Supplement of

Gas-phase chemistry in the online multiscale NMMB/BSC Chemical Transport Model: Description and evaluation at global scale

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1 Statistical Measures

There are several metrics that are used by the modeling community to evaluate performances of AQMs (U.S.EPA, 1991; Cox and Tikvart, 1990; Russell and Dennis, 2000). The statistical indicators selected in this study are: Correlation coefficient (r: Eq. 1), Mean Bias (MB: Eq. 2) and Root Mean Square Error (RMSE: Eq.3).

$$r = \frac{1}{N} \frac{\sum_{i=1}^{N} (O_i - \overline{O}) \Delta(P_i - \overline{P})}{\sigma_O \Delta \sigma_P} \tag{1}$$

$$MB = \frac{\sum_{i=1}^{N} (P_i - O_i)}{N} \tag{2}$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (P_i - O_i)^2}$$
(3)

where σ is the standard deviation and *P* and *O* denote the vector of model output and the vector observations, respectively. No threshold has been applied in the computation of the statistics.

2 Figures



Figure S1: Biogenic emisions of isoprene (upper panel) and monoterpene (middle panel), from the on-line model MEGAN, and anthropogenic emissions of NO, from ACCMIP inventory, for January and July 2004 used in this model simulation



Figure S2: CO vertical profile seasonal averages over Portland, Abu Zabi and Niamey (from left to right) for the whole year 2004. Observations are in a solid red line and model data in a solid black line. The number of observations flights is given on the top of each plot.



Figure S3: Comparison of modeled NMMB/BSC-CTM CO mixing ratio at 500hPa against satellite data (MOPITT) for (from top) DJF, MAM, JJA, and SON for the whole year 2004 in ppb. NMMB/BSC-CTM data is displayed in the left panel, MOPITT data in the middle panel and the bias in the right panel.



Figure S4: Scatter plots of the simulated HNO_3 versus nitrate measurements for three networks: Europe (left panel), USA (middle panel) and Asia (right panel). Dashed lines have slopes equal to 2 and 0.5. The dotted line is the result of the linear regression fitting through the origin.



Figure S5: Comparison of ozonesonde measurements (red lines) and simulated (black lines) seasonal vertical profiles of O_3 (ppb) and standard deviations (horizontal lines). The region name and the number of stations, using brackets, are given above each plot.

3 Tables

Table S1: The chemical trace species for the CB05 chemical mechanism included in gasphase tropospheric chemistry version of NMMB/BSC-CTM.

Species name	Description	Species name	Description
NO	Nitric oxide	SO ₂	Sulfur dioxide
NO ₂	Nitrogen dioxide	MEO ₂	Methylperoxy radical
O3	Ozone	MEOH	Methanol
0	Oxygen atom in the $O^{3}(P)$ electronic state	MEPX	Methylhydroperoxide
O^1D	Oxygen atom in the O ¹ (D) electronic state	FACD	Formic acid
OH	Hydroxyl radical	ETHA	Ethane
HO_2	Hydroperoxy radical	ROOH	Higher organic peroxide
H_2O_2	Hydrogen peroxide	AACD	Acetic and higher carboxylic acids
NO ₃	Nitrate radical	PACD	Peroxyacetic and higher peroxycarboxylic acids
N_2O_5	Dinitrogen pentoxide	PAR	Paraffin carbon bond (C-C)
HONO	Nitrous acid	ROR	Secondary alkoxy radical
HNO ₃	Nitric acid	ETH	Ethene
PNA	Peroxynitric acid (HNO ₄)	OLE	Terminal olefin carbon bond (R-C=C)
CO	Carbon monoxide	IOLE	Internal olefin carbon bond (R-C=C-R)
FORM	Formaldehyde	ISOP	Isoprene
ALD2	Acetaldehyde	ISPD	Isoprene product (lumped methacrolein, methyl vinyl ketone, etc.)
C_2O_3	Acetylperoxy radical		
PAN	Peroxyacetyl nitrate	TERP	Terpene
ALDX	Propionaldehyde and higher aldehydes	TOL	Toluene and other monoalkyl aromatics
CXO ₃	C3 and higher acylperoxy radicals	XYL	Xylene and other polyalkyl aromatics
PANX	C3 and higher peroxyacyl nitrates	CRES	Cresol and higher molecular weight phenols
XO ₂	NO to NO ₂ conversion from alkylperoxy (RO ₂) radical	TO ₂	Toluene-hydroxyl radical adduct
XO_2N	NO to organic nitrate conversion from alkylperoxy (RO ₂) radical	OPEN	Aromatic ring opening product
NTR	Organic nitrate (RNO ₃)	CRO	Methylphenoxy radical
ETOH	Ethanol	MGLY	Methylglyoxal and other aromatic products
SULF	Sulfuric acid (gaseous)		

Products Reactants Rate expression 6.0E-34*(300/T)^{2.4} $O_3 + M$ $O + O_2 + M$ \rightarrow $O_3 + NO$ NO_2 3.0E-12*exp(T/1500) \rightarrow NO 5.6E-12*exp(180/T) $O + NO_2$ \rightarrow NO₃ $K_0 = 2.5E-31 \exp(300/T)^{1.8}$ $O + NO_2$ \rightarrow $K_{\infty}=2.2E-11*exp(300/T)^{0.7}$ K₀=9.0E-32*exp(300/T)^{1.5} O + NO NO_2 \rightarrow K_∞=3.0E-11 1.2E-13*exp(T/2450) $NO_2 + O_3$ NO₃ \rightarrow O(1)D + MO + M2.1E-11*exp(102/T) \rightarrow 2.000*OH 2.2E-10 $O(^{1})D + H_{2}O$ \rightarrow $O_3 + OH$ HO_2 1.7E-12*exp(T/940) \rightarrow 1.0E-14*exp(T/490) $O_3 + HO_2$ OH \rightarrow 2.000*NO2 1.5E-11*exp(170/T) $NO_3 + NO$ \rightarrow $NO + NO_2$ 4.5E-14*exp(T/1260) $NO_3 + NO_2$ \rightarrow $NO_3 + NO_2$ $N2O_5$ $K_0 = 2.0E-30 * (300/T)^{4.4}$ \rightarrow $K_{\infty} = 1.4E - 12*(300/T)^{0.7}$ 2.000*HNO3 2.5E-22 $N_2O_5 + H_2O$ \rightarrow 2.000*HNO3 1.8E-39 $N_2O_5 + H_2O + H_2O$ \rightarrow $NO_3 + NO_2$ $K_0 = 1.0E - 03 \exp(11000/T)^{3.5}$ N_2O_5 \rightarrow $K_{\infty} = 9.7E + 14 \exp(T/11080)^{0.1}$ $F_c = 0.45$ n= 1.0 $NO + NO + O_2$ 2.000*NO2 3.3E-39*exp(530/T) \rightarrow $NO + NO_2 + H_2O$ 2.000*HONO 5.0E-40 \rightarrow NO + OHHONO 7.0E-31*exp(300/T)^{2.6} \rightarrow 3.6E-11*exp(300/T)-0.1 1.8E-11*exp(T/390) OH + HONO NO_2 \rightarrow $NO + NO_2$ 1.0E-20 HONO + HONO \rightarrow $NO_2 + OH$ HNO₃ K₀=2.0E-30*exp(300/T)^{3.0} \rightarrow K_∞=2.5E-11 $K_0=2.4E-14*exp(460/T)$ OH+ HNO₃ NO₃ \rightarrow K₂= 2.7E-17*exp(2199/T) $K_3 = 6.5E-34 \exp(1335/T)$ $OH + NO_2$ K₀=3.5E-12*exp(250/T) $HO_2 + NO$ \rightarrow $HO_2 + NO_2$ PNA K₀=1.8E-31*exp(300/T)^{3.2} \rightarrow K∞=4.7E-12 $F_c = 0.6$ HO₂+NO₂ K₀=4.1E-5*exp(T/10650) PNA \rightarrow K_{∞} =4.8E15*exp(T/11170) $F_c = 0.6$ 1.3E-12*exp(380/T) OH + PNA NO_2 \rightarrow $HO_2 + HO_2$ H_2O_2 K₁=2.3E-13*exp(600/T) $K_2 = 1.7E - 33 \exp(1000/T)$ HO₂+HO₂+H₂O H_2O_2 K1=3.22E-34*exp(2800/T) \rightarrow K2=2.38E-54*exp(3200/T)

Table S2: The gas-phase CB05 chemical mechanism reactions applied in the NMMB/BSC-CTM. The first column describes the reactants, the second the products and the third displays the coefficients to compute the full rate expressions for each reaction.

Reactants		Products	Rate expression
$OH + H_2O_2$	\rightarrow	HO ₂	2.9E-12*exp(T/160)
$O^1D + H_2$	\rightarrow	$OH + HO_2$	1.1E-10
$OH + H_2$	\rightarrow	HO ₂	5.5E-12*exp(T/2000)
$OH + O_2$	\rightarrow	HO ₂	2.2E-11*exp(120/T)
OH + OH	\rightarrow	0	4.2E-12*exp(T/240)
OH + OH	\rightarrow	HaOa	$K_0 = 6.9E_{-31*exp}(300/T)^{1.0}$
011 + 011	/	1202	$K_{1}=2.5E-31$ exp(300/1) $K_{2}=2.6E-11$
$OH + HO_2$	\rightarrow		4.8E-11*exp(250/T)
$HO_2 + O_2$	\rightarrow	OH	3.0E-11*exp(200/T)
$H_{2}O_{2} + O$	\rightarrow	$OH + HO_2$	1.4E-12*exp(-2000/T)
$NO_2 + O$	\rightarrow	NO ₂	1.0E-11
$NO_2 + OH$	\rightarrow	$HO_2 + NO_2$	2.2E-11
$NO_2 + HO_2$	\rightarrow	HNO ₂	3 5E-12
$NO_2 + O_2$	\rightarrow	NO ₂	1 0E-17
$NO_3 + NO_2$	\rightarrow	2,000*NO2	8.5E-13*exp(T/2450)
$XO_2 \pm NO_3$		NO ₂	2.6E-12*exp(365/T)
$XO_2 N + NO$	\rightarrow	NTR	2.6E-12*exp(365/T)
$XO_2 + HO_2$	\rightarrow	ROOH	7.5E-13*exp(700/T)
$XO_2 + HO_2$ $XO_2N + HO_2$		ROOH	7.5E-13*exp(700/T)
$XO_2 + XO_2$		Room	6 8E-14
$XO_2 + XO_2$ $XO_2N + XO_2N$			6.8E-14
$XO_2 + XO_2 N$	\rightarrow		6.8E-14
A02 + A021	/	HNO_3 + HO_2 + 0.330 *FORM+	
NTR + OH	\rightarrow	0.330*ALD2+ 0.330*ALDX- 0.660*PAR	5.9E-13*exp(360/T)
ROOH + OH	\rightarrow	XO ₂ + 0.500*ALD2 + 0.500*ALDX	3.01E-12*exp(190/T)
OH + CO	\rightarrow	HO ₂	$K_1 = 1.44E-13$
			K ₂ =3.43E-33
OH + CH4	\rightarrow	MEO ₂	2.45E-12*exp(T/1775)
$MEO_2 + NO$	\rightarrow	$FORM + HO_2 + NO_2$	2.8E-12*exp(300/T)
$MEO_2 + HO_2$	\rightarrow	MEPX	4.1E-13*exp(750/T)
$MEO_2 + MEO_2$	\rightarrow	1.370*FORM+ 0.740*HO ₂ + 0.630*MEOH	9.5E-14*exp(390/T)
MEPX + OH	\rightarrow	0.700*MEO ₂ + 0.300*XO ₂ + 0.300*HO ₂	3.8E-12*exp(200/T)
MEOH + OH	\rightarrow	$FORM + HO_2$	7.3E-12*exp(T/620)
FORM + OH	\rightarrow	$HO_2 + CO$	9.0E-12
FORM + O	\rightarrow	$OH + HO_2 + CO$	3.4E-11*exp(T/1600)
$FORM + NO_3$	\rightarrow	HNO_3+HO_2+CO	5.8E-16
$FORM + HO_2$	\rightarrow	HCO ₃	9.7E-15*exp(625/T)
HCO ₃	\rightarrow	$FORM + HO_2$	2.4E+12*exp(T/7000)
$HCO_3 + NO$	\rightarrow	$FACD + NO_2 + HO_2$	5.6E-12
$HCO_3 + HO_2$	\rightarrow	MEPX	5.6E-15*exp(2300/T)
FACD + OH	\rightarrow	HO ₂	4.0E-13
ALD2 + O	\rightarrow	$C_2O_3 + OH$	1.8E-11*exp(T/1100)
ALD2 + OH	\rightarrow	C_2O_3	5.6E-12*exp(270/T)
$ALD2 + NO_3$	\rightarrow	C_2O_3 + HNO ₃	1.4E-12*exp(T/1900)
$C_2O_3 + NO$	\rightarrow	$MEO_2 + NO_2$	8.1E-12*exp(270/T)
PAN	\rightarrow	$C_2O_3 + NO_2$	$K_0 = 4.9E-3*exp(12100/T)$
			$K_{\infty} = 5.4E16 * exp(T/13830)$
			$F_c = 0.3$
$C_2O_3 + HO_2$	\rightarrow	0.800*PACD+ 0.200*AACD+ 0.200*O ₃	4.3E-13*exp(1040/T)
$C_2O_3 + MEO_2$	\rightarrow	0.900*MEO ₂ + 0.900*HO ₂ + FORM+ 0.100*AACD	2.0E-12*exp(500/T)

Table S2: Continued from previous page

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$\begin{array}{rcl} AACD + OH & \rightarrow & MEO_2 & 4.0E-13^{*}exp(200/T) \\ ALDX + O & \rightarrow & CXO_3 + OH & 1.3E-11^{*}exp(T/870) \\ ALDX + OH & \rightarrow & CXO_3 & 5.1E-12^{*}exp(405/T) \\ ALDX + NO_3 & \rightarrow & CXO_3 + HNO_3 & 6.5E-15 \\ CXO_3 + NO & \rightarrow & ALD2 + NO_2 + HO_2 + XO_2 & 6.7E-12^{*}exp(340/T) \\ CXO_3 + NO_2 & \rightarrow & PANX & K_{a}=1.2E-11^{*}exp(300/T)^{7.1} \\ K_{a}=1.2E-11^{*}exp(300/T)^{0.9} \\ F_{c}=0.3 \\ PANX + OH & \rightarrow & ALD2 + NO_2 & 3.0E-13 \\ CXO_3 + HO_2 & 0.900^{*}ALD2 + 0.200^{*}AACD + 0.200^{*}O_3 & 4.3E-13^{*}exp(1040/T) \\ CXO_3 + MEO_2 & \rightarrow & 0.900^{*}ALD2 + 0.900^{*}XO_2 + HO_2 + \\ O.100^{*}AACD + 0.100^{*}AACD & 4.4E-13^{*}exp(1040/T) \\ CXO_3 + XO_2 & \rightarrow & 0.900^{*}ALD2 + 0.100^{*}AACD & 4.4E-13^{*}exp(1070/T) \\ CXO_3 + C2O_3 & \rightarrow & 2.000^{*}ALD2 + 0.200^{*}XO_2 + HO_2 + \\ O.500^{*}ALD2 & - 0.900^{*}ALD2 + 0.200^{*}O_2 + HO_2 + \\ O.100^{*}AACD + 0.100^{*}AACD & 4.4E-13^{*}exp(1070/T) \\ CXO_3 + C2O_3 & \rightarrow & 2.000^{*}ALD2 + 0.200^{*}RO_2 + 0.200^{*}HO_2 + \\ O.500^{*}ALDX & 0.900^{*}ALD2 + 0.200^{*}ROR + \\ 0.050^{*}ALDX & 0.900^{*}ALD2 + 0.940^{*}HO_2 - \\ ROR & \rightarrow & 2.100^{*}PAR + 0.040^{*}XO_2 N + 0.110^{*}HO_2 + \\ O + OLE & \rightarrow & 0.200^{*}ALD2 + 0.300^{*}ALD2 + 0.200^{*}FORM + \\ 0.010^{*}XO_2 N + 0.200^{*}FAR + 0.100^{*}OR + \\ 0.010^{*}XO_2 N + 0.200^{*}FAR + 1.6E+13 \\ COD^{*}ALDX & 0.800^{*}FOR + \\ 0.100^{*}XD_2 N + 0.200^{*}FAR + 1.00^{*}OR + \\ 0.100^{*}XD_2 N + 0.200^{*}FAR + 1.00^{*}OR + \\ 0.100^{*}XO_2 N + 0.200^{*}FAR + 1.00^{*}FORM + \\ 0.100^{*}XO_2 N + 0.200^{*}FAR + 1.00^{*}FORM + \\ 0.300^{*}FORM + & 0.330^{*}ALD2 + 0.500^{*}HO_2 - \\ 0.700^{*}PAR & 0.140^{*}HO_2 - 1.000^{*}PAR + \\ 0.100^{*}ALDX + 0.800^{*}XO_2 N + 0.200^{*}FORM + \\ 0.300^{*}ALDX + 0.300^{*}ALDX + 0.300^{*}HO_2 - \\ 0.700^{*}PAR & 0.100^{*}OH + \\ 0.300^{*}ALDX + 0.300^{*}ALDX + 0.100^{*}OH + \\ 0.300^{*}ALDX + 0.200^{*}XO_2 N + \\ 0.950^{*}ALDX + 0.200^{*}XO_2 N + \\ 0.950^{*}ALDX + 0.200^{*}XO_2 N + \\ 0.950^{*}ALDX + 0.500^{*}ADZ + 0.100^{*}OH + \\ 0.50^{*}ALDX + 0.500^{*}ALDX + 0.500^{*}ADZ + \\ 0.65E^{*}ALDX + 0.500^{*}ALDX + \\ 0.65E^{*}ALDX + 0.500^{*}ALDX + \\ 0.65$
$\begin{array}{rcl} ALDX + OH & \rightarrow & CXO_3 + OH & 1.3E + 11 \exp(7870) \\ ALDX + OH & \rightarrow & CXO_3 + OH & 1.3E + 11 \exp(7870) \\ ALDX + NO_3 & \rightarrow & CXO_3 + HNO_3 & 6.5E + 15 \\ CXO_3 + NO & \rightarrow & ALD2 + NO_2 + HO_2 + XO_2 & 6.7E + 12^*\exp(340/T) \\ CXO_3 + NO_2 & \rightarrow & PANX & K_0 = 2.7E + 28^*\exp(300/T)^{7.1} \\ K_{\infty} = 1.2E + 11^*\exp(300/T)^{0.9} \\ F_c = 0.3 \\ PANX + OH & \rightarrow & ALD2 + NO_2 & 3.0E + 13 \\ CXO_3 + HO_2 & \rightarrow & 0.800^*PACD + 0.200^*AACD + 0.200^*O_3 & 4.3E + 13^*\exp(140/T) \\ 0.900^*ALD2 + & 0.900^*XO_2 + HO_2 + \\ 0.100^*AACD + 0.100^*FORM & 2.0E + 12^*\exp(500/T) \\ CXO_3 + XO_2 & \rightarrow & 0.900^*ALD2 + 0.100^*FORM & 2.0E + 12^*\exp(500/T) \\ CXO_3 + XO_2 & \rightarrow & 0.900^*ALD2 + 0.000^*XO_2 + 2.000^*HO_2 & 2.9E + 12^*\exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E + 12^*\exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E + 12^*\exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E + 12^*\exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E + 12^*\exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E + 12^*\exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + 0.100^*HO_2 + \\ PAR + OH & \rightarrow & 0.600^*ALD2 + 0.100^*ROR + \\ 0.050^*ALDX & 0.960^*XO_2 + 0.000^*ROR + \\ 0.050^*ALDX & 0.960^*XO_2 + 0.000^*ROR + \\ 0.050^*ALDX & 0.960^*XO_2 + 0.000^*ROR + \\ 0.010^*XO_2 + 0.200^*ALD2 + 0.300^*HO_2 + \\ O + OLE & \rightarrow & 0.200^*XO_2 + 0.200^*FORM + \\ 0.110^*XO_2 + 0.200^*ALDX + 0.300^*HO_2 + \\ OH + OLE & \rightarrow & 0.620^*ALDX + 0.200^*COH + 0.200^*FORM + \\ 0.180^*ALD2 + 0.200^*ALDX + 0.200^*FORM + \\ 0.180^*ALD2 + 0.300^*ALD2 + 0.900^*RN + \\ NO_3 + OLE & \rightarrow & 0.320^*ALDX + 0.200^*XO_2 + 0.100^*OH + \\ 0.330^*CO + 0.440^*HO_2 - 1.000^*PAR + \\ NO_3 + OLE & \rightarrow & 0.320^*ALDX + 0.200^*XO_2 + 0.100^*OH + \\ 0.330^*CO + 0.440^*HO_2 - 1.000^*PAR + \\ NO_2 + FORM + 0.910^*XO_2 + 0.090^*XO_2 N + \\ 0.90^*ALDX + 0.300^*ALDX + 0.300^*ALDX + \\ 0.90^*ALDX + 0.300^*ALDX + \\ 0.90^$
$\begin{array}{rcl} ALDX + OH & \rightarrow & CXO_3 & HNO_3 & HIL = 124 \exp(405/T) \\ ALDX + NO_3 & \rightarrow & CXO_3 + HNO_3 & 6.5E-15 \\ CXO_3 + NO & \rightarrow & ALD2 + NO_2 + HO_2 + XO_2 & 6.7E-12*\exp(340/T) \\ CXO_3 + NO_2 & \rightarrow & PANX & K_0 = 2.7E-28*\exp(300/T)^{7.1} \\ K_{\infty} = 1.2E-11*\exp(300/T)^{0.9} \\ F_c = 0.3 \\ PANX + OH & \rightarrow & ALD2 + NO_2 & 3.0E-13 \\ CXO_3 + HO_2 & \rightarrow & 0.800*PACD + 0.200*AACD + 0.200*O_3 & 4.3E-13*\exp(1040/T) \\ 0.900*ALD2 + & 0.900*XO_2 + HO_2 + 2 \\ 0.100*AACD + 0.100*FORM & 4.4E-13*\exp(1070/T) \\ CXO_3 + XO_2 & \rightarrow & 0.900*ALD2 + 0.010*ACD & 4.4E-13*\exp(1070/T) \\ CXO_3 + CQO_3 & \rightarrow & 2.000*ALD2 + 2.000*XO_2 + 2.000*HO_2 & 2.9E-12*\exp(500/T) \\ CXO_3 + CQO_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E-12*\exp(500/T) \\ CXO_3 + CQO_3 & \rightarrow & MEO_2 + XO_2 + 0.10*PAR + 0.760*ROR + \\ 0.500*ALDX & 0.500*ALDX & 0.900*ALD2 + 0.940*HO_2 + \\ O.500*ALDX & 0.500*ALDX & 0.300*ALD2 + 1.E+15*\exp(T/8000) \\ 0.500*ALDX & 0.200*CO + 0.200*FORM + \\ 0.100*XO_2N + 0.200*CO + 0.200*FORM + \\ 0.010*XO_2N + 0.200*CO + 0.200*FORM + \\ 0.010*XO_2N + 0.200*CO + 0.200*FORM + \\ 0.010*XO_2N + 0.200*PAR + 0.100*HO_2 + \\ O+OLE & \rightarrow & 0.620*ALDX + 0.300*ALD2 + 0.940*HO_2 - \\ OH + OLE & \rightarrow & 0.620*ALDX + 0.800*XO_2 + 0.900*XO_2 + \\ 0.40*ALDX + 0.800*ALDX + 0.300*HO_2 + \\ 0.500*ALDX + 0.200*CO + 0.200*FORM + \\ 0.110*XO_2N + 0.200*CO + 0.200*FORM + \\ 0.110*XO_2N + 0.200*CO + 0.200*FORM + \\ 0.110*XO_2N + 0.200*CO + 0.200*FORM + \\ 0.110*ALDX + 0.300*ALD2 + \\ 0.40*ALDX + 0.800*XO_2 + 0.950*HO_2 - \\ 0.700*PAR & 0.100*OH + \\ 0.330*CO + 0.440*HO_2 - 1.000*PAR \\ NO_3 + OLE & \rightarrow & 0.520*ALDX + 0.200*XO_2N + \\ 0.560*ALDX + 0.200*XO_2 + 0.100*OH + \\ 0.330*CO + 0.440*HO_2 - 1.000*PAR \\ NO_3 + OLE & \rightarrow & 0.520*ALDX + 0.200*XO_2N + \\ 0.560*ALDX + 0.200*XO_2 + 0.100*OH + \\ 0.530*ALDX + 0.200*XO_2 + 0.100*OH + \\ 0.530*CO + 0.440*HO_2 - 1.000*PAR \\ NO_3 + OLE & \rightarrow & 0.520*ALDX + 0.200*XO_2N + \\ 0.560*ALDX + 0.500*XO_2 + 0.100*OH + \\ 0.550*ALDX + 0.200*XO_2 + 0.100*OH + \\ 0.550*ALDX + 0.200*XO_2 + 0.100*OH + \\ 0.550*ALDX + 0.500*ALD2 + 0.100*PAR \\ NO_2 + FORM + 0.110*XO_2 + 0.00*XO_2N + \\ 0.560*ALDX + 0.500*XO_2 + 0.0$
$\begin{array}{rcl} ALDX + ON & \rightarrow & CXO_3 + HNO_3 & & G.SE - 15 \\ CXO_3 + NO & \rightarrow & ALD2 + NO_2 + HO_2 + XO_2 & & G.SE - 15 \\ CXO_3 + NO & \rightarrow & ALD2 + NO_2 + HO_2 + XO_2 & & G.SE - 15 \\ CXO_3 + NO_2 & \rightarrow & PANX & & K_0 = 2.7E - 28^* exp(300/T)^{7.1} \\ K_w = 1.2E - 11^* exp(300/T)^{0.9} \\ F_c = 0.3 \\ PANX & \rightarrow & CXO_3 + NO_2 & & 3.0E - 13 \\ CXO_3 + HO_2 & \rightarrow & 0.800^*PACD + 0.200^*AACD + 0.200^*O_3 & & 4.3E - 13^* exp(1040/T) \\ 0.900^*ALD2 + & 0.900^*XO_2 + & HO_2 + \\ 0.100^*AACD & - 0.100^*PORM & & 4.4E - 13^* exp(1070/T) \\ CXO_3 + XO_2 & \rightarrow & 0.900^*ALD2 + 0.100^*PORM & & 4.4E - 13^* exp(1070/T) \\ CXO_3 + CQ_3 & \rightarrow & 0.900^*ALD2 + 0.100^*PORM & & 2.9E - 12^* exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & 0.000^*ALD2 + 0.100^*AACD & & 4.4E - 13^* exp(1070/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & & 2.9E - 12^* exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & & 2.9E - 12^* exp(500/T) \\ CXO_3 + CQ_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + 0.100^*RORH & & 8.1E - 13 \\ & 0.050^*ALD2 & 0.110^*PAR + 0.760^*RORH & & 8.1E - 13 \\ & 0.500^*ALD2 & 0.100^*PAR + 0.020^*RORH & & 1.E + 15^* exp(T/8000) \\ & 0.500^*ALDX & & 0.500^*ALDX + 0.300^*ALD2 + & 1.000^*HO_2 + \\ O + OLE & \rightarrow & 0.200^*ALD2 + 0.200^*CO + 0.200^*FORM + & 1.5E - 11 \\ & 0.200^*ALDX + 0.200^*PAR + 0.100^*OH \\ & 0.800^*FORM + & 0.330^*ALD2 + & 3.2E - 11 \\ & 0.100^*XO_2 + 0.200^*CO + 0.200^*FORM + & 1.E - 11^* exp(T/280) \\ & 0.100^*XO_2 + 0.200^*CO + 0.200^*FORM + & 0.330^*ALD2 + & 3.2E - 11 \\ & 0.100^*XO_2 + 0.200^*XO_2 + 0.950^*HO_2 - & 3.2E - 11 \\ & 0.100^*XO_2 + 0.200^*XO_2 + 0.950^*HO_2 - & 3.2E - 11 \\ & 0.100^*XO_2 + 0.200^*XO_2 + 0.900^*XO_2 + & 3.2E - 11 \\ & 0.100^*XO_2 + 0.200^*XO_2 + 0.900^*XO_2 + & 0.500^*HO_2 - & 0.700^*PAR \\ & 0.180^*ALD2 + & 0.740^*FORM + & 0.330^*ALD2 + & 0.740^*FORM + \\ & 0.330^*CO + 0.440^*HO_2 1.000^*PAR & & 7.0E - 13^* exp(T/2160) \\ \end{array}$
$\begin{array}{rcl} \text{ALD} X + \text{NO}_3 & \rightarrow & \text{ALD}^2 + \text{NO}_2 + \text{NO}_2 + \text{AO}_2 + \text$
$\begin{array}{ccccccc} CXO_3 + NO & \rightarrow & PANX & & & \\ CXO_3 + NO_2 & \rightarrow & PANX & & & \\ ROR & + OL & & & \\ PANX + OH & \rightarrow & ALD2 + NO_2 & & \\ ALD2 + NO_2 & & & \\ PANX + OH & \rightarrow & ALD2 + NO_2 & & \\ ALD2 + NO_2 & & & \\ O.800^{*PACD+0.200^*AACD+0.200^*O_3} & & & \\ A.3E-13^*exp(1040/T) & & \\ O.900^*ALD2 + & & 0.900^*XO_2 + & HO_2 + & \\ O.100^*AACD + 0.100^*AACD & & \\ A.4E-13^*exp(1040/T) & & \\ 2.0E-12^*exp(500/T) & & \\ CXO_3 + XO_2 & \rightarrow & 0.900^*ALD2 + 0.100^*ACD & & \\ A.4E-13^*exp(1070/T) & & \\ CXO_3 + CQ_3 & \rightarrow & 2.000^*ALD2 + 0.200^*XO_2 + 2.000^*HO_2 + & \\ O.500^*ALD2 & & & \\ O.600^*ALD2 + 0.100^*ACD & & \\ A.4E-13^*exp(500/T) & & \\ CXO_3 + CQ_3 & \rightarrow & \\ O.600^*ALD2 + 0.100^*ACD & & \\ A.4E-13^*exp(500/T) & & \\ CXO_3 + CQ_3 & \rightarrow & \\ O.600^*ALD2 + 0.100^*ACD & & \\ O.600^*ALD2 + 0.110^*PAR + 0.760^*ROR + & \\ O.500^*ALDX & & \\ O.960^*XO_2 + 0.600^*ALD2 + 0.940^*HO_2 - & \\ ROR & \rightarrow & \\ O.500^*ALDX & & \\ O.500^*ALDX & & \\ O.500^*ALDX & & \\ O.500^*ALDX & & \\ O.600^*ALD2 + 0.200^*CO + 0.200^*FORM + & \\ O.500^*ALDX & & \\ O.10^*XO_2 + 0.200^*CO + 0.200^*FORM + & \\ O.200^*ALD2 + 0.200^*CO + 0.200^*FORM + & \\ O.100^*XO_2 + 0.200^*CO + 0.200^*FORM + & \\ O.100^*XO_2 + 0.200^*CO + 0.200^*FORM + & \\ O.100^*XO_2 + 0.200^*CO_2 + 0.950^*HO_2 - & \\ O.740^*FORM + & \\ O.310^*ALD2 + & \\ O.740^*FORM + & \\ O.320^*ALDX + 0.200^*XO_2 + 0.100^*OH + & \\ O.500^*ALDX + 0.200^*XO_2 + 0.100^*OH + & \\ O.500^*ALDX + 0.200^*XO_2 + 0.100^*OH + & \\ O.740^*FORM + & \\ O.300^*CO + 0.440^*HO_2 - & \\ O.740^*FORM + \\ O.300^*CO + & \\ O.500^*ALDX + \\ O.500^*A$
$\begin{array}{rcl} CXO_3 + NO_2 & \rightarrow & IAAA & K_{0=1,22-11}^{CZO} (CxD(SOOT)^{0.9} \\ F_c=0.3 \\ \\ PANX + OH & \rightarrow & ALD2 + NO_2 & SOOFPC \\ PANX + OH & \rightarrow & ALD2 + NO_2 & SOOFPC \\ O + OBO^* + OL2 & O & SOOPACDP \\ O + OLD2 + & O.SOOPACDP \\ O + OLD2 + & O.SOOPACDP \\ O + OLD2 + & O.OOO^*ACDP \\ O + OLD2 + & O.OOO^*ACDP \\ O + OLD2 & \rightarrow & O.OOO^*ALD2 + & O.OO^*OCP \\ O + OL2 & \rightarrow & O.OO^*ALD2 + O.OO^*ACDP \\ O + OL2 & \rightarrow & O.OO^*ALD2 + O.OO^*ACDP \\ O + OL2 & \circ & O.O^*OALD2 + O.OO^*ACDP \\ O + OL2 & \circ & O.O^*OALD2 + O.OO^*ACDP \\ O + OO + ALD2 \\ O + OC & \rightarrow & O.OO^*ALD2 + O.OO^*ACP \\ O + OO & ALD2 \\ O & O & O & ALD2 \\ O + O \\ O & O & O & ALDX \\ O & O & O & ALDX \\ O & O & O & O \\ A \\ O \\ \mathsf$
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$\begin{array}{rcl} {\rm PANX} & \rightarrow & {\rm CAO_3} + {\rm NO_2} \\ {\rm PANX} + {\rm OH} & \rightarrow & {\rm ALD2} + {\rm NO_2} & {\rm 3.0E-13} \\ {\rm CXO_3} + {\rm HO_2} & \rightarrow & {\rm 0.800^*{\rm PACD} + 0.200^*{\rm AACD} + 0.200^*{\rm O_3} & {\rm 4.3E-13^*{\rm exp}(1040/{\rm T})} \\ {\rm 0.900^*{\rm ALD2} + & 0.900^*{\rm XO_2} + & {\rm HO_2} + \\ {\rm 0.100^*{\rm AACD} + 0.100^*{\rm FORM} & {\rm 4.4E-13^*{\rm exp}(1070/{\rm T})} \\ {\rm CXO_3} + {\rm XO_2} & \rightarrow & {\rm 0.900^*{\rm ALD2} + 0.100^*{\rm AACD} & {\rm 4.4E-13^*{\rm exp}(1070/{\rm T})} \\ {\rm CXO_3} + {\rm CXO_3} & \rightarrow & {\rm 2.000^*{\rm ALD2} + 0.200^*{\rm XO_2} + 2.000^*{\rm HO_2} & {\rm 2.9E-12^*{\rm exp}(500/{\rm T})} \\ {\rm CXO_3} + {\rm C2O_3} & \rightarrow & {\rm MEO_2 + {\rm XO_2} + {\rm HO_2} + {\rm ALD2} & {\rm 2.9E-12^*{\rm exp}(500/{\rm T})} \\ {\rm 0.870^*{\rm XO_2} + & 0.130^*{\rm XO_2}{\rm N} + & 0.110^*{\rm HO_2} + \\ {\rm PAR} + {\rm OH} & \rightarrow & {\rm 0.060^*{\rm ALD2} - & 0.110^*{\rm PAR} + & 0.760^*{\rm ROR} + \\ {\rm 0.960^*{\rm XO_2} + & 0.600^*{\rm ALD2} + & 0.940^*{\rm HO_2} - \\ \\ {\rm ROR} & \rightarrow & {\rm 0.600^*{\rm ALDX} - & 0.010^*{\rm PAR} + & 0.760^*{\rm ROR} + \\ {\rm 0.500^*{\rm ALDX} & 0.960^*{\rm XO_2} + & 0.020^*{\rm ROR} + \\ {\rm 0.500^*{\rm ALDX} & 0.900^*{\rm ALDX} + & 0.300^*{\rm HO_2} + \\ \\ {\rm O} + {\rm OLE} & \rightarrow & {\rm NTR} & {\rm 1.5E-11} \\ {\rm 0.200^*{\rm XO_2} + & 0.200^*{\rm CO} + & 0.200^*{\rm FORM} + \\ {\rm 0.800^*{\rm FORM} + & 0.330^*{\rm ALD2} + \\ 0.010^*{\rm XO_2} {\rm N} + 0.200^*{\rm PAR} + & 0.100^*{\rm OH} \\ {\rm 0.800^*{\rm FORM} + & 0.330^*{\rm ALD2} + \\ 0.180^*{\rm ALD2} + & 0.200^*{\rm XO_2} + & 0.950^*{\rm HO_2} - \\ {\rm 0.700^*{\rm PAR} & 0.180^*{\rm ALD2} + \\ 0.330^*{\rm CO} + {\rm 0.440^*{\rm HO_2} - 1.000^*{\rm OH} \\ {\rm 0.330^*{\rm CO} + 0.440^*{\rm HO_2} - 1.000^*{\rm PAR} \\ \\ 0.180^*{\rm ALD2} + & 0.300^*{\rm ALD2} + \\ 0.090^*{\rm XO_2} + 0.220^*{\rm XO_2} {\rm NO_2} + \\ {\rm 0.950^*{\rm ALDX} + 0.300^*{\rm ALD2} + \\ 0.950^*{\rm ALDX} + \\ 0.560^*{\rm ALDX} + 0.350^*{\rm ALD2} - 1.000^*{\rm PAR} \\ \end{array} \right $
$\begin{array}{rcl} AAA + OIT & \rightarrow & ALD2 + OI20^{\circ} AAACD + 0.200^{\circ} AAACD + 0.200^{\circ} O_3 & 4.3E + 13^{\circ} exp(1040/T) \\ CXO_3 + MEO_2 & \rightarrow & 0.900^{\circ} ALD2 + 0.900^{\circ} XO_2 + HO_2 + \\ CXO_3 + XO_2 & \rightarrow & 0.900^{\circ} ALD2 + 0.100^{\circ} FORM & 2.0E - 12^{\circ} exp(500/T) \\ CXO_3 + CXO_3 & \rightarrow & 2.000^{\circ} ALD2 + 2.000^{\circ} XO_2 + 2.000^{\circ} HO_2 & 2.9E + 12^{\circ} exp(500/T) \\ CXO_3 + C_2O_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E + 12^{\circ} exp(500/T) \\ CXO_3 + C_2O_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E + 12^{\circ} exp(500/T) \\ 0.870^{\circ} XO_2 + 0.130^{\circ} XO_2 N + 0.110^{\circ} HO_2 + \\ PAR + OH & \rightarrow & 0.060^{\circ} ALD2 - 0.110^{\circ} PAR + 0.760^{\circ} ROR + \\ 0.500^{\circ} ALDX & 0.960^{\circ} XO_2 + 0.600^{\circ} ALD2 + 0.940^{\circ} HO_2 - \\ ROR & \rightarrow & 2.100^{\circ} PAR + 0.040^{\circ} XO_2 N + 0.020^{\circ} ROR + \\ 0.500^{\circ} ALDX & 1.5E + 11 \\ 0.200^{\circ} ALDX & 1.5E + 11 \\ 0.200^{\circ} ALD2 + 0.200^{\circ} CO + 0.200^{\circ} FORM + \\ 0.101^{\circ} XO_2 N + 0.200^{\circ} PAR + 0.100^{\circ} OH + \\ 0.800^{\circ} FORM + & 0.300^{\circ} ALD2 + \\ O + OLE & \rightarrow & 0.620^{\circ} ALDX + 0.200^{\circ} PAR + 0.100^{\circ} OH + \\ 0.100^{\circ} XO_2 N + 0.200^{\circ} PAR + 0.100^{\circ} OH + \\ 0.100^{\circ} XO_2 N + 0.200^{\circ} PAR + 0.100^{\circ} OH + \\ 0.100^{\circ} XO_2 N + 0.200^{\circ} PAR + 0.100^{\circ} OH + \\ 0.300^{\circ} COH + 0.200^{\circ} ALDX + 0.200^{\circ} FORM + \\ 0.300^{\circ} COH + 0.910^{\circ} XO_2 N + 0.100^{\circ} OH + \\ 0.300^{\circ} COH + 0.910^{\circ} XO_2 + 0.900^{\circ} XO_2 N + \\ 0.500^{\circ} ALDX + 0.300^{\circ} ALD2 + 0.100^{\circ} PAR + \\ 0.500^{\circ} ALDX + 0.200^{\circ} XO_2 N + \\ 0.500^{\circ} ALDX + 0.300^{\circ} XO_2 N + \\ 0.500^{\circ} ALDX + 0.300^{\circ} XO_2 N + \\ 0.500^{\circ} ALDX + 0.200^{\circ} XO_2 N + \\ 0.500^{\circ} ALDX + 0.300^{\circ} XO_2 N + \\ 0.500^{\circ} A$
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$\begin{array}{rcl} CXO_3 + RO_2 & \rightarrow & 2.000^* ALD2 + 2.000^* XO_2 + 2.000^* HO_2 & 2.9E-12^* exp(500/T) \\ CXO_3 + C_2O_3 & \rightarrow & MEO_2 + XO_2 + HO_2 + ALD2 & 2.9E-12^* exp(500/T) \\ 0.870^* XO_2 + & 0.130^* XO_2 N + & 0.110^* HO_2 + \\ PAR + OH & \rightarrow & 0.060^* ALD2 - & 0.110^* PAR + & 0.760^* ROR + \\ & 0.050^* ALDX & 0.960^* XO_2 + & 0.020^* ROR + \\ & 0.960^* XO_2 + & 0.600^* ALD2 + & 0.940^* HO_2 - \\ ROR & \rightarrow & 2.100^* PAR + & 0.040^* XO_2 N + & 0.020^* ROR + \\ & 0.500^* ALDX & 0.960^* XO_2 N + & 0.020^* ROR + \\ & 0.500^* ALDX & 0.200^* ROR + \\ ROR & \rightarrow & HO_2 & 1.6E+3 \\ ROR + NO_2 & \rightarrow & NTR & 1.5E-11 \\ & 0.200^* ALD2 + & 0.300^* ALDX + & 0.300^* HO_2 + \\ O + OLE & \rightarrow & 0.200^* XO_2 + & 0.200^* CO + & 0.200^* FORM + \\ & 0.10^* XO_2 N + & 0.200^* PAR + & 0.100^* OH \\ & 0.800^* FORM + & 0.330^* ALD2 + \\ OH + OLE & \rightarrow & 0.620^* ALDX + & 0.800^* XO_2 + & 0.950^* HO_2 - \\ & 0.700^* PAR & 0.180^* ALD2 + & 0.740^* FORM + \\ O_3 + OLE & \rightarrow & 0.320^* ALDX + & 0.220^* XO_2 + & 0.100^* OH \\ & 0.330^* CO + & 0.440^* HO_2 - 1.000^* PAR \\ NO_3 + OLE & \rightarrow & NO_2 + FORM + & 0.910^* XO_2 + & 0.900^* XO_2 N + \\ & NO_3 + OLE & \rightarrow & 0.560^* ALDX + & 0.350^* ALD2 - 1.000^* PAR \\ NO_3 + OLE & \rightarrow & 0.560^* ALDX + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.910^* XO_2 + & 0.900^* XO_2 N + \\ & 0.560^* ALDX + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.910^* XO_2 + & 0.900^* XO_2 N + \\ & 0.560^* ALDX + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.910^* XO_2 + & 0.900^* XO_2 N + \\ & 0.560^* ALDX + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.910^* XO_2 + & 0.900^* XO_2 N + \\ & 0.560^* ALDX + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.910^* XO_2 + & 0.900^* XO_2 N + \\ & 0.560^* ALDX + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.910^* XO_2 + & 0.900^* XO_2 N + \\ & 0.560^* ALDX + & 0.350^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.910^* XO_2 + & 0.900^* XO_2 N + \\ & 0.560^* ALDX + & 0.550^* ALD2 - 1.000^* PAR \\ & NO_2 + FORM + & 0.9$
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$\begin{array}{rcl} \text{ROR} & \rightarrow & \text{HO}_2 & 1.6\text{E}+3 \\ \text{ROR} & \rightarrow & \text{NTR} & 1.5\text{E}-11 \\ & 0.200^*\text{ALD2} + 0.300^*\text{ALD2} + 0.300^*\text{ROR} + \\ & 0.200^*\text{ALD2} + 0.300^*\text{ALD2} + 0.200^*\text{FORM} + \\ & 0.200^*\text{ALD2} + 0.200^*\text{FORM} + \\ & 0.010^*\text{XO}_2\text{N} + 0.200^*\text{FORM} + \\ & 0.800^*\text{FORM} + \\ & 0.300^*\text{FORM} + \\ & 0.300^*\text{ALD2} + \\ \text{OH} + \text{OLE} & \rightarrow & 0.620^*\text{ALDX} + 0.800^*\text{XO}_2 + 0.950^*\text{HO}_2 - \\ & 0.700^*\text{PAR} \\ & 0.180^*\text{ALD2} + \\ & 0.700^*\text{PAR} \\ & 0.180^*\text{ALD2} + \\ & 0.320^*\text{ALDX} + 0.220^*\text{XO}_2 + 0.100^*\text{OH} + \\ & 0.320^*\text{ALDX} + 0.220^*\text{XO}_2 + 0.100^*\text{OH} + \\ & 0.330^*\text{CO} + 0.440^*\text{HO}_2 - 1.000^*\text{PAR} \\ & \text{NO}_3 + \text{OLE} & \rightarrow & \frac{\text{NO}_2 + \text{FORM} + 0.910^*\text{XO}_2 + 0.090^*\text{XO}_2\text{N} + \\ & 0.560^*\text{ALDX} + 0.350^*\text{ALD2} - 1.000^*\text{PAR} \\ \end{array}$
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$\begin{array}{cccc} 0.180^* ALD2+ & 0.740^* FORM+ \\ O_3 + OLE & \rightarrow & 0.320^* ALDX+ & 0.220^* XO_2 + & 0.100^* OH + & 6.5E-15^* exp(T/1900) \\ & & 0.330^* CO + & 0.440^* HO_2 - & 1.000^* PAR \\ NO_3 + OLE & \rightarrow & \frac{NO_2 + FORM + & 0.910^* XO_2 + & 0.090^* XO_2N + }{0.560^* ALDX + & 0.350^* ALD2 - & 1.000^* PAR } & 7.0E-13^* exp(T/2160) \end{array}$
$\begin{array}{llllllllllllllllllllllllllllllllllll$
NO ₃ + OLE $\rightarrow \begin{cases} 0.330*CO+0.440*HO_2 - 1.000*PAR \\ NO_2 + FORM + 0.910*XO_2 + 0.090*XO_2N + \\ 0.560*ALDX + 0.350*ALD2 - 1.000*PAR \end{cases}$ 7.0E-13*exp(T/2160)
$NO_3 + OLE \rightarrow \frac{NO_2 + FORM + 0.910^* XO_2 + 0.090^* XO_2 N +}{0.560^* ALDX + 0.350^* ALD2 - 1.000^* PAR} 7.0E-13^* exp(T/2160)$
0.560*ALDX + 0.350*ALD2 - 1.000*PAR
$O + ETH \rightarrow FORM + 1.700 * HO_2 + CO + 0.700 * XO_2 + 1.04E - 11 * exp(T/792)$
0.300*OH
$OH + ETH \rightarrow XO_2 + 1.560*FORM + 0.220*ALDX + HO_2 K_0 = 1.0E-28*exp(300/T)^{0.6}$
$K_{\infty} = 8.8E - 12$
$O_3 + ETH \rightarrow 1.0630 \times CO^+ 0.130 \times HO_2 + 1.2E \cdot 14 \times exp(T/2630)$
$0.130 \times OH + 0.3 / 0^{+} FACD$ 2.2E 12*-cm (7/280)
$NO_3 + ETH \rightarrow NO_2 + XO_2 + ZO^* FORM$ 5.3E-12*exp(1/2880)
IOLE + O \rightarrow 0.100*VO + 0.100*PADA 0.100*PADA 2.3E-11
$0.100^{\circ} AO_2^{\circ} + 0.100^{\circ} CO^{\circ} 0.100^{\circ} rAK$
$IULE + UE \rightarrow I.JUU^{(ALD_2 + U, UU^{(ALD_A + EU)} + AU)} + AU^{(ALD_A + EU)} + AU^{(ALD_A + EU)}$
$0.650* \Delta I D^2 + 0.350* \Delta I D^2 +$
$0.650^{*}ALD2 + 0.350^{*}ALDX + 0.250^{*}CO + 0.500^{*}O - 8.4F_{-}15^{*}exp(T/1100)$

Table S2: Continued from previous page

Reactants		Products	Rate expression
$IOLE + NO_3$	\rightarrow	1.180*ALD2 + 0.640*ALDX + HO ₂ + NO ₂	9.6E-13*exp(T/270)
		0.440*HO ₂ + 0.080*XO ₂ + 0.360*CRES +	1 0F 10* (255/TF)
TOL + OH	\rightarrow	$0.560*TO_2 + 0.765*TOLRO_2$	$1.8E-12^{*}\exp(355/1)$
$TO_2 + NO$	\rightarrow	0.900*NO ₂ + 0.900*HO ₂ + 0.900*OPEN + 0.100*NTR	8.1E-12
TO	\rightarrow	$CRES + HO_2$	4.2
102	/	0.400° CRO + 0.600° XO ₂ + 0.600° HO ₂ +	
OH + CRES	\rightarrow	0.300*OPEN	4.1E-11
$CRES + NO_3$	\rightarrow	$CRO + HNO_3$	2.2E-11
$CRO + NO_2$	\rightarrow	NTR	1.4E-11
$CRO + HO_2$	\rightarrow	CRES	5.5E-12
		$XO_2 + 2.000*CO + 2.000*HO_2 + C_2O_3 +$	2 OF 11
OPEN + OH	\rightarrow	FORM	3.0E-11
		$0.030^{*}ALDX + 0.620^{*}C_{2}O_{3} +$	
$OPEN + O_3$	\rightarrow	$0.700*FORM + 0.030*XO_2 + 0.690*CO +$	5.4E-17*exp(T/500)
		0.080*OH + 0.760*HO ₂ + 0.200*MGLY	
		$0.700*HO_2 + 0.500*XO_2 + 0.200*CRES +$	
OH + XYL	\rightarrow	$0.800*MGLY + 1.100*PAR + 0.300*TO_2 +$	1.7E-11*exp(116/T)
		$0.804*XYLRO_2$	
OH + MGLY	\rightarrow	$XO_2 + C_2O_3$	1.8E-11
O + ISOP	\rightarrow	0.750*ISPD + $0.500*$ FORM + $0.250*$ XO ₂	3.6E-11
		$+ 0.250*HO_2 + 0.250*CXO_3 + 0.250*PAR$	
OH + ISOP	\rightarrow	$0.912*15PD + 0.029*FOKM + 0.991*AO_2$	2.54E-11*exp(407.6/T)
		$+ 0.912*HO_2 + 0.088*AO_2N + 150PKAN 0.650*ISPD + 0.600*EORM + 0.200*XO_2$	-
O I ISOD	,	$+ 0.066*HO_{2} + 0.266*OH + 0.200*CVO_{2}$	7.86E 15*exp(T/1012)
$0_3 + 150P$	\rightarrow	$+ 0.000^{\circ} \text{HO}_2 + 0.200^{\circ} \text{OH} + 0.200^{\circ} \text{CAO}_3 + 0.150^{\circ} \text{ALDY} + 0.250^{\circ} \text{DAP} + 0.066^{\circ} \text{CO}$	$7.80E-13^{-1}\exp(1/1912)$
		$0.150^{\circ}\text{ALDA} + 0.550^{\circ}\text{FAR} + 0.000^{\circ}\text{CO}$ $0.200^{\circ}\text{ISPD} + 0.800^{\circ}\text{NTR} + XO_{2} + 0.000^{\circ}\text{CO}$	
$NO_2 \pm ISOP$	_	$0.800*HO_2 + 0.200*NO_2 + 0.800*AUDX +$	3.03E-12*exp(T/448)
103 + 1501		2 400*PAR	5.05E 12 exp(1/110)
		$1.565*PAR + 0.167*FORM + 0.713*XO_2 +$	
		$0.503*HO_2 + 0.334*CO + 0.168*MGLY +$	2.2/E 11
OH + ISPD	\rightarrow	$0.252*ALD2 + 0.210*C_2O_3 + 0.250*CXO_3$	3.36E-11
		+ 0.120*ALDX	
		0.114*C ₂ O ₃ + 0.150*FORM +	
		0.850*MGLY + 0.154*HO ₂ + 0.268*OH +	7 1E 19
$O_3 + ISPD$	\rightarrow	0.064*XO ₂ + 0.020*ALD2 + 0.360*PAR +	/.IE-18
		0.225*CO	
		0.357*ALDX + 0.282*FORM + 1.282*PAR	
$NO_3 + ISPD$	\rightarrow	$+ 0.925*HO_2 + 0.643*CO + 0.850*NTR +$	1.0E-15
		$0.075 * CXO_3 + 0.075 * XO_2 + 0.150 * HNO_3$	
TERP + O	\rightarrow	0.150*ALDX + 5.12*PAR + TRPRXN	3.6E-11
		$0.750*HO_2 + 1.250*XO_2 + 0.250*XO_2N +$	
TERP + OH	\rightarrow	0.280*FORM + 1.66* PAR + 0.470*ALDX	1.5E-11*exp(449/T)
		+ TRPRXN	
		$0.5/0^{\circ}OH + 0.0/0^{\circ}HO_2 + 0./60^{\circ}XO_2 + 0.180^{\circ}XO_1 + 0.240^{\circ}EODM + 0.001^{\circ}CO$	
TERP + O ₃	\rightarrow	$0.180^{+}AO_{2}N + 0.240^{+}FOKM + 0.001^{+}CO + 7.000^{+}DAD + 0.210^{+}ALDN + 0.200^{+}CNO$	1.2E-15*exp(T/821)
- 5		7.000*PAK + 0.210*ALDA + 0.390*CAO ₃	L × /
		+ 1 Kr KAN 0 470*NO2 + 0 280*HO2 + 1 020*VO	
TEDD I NO		$0.250*XO_2N \pm 0.470*AUDY \pm 0.520*NTP$	$3.7E_{-}12*exp(175/T)$
$1 \text{EKP} + \text{NO}_3$	\rightarrow	+ TRPRXN	$5.12^{-12} \exp(1/5/1)$

Table S2: Continued from previous page

Reactants		Products	Rate expression
$SO_2 + OH$	\rightarrow	$SULF + HO_2 + SULRXN$	K_0 = 3.0E-31*exp(300/T) ^{3.3} K_{∞} = 1.5E-12
OH + ETOH	\rightarrow	HO ₂ + 0.900*ALD2 + 0.050*ALDX + 0.100*FORM + 0.100*XO ₂	6.9E-12*exp(T/230)
OH + ETHA	\rightarrow	0.991*ALD2 + 0.991*XO ₂ + 0.009*XO ₂ N + HO ₂	8.7E-12*exp(T/1070)
$NO_2 + ISOP$	\rightarrow	0.200 [*] ISPD + 0.800*NTR + XO ₂ + 0.800*HO ₂ + 0.200*NO + 0.800*ALDX + 2.400*PAR	1.5E-19

Table S2: Continued from previous page

Reactants		Products
NO ₂ +hv	\rightarrow	NO + O
O ₃ +hv	\rightarrow	0
O ₃ +hv	\rightarrow	O ¹ D
NO ₃ +hv	\rightarrow	$NO_2 + O$
NO ₃ +hv	\rightarrow	NO
HONO +hv	\rightarrow	NO + OH
H_2O_2 +hv	\rightarrow	2.000*OH
PNA +hv	\rightarrow	$0.610*HO_2 + 0.610*NO_2 + 0.390*OH+$ 0.390*NO ₂
HNO ₃ +hv	\rightarrow	$OH + NO_2$
N2O5 +hv	\rightarrow	$NO_2 + NO_3$
NTR +hv	\rightarrow	NO ₂ + HO ₂ + 0.330*FORM+ 0.330*ALD2+ 0.330*ALDX- 0.660*PAR
FORM +hv	\rightarrow	$2.000*HO_2 + CO$
FORM +hv	\rightarrow	СО
ALD2 +hv	\rightarrow	$MEO_2 + CO + HO_2$
PAN +hv	\rightarrow	$C_2O_3 + NO_2$
PANX +hv	\rightarrow	$CXO_3 + NO_2$
PACD +hv	\rightarrow	$MEO_2 + OH$
ALDX +hv	\rightarrow	$MEO_2 + CO + HO_2$

Table S3: Photolysis reactions applied in the NMMB/BSC-CTM

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