Supporting Information:

Comprehensive Treatment of C_4-C_6 Alkanes and Their Oxidation Products in CAM-chem: The MOZART-T3 Mechanism

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Table S1. Kinetic reactions added in MOZART-T3 mechanism. Mechanism label denotes the reaction tag used in CAM-chem reaction files. Details can be found in Sect. 2.

Mechanism label	Reactants		Products	Rate	Reference
			C_1		
CH3O2_NO3	CH3O2 + NO3	→	CH2O + NO2 + HO2	8.90E-12 exp(-600/T)	Jenkin et al. (2019)
			C_2		
usr_C2H5O2_NOa	C2H5O2 + NO	→	CH3CHO + HO2 + NO2	2.60E-12 exp(365/T) * (1 - **α**)	JPL19; Jenkin et al. (2019)
usr_C2H5O2_NOn	C2H5O2 + NO	→	ALKNIT	2.60E-12 exp(365/T) * **α**	JPL19; Jenkin et al. (2019)
C2H5O2_NO3	C2H5O2 + NO3	→	CH3CHO + NO2 + HO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
CH3CO3_NO3	CH3CO3 + NO3	→	CH3O2 + CO2 + NO2	8.90E-12 exp(-305/T)	Jenkin et al. (2019)
CH3CO3_HO2a	CH3CO3 + HO2	→	CH3COOOH	1.50E-12 exp(480/T)	IUPAC
CH3CO3_HO2b	CH3CO3 + HO2	→	CH3COOH + O3	4.40E-15 exp(1910/T)	IUPAC
CH3CO3_HO2c	CH3CO3 + HO2	→	CH3O2 + CO2 + OH	4.66E-12 exp(235/T)	IUPAC
			C_3		
C3H8_OH_N	C3H8 + OH	→	NC3H7O2 + H2O	1.06E-11 exp(-1071/T)	IUPAC; Droege and Tully (1986)
C3H8_OH_I	C3H8 + OH	→	IC3H7O2 + H2O	3.40E-12 exp(-442/T)	IUPAC; Droege and Tully (1986)
usr_NC3H7O2_NOa	NC3H7O2 + NO	→	PROPANAL + NO2 + HO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_NC3H7O2_NOn	NC3H7O2 + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
usr_IC3H7O2_NOa	IC3H7O2 + NO	→	CH3COCH3 + NO2 + HO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_IC3H7O2_NOn	IC3H7O2 + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
NC3H7O2_HO2	NC3H7O2 + HO2	→	NC3H7OOH	1.41E-13 exp(1300/T)	Wennberg et al. (2018)
IC3H7O2_HO2	IC3H7O2 + HO2	→	IC3H7OOH	1.41E-13 exp(1300/T)	Wennberg et al. (2018)
NC3H7O2_CH3O2	NC3H7O2 + CH3O2	→	0.80*CH2O + 0.80*PROPANAL + 0.20*PROPANOL + 1.2*HO2 + 0.20*CH3OH	1.00E-13 exp(557/T)	IUPAC; Jenkin et al. (2019)
IC3H7O2_CH3O2	IC3H7O2 + CH3O2	→	PROPANAL + HO2 + CH3O2 + CO2	100E-13 exp(-293/T)	IUPAC; Jenkin et al. (2019)
NC3H7O2_CH3CO3	NC3H7O2 + CH3CO3	→	0.80*CH2O + 0.80*PROPANAL + 0.20*PROPANOL + 1.2*HO2 + 0.20*CH3OH	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
IC3H7O2_CH3CO3	IC3H7O2 + CH3CO3	→	CH3COCH3 + HO2 + CH3O2 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
NC3H7O2_NO3	NC3H7O2 + NO3	→	PROPANAL + NO2 + HO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
IC3H7O2_NO3	IC3H7O2 + NO3	→	CH3COCH3 + NO2 + HO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
NC3H7OOH_OH	NC3H7OOH + OH	→	H2O + NC3H7O2	1.90E-12 exp(190/T)	MCMv3.3.1
NC3H7OOH_OH_C	NC3H7OOH + OH	→	H2O + PROPANAL + OH	1.10E-11	MCMv3.3.1
IC3H7OOH_OH	IC3H7OOH + OH	→	H2O + IC3H7O2	1.90E-12 exp(190/T)	MCMv3.3.1

IC3H7OOH_OH_C	IC3H7OOH + OH	→	H2O + CH3COCH3 + OH	1.66E-11	MCMv3.3.1
PROPANAL_OH	PROPANAL + OH	→	C2H5CO3 + H2O	4.80E-12 exp(405/T)	Calvert et al. (2015)
PROPANOL_OH	PROPANOL + OH	→	PROPANAL + HO2 + H2O	4.60E-12 exp(70/T)	IUPAC
IPROPANOL_OH	IPROPANOL + OH	→	CH3COCH3 + HO2 + H2O	2.60E-12 exp(200/T)	IUPAC
tag_C2H5CO3_NO2	C2H5CO3 + NO2 + M	→	PPN + M	9.6e-28, 8.9, 7.7e-12, 0.2, 0.6	JPL19
usr_PPN_M	PPN + M	→	C2H5CO3 + NO2 + M	9.0e-29 exp(14000/T)	JPL19
C2H5CO3_HO2a	C2H5CO3 + HO2	→	CH3COOOH	1.50E-12 exp(480/T)	IUPAC (same as CH3CO3 + HO2)
C2H5CO3_HO2b	C2H5CO3 + HO2	→	CH3COOH + O3	4.40E-15 exp(1910/T)	IUPAC (same as CH3CO3 + HO2)
C2H5CO3_HO2c	C2H5CO3 + HO2	→	C2H5O2 + CO2 + OH	4.66E-12 exp(235/T)	IUPAC (same as CH3CO3 + HO2)
C2H5CO3_NO	C2H5CO3 + NO	→	C2H5O2 + NO2 + CO2	6.70E-12 exp(340/T)	IUPAC for C2H5CO3
C2H5CO3_CH3O2	C2H5CO3 + CH3O2	→	C2H5O2 + HO2 + CH2O + CO2	2.00E-12 exp(500/T)	JPL19 (Same as CH3CO3 + CH3O2)
C2H5CO3_CH3CO3	C2H5CO3 + CH3CO3	→	C2H5O2 + CH3O2 + 2*CO2	2.90E-12 exp(500/T)	JPL19 (Same as CH3CO3 + CH3CO3)
C2H5CO3_NO3	C2H5CO3 + NO3	→	C2H5O2 + CO2 + NO2	8.90E-12 exp(-305/T)	Jenkin et al. (2019)
			C_4		
NBUTANE_OH_N	NBUTANE + OH	→	NBUPO2 + H2O	6.89E-12 exp(-893/T)	IUPAC; Droege and Tully (1986)
NBUTANE_OH_I	NBUTANE + OH	→	NBUO2 + H2O	6.76E-12 exp(-362/T)	IUPAC; Droege and Tully (1986)
ISOBUTANE_OH	ISOBUTANE + OH	→	TBUO2 + H2O	7.00E-12 exp(-350/T)	Calvert et al. (2008)
NBUPO2_HO2	NBUPO2 + HO2	→	NBUPOOH	1.70E-13 exp(1300/T)	Wennberg et al. (2018)
NBUO2_HO2	NBUO2 + HO2	→	NBUOOH	1.70E-13 exp(1300/T)	Wennberg et al. (2018)
TBUO2_HO2	TBUO2 + HO2	→	TBUOOH	1.70E-13 exp(1300/T)	Wennberg et al. (2018)
usr_NBUPO2_NOa	NBUPO2 + NO	→	NBUPO + NO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_NBUPO2_NOn	NBUPO2 + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
usr_NBUO2_NOa	NBUO2 + NO	→	NBUO + NO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_NBUO2_NOn	NBUO2 + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
usr_TBUO2_NOa	TBUO2 + NO	→	CH3O2 + CH3COCH3 + NO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_TBUO2_NOn	TBUO2 + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
NBUPO2_CH3O2	NBUPO2 + CH3O2	→	NBUPO + CH2O + HO2	6E-14 exp(600/T)	IUPAC; Glover and Miller (2005); Jenkin et al. (2019)
NBUPO2_CH3O2_2	NBUPO2 + CH3O2	→	BUTANAL + 0.5*CH3OH + 0.5*CH2O	4E-14 exp(600/T)	IUPAC; Glover and Miller (2005); Jenkin et al. (2019)
NBUO2_CH3O2	NBUO2 + CH3O2	→	NBUO + CH2O + HO2	6E-14 exp(340/T)	IUPAC; Glover and Miller (2005); Jenkin et al. (2019)
NBUO2_CH3O2_2	NBUO2 + CH3O2	→	0.5*BUTOL2 + 0.5*MEK + 0.5*CH3OH + 0.5*CH2O	4E-14 exp(340/T)	IUPAC; Glover and Miller (2005); Jenkin et al. (2019)
TBUO2_CH3O2	TBUO2 + CH3O2	→	CH3O2 + CH3COCH3 + CH2O + HO2	3.04E-13 exp(-1430/T)	IUPAC; Jenkin et al. (2019)
TBUO2_CH3O2_2	TBUO2 + CH3O2	→	TBUOH + CH2O	7.60E-14 exp(-1430/T)	IUPAC; Jenkin et al. (2019)
NBUPO2_CH3CO3	NBUPO2 + CH3CO3	→	NBUPO + CH3O2 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
NBUO2_CH3CO3	NBUO2 + CH3CO3	→	NBUO + CH3O2 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)

TBUO2_CH3CO3	TBUO2 + CH3CO3	→	2*CH3O2 + CH3COCH3 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
NBUPO2_NO3	NBUPO2 + NO3	→	NBUPO + NO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
NBUO2_NO3	NBUO2 + NO3	→	NBUO + NO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
TBUO2_NO3	TBUO2 + NO3	→	CH3O2 + CH3COCH3 + NO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
NBUPO_O2	NBUPO + O2	→	BUTANAL + HO2	2.50E-14 exp(-300/T)	Atkinson (2007)
NBUO_O2	NBUO + O2	→	MEK + HO2	2.50E-14 exp(-300/T)	Atkinson (2007)
NBUPO_I	NBUPO	→	NBUPOHO2	1.20E+11 exp(-3825/T)	Atkinson (2007)
usr_NBUO	NBUO	→	CH3CHO + C2H5O2	1.12E+9 T^(1.7) exp(-6139.3/T)	Vereecken and Peeters (2009)
NBUPOHO2_HO2	NBUPOHO2 + HO2	→	NBUPOOH	1.93E-13 exp(1300/T)	Wennberg et al. (2018)
usr_NBUPOHO2_NOa	NBUPOHO2 + NO	→	OHBUTANAL + HO2 + NO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_NBUPOHO2_NOn	NBUPOHO2 + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
NBUPOHO2_CH3O2	NBUPOHO2 + CH3O2	→	OHBUTANAL + 2*HO2 + CH2O	6E-14 exp(600/T)	Same as NBUPO2
NBUPOHO2_CH3O2_2	NBUPOHO2 + CH3O2	→	OHBUTANAL + 0.5*CH3OH + 0.5*CH2O	4E-14 exp(600/T)	Same as NBUPO2
NBUPOHO2_CH3CO3	NBUPOHO2 + CH3CO3	→	OHBUTANAL + HO2 + CH3O2 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
NBUPOHO2_NO3	NBUPOHO2 + NO3	→	OHBUTANAL + HO2 + NO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
NBUPOOH_OH	NBUPOOH + OH	→	NBUPO2 + H2O	1.90E-12 exp(190/T)	MCMv3.3.1
NBUPOOH_OH_C	NBUPOOH + OH	→	BUTANAL + H2O + OH	1.24E-11	MCMv3.3.1
NBUOOH_OH	NBUOOH + OH	→	NBUO2 + H2O	1.90E-12 exp(190/T)	MCMv3.3.1
NBUOOH_OH_C	NBUOOH + OH	→	MEK + H2O + OH	2.15E-11	MCMv3.3.1
TBUOOH_OH	TBUOOH + OH	→	TBUO2 + H2O	7.00E-13 exp(485/T)	Baasandorj et al. (2010)
BUTANAL_OH	BUTANAL + OH	→	NC3H7O2 + CO2	5.97E-12 exp(411/T)	Calvert et al. (2015)
OHBUTANAL_OH	OHBUTANAL + OH	→	NC3H7O2 + CO2	2.95E-11	Calvert et al. (2015) (Same as 3-hydroxy butanal)
BUTOL2_OH	BUTOL2 + OH	→	MEK + HO2 + H2O	2.70E-12 exp(329/T)	Calvert et al. (2015)
TBUOH_OH	TBUOH + OH	→	CH3COCH3 + CH2O + HO2 + H2O	1.60E-12 exp(-124/T)	Calvert et al. (2015)
			C_5		
NPENTANE_OH_A	NPENTANE + OH	→	NPENTO2A + H2O	7.40E-12 exp(-452/T)	Calvert et al. (2015)
NPENTANE_OH_B	NPENTANE + OH	→	NPENTO2B + H2O	1.07E-11 exp(-452/T)	Calvert et al. (2015)
IPENTANE_OH_A	IPENTANE + OH	→	IPENTO2A + H2O	6.45E-12 exp(-296/T)	Calvert et al. (2015)
IPENTANE_OH_B	IPENTANE + OH	→	IPENTO2B + H2O	3.65E-12 exp(-296/T)	Calvert et al. (2015)
NPENTO2A_HO2	NPENTO2A + HO2	→	NPENTOOHA	1.93E-13 exp(1300/T)	Wennberg et al. (2018)
NPENTO2B_HO2	NPENTO2B + HO2	→	NPENTOOHB	1.93E-13 exp(1300/T)	Wennberg et al. (2018)
IPENTO2A_HO2	IPENTO2A + HO2	→	IPENTOOHA	1.93E-13 exp(1300/T)	Wennberg et al. (2018)
IPENTO2B_HO2	IPENTO2B + HO2	→	IPENTOOHB	1.93E-13 exp(1300/T)	Wennberg et al. (2018)
usr_NPENTO2A_NOa	NPENTO2A + NO	→	NPENTOA + NO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_NPENTO2A_NOn	NPENTO2A + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)

usr_NPENTO2B_NOa	NPENTO2B + NO	→	NPENTOB + NO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_NPENTO2B_NOn	NPENTO2B + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
usr_IPENTO2A_NOa	IPENTO2A + NO	→	CH3COCH3 + C2H5O2 + NO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_IPENTO2A_NOn	IPENTO2A + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
usr_IPENTO2B_NOa	IPENTO2B + NO	→	IPENTOB + NO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_IPENTO2B_NOn	IPENTO2B + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
NPENTO2A_CH3O2	NPENTO2A + CH3O2	→	NPENTOA + CH2O + HO2	6E-14 exp(228/T)	IUPAC; Jenkin et al. (2019)
NPENTO2A_CH3O2_2	NPENTO2A + CH3O2	→	0.5*CH3OH + 0.5*CH2O + 0.5*PENTANONE3 + 0.5*PENTANOL3	4E-14 exp(228/T)	IUPAC; Jenkin et al. (2019)
NPENTO2B_CH3O2	NPENTO2B + CH3O2	→	NPENTOB + CH2O + HO2	6E-14 exp(228/T)	IUPAC; Jenkin et al. (2019)
NPENTO2B_CH3O2_2	NPENTO2B + CH3O2	→	0.5*CH3OH + 0.5*CH2O + 0.5*PENTANONE2 + 0.5*PENTANOL2	4E-14 exp(228/T)	IUPAC; Jenkin et al. (2019)
IPENTO2A_CH3O2	IPENTO2A + CH3O2	→	CH3COCH3 + C2H5O2 + CH2O + HO2	3.04E-13 exp(-1430/T)	Same as TBUO2 + CH3O2
IPENTO2A_CH3O2_2	IPENTO2A + CH3O2	→	IPENTOL + CH2O	7.60E-14 exp(-1430/T)	Same as TBUO2 + CH3O2
IPENTO2B_CH3O2	IPENTO2B + CH3O2	→	IPENTOB + CH2O + HO2	6E-14 exp(228/T)	IUPAC (CH3O2 self); Jenkin et al. (2019) (sec-C4H9O2 self)
IPENTO2B_CH3O2_2	IPENTO2B + CH3O2	→	0.5*CH3OH + 0.5*CH2O + 0.5*M2BUTOL + 0.5*NELSON	4E-14 exp(228/T)	IUPAC (CH3O2 self); Jenkin et al. (2019) (sec-C4H9O2 self)
NPENTO2A_CH3CO3	NPENTO2A + CH3CO3	→	NPENTOA + CH3O2 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
NPENTO2B_CH3CO3	NPENTO2B + CH3CO3	→	NPENTOB + CH3O2 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
IPENTO2A_CH3CO3	IPENTO2A + CH3CO3	→	CH3COCH3 + C2H5O2 + CH3O2 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
IPENTO2B_CH3CO3	IPENTO2B + CH3CO3	→	NPENTOB + CH3O2 + CO2	4.4E-13 exp(1070/T)	IUPAC (Same as C2H5O2 + CH3CO3)
NPENTO2A_NO3	NPENTO2A + NO3	→	NPENTOA + NO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
NPENTO2B_NO3	NPENTO2B + NO3	→	NPENTOB + NO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
IPENTO2A_NO3	IPENTO2A + NO3	→	CH3COCH3 + C2H5O2 + NO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
IPENTO2B_NO3	IPENTO2B + NO3	→	IPENTOB + NO2	8.90E-12 exp(-390/T)	Jenkin et al. (2019)
NPENTOA_O2	NPENTOA + O2	→	PENTANONE3 + HO2	2.50E-14 exp(-300/T)	Atkinson (2007)
NPENTOB_O2	NPENTOB + O2	→	PENTANONE2 + HO2	2.50E-14 exp(-300/T)	Atkinson (2007)
IPENTOB_O2	IPENTOB + O2	→	NELSON + HO2	2.50E-14 exp(-300/T)	Atkinson (2007)
usr_NPENTOA	NPENTOA	→	PROPANAL + C2H5O2	2.24E+9 T^(1.7) exp(-6139.3/T)	Vereecken and Peeters (2009)
NPENTOB_I	NPENTOB	→	HYDROXYKETONE + HO2	1.20E+11 exp(-3825/T)	Atkinson (2007)
usr_IPENTOB	IPENTOB	→	CH3CHO + IC3H7O2	1.12E+9 T^(1.7) exp(-4428.3/T)	Vereecken and Peeters (2009)
NPENTOOHA_OH	NPENTOOHA + OH	→	NPENTO2A + H2O	1.90E-12 exp(190/T)	MCMv3.3.1

NPENTOOHA_OH_C	NPENTOOHA + OH	→	PENTANONE3 + H2O + OH	2.73E-11	MCMv3.3.1
NPENTOOHB_OH	NPENTOOHB + OH	→	NPENTO2B + H2O	1.90E-12 exp(190/T)	MCMv3.3.1
NPENTOOHB_OH_C	NPENTOOHB + OH	→	PENTANONE2 + H2O + OH	2.30E-11	MCMv3.3.1
IPENTOOHA_OH	IPENTOOHA + OH	→	IPENTO2A + H2O	5.25E-12	MCMv3.3.1
IPENTOOHB_OH	IPENTOOHB + OH	→	IPENTO2B + H2O	1.90E-12 exp(190/T)	MCMv3.3.1
IPENTOOHB_OH_C	IPENTOOHB + OH	→	NELSON + H2O + OH	2.29E-11	MCMv3.3.1
PENTANOL3_OH	PENTANOL3 + OH	→	PENTANONE3 + HO2 + H2O	1.30E-11	Calvert et al. (2015)
PENTANOL2_OH	PENTANOL2 + OH	→	PENTANONE2 + HO2 + H2O	1.10E-11	Calvert et al. (2015)
IPENTOL_OH	IPENTOL + OH	→	CH3CHO + CH3COCH3 + HO2 + H2O	2.00E-12 exp(160/T)	Calvert et al. (2015)
M2BUTOL_OH	M2BUTOL + OH	→	NELSON + HO2 + H2O	2.50E-12 exp(464/T)	Calvert et al. (2015)
PENTANONE3_OH	PENTANONE3 + OH	→	C2H5CO3 + CH3CHO + H2O	2.00E-12	Calvert et al. (2015)
PENTANONE2_OH	PENTANONE2 + OH	→	CH3CHO + CH2O + CH3CO3 + H2O	3.80E-13 exp(705/T)	Calvert et al. (2015)
NELSON_OH	NELSON + OH	→	CH3COCH3 + CH3CO3 + H2O	1.45E-12 exp(219/T)	Calvert et al. (2015)
ALKNIT_OH	ALKNIT + OH	→	H2O + NO2 + CH3CHO + 0.5*CH3COCH3 + 0.5*PROPANAL	2.20E-12	Calvert et al. (2011)
			C_6		
C6ALKANES_OH	C6ALKANES + OH	→	C6ALKO2 + H2O	2.00E-11 exp(-350/T)	Calvert et al. (2015) (Averaged from >=C6 Alkanes)
C6ALKO2_HO2	C6ALKO2 + HO2	→	C6ALKOOH	2.11E-13 exp(1300/T)	Wennberg et al. (2018)
usr_C6ALKO2_NOa	C6ALKO2 + NO	→	NO2 + 0.60*C6ALKOHO2 + 0.40*IPENTOB	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_C6ALKO2_NOn	C6ALKO2 + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
C6ALKOOH_OH	C6ALKOOH + OH	→	C6ALKO2 + H2O	1.90E-12 exp(190/T)	MCMv3.3.1
C6ALKOOH_OH_C	C6ALKOOH + OH	→	HYDROXYKETONE + OH + H2O	3.53E-11	MCMv3.3.1
C6ALKOHO2_HO2	C6ALKOHO2 + HO2	→	C6ALKOOH	2.26E-13 exp(1300/T)	Wennberg et al. (2018)
usr_C6ALKOHO2_NOa	C6ALKOHO2 + NO	→	NO2 + HYDROXYKETONE + HO2	2.70E-12 exp(360/T) * (1 - **α**)	Jenkin et al. (2019)
usr_C6ALKOHO2_NOn	C6ALKOHO2 + NO	→	ALKNIT	2.70E-12 exp(360/T) * **α**	Jenkin et al. (2019)
usr_C6ALKOHO2	C6ALKOHO2	→	C6KETOOH + HO2	0.303 T^(3.39) exp(-5905/T)	Vereecken and Nozière (2020)
C6KETOOH_OH	C6KETOOH + OH	→	C6ALKOHO2 + H2O	1.90E-12 exp(190/T)	MCMv3.3.1
C6KETOOH_OH_C	C6KETOOH + OH	→	C6DIKETONE + OH + H2O	3.66E-11	MCMv3.3.1
HYDROXYKETONE_OH	HYDROXYKETONE + OH	→	C6DIKETONE + H2O + HO2	2.20E-11	Calvert et al. (2011)
C6DIKETONE_OH	C6DIKETONE + OH	→	H2O + 2*CH3CO3 + CO2 + CH2O	1.49E-12 exp(-450/T)	Calvert et al. (2011)

1) For third body reactions, parameters are shown in this order: k_0, n, k_inf, m, f. See Sect. 2 and Table 2-1 in JPL19.
2) For decomposition reactions, equilibrium constant is presented.
3) RO2 + CH3O2 rates are estimated using the geometric mean of CH3O2 + CH3O2 and RO2 + RO2 reactions
4) Nitrate yield (**α**) is calculated based on the method presented by Jenkin et al. (2019).

Table S2. Photolytic reactions added in MOZART-T3 mechanism. Mechanism label denotes the reaction tag used in CAM-chem reaction files. Details can be found in Sect. 2.

Mechanism label	Molecule		Products
		C_3	
[jnc3h7ooh->,jch3ooh]	NC3H7OOH	→	PROPANAL + OH + HO2
[jic3h7ooh->,jch3ooh]	IC3H7OOH	→	CH3COCH3 + OH + HO2
[jppn->,jpan]	PPN	→	0.6*C2H5CO3 + 0.6*NO2 + 0.4*C2H5O2 + 0.4*NO3 + 0.4*CO2
[jpropanal->,2.0*jch3cho]	PROPANAL	→	C2H5O2 + HO2 + CO
		C_4	
[jnbupooh->,jch3ooh]	NBUPOOH	→	NBUPO + OH
[jnbuooh->,jch3ooh]	NBUOOH	→	NBUO + OH
[jtbuooh->,jch3ooh]	TBUOOH	→	CH3O2 + CH3COCH3 + OH
[jbutanal->,2.0*jch3cho]	BUTANAL	→	NC3H7O2 + HO2 + CO
[johbutanal->,2.0*jch3cho]	OHBUTANAL	→	NC3H7O2 + HO2 + CO
		C_5	
[jnpentooha->,jch3ooh]	NPENTOOHA	→	NPENTOA + OH
[jnpentoohb->,jch3ooh]	NPENTOOHB	→	NPENTOB + OH
[jipentooha->,jch3ooh]	IPENTOOHA	→	CH3COCH3 + C2H5O2 + OH
[jipentoohb->,jch3ooh]	IPENTOOHB	→	IPENTOB + OH
[jpentanone3->,5.0*jacet]	PENTANONE3	→	C2H5CO3 + C2H5O2
[jpentanone2->,5.0*jacet]	PENTANONE2	→	CH3CO3 + NC3H7O2
[jnelson->,5.0*jacet]	NELSON	→	CH3CO3 + IC3H7O2
[jalknit->,jch3ooh]	ALKNIT	→	NO2 + 0.2*PROPANAL + 0.5*C2H5O2 + 0.5*CH3CHO + 0.3*NC3H7O2 + 0.3*CH3COCH3 + 0.2*IC3H7O2
		C_6	
[jc6alkooh->,jch3ooh]	C6ALKOOH	→	OH + HO2 + HYDROXYKETONE
[jc6ketooh->,jch3ooh]	C6KETOOH	→	OH + HO2 + C6DIKETONE
[jhydroxyketone->,5.0*jacet]	HYDROXYKETONE	→	CH3CO3 + 2*CH2O + HO2 + CH3CHO
[jc6diketone->,10.0*jacet]	C6DIKETONE	→	2*CH3CO3 + 2*CH2O

Table S3. C_3-C_6 alkanes and their oxidation products used in this study. Species newly added in T3 are shown in **bold**. Species used only in T1/T2 are shown in *italic*. Species used across all mechanisms (T1/T2/T3) are shown in normal font.

Species name	Chemical Formula	Description
	C_3	
C3H8	C3H8	propane
C3H7O2	*C3H7O2*	*propyl peroxy radical*
NC3H7O2	**C3H7O2**	**n-propyl peroxy radical**
IC3H7O2	**C3H7O2**	**isopropyl peroxy radical**
CH3COCH3	CH3COCH3	acetone
PROPANAL	**C2H5CHO**	**propanal**
PROPANOL	**C3H8O**	**n-propanol**
IPROPANOL	**C3H8O**	**isopropanol**
C2H5CO3	**C2H5CO3**	**propionyl peroxy radical**
C3H7OOH	*C3H7OOH*	*propyl hydroperoxide*
NC3H7OOH	**C3H7OOH**	**n-propyl hydroperoxide**
IC3H7OOH	**C3H7OOH**	**isopropyl hydroperoxide**
CH3COOOH	CH3COOOH	peracetic acid
CH3OOH	CH3OOH	methyl hydroperoxide
PPN	**C2H5CO3NO2**	**peroxy propionyl nitrate**
	C_4	
NBUTANE	**C4H10**	**n-butane**
IBUTANE	**C4H10**	**isobutane**
NBUPO2	**C4H9O2**	**1-butyl peroxy radical**
NBUO2	**C4H9O2**	**2-butyl peroxy radical**
TBUO2	**C4H9O2**	**t-butyl peroxy radical**
NBUPOOH	**C4H10O2**	**n-butyl hydroperoxide**
NBUOOH	**C4H10O2**	**s-butyl hydroperoxide**
TBUOOH	**C4H10O2**	**t-butyl hydroperoxide**
NBUPO	**C4H9O**	**n-butoxy radical**
NBUO	**C4H9O**	**s-butoxy radical**
BUTANAL	**C4H8O**	**butanal**
MEK	*C4H8O*	*methyl ethyl ketone*
BUTOL2	**C4H10O**	**2-butanol**
TBUOH	**C4H10O**	**t-butanol**
NBUPOHO2	**C4H9O3**	**4-hydroxy butyl peroxy radical**
OHBUTANAL	**C4H8O2**	**4-hydroxy butanal**
	C_5	
BIGALK	*C5H12*	*lumped alkanes (≥C_4)*
NPENTANE	**C5H12**	**n-pentane**
IPENTANE	**C5H12**	**isopentane**
ALKO2	*C5H11O2*	*lumped alkane peroxy radical from BIGALK*
NPENTO2A	**C5H11O2**	**3-pentyl peroxy radical**
NPENTO2B	**C5H11O2**	**2-pentyl peroxy radical**

IPENTO2A	**C5H11O2**	**t-pentyl peroxy radical**
IPENTO2B	**C5H11O2**	**3-methyl-2-butyl peroxy radical**
ALKOOH	*C5H12O2*	*lumped alkane hydroperoxide*
NPENTOOHA	**C5H12O2**	**3-hydroperoxy pentane**
NPENTOOHB	**C5H12O2**	**2-hydroperoxy pentane**
IPENTOOHA	**C5H12O2**	**1,1-dimethylpropyl hydroperoxide**
IPENTOOHB	**C5H12O2**	**2-hydroperoxy-3-methyl butane**
NPENTOA	**C5H11O**	**3-pentoxy radical**
NPENTOB	**C5H11O**	**2-pentoxy radical**
IPENTOB	**C5H11O**	**3-methyl 2-butyl alkoxy radical**
PENTANONE3	**C5H10O**	**3-pentanone**
PENTANONE2	**C5H10O**	**2-pentanone**
NELSON	**C5H10O**	**methyl isopropyl ketone**
PENTANOL3	**C5H12O**	**3-pentanol**
PENTANOL2	**C5H12O**	**2-pentanol**
IPENTOL	**C5H12O**	**t-pentyl alcohol**
M2BUTOL	**C5H12O**	**2-methyl-3-butanol**
ALKNIT	C5H11ONO2	lumped alkyl nitrates
	C_6	
C6ALKANES	**C6H14**	**lumped alkanes (≥C_6)**
C6ALKO2	**C6H13O2**	**peroxy radical from C6ALKANES**
C6ALKOOH	**C6H14O2**	**lumped hydroperoxide from C6ALKO2 + HO2**
C6KETOOH	**C6H12O3**	**2-hydroperoxy-5-hexanone**
C6ALKOHO2	**C6H13O3**	**peroxy radical from C6ALKANES after H-shift**
HYDROXYKETONE	**C6H12O2**	**lumped hydroxyketones (2-hydroperoxy 5-hexanone)**
C6DIKETONE	**C6H10O2**	**lumped diketones (2,5-hexanedione)**

Table S4. Molecular weights, effective Henry's law constants, and reactivity factors (F0) for newly added species in T3.

Species name	Molecular weight (g mol^{-1})	KH_{298} (M atm^{-1})	$\Delta H/R$ (K)	F0	Reference
			C_3		
PROPANAL	58.079257	1.00E+01	4330	0.1	JPL19
PROPANOL	60.09055	1.42E+02	7370	0.1	JPL19
IPROPANOL	60.09055	1.32E+02	7100	0.1	JPL19
NC3H7OOH	76.094544	2.34E+02	6014	0.1	GROMHE (GECKO-A)
IC3H7OOH	76.094544	2.34E+02	6014	0.1	GROMHE (GECKO-A)
PPN	135.075639	2.94E+00	5730	0.1	JPL19 (same as PAN)
			C_4		
NBUTANE	58.122351	1.19E-03	3740	1E-36	JPL19
IBUTANE	58.122351	9.18E-04	3340	1E-36	JPL19
NBUPOOH	90.121161	1.78E+02	6014	0.1	GROMHE (GECKO-A)
NBUOOH	90.121161	1.78E+02	6014	0.1	GROMHE (GECKO-A)
TBUOOH	90.121161	1.78E+02	6014	0.1	GROMHE (GECKO-A)
BUTANAL	72.105875	9.60E+00	6220	0.1	JPL19
BUTOL2	74.121756	1.11E+02	7095	0.1	JPL19
TBUOH	74.121756	7.05E+01	8310	0.1	JPL19
OHBUTANAL	88.105279	3.24E+05	6014	1	GROMHE (GECKO-A)
			C_5		
NPENTANE	72.148969	8.11E-04	3400	1E-36	Sander (2015); Abraham and Matteoli (1988)
IPENTANE	72.148969	7.34E-04	6014	1E-36	Sander (2015); Mackay and Shiu (1981)
NPENTOOHA	104.147778	1.35E+02	6014	0.1	GROMHE (GECKO-A)
NPENTOOHB	104.147778	1.35E+02	6014	0.1	GROMHE (GECKO-A)
IPENTOOHA	104.147778	1.35E+02	6014	0.1	GROMHE (GECKO-A)
IPENTOOHB	104.147778	1.35E+02	6014	0.1	GROMHE (GECKO-A)
PENTANONE3	86.132492	1.62E+01	5600	0.1	Sander (2015); Ji and Evans (2007)
PENTANONE2	86.132492	1.62E+01	5700	0.1	Sander (2015); Ji and Evans (2007)
NELSON	86.132492	8.82E+00	5700	0.1	Sander (2015); Bagno et al. (1991)
PENTANOL3	88.148373	6.38E+01	7900	0.1	Sander (2015); Cabani et al. (1975)
PENTANOL2	88.148373	6.79E+01	7600	0.1	Sander (2015); Butler et al. (1935); Kühne et al. (2005)
IPENTOL	88.148373	7.19E+01	7600	0.1	Sander (2015); Butler et al. (1935); Kühne et al. (2005)
M2BUTOL	88.148373	7.19E+01	7600	0.1	Sander (2015); Butler et al. (1935); Kühne et al. (2005)
			C_6		
C6ALKANES	86.175586	6.18E-04	3800	1E-36	Sander (2015); Abraham and Matteoli (1988)
C6ALKOOH	118.16542	1.02E+02	6014	0.1	GROMHE (GECKO-A)
C6KETOOH	132.157919	5.50E+05	6014	1	GROMHE (GECKO-A)
HYDROXYKETONE	116.158514	2.75E+05	6014	1	GROMHE (GECKO-A)
C6DIKETONE	114.142633	4.37E+04	6014	1	GROMHE (GECKO-A)

Table S5. Kinetic and photolysis reactions updated or added in T1.3 relative to T1.2. Bold values indicate updated reaction rate constants or branching ratios. Note that some reactions unrelated to alkane chemistry are also included, as they were incorporated from separate ongoing development of the T1.3 mechanism.

Mechanism label	Reactants		Products	Rate	Updated/Added
			Photolysis		
[jmek->,**5.0***jacet]	MEK	→	CH3CO3 + C2H5O2	jacet	Updated
			Kinetics		
CH3O2_NO3	CH3O2 + NO3	→	CH2O + NO2 + HO2	8.9E-12 exp(-600/T)	Added
C2H5O2_NO3	C2H5O2 + NO3	→	CH3CHO + NO2 + HO2	8.9E-12 exp(-390/T)	Added
CH3CO3_HO2	CH3CO3 + HO2	→	**0.36***CH3COOOH + 0.15*CH3COOH + 0.15*O3 + **0.49***OH + **0.49***CH3O2	4.2E-13 exp(1040/T)	Updated
CH3CO3_NO3	CH3CO3 + NO3	→	CH3O2 + CO2 + NO2	8.9E-12 exp(-305/T)	Added
C3H7O2_CH3O2	C3H7O2 + CH3O2	→	CH2O + HO2 + 0.82*CH3COCH3	**1.0E-13 exp(557/T)**	Updated
C3H7O2_HO2	C3H7O2 + HO2	→	C3H7OOH + O2	**1.41E-13 exp(1300/T)**	Updated
C3H7O2_NO	C3H7O2 + NO	→	0.82*CH3COCH3 + NO2 + HO2 + 0.27*CH3CHO	**2.7E-12 exp(360/T)**	Updated
ALKNIT_OH	ALKNIT + OH	→	0.4*CH2O + 0.8*CH3CHO + 0.8*CH3COCH3 + NO2	**2.20E-12**	Updated
OH_HONO	HONO + OH	→	H2O + NO2	3E-12 exp(250/T)	Added
OH_NO_M	OH + NO + M	→	HONO + M	7e-31, 2.6, 3.6e-11, 0.1, 0.6	Added
O1D_O3a	O1D + O3	→	O2 + 2*O	1.20E-10	Added
usr_NO2_aer	NO2	→	0.5*OH + 0.5*NO + 0.5*HNO3	heterogeneous reaction	Added

Table S6. Iso-to-normal (i/n) ratios for butanes and pentanes anthropogenic emissions used in this study. Ratios are calculated from average values shown in Table S7. Note that calculation methods based on continental averages versus global averaging from each study show minimal differences (<2%).

i/n Ratio	Emission Sector		
	Transportation	Industrial/Energy	Other
Butanes	0.482	0.523	0.564
Pentanes	2.734	1.027	2.037

Table S7. Literature compilation of iso-to-normal (i/n) ratios and iso-fractions [i/(n+i)] for butanes and pentanes across different emission sectors and geographic regions. Some values are for report only and excluded from global averaging (Table S6) to prevent oversampling from similar sources or mixed emission signatures, as indicated by footnote markers.

					i/n ratio		i/(n+i)	
Sector	Region		Study	Detail	Butane	Pentane	Butane	Pentane
Transport	North America	California, US	Pang et al. (2014)	1995 Fleet tailpipe	0.647	3.070	0.393	0.754
				1999 Fleet tailpipe	0.232	2.855	0.188	0.741
				2001 Fleet tailpipe	0.132	2.764	0.117	0.734
				2003 Fleet tailpipe	0.250	3.094	0.200	0.756
		Georgia, US	Conner et al. (1995)	Roadway in Atlanta	0.273	3.248	0.214	0.765
				Weighted gasoline avg[a]	0.185	2.670	0.156	0.728
				87 Octane gasoline[a]	0.187	2.429	0.158	0.708
				89 Octane gasoline[a]	0.188	2.920	0.158	0.745
		California, US	Gentner et al. (2013)	on-road	0.094	3.894	0.086	0.796
				Fuel composition based[a]	0.078	3.386	0.072	0.772
		US cities (roadside)	Baker et al. (2008)	New York City	1.412	2.900	0.585	0.744
				Philadelphia	0.800	2.222	0.444	0.690
				Salt Lake City	0.403	1.935	0.287	0.659
		Mexico	Araizaga et al. (2013)	Tunnel in Monterrey	0.415	1.816	0.293	0.645
	Asia	South Korea	Simpson et al. (2020)	Aircraft measurements over Seoul, below 500 m[a]	0.560	1.403	0.359	0.584
		China	Zhang et al. (2018)	Tunnel in Guangzhou	0.583	2.205	0.368	0.688
			Song et al. (2020)	Tunnel in Beijing	0.280	2.962	0.219	0.748
				Tunnel in Tianjin	0.357	2.918	0.263	0.745
				Tunnel in Nanjing	0.942	3.644	0.485	0.785
			Deng et al. (2018)	Tunnel in Hefei	0.442	5.096	0.307	0.836
			Ho et al. (2009)	Tunnel in Hong Kong	0.632	3.294	0.387	0.767
		Taiwan	Hwa et al. (2002)	Tunnel in Taifei	0.697	1.313	0.411	0.568
	South America	Brazil	Santos and Azevedo (2021)	Tunnel in Rio de Janeiro (Oct 2018)	0.592	1.434	0.372	0.589
				Tunnel in Rio de Janeiro (May 2019)	0.379	1.597	0.275	0.615
			Dominutti et al. (2016)	Urban background site in São Paulo (2013 annual mean)[a]	0.497	1.327	0.332	0.570

			Dominutti et al. (2020)	Urban background site in São Paulo (summer, mean VOC/C_2H_2)[a]	0.641	1.290	0.391	0.563
				Urban background site in São Paulo (summer, mean VOC/CO)	0.678	0.954	0.404	0.488
				Urban background site in São Paulo (winter, mean VOC/C_2H_2)[a]	0.527	1.320	0.345	0.569
				Urban background site in São Paulo (winter, mean VOC/CO)	0.600	1.154	0.375	0.536
			Martins et al. (2006)	Tunnel in São Paulo	0.279	-	0.218	-
	Europe	France	Baudic et al. (2016)	Urban background sites in Paris	0.585	2.154	0.369	0.683
			Ammoura et al. (2014)	Tunnel in Thiais	-	2.722	-	0.731
		Switzerland	Lanz et al. (2008)	Urban background site in Zurich (1993–1994)	0.341	3.149	0.254	0.759
				Urban background site in Zurich (2005–2006)	0.596	2.583	0.373	0.721
			Stemmler et al. (2005)	Tunnel near Zurich	0.346	3.875	0.257	0.795
		Belgium	Ait-Helal et al. (2015)	Tunnel in Brussels	0.369	2.970	0.270	0.748
	Middle East	Saudi Arabia	Simpson et al. (2014)	Saudi background	0.409	2.643	0.290	0.726
				Urban Mecca	0.446	3.621	0.308	0.784
				Pilgrimage route	0.359	3.078	0.264	0.755
				Tunnels in Mecca	0.370	3.586	0.270	0.782
Energy	North America	Colorado, US	Gilman et al. (2013)	Tower near oil & natural gas operations in Erie; ratios from maximum observed values[b]	0.462	0.877	0.316	0.467
				Tower near oil & natural gas operations in Erie; ratios from mean observed values[a]	0.429	0.894	0.300	0.472
			Swarthout et al. (2013)	Tower near oil & natural gas operations in Erie; ratios from mean observed values[b]	0.409	0.985	0.290	0.496
			Hecobian et al. (2019)	Oil & natural gas in the Denver-Julesburg Basin during production activity	0.382	0.769	0.276	0.435
		Pennsylvania, US	Swarthout et al. (2015)	Night samples near wells; atios from maximum observed values	0.687	1.222	0.407	0.550

				Night samples near wells; ratios from mean observed values[a]	0.579	0.900	0.367	0.474
		Alberta, Canada	Simpson et al. (2010)	Near oil sands; ratios from maximum values	0.379	1.106	0.275	0.525
	Europe	Arctic	Gilman et al. (2010)	Arctic ship measurements of air mass likely from natural gas processing in Russia	0.328	0.889	0.247	0.471
		The North Sea	Wilde et al. (2021)	Northern UK	0.398	0.890	0.285	0.471
				Norwegian sector	0.755	1.120	0.430	0.528
				West Shetland	0.665	1.080	0.399	0.519
				Southern UK	0.680	1.240	0.405	0.554
All general		28 US cities mean	Baker et al. (2008)	Well-ventilated areas removed from roadsides such as parks, schools and cemeteries[c]	0.606	2.262	0.377	0.693
		16 US cities mean	Rossabi and Helmig (2018)	10 PALMS[d] type 2 sites and 6 GGGRN[e] sites	0.522	1.811	0.343	0.644

[a] Values excluded from the calculation in Table S5 to avoid oversampling or when emission sources are suspected to be mixed for the measurement.

[b] Average values calculated first for measurements at the same site and time period before calculating the global average in Table S5.

[c] Roadside locations are excluded from this table.

[d] PALMS: Photochemical Assessment Monitoring Stations.

[e] GGGRN: Global Greenhouse Gas Reference Network.

Table S8. OVOC speciation profiles for anthropogenic emissions, including alcohols, aldehydes, and ketones across different MOZART chemical mechanism versions.

OVOCs	CAM-chem Species	MOZART Mechanism[a]		
		T1.2	T1.3	T3
Alcohols (VOC01-alcohols)	CH3OH	0.15	0.60 (0.50)	0.60 (0.50)
	C2H5OH	0.85	0.40 (0.50)	0.38 (0.48)
	IPROPANOL	N/A	N/A	0.02
Aldehydes (VOC22-other-alkanals)	CH3CHO	1.00	1.00	0.85
	PROPANAL	N/A	N/A	0.10
	BUTANAL	N/A	N/A	0.05
Ketones (VOC23-ketones)	CH3COCH3	0.20	0.80	0.80
	MEK	0.80	0.20	0.20

[a] The default "T1.2" values are from Emmons et al. (2020), and the updated "T1.3" and "T3" values are derived from the NSF NCAR Trace Organic Gas Analyzer (TOGA) measurements from multiple field campaigns over source regions, including the Front Range Air Pollution and Photochemistry Éxperiment (FRAPPÉ) (Flocke et al., 2020), the Wintertime Investigation of Transport, Emissions, and Reactivity (WINTER) (McDuffie et al., 2018), ATom (Thompson et al., 2022), the Asian Summer Monsoon Chemical and Climate Impact Project (ACCLIP) (Pan et al., 2025), and the Atmospheric Science and Chemistry mEasurement NeTwork (ASCENT) campaigns. Values represent global averages, with South American regional values shown in parentheses for alcohols.

Table S9. Scaling factors applied to BIGALK emissions to create speciated MOZART-T3 alkane emissions for biomass burning sources across different land cover types. Factors represent the fractional contribution of each alkane species to the total BIGALK emission category and sum to unity for each ecosystem.

Species	Tropical Forest	Savanna	Croplands	Boreal Forest	Temperate Forest
NBUTANE	0.47	0.39	0.35	0.34	0.34
ISOBUTANE	0.13	0.11	0.12	0.12	0.12
NPENTANE	0.08	0.06	0.10	0.20	0.20
IPENTANE	0.10	0.04	0.08	0.09	0.09
C6ALKANES	0.22	0.40	0.35	0.25	0.25

Table S10. Annual global budgets for ketone species including emissions (anthropogenic, biomass burning, and biogenic), chemical production and loss rates, dry and wet depositions, source totals (emission + chemical production) and loss totals (chemical loss + deposition), atmospheric burden, and atmospheric lifetime across different simulation cases. All emission, production, loss, and deposition values are in Tg yr^{-1}, burden in Tg, and lifetime in days.

Species	Case	Emission (Anth.)	Emission (BB)	Emission (Biog.)	Chem. Prod.	Chem. Loss.	Dry Dep.	Wet Dep.	Emission (All)	Source (All)	Loss (All)	Burden	Lifetime
KETONE	CEDS_T1.2	3.50	16.17	42.31	128.88	131.86	57.68	1.43	61.98	190.86	190.97	5.40	10.32
	CEDS_T1.3	3.08	16.17	42.26	129.41	132.18	56.77	1.40	61.51	190.92	190.35	5.09	9.77
	CEDS_T2.3	3.08	16.17	42.29	95.24	108.75	47.41	1.09	61.54	156.78	157.25	3.93	9.12
	CEDS_T1.3_T3	3.08	16.17	42.65	163.69	158.09	57.24	9.85	61.89	225.58	225.18	4.98	8.07
	CEDS_T2.3_T3	3.08	16.17	42.67	127.10	132.55	47.87	8.83	61.92	189.02	189.25	3.83	7.38
	CAMS_T1.2	7.60	16.17	42.34	116.02	123.04	57.87	1.41	66.11	182.13	182.32	5.26	10.53
	CAMS_T1.3	6.68	16.17	42.33	117.05	122.74	57.15	1.40	65.18	182.23	181.29	5.04	10.15
	CAMS_T2.3	6.68	16.17	42.34	82.42	99.21	47.77	1.09	65.18	147.60	148.08	3.86	9.51
	CAMS_T1.3_T3	6.68	16.17	42.71	149.06	147.09	57.71	9.39	65.55	214.62	214.19	4.88	8.32
	CAMS_T2.3_T3	6.68	16.17	42.75	112.32	121.50	48.32	8.36	65.59	177.92	178.17	3.72	7.63
CH3COCH3	CEDS_T1.2	0.59	5.63	42.31	83.57	84.38	46.04	1.27	48.53	132.10	131.69	4.59	12.73
	CEDS_T1.3	2.35	5.63	42.26	84.67	85.32	47.19	1.28	50.24	134.91	133.80	4.59	12.52
	CEDS_T2.3	2.35	5.63	42.29	51.88	63.20	37.90	0.98	50.27	102.15	102.07	3.44	12.29
	CEDS_T1.3_T3	2.35	5.63	42.26	87.47	87.44	48.34	1.32	50.25	137.71	137.10	4.73	12.58
	CEDS_T2.3_T3	2.35	5.63	42.29	55.43	65.52	39.07	1.02	50.27	105.70	105.61	3.58	12.38
	CAMS_T1.2	1.27	5.63	42.34	81.74	83.09	46.22	1.27	49.25	130.99	130.58	4.57	12.77
	CAMS_T1.3	5.10	5.63	42.33	83.18	85.19	48.30	1.30	53.06	136.24	134.80	4.63	12.53
	CAMS_T2.3	5.10	5.63	42.34	49.95	62.97	38.99	0.99	53.07	103.01	102.95	3.46	12.26
	CAMS_T1.3_T3	5.10	5.63	42.32	83.43	85.60	48.89	1.32	53.05	136.48	135.81	4.66	12.54
	CAMS_T2.3_T3	5.10	5.63	42.36	51.25	63.64	39.61	1.01	53.09	104.34	104.27	3.51	12.29
MEK	CEDS_T1.2	2.92	10.54		45.31	47.48	11.64	0.16	13.45	58.76	59.28	0.80	4.94
	CEDS_T1.3	0.73	10.54		44.75	46.85	9.58	0.12	11.26	56.01	56.55	0.50	3.25
	CEDS_T2.3	0.73	10.54		43.36	45.55	9.51	0.11	11.26	54.63	55.18	0.49	3.26
	CEDS_T1.3_T3	0.73	10.54		9.50	15.38	5.71	0.04	11.26	20.76	21.13	0.15	2.64
	CEDS_T2.3_T3	0.73	10.54		9.49	15.39	5.70	0.04	11.26	20.75	21.12	0.15	2.63
	CAMS_T1.2	6.33	10.54		34.28	39.95	11.65	0.14	16.86	51.14	51.74	0.69	4.86
	CAMS_T1.3	1.58	10.54		33.87	37.54	8.85	0.10	12.12	45.99	46.49	0.41	3.25

	CAMS_T2.3	1.58	10.54		32.48	36.25	8.79	0.10	12.12	44.59	45.13	0.40	3.26
	CAMS_T1.3_T3	1.58	10.54		7.49	14.05	5.90	0.04	12.12	19.61	19.98	0.14	2.63
	CAMS_T2.3_T3	1.58	10.54		7.49	14.07	5.88	0.04	12.12	19.60	19.98	0.14	2.63
PENTANONE2	CEDS_T1.3_T3				2.38	2.33	0.05	0.002		2.38	2.38	0.01	1.41
	CEDS_T2.3_T3				2.38	2.32	0.05	0.002		2.38	2.38	0.01	1.41
	CAMS_T1.3_T3				0.89	0.86	0.02	0.001		0.89	0.89	0.00	1.68
	CAMS_T2.3_T3				0.89	0.86	0.02	0.001		0.89	0.89	0.00	1.69
PENTANONE3	CEDS_T1.3_T3				2.59	2.47	0.11	0.005		2.59	2.58	0.02	2.98
	CEDS_T2.3_T3				2.58	2.47	0.11	0.005		2.58	2.58	0.02	2.99
	CAMS_T1.3_T3				0.98	0.93	0.05	0.002		0.98	0.98	0.01	3.46
	CAMS_T2.3_T3				0.98	0.93	0.05	0.002		0.98	0.98	0.01	3.47
NELSON	CEDS_T1.3_T3				1.71	1.67	0.04	0.001		1.71	1.71	0.01	1.97
	CEDS_T2.3_T3				1.69	1.65	0.04	0.001		1.69	1.69	0.01	1.98
	CAMS_T1.3_T3				0.71	0.69	0.02	0.001		0.71	0.71	0.00	2.36
	CAMS_T2.3_T3				0.69	0.67	0.02	0.001		0.69	0.69	0.00	2.39
HYDROXYKETONE	CEDS_T1.3_T3				25.09	20.81	0.98	3.28		25.09	25.07	0.02	0.27
	CEDS_T2.3_T3				22.86	18.98	0.94	2.91		22.86	22.84	0.02	0.26
	CAMS_T1.3_T3				23.10	19.00	0.89	3.19		23.10	23.08	0.02	0.27
	CAMS_T2.3_T3				20.85	17.15	0.86	2.82		20.85	20.83	0.02	0.27
C6KETOOH	CEDS_T1.3_T3				9.03	7.95	0.38	0.70		9.03	9.02	0.003	0.12
	CEDS_T2.3_T3				8.70	7.68	0.36	0.65		8.70	8.69	0.003	0.12
	CAMS_T1.3_T3				8.60	7.57	0.36	0.66		8.60	8.59	0.003	0.12
	CAMS_T2.3_T3				8.27	7.31	0.34	0.61		8.27	8.26	0.003	0.12
C6DIKETONE	CEDS_T1.3_T3			0.38	25.93	20.04	1.65	4.51	0.38	26.31	26.20	0.04	0.52
	CEDS_T2.3_T3			0.38	23.97	18.54	1.61	4.20	0.38	24.36	24.34	0.03	0.52
	CAMS_T1.3_T3			0.38	23.86	18.38	1.59	4.18	0.38	24.25	24.15	0.03	0.52
	CAMS_T2.3_T3			0.38	21.91	16.86	1.55	3.87	0.38	22.30	22.28	0.03	0.52

Table S11. Annual global budgets for aldehydes and organic nitrates including emissions (anthropogenic, biomass burning, and biogenic), chemical production and loss rates, dry and wet depositions, source totals (emission + chemical production) and loss totals (chemical loss + deposition), atmospheric burden, and atmospheric lifetime across different simulation cases. All emission, production, loss, and deposition values are in Tg yr^{-1}, burden in Tg, and lifetime in days.

Species	Case	Emission (Anth.)	Emission (BB)	Emission (Biog.)	Chem. Prod.	Chem. Loss.	Dry Dep.	Wet Dep.	Emission (All)	Source (All)	Loss (All)	Burden	Lifetime
CH3CHO	CEDS_T1.2	1.16	14.84	20.45	135.60	155.94	16.07	0.07	36.44	172.05	172.08	0.239	0.51
	CEDS_T1.3	1.16	14.84	20.40	134.70	155.16	15.93	0.07	36.40	171.10	171.15	0.225	0.48
	CEDS_T2.3	1.16	14.84	20.43	130.17	150.21	15.57	0.07	36.43	166.59	165.84	0.211	0.47
	CEDS_T1.3_T3	0.98	14.84	20.41	120.35	140.79	15.76	0.07	36.23	156.58	156.62	0.208	0.49
	CEDS_T2.3_T3	0.98	14.84	20.43	116.14	136.80	15.41	0.06	36.25	152.39	152.27	0.195	0.47
	CAMS_T1.2	9.33	14.84	20.48	135.11	161.44	18.33	0.08	44.65	179.76	179.85	0.251	0.51
	CAMS_T1.3	9.33	14.84	20.48	129.19	155.84	18.04	0.07	44.65	173.84	173.96	0.233	0.49
	CAMS_T2.3	9.33	14.84	20.47	124.56	150.74	17.69	0.07	44.64	169.21	168.50	0.218	0.47
	CAMS_T1.3_T3	7.93	14.84	20.47	117.05	142.72	17.58	0.07	43.24	160.28	160.38	0.216	0.49
	CAMS_T2.3_T3	7.93	14.84	20.50	112.89	138.75	17.22	0.07	43.27	156.16	156.03	0.203	0.47
PROPANAL	CEDS_T1.3_T3	0.15			7.03	7.11	0.07	0.001	0.15	7.19	7.18	0.007	0.36
	CEDS_T2.3_T3	0.15			6.98	7.06	0.07	0.001	0.15	7.13	7.13	0.007	0.36
	CAMS_T1.3_T3	1.23			6.78	7.81	0.21	0.001	1.23	8.01	8.01	0.008	0.37
	CAMS_T2.3_T3	1.23			6.73	7.75	0.21	0.001	1.23	7.96	7.96	0.008	0.37
BUTANAL	CEDS_T1.3_T3	0.09			1.07	1.15	0.02	0.000	0.09	1.17	1.16	0.001	0.28
	CEDS_T2.3_T3	0.09			1.07	1.15	0.02	0.000	0.09	1.17	1.17	0.001	0.28
	CAMS_T1.3_T3	0.76			0.83	1.50	0.09	0.000	0.76	1.59	1.59	0.001	0.34
	CAMS_T2.3_T3	0.76			0.83	1.50	0.09	0.000	0.76	1.59	1.60	0.001	0.34
PAN	CEDS_T1.2				971.6	966.9	5.23	0.024	0.0	971.6	972.1	2.282	0.86
	CEDS_T1.3				1065.0	1059.0	5.85	0.024	0.0	1065.0	1064.9	2.330	0.80
	CEDS_T2.3				1092.5	1086.3	5.76	0.024	0.0	1092.5	1092.1	2.239	0.75
	CEDS_T1.3_T3				993.2	988.3	5.61	0.022	0.0	993.2	994.0	2.115	0.78
	CEDS_T2.3_T3				1018.7	1013.3	5.52	0.022	0.0	1018.7	1018.9	2.029	0.73
	CAMS_T1.2				986.7	981.8	5.37	0.023	0.0	986.7	987.2	2.217	0.82
	CAMS_T1.3				1061.3	1055.2	5.87	0.023	0.0	1061.3	1061.1	2.226	0.77
	CAMS_T2.3				1089.2	1083.0	5.78	0.022	0.0	1089.2	1088.8	2.135	0.72
	CAMS_T1.3_T3				990.3	985.4	5.60	0.020	0.0	990.3	991.0	2.035	0.75
	CAMS_T2.3_T3				1016.7	1011.3	5.52	0.020	0.0	1016.7	1016.8	1.951	0.70

PPN	CEDS_T1.3_T3	16.42	16.35	0.08	0.001	0.0	16.4	16.4	0.052	1.14
	CEDS_T2.3_T3	16.27	16.18	0.08	0.001	0.0	16.3	16.3	0.051	1.14
	CAMS_T1.3_T3	16.44	16.36	0.09	0.001	0.0	16.4	16.5	0.045	0.99
	CAMS_T2.3_T3	16.26	16.17	0.09	0.001	0.0	16.3	16.3	0.044	0.99
ALKNIT	CEDS_T1.2	16.5	15.2	1.27	0.001	0.0	16.5	16.4	0.116	2.58
	CEDS_T1.3	16.5	15.4	1.15	0.001	0.0	16.5	16.5	0.098	2.16
	CEDS_T2.3	15.9	14.9	1.13	0.001	0.0	15.9	16.0	0.095	2.18
	CEDS_T1.3_T3	13.8	12.5	1.32	0.001	0.0	13.8	13.8	0.088	2.32
	CEDS_T2.3_T3	13.6	12.2	1.30	0.001	0.0	13.6	13.5	0.087	2.34
	CAMS_T1.2	12.3	11.2	0.98	0.001	0.0	12.3	12.2	0.089	2.67
	CAMS_T1.3	12.3	11.4	0.89	0.001	0.0	12.3	12.3	0.076	2.24
	CAMS_T2.3	11.7	10.9	0.88	0.001	0.0	11.7	11.8	0.073	2.27
	CAMS_T1.3_T3	11.1	10.0	1.08	0.001	0.0	11.1	11.1	0.071	2.35
	CAMS_T2.3_T3	10.9	9.8	1.06	0.001	0.0	10.9	10.8	0.070	2.37

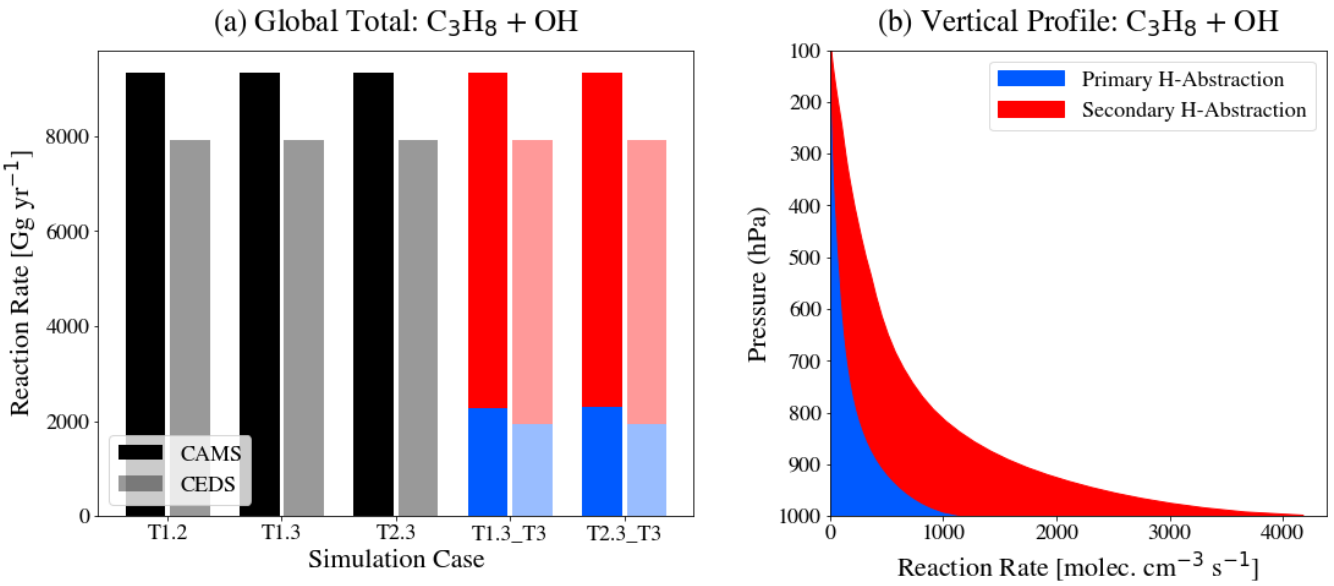

Figure S1. Annual global C3H8 + OH reaction rates across different simulation cases. (a) Total reaction rates showing CAMS (black) and CEDS (gray) emission inventories, with T3 mechanisms displaying primary (blue) and secondary (red) carbon hydrogen abstraction pathways. (b) Vertical profile of reaction pathways for the CEDS_T2.3_T3 case.

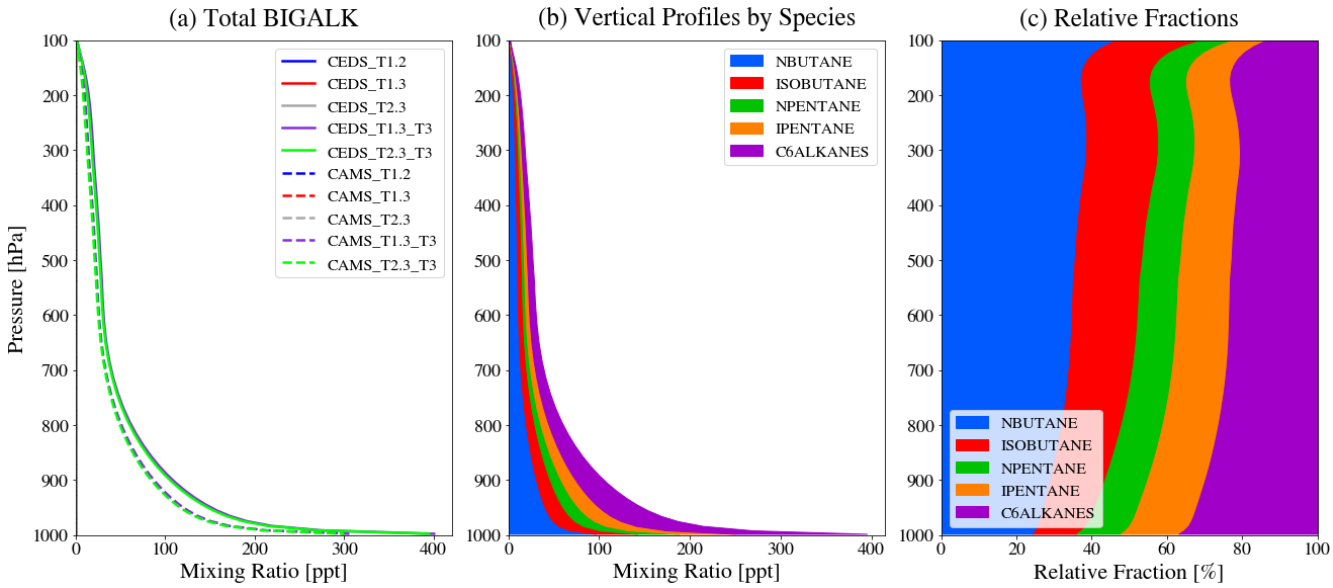

Figure S2. Vertical profiles of BIGALK species mixing ratios. (a) Total BIGALK across different mechanisms and emission inventories (solid lines: CEDS, dashed lines: CAMS). (b) Individual C_4–C_6 alkane species contributions in the CEDS_T2.3_T3 case. (c) Relative fractions of each alkane species as a function of altitude.

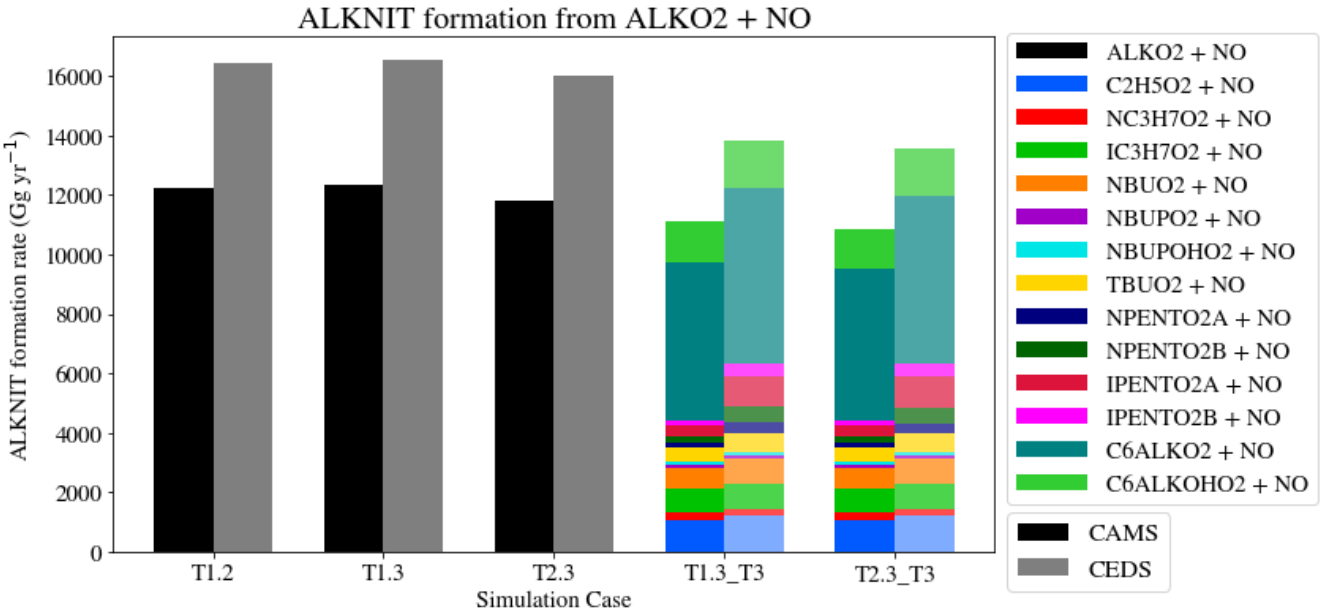

Figure S3. Annual total ALKNIT formation rates from alkyl RO_2 + NO reactions across different mechanism and emission inventory cases. Formation rates from individual peroxy radicals are normalized by their respective molecular weights and multiplied by ALKNIT molecular weight to enable direct mass flux comparison. T1 and T2 use lumped ALKO2 species (black), while T3 explicitly represents individual alkane-derived peroxy radicals (colored). Dark shading represents CAMS inventory and light shading represents CEDS inventory cases.

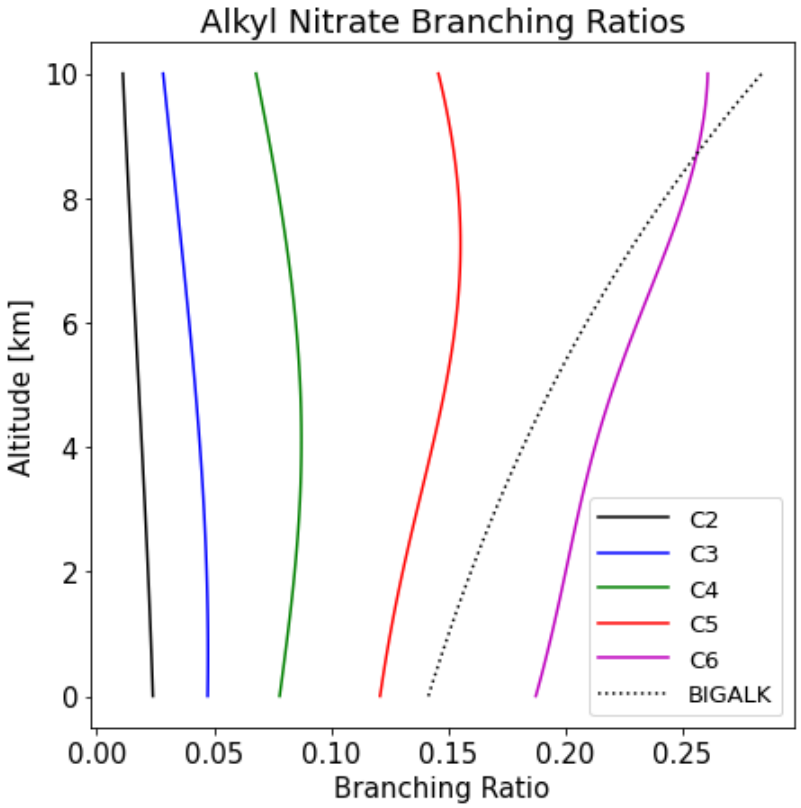

Figure S4. Altitude dependence of alkyl nitrate branching ratios from alkyl RO_2 + NO reactions. Solid lines show branching ratios for individual C_2–C_6 alkanes using the temperature and pressure dependent parameterization from Jenkin et al. (2019) implemented in T3. Dotted line shows the lumped BIGALK branching ratio in T1/T2, calculated from temperature-dependent rate constants (Emmons et al., 2020). Atmospheric temperature and pressure profiles are from the International Standard Atmosphere 1993.

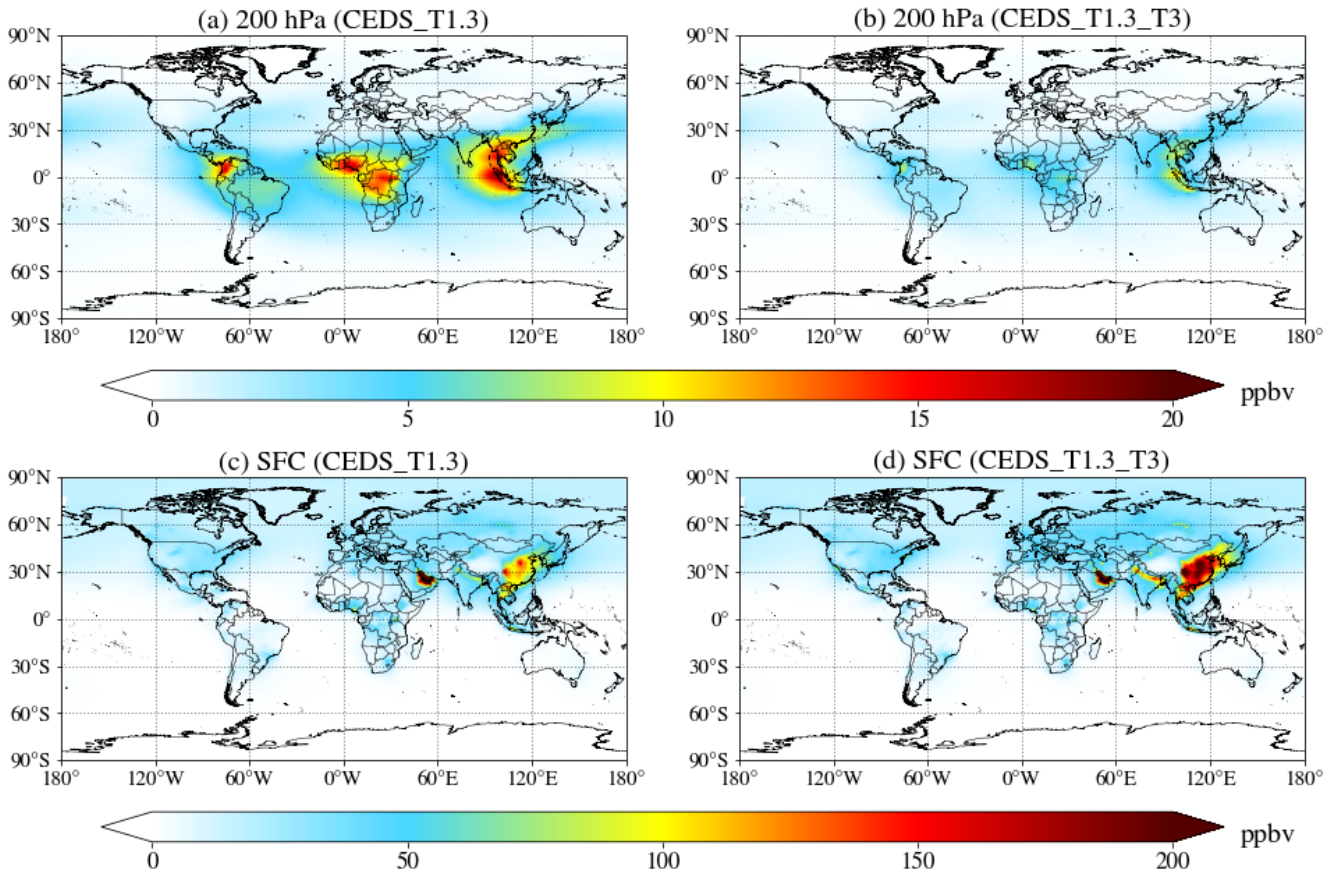

Figure S5. Annual mean ALKNIT mixing ratios at 200 hPa for (a) CEDS_T1.3 and (b) CEDS_T1.3_T3, and at the surface for (c) CEDS_T1.3 and (d) CEDS_T1.3_T3. Note the different color scales for upper troposphere (0-20 ppbv) and surface (0-200 ppbv).

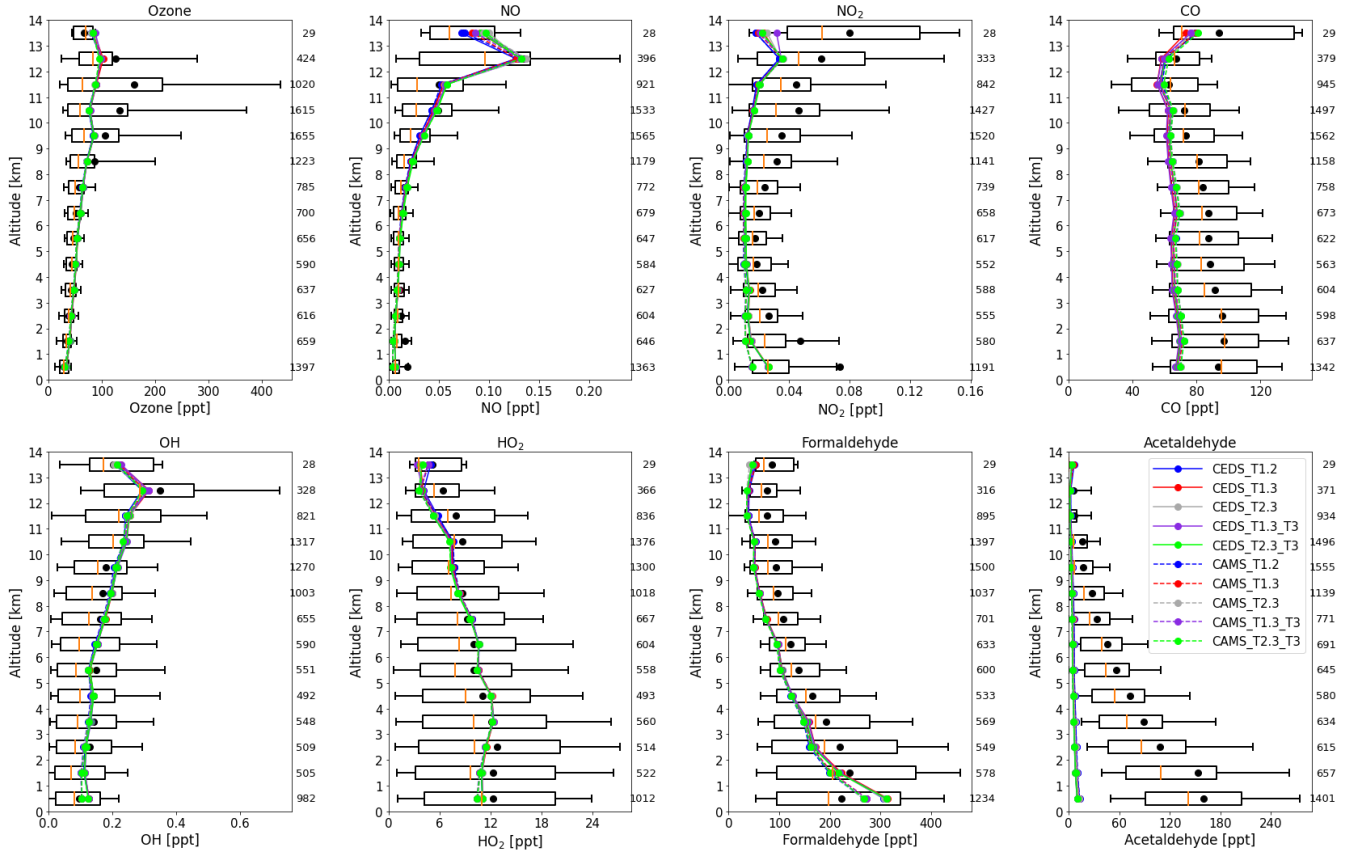

Figure S6. Vertical profiles of major air pollutants compared with ATom observations across all four campaigns (ATom-1 through ATom-4). Box-and-whisker plots show the distribution of ATom measurements at each altitude bin, with the box representing the interquartile range, the orange line indicating the median, and whiskers extending to the 10th and 90th percentiles. Black dots represent the mean of observations. Model median values from different mechanism and emission inventory combinations are shown as colored lines and symbols. Numbers on the right *y*-axis indicate the number of observations in each altitude bin.

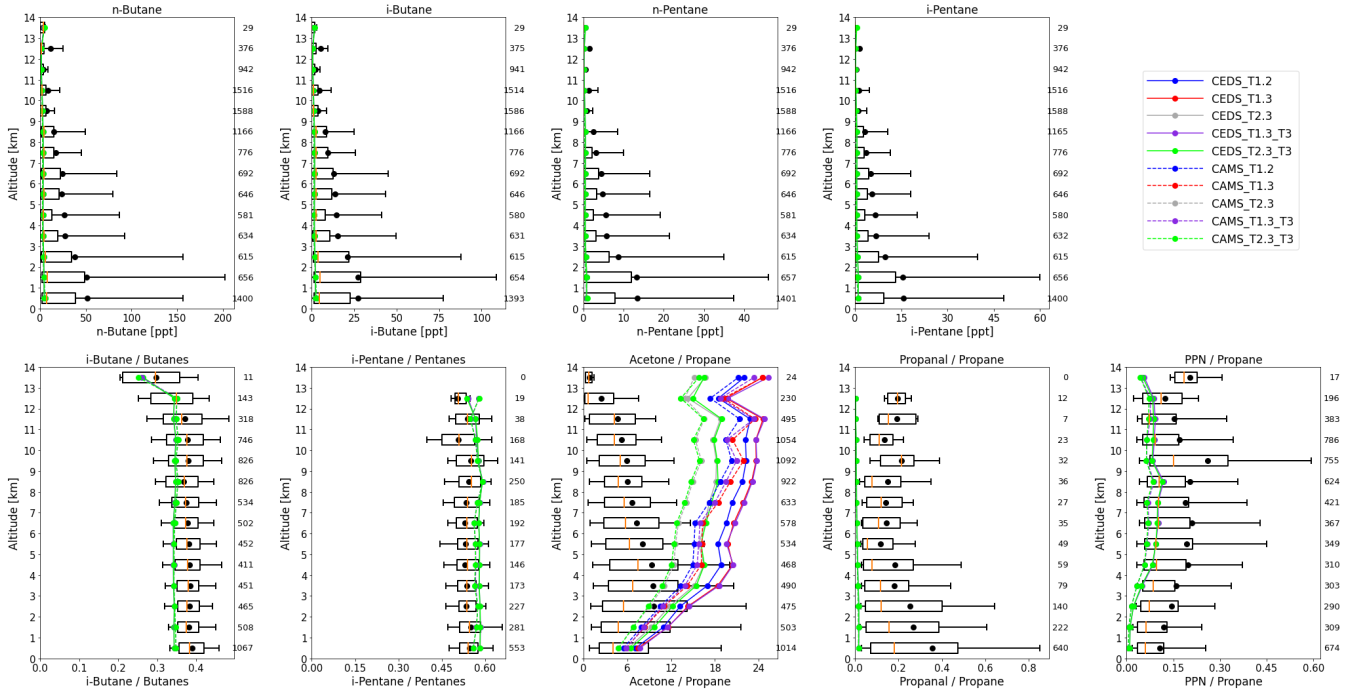

Figure S7. Same as Figure S6 but for explicit C_4–C_5 alkane species (n-butane, i-butane, n-pentane, i-pentane), ratios of isomers to total alkanes (i-butane/butanes, i-pentane/pentanes), and OVOCs to parent hydrocarbons (acetone/propane, propanal/propane, PPN/propane).

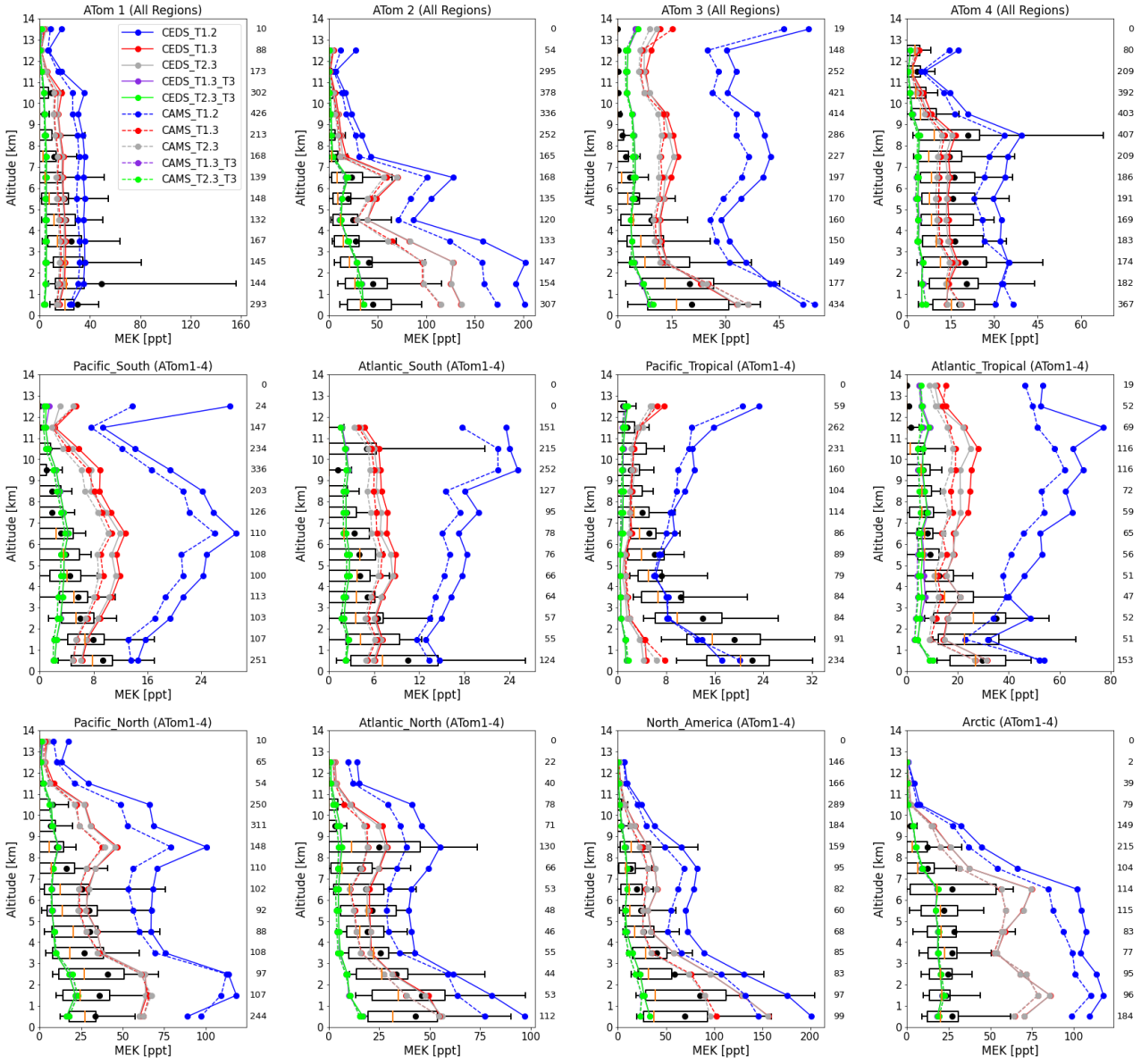

Figure S8. Vertical profiles of MEK for individual ATom campaigns (ATom-1 through ATom-4) and by region. Regional definitions are shown in Figure S9. Box-and-whisker plots show the distribution of ATom measurements at each altitude bin, with the box representing the interquartile range, the orange line indicating the median, and whiskers extending to the 10th and 90th percentiles. Black dots represent the mean of observations. Model median values from different mechanism and emission inventory combinations are shown as colored lines and symbols. Numbers on the right *y*-axis indicate the number of observations in each altitude bin.

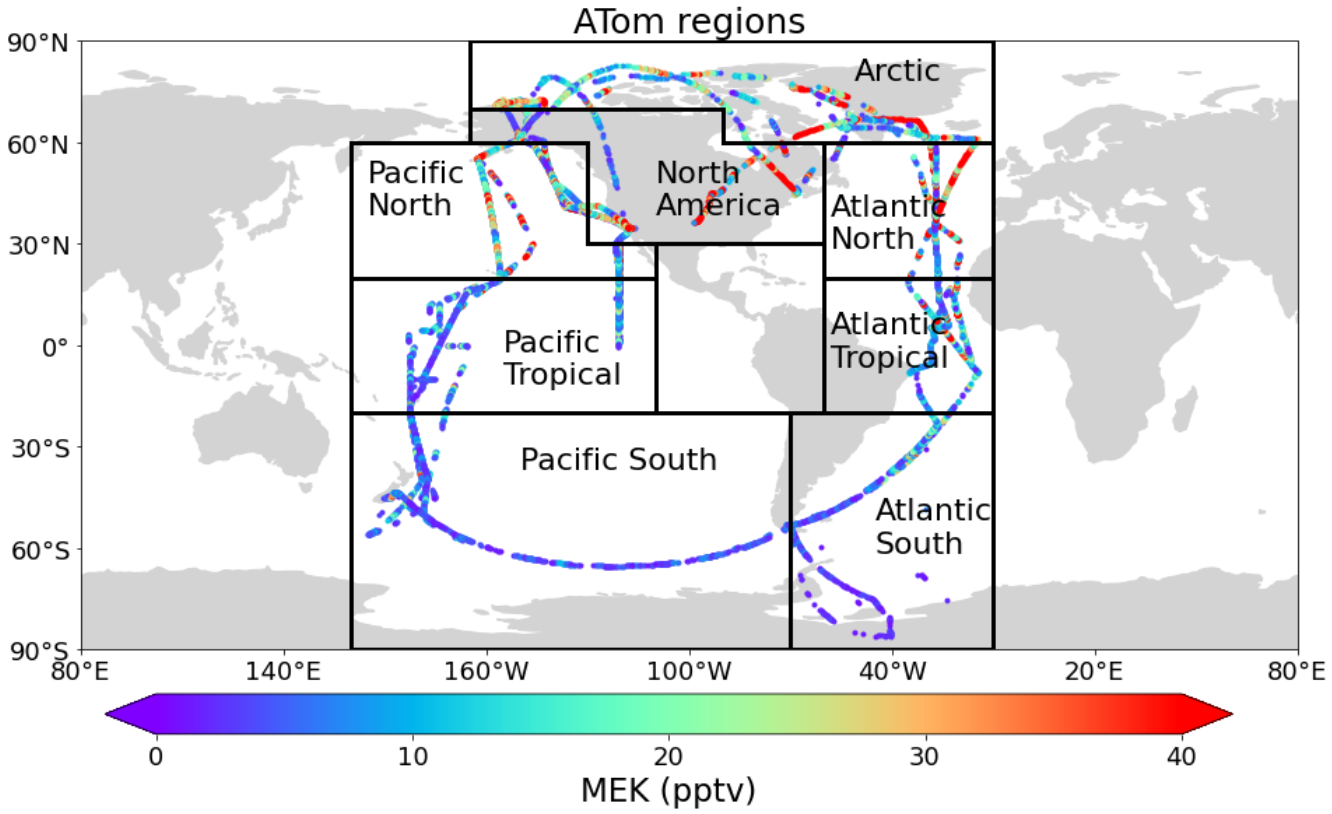

Figure S9. Spatial distribution of observed MEK concentrations along ATom flight tracks, divided into regional boxes. The color scale indicates MEK mixing ratios in pptv.

References

References cited in this supplement are listed in the main text reference list.