T)	[3]	[1]
HC5OO + MEO2 = 0.117*HOCCHO + 0.117*MGLY + 0.108*GLY + 0.108*HACET + 0.145*DHMOB + 0.085*RCOOH + 0.045*PRD2 + 0.045*CO + 0.5*HO2 + 0.5*PRD2 + 0.25*HCHO + 0.25*MEOH + 0.5*HO2 + 0.5*HCHO - 0.42*XC	2.00E-13	[1]	[1],[2]
HC5OO + RO2C = 0.117*HOCCHO + 0.117*MGLY + 0.108*GLY +	3.50E-14	[1]	[1],[2]

$0.108 \cdot \text{HACET} + 0.145 \cdot \text{DHMOB} + 0.085 \cdot \text{RCOOH} + 0.045 \cdot \text{PRD2} + 0.045 \cdot \text{CO} + 0.5 \cdot \text{HO2} + 0.5 \cdot \text{PRD2} - 0.42 \cdot \text{XC}$			
$\text{HC5OO} + \text{MECO3} = \text{MEO2} + \text{CO2} + 0.234 \cdot \text{HOCCHO} + 0.234 \cdot \text{MGLY} + 0.216 \cdot \text{GLY} + 0.216 \cdot \text{HACET} + 0.29 \cdot \text{DHMOB} + 0.17 \cdot \text{RCOOH} + 0.09 \cdot \text{PRD2} + 0.09 \cdot \text{CO} + \text{HO2} + 0.16 \cdot \text{XC}$	4.40E-13*exp(1070/T)	[1]	[1],[2]
$\text{HC5} + \text{O3} = 0.50 \cdot \text{MGLY} + 0.35 \cdot \text{GLY} + 0.79 \cdot \text{OH} + 0.02 \cdot \text{HCHO} + 0.35 \cdot \text{HOCCHO} + 0.59 \cdot \text{CO} + 0.15 \cdot \text{HACET} + 0.13 \cdot \text{RCOOH} + 0.08 \cdot \text{CO2} + 0.6 \cdot \text{HO2} + 0.35 \cdot \text{MECO3} - 0.13 \cdot \text{XC}$	3.94E-15*exp(-1520/T)	[9],[5]	[1],[5],[11]
$\text{DIBOO} + \text{NO} = \text{NO2} + \text{HO2} + 0.52 \cdot \text{HOCCHO} + 0.52 \cdot \text{MGLY} + 0.48 \cdot \text{GLY} + 0.48 \cdot \text{HACET}$	2.60E-12*exp(380/T)	[1]	[2]
$\text{DIBOO} + \text{HO2} = \text{R6OOH} - \text{XC}$	2.06E-13*exp(1300/T)	[3]	[1]
$\text{DIBOO} + \text{MEO2} = 0.5 \cdot \text{HO2} + 0.26 \cdot \text{HOCCHO} + 0.26 \cdot \text{MGLY} + 0.24 \cdot \text{GLY} + 0.24 \cdot \text{HACET} + 0.5 \cdot \text{PRD2} + 0.25 \cdot \text{HCHO} + 0.25 \cdot \text{MEOH} + 0.5 \cdot \text{HCHO} + 0.50 \cdot \text{HO2} - 0.5 \cdot \text{XC}$	2.00E-13	[1]	[1],[2]
$\text{DIBOO} + \text{RO2C} = 0.5 \cdot \text{HO2} + 0.26 \cdot \text{HOCCHO} + 0.26 \cdot \text{MGLY} + 0.24 \cdot \text{GLY} + 0.24 \cdot \text{HACET} + 0.5 \cdot \text{PRD2} - 0.5 \cdot \text{XC}$	3.50E-14	[1]	[1],[2]
$\text{DIBOO} + \text{MECO3} = \text{HO2} + 0.52 \cdot \text{HOCCHO} + 0.52 \cdot \text{MGLY} + 0.48 \cdot \text{GLY} + 0.48 \cdot \text{HACET} + \text{MEO2} + \text{CO2}$	4.40E-13*exp(1070/T)	[1]	[1],[2]
<b>miscellaneous changes</b>			
$\text{MAPAN} + \text{OH} = \text{HACET} + \text{CO} + \text{NO2}$	2.90E-11	[9]	[9]
$\text{HOCCHO} + \text{OH} = 0.75 \cdot \text{HO2} + 0.25 \cdot \text{OH} + 0.13 \cdot \text{GLY} + 0.52 \cdot \text{CO} + 0.35 \cdot \text{CO2} + 0.16 \cdot \text{HCOOH} + 0.71 \cdot \text{HCHO}$	8.00E-12	[2]	[2][20]
$\text{DHMOB} + \text{OH} = 1.5 \cdot \text{CO} + 0.5 \cdot \text{HO2} + 0.5 \cdot \text{HACET} + 0.5 \cdot \text{PRD2} - \text{XC}$	1.00E-11	[2]	[2]
$\text{PYRUACD} = \text{CCHO} + \text{CO2}$	$J_{\text{MGLY}}$	[5]	[17]
$\text{HACET} + \text{OH} = 0.75 \cdot \text{MGLY} + 0.825 \cdot \text{HO2} + 0.125 \cdot \text{HCOOH} + 0.1 \cdot \text{OH} + 0.125 \cdot \text{MEO2} + 0.20 \cdot \text{CO2} + 0.05 \cdot \text{CO} + 0.125 \cdot \text{CCOOH}$	2.15E-12*exp(305/T)	[2],[16]	[2][20]
$\text{HACET} = \text{HO2} + \text{MECO3} + \text{HCHO}$	1.75E-1* $J_{\text{MEK}}$	[1]	[1]

1

2 Notes:

3 [1]: SAPRC-07 (Carter, 2010)

4 [2]: Paulot et al. (2009a)

5 [3]: Saunders et al. (2003)

6 [4]: Paulot et al. (2009b)

7 [5]: this work

8 [6]: Crouse et al. (2011)

9 [7]: Peeters and Müller (2010)

10 [8]: Rollins et al. (2009)

11 [9]: Master Chemical Mechanism (MCM V3.2, <http://mcm.leeds.ac.uk/MCM/>) (Saunders et al.,  
12 2003)

13 [10]: Lockwood et al. (2010)

14 [11]: SAPRC-99 (Carter, 2000)

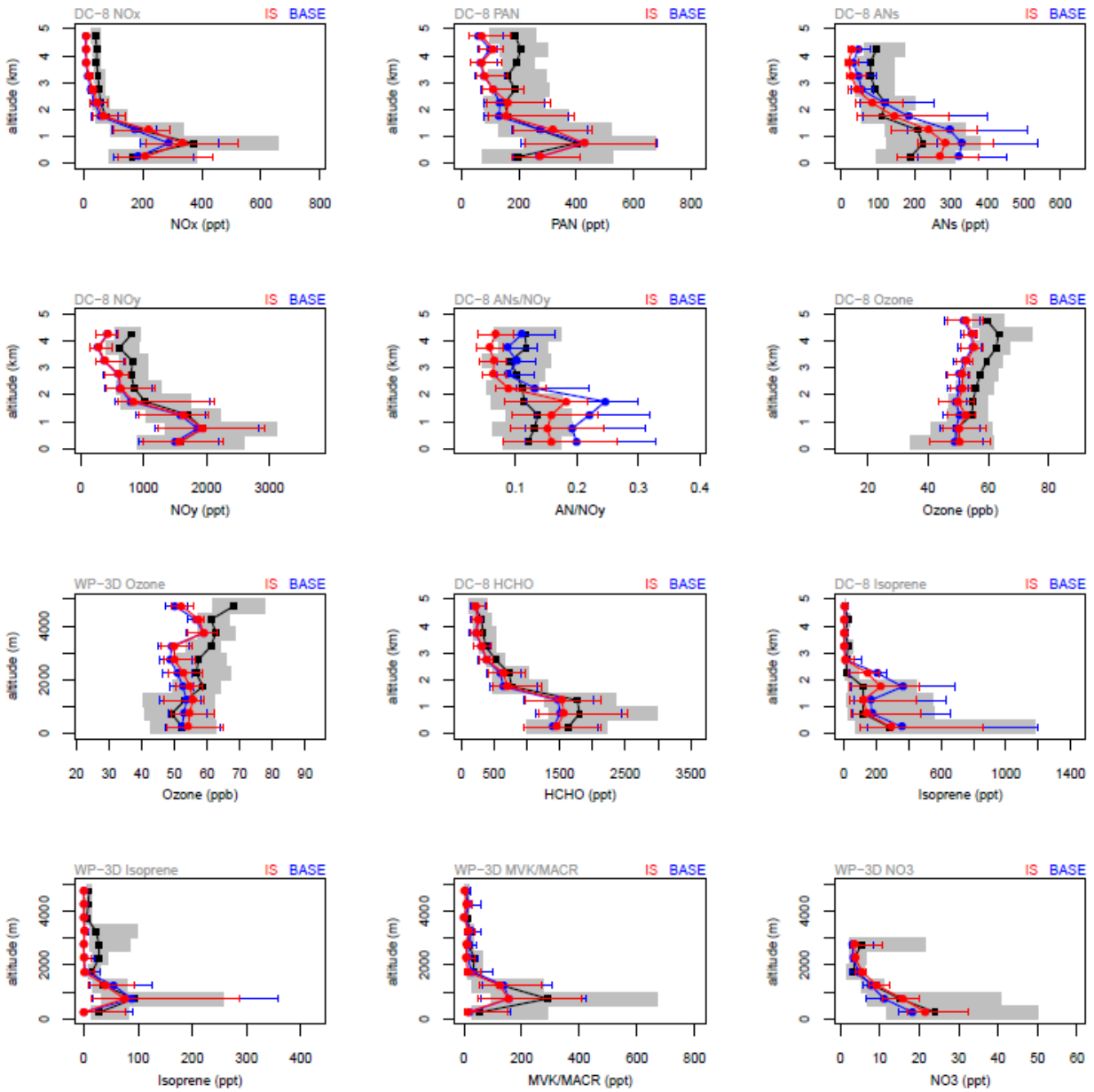
15 [12]: Paulot et al. (2012)

16 [13]: Zhu et al. (1991)

1 [14]: Roberts and Fajer (1989)  
2 [15]: Barnes et al. (1993)  
3 [16]: Dillon et al. (2006)  
4 [17]: Yamamoto and Back (1985)  
5 [18]: Jenkin et al. (1997)  
6 [19]: Hutzell et al. (2012)  
7 [20]: Butkovskaya et al. (2006a, b) (Recent work by Orlando et al. (2012) suggests limited acid  
8 formation from glycolaldehyde and hydroxyacetone oxidation under atmospheric conditions.  
9 Therefore, our study likely represents an upper limit for the amount of formic and acetic acid  
10 originated from isoprene oxidation.  
11  
12

1 Figure S1. Comparisons of vertical profiles of selected modeled species with observations within  
 2 5 km of the surface. Measurements are from the same datasets as those shown in Fig. 2 except  
 3 for extended elevation. The black squares and lines are observed median concentrations. The  
 4 red (blue) circles and lines are modeled median concentrations from the SI (base) simulation.  
 5 The grey boxes show the interquartile ranges of observations, and the colored error bars show  
 6 those for the model results.

7



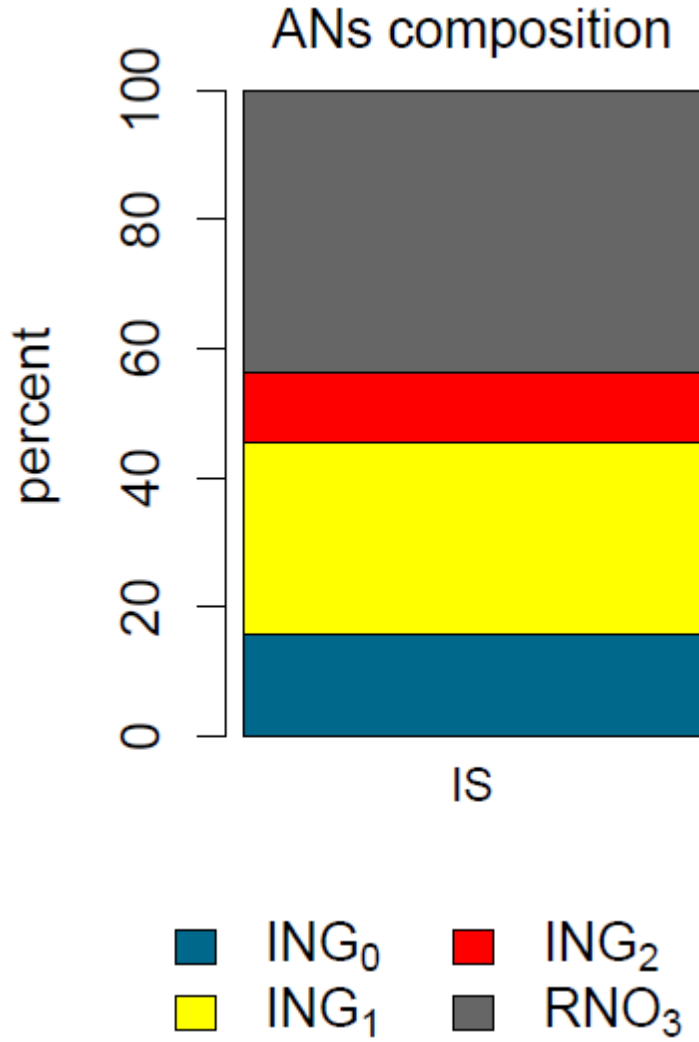
8

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1 Figure S2. Composition of ANs from the IS simulation. Results are summarized over the entire  
2 modeling period for the southeastern US within 2 km of the surface.

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1 **References**

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